Supporting Information

Chapter 2 Supporting Information:

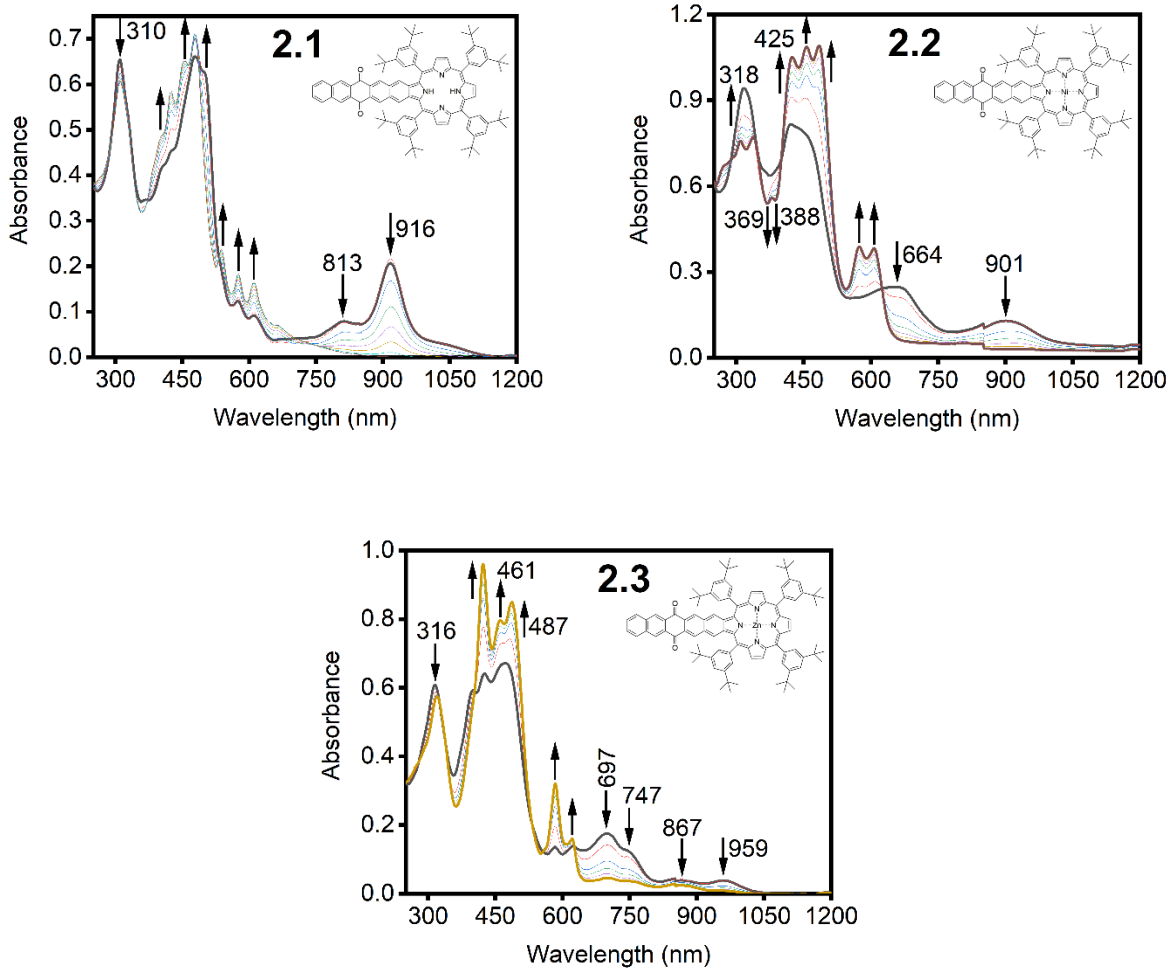


Figure S2.1. Reduction of [**2.1**-**2.3**]$^{+\bullet}$ cation-radicals to neutral **2.1**-**2.3** under spectroelectrochemical conditions in DCM/0.3M TBAP system.

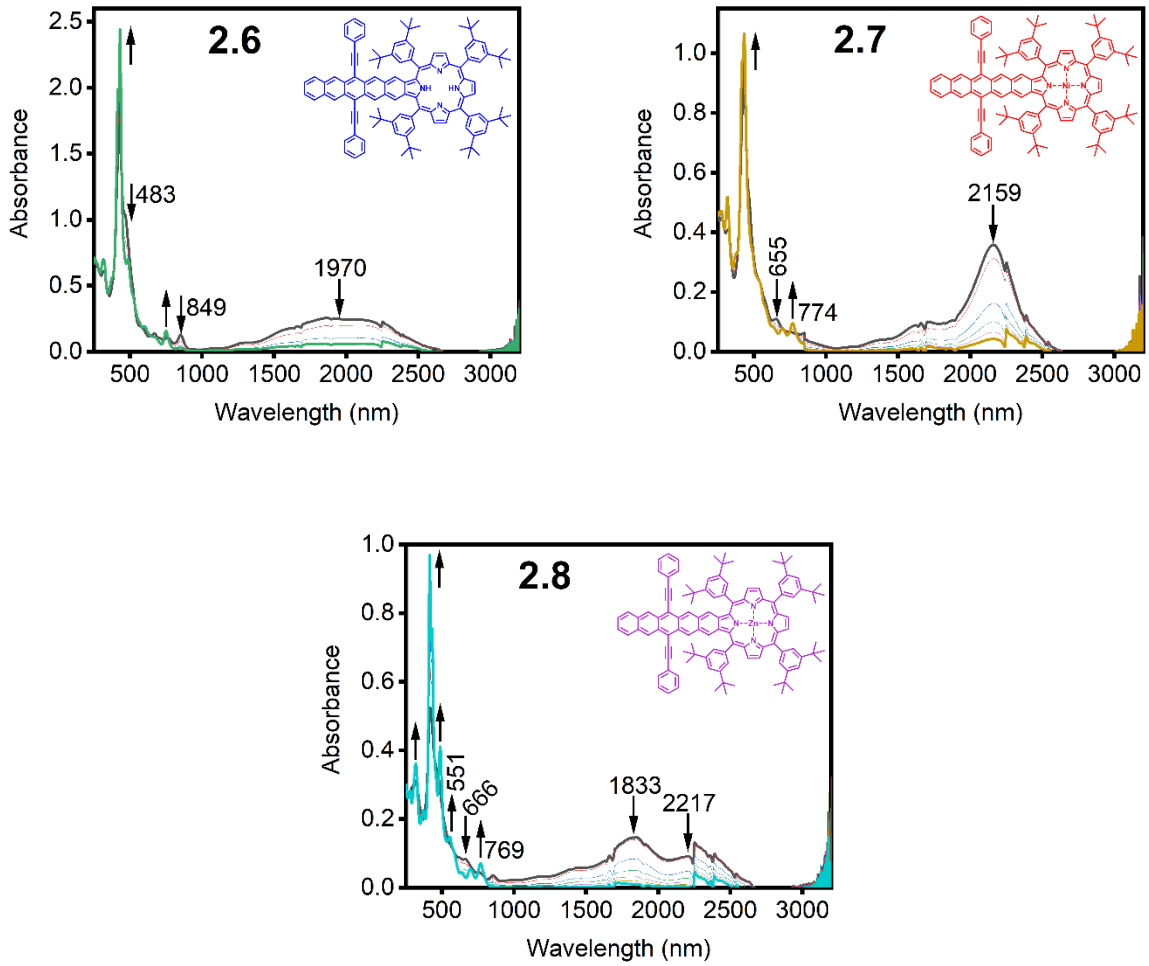


Figure S2.2. Reduction of [**2.6**-**2.8**]$^{+\bullet}$ cation-radicals to neutral **2.6**-**2.8** under spectroelectrochemical conditions in DCM/0.3M TBAP system.

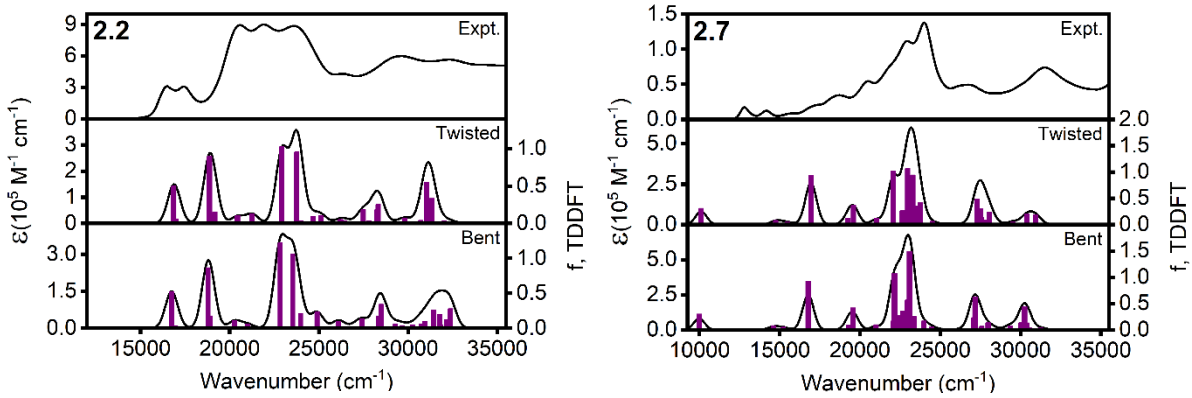


Figure S2.3. TDDFT-predicted UV-vis spectra of **2.2** and **2.7** using the B3LYP exchange correlation functional.

Table S2.1. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.7** using the B3LYP exchange correlation functional and bent geometry.

```
Excited State   1:      Singlet-A"     1.2373 eV 1002.07 nm  f=0.2973  <S**2>=0.000
    291 -> 292        0.71068
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4804.20241833
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A'     1.7572 eV  705.59 nm  f=0.0002  <S**2>=0.000
    282 -> 295        0.10911
    284 -> 295        0.69216
    284 <- 295       -0.15006

 Excited State   3:      Singlet-A"     1.8114 eV  684.47 nm  f=0.0808  <S**2>=0.000
    290 -> 292        0.69954

 Excited State   4:      Singlet-A"     1.8508 eV  669.89 nm  f=0.0003  <S**2>=0.000
    265 -> 295        0.32577
    285 -> 295        0.31923
    287 -> 295       -0.14158
    288 -> 295        0.49026
    291 -> 295       -0.13273

 Excited State   5:      Singlet-A"     1.8775 eV  660.35 nm  f=0.0123  <S**2>=0.000
    289 -> 294       -0.10888
    291 -> 293        0.68822

 Excited State   6:      Singlet-A'     1.8891 eV  656.30 nm  f=0.0503  <S**2>=0.000
    289 -> 292        0.68495
    291 -> 294        0.12782

 Excited State   7:      Singlet-A'     1.9397 eV  639.20 nm  f=0.0003  <S**2>=0.000
    266 -> 295        0.21258
    270 -> 295       -0.23656
    278 -> 295        0.11879
    286 -> 295        0.58586

 Excited State   8:      Singlet-A'     2.0795 eV  596.23 nm  f=0.9256  <S**2>=0.000
    289 -> 292       -0.14263
    289 -> 293        0.14063
    291 -> 294        0.66872

 Excited State   9:      Singlet-A"     2.3945 eV  517.79 nm  f=0.0916  <S**2>=0.000
    288 -> 292        0.10308
    289 -> 294       -0.34694
    290 -> 293        0.58895
```

291 -> 293 -0.11149

Excited State 10: Singlet-A' 2.4244 eV 511.40 nm f=0.4142 <S**2>=0.000
289 -> 293 0.56762
290 -> 294 0.36726
291 -> 294 -0.17166

Excited State 11: Singlet-A" 2.5173 eV 492.53 nm f=0.0001 <S**2>=0.000
262 -> 295 0.33165
288 -> 295 0.10847
290 -> 295 0.28175
291 -> 295 0.53189

Excited State 12: Singlet-A" 2.5351 eV 489.08 nm f=0.0014 <S**2>=0.000
287 -> 292 0.13387
288 -> 292 0.63897
288 -> 293 0.13298
291 -> 296 0.13414

Excited State 13: Singlet-A" 2.6050 eV 475.95 nm f=0.0981 <S**2>=0.000
285 -> 292 0.10888
287 -> 292 0.64884
291 -> 296 -0.14743
291 -> 297 0.14069

Excited State 14: Singlet-A" 2.6396 eV 469.71 nm f=0.0011 <S**2>=0.000
262 -> 295 0.59158
291 -> 295 -0.31961

Excited State 15: Singlet-A" 2.6834 eV 462.04 nm f=0.0110 <S**2>=0.000
285 -> 292 -0.39191
287 -> 292 0.13817
288 -> 292 -0.12955
288 -> 293 -0.17730
291 -> 296 0.50029

Excited State 16: Singlet-A' 2.7369 eV 453.00 nm f=0.1679 <S**2>=0.000
284 -> 292 0.58467
284 -> 293 0.35615

Excited State 17: Singlet-A' 2.7464 eV 451.44 nm f=1.0725 <S**2>=0.000
282 -> 292 -0.15004
284 -> 293 -0.10070
286 -> 292 0.58074
289 -> 293 0.14876
289 -> 295 -0.19515

290 -> 294 -0.19212

Excited State 18: Singlet-A" 2.7890 eV 444.54 nm f=0.2697 <S**2>=0.000
285 -> 292 0.48732
288 -> 293 0.21619
291 -> 296 0.42904

Excited State 19: Singlet-A' 2.8092 eV 441.36 nm f=0.3530 <S**2>=0.000
289 -> 293 0.12779
289 -> 295 0.63072
290 -> 294 -0.20655

Excited State 20: Singlet-A' 2.8475 eV 435.41 nm f=0.5671 <S**2>=0.000
286 -> 292 0.32470
289 -> 293 -0.29004
289 -> 295 0.18060
290 -> 294 0.48096

Excited State 21: Singlet-A" 2.8620 eV 433.21 nm f=1.4913 <S**2>=0.000
288 -> 293 -0.13155
289 -> 294 0.57079
290 -> 293 0.35212

Excited State 22: Singlet-A" 2.8968 eV 428.00 nm f=0.2502 <S**2>=0.000
287 -> 292 -0.14694
291 -> 297 0.68000

Excited State 23: Singlet-A" 2.9731 eV 417.02 nm f=0.1682 <S**2>=0.000
285 -> 292 -0.27558
285 -> 293 0.21011
287 -> 293 -0.11112
288 -> 292 -0.17954
288 -> 293 0.53695
289 -> 294 0.13275

Excited State 24: Singlet-A' 3.0353 eV 408.48 nm f=0.0575 <S**2>=0.000
282 -> 292 -0.20338
283 -> 292 0.63687
291 -> 299 -0.19429

Excited State 25: Singlet-A" 3.0872 eV 401.61 nm f=0.0000 <S**2>=0.000
290 -> 295 0.62404
291 -> 295 -0.29460

Excited State 26: Singlet-A' 3.0914 eV 401.06 nm f=0.0067 <S**2>=0.000
278 -> 292 0.11780

```
   282 -> 292        0.39842
   283 -> 292        0.17679
   284 -> 292       -0.15520
   284 -> 293        0.27831
   286 -> 292        0.10659
   286 -> 293        0.18565
   288 -> 294       -0.10275
   290 -> 294       -0.12263
   291 -> 298       -0.21663
   291 -> 299        0.18287
   291 -> 300       -0.11154

Excited State  27:      Singlet-A'     3.1310 eV  395.99 nm  f=0.0052  <S**2>=0.000
   282 -> 292       -0.12748
   284 -> 292       -0.32608
   284 -> 293        0.47869
   286 -> 293       -0.29997
   288 -> 294        0.13977

Excited State  28:      Singlet-A'     3.1837 eV  389.43 nm  f=0.0049  <S**2>=0.000
   282 -> 292       -0.21296
   283 -> 292       -0.10292
   284 -> 292       -0.10384
   284 -> 293        0.20004
   285 -> 294       -0.10921
   286 -> 292       -0.15484
   286 -> 293        0.42549
   288 -> 294       -0.29360
   289 -> 296        0.10324
   291 -> 298        0.20707

Excited State  29:      Singlet-A"     3.2481 eV  381.71 nm  f=0.0045  <S**2>=0.000
   284 -> 294        0.54517
   286 -> 294       -0.43970

Excited State  30:      Singlet-A'     3.2717 eV  378.97 nm  f=0.0149  <S**2>=0.000
   282 -> 292        0.11223
   283 -> 292        0.16135
   291 -> 298        0.57424
   291 -> 299        0.31766

Excited State  31:      Singlet-A"     3.2720 eV  378.93 nm  f=0.0063  <S**2>=0.000
   284 -> 294        0.43974
   286 -> 294        0.53909

Excited State  32:      Singlet-A"     3.3465 eV  370.48 nm  f=0.0076  <S**2>=0.000
```

```
   279 -> 292        0.10750
   290 -> 296        0.67636

Excited State  33:      Singlet-A'     3.3570 eV  369.33 nm  f=0.2310  <S**2>=0.000
   282 -> 292        0.16413
   285 -> 294        0.10130
   286 -> 293        0.32638
   288 -> 294        0.50809
   291 -> 298        0.10185
   291 -> 299       -0.23864

Excited State  34:      Singlet-A'     3.3685 eV  368.07 nm  f=0.6285  <S**2>=0.000
   282 -> 292       -0.34067
   286 -> 293        0.20632
   288 -> 294        0.21878
   291 -> 298       -0.16408
   291 -> 299        0.46869

Excited State  35:      Singlet-A"     3.3868 eV  366.08 nm  f=0.0302  <S**2>=0.000
   279 -> 292        0.46325
   285 -> 293        0.44015
   287 -> 293       -0.16651
   288 -> 293       -0.19877

Excited State  36:      Singlet-A'     3.4000 eV  364.66 nm  f=0.0070  <S**2>=0.000
   274 -> 292       -0.14831
   277 -> 292       -0.18680
   281 -> 292        0.62258
   289 -> 296        0.19038

Excited State  37:      Singlet-A'     3.4164 eV  362.91 nm  f=0.0141  <S**2>=0.000
   278 -> 292        0.12518
   281 -> 292       -0.17536
   285 -> 294        0.12126
   289 -> 296        0.62463

Excited State  38:      Singlet-A"     3.4211 eV  362.41 nm  f=0.0662  <S**2>=0.000
   279 -> 292        0.50353
   285 -> 293       -0.38648
   287 -> 293        0.15724
   288 -> 293        0.18855
   290 -> 296       -0.11732

Excited State  39:      Singlet-A'     3.4693 eV  357.38 nm  f=0.1330  <S**2>=0.000
   274 -> 292       -0.22033
   277 -> 292        0.11163
```

```
   278 -> 292        0.58872
   282 -> 292       -0.10163
   289 -> 296       -0.11509
   291 -> 299       -0.13770
   291 -> 300       -0.10242

Excited State  40:      Singlet-A"     3.5071 eV  353.52 nm  f=0.0094  <S**2>=0.000
   275 -> 292        0.29016
   276 -> 292       -0.16332
   280 -> 292        0.60669

Excited State  41:      Singlet-A"     3.5497 eV  349.28 nm  f=0.0194  <S**2>=0.000
   275 -> 292        0.33302
   276 -> 292       -0.17797
   280 -> 292       -0.18983
   285 -> 293        0.16699
   287 -> 293        0.53154

Excited State  42:      Singlet-A"     3.5512 eV  349.13 nm  f=0.0000  <S**2>=0.000
   275 -> 292        0.42181
   276 -> 292       -0.22583
   280 -> 292       -0.26513
   285 -> 293       -0.22254
   287 -> 293       -0.37262

Excited State  43:      Singlet-A'     3.5791 eV  346.41 nm  f=0.0011  <S**2>=0.000
   273 -> 292       -0.34771
   274 -> 292       -0.22256
   277 -> 292        0.50563
   281 -> 292        0.12056

Excited State  44:      Singlet-A'     3.6376 eV  340.84 nm  f=0.0387  <S**2>=0.000
   274 -> 292       -0.30324
   278 -> 292       -0.10632
   285 -> 294        0.51442
   287 -> 294       -0.22879
   288 -> 294       -0.18477

Excited State  45:      Singlet-A'     3.6389 eV  340.72 nm  f=0.0048  <S**2>=0.000
   274 -> 292        0.48545
   277 -> 292        0.27230
   281 -> 292        0.21027
   285 -> 294        0.27003
   287 -> 294       -0.10327
   288 -> 294       -0.10729
```

Excited State 46: Singlet-A" 3.6405 eV 340.57 nm f=0.0716 <S**2>=0.000
290 -> 297 0.68784

Excited State 47: Singlet-A" 3.6653 eV 338.26 nm f=0.0000 <S**2>=0.000
272 -> 292 0.69215
291 -> 304 0.10416

Excited State 48: Singlet-A' 3.6655 eV 338.25 nm f=0.0085 <S**2>=0.000
271 -> 292 0.69059
291 -> 303 -0.10454

Excited State 49: Singlet-A" 3.6945 eV 335.59 nm f=0.0018 <S**2>=0.000
275 -> 292 0.33199
276 -> 292 0.60797

Excited State 50: Singlet-A' 3.7249 eV 332.85 nm f=0.1332 <S**2>=0.000
273 -> 292 0.41226
274 -> 292 -0.12783
277 -> 292 0.29282
278 -> 292 -0.23503
282 -> 293 -0.15546
291 -> 300 -0.32549

Excited State 51: Singlet-A" 3.7472 eV 330.87 nm f=0.0000 <S**2>=0.000
268 -> 292 0.69742

Excited State 52: Singlet-A' 3.7521 eV 330.44 nm f=0.4430 <S**2>=0.000
273 -> 292 0.33938
274 -> 292 -0.12710
287 -> 294 0.10436
289 -> 297 -0.27653
291 -> 300 0.47662

Excited State 53: Singlet-A' 3.7641 eV 329.39 nm f=0.0029 <S**2>=0.000
285 -> 294 0.27573
287 -> 294 0.62360
291 -> 300 -0.13213

Excited State 54: Singlet-A' 3.7672 eV 329.12 nm f=0.1304 <S**2>=0.000
287 -> 294 0.10512
289 -> 297 0.63268
291 -> 300 0.23789

Excited State 55: Singlet-A" 3.7789 eV 328.10 nm f=0.0000 <S**2>=0.000
291 -> 301 0.67594
291 -> 304 -0.10042

Excited State 56: Singlet-A' 3.7870 eV 327.40 nm f=0.0329 <S**2>=0.000
273 -> 292 0.22462
273 -> 293 -0.10283
278 -> 293 -0.22960
282 -> 293 0.51043
283 -> 293 0.26129
291 -> 300 -0.10288

Excited State 57: Singlet-A' 3.8308 eV 323.65 nm f=0.0003 <S**2>=0.000
266 -> 292 -0.20264
267 -> 292 0.66436

Excited State 58: Singlet-A" 3.8536 eV 321.73 nm f=0.0205 <S**2>=0.000
269 -> 292 0.22706
291 -> 302 -0.37991
291 -> 304 -0.13895
291 -> 306 0.50562

Excited State 59: Singlet-A' 3.8783 eV 319.69 nm f=0.0415 <S**2>=0.000
281 -> 293 0.15773
290 -> 298 0.18583
291 -> 303 0.48889
291 -> 305 -0.15453
291 -> 307 -0.34953

Excited State 60: Singlet-A" 3.8936 eV 318.43 nm f=0.0001 <S**2>=0.000
272 -> 292 -0.11837
291 -> 301 0.10264
291 -> 302 -0.11370
291 -> 304 0.65953

Table S2.2. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.7** using the B3LYP exchange correlation functional and twisted geometry.

Excited State 1: Singlet-B 1.2525 eV 989.86 nm f=0.3079 <S**2>=0.000
291 -> 292 0.71061
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4804.20500100
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-B 1.8294 eV 677.71 nm f=0.0766 <S**2>=0.000
290 -> 292 0.68885
291 -> 293 -0.13055

```
Excited State   3:      Singlet-B      1.8648 eV  664.88 nm  f=0.0207  <S**2>=0.000
    290 -> 292        0.13694
    291 -> 293        0.68163

Excited State   4:      Singlet-A      1.9205 eV  645.57 nm  f=0.0512  <S**2>=0.000
    289 -> 292        0.68237
    291 -> 294       -0.14538

Excited State   5:      Singlet-A      2.0491 eV  605.08 nm  f=0.0241  <S**2>=0.000
    284 -> 297        0.13226
    285 -> 297        0.67105
    291 -> 294       -0.14186
    285 <- 297       -0.12446

Excited State   6:      Singlet-A      2.1008 eV  590.17 nm  f=0.9394  <S**2>=0.000
    285 -> 297        0.15064
    289 -> 292        0.16250
    289 -> 293       -0.13456
    291 -> 294        0.64362

Excited State   7:      Singlet-A      2.1587 eV  574.34 nm  f=0.0182  <S**2>=0.000
    266 -> 297        0.30335
    284 -> 297       -0.26521
    286 -> 297       -0.12050
    288 -> 297        0.52482
    291 -> 297       -0.12108

Excited State   8:      Singlet-B      2.2331 eV  555.21 nm  f=0.0002  <S**2>=0.000
    264 -> 297        0.11761
    267 -> 297        0.19358
    270 -> 297        0.24355
    279 -> 297        0.12603
    287 -> 297        0.59972

Excited State   9:      Singlet-B      2.3871 eV  519.40 nm  f=0.1219  <S**2>=0.000
    288 -> 292       -0.10413
    289 -> 294       -0.32690
    290 -> 293        0.60019
    291 -> 293        0.10679

Excited State  10:      Singlet-A      2.4298 eV  510.27 nm  f=0.3699  <S**2>=0.000
    289 -> 293        0.56898
    290 -> 294        0.35957
    291 -> 294        0.17565

Excited State  11:      Singlet-B      2.5240 eV  491.22 nm  f=0.0007  <S**2>=0.000
```

```
   288 -> 292        0.63827
   288 -> 293        0.20523
   290 -> 293        0.10235

Excited State  12:      Singlet-B      2.6069 eV  475.59 nm  f=0.1175  <S**2>=0.000
   262 -> 297        0.10625
   286 -> 292        0.65339
   291 -> 296        0.13972

Excited State  13:      Singlet-B      2.6152 eV  474.08 nm  f=0.0019  <S**2>=0.000
   262 -> 297       -0.47296
   270 -> 297       -0.15849
   279 -> 297        0.15813
   286 -> 292        0.13950
   289 -> 297        0.38216

Excited State  14:      Singlet-B      2.6428 eV  469.15 nm  f=0.0015  <S**2>=0.000
   285 -> 292        0.57327
   285 -> 293        0.39129

Excited State  15:      Singlet-B      2.6954 eV  459.98 nm  f=0.0048  <S**2>=0.000
   284 -> 292        0.43745
   288 -> 293       -0.20081
   291 -> 295        0.49036

Excited State  16:      Singlet-A      2.7347 eV  453.37 nm  f=1.0238  <S**2>=0.000
   282 -> 292        0.13091
   287 -> 292        0.63604
   289 -> 293        0.12558
   290 -> 294       -0.15687

Excited State  17:      Singlet-B      2.8071 eV  441.68 nm  f=0.2677  <S**2>=0.000
   284 -> 292       -0.40158
   288 -> 292       -0.14616
   288 -> 293        0.27760
   291 -> 295        0.46004

Excited State  18:      Singlet-A      2.8478 eV  435.37 nm  f=1.0686  <S**2>=0.000
   282 -> 292       -0.13901
   287 -> 292        0.21574
   287 -> 293        0.10078
   289 -> 293       -0.31912
   290 -> 294        0.54095

Excited State  19:      Singlet-B      2.8885 eV  429.23 nm  f=0.9434  <S**2>=0.000
   284 -> 292        0.16488
```

```
   288 -> 292       -0.13021
   288 -> 293        0.25072
   289 -> 294        0.52676
   290 -> 293        0.30895

Excited State  20:      Singlet-B      2.9072 eV  426.47 nm  f=0.3512  <S**2>=0.000
   286 -> 292       -0.13294
   288 -> 293        0.11429
   291 -> 296        0.66531

Excited State  21:      Singlet-A      2.9290 eV  423.29 nm  f=0.0363  <S**2>=0.000
   288 -> 297        0.11442
   290 -> 297       -0.30293
   291 -> 297        0.61836

Excited State  22:      Singlet-B      2.9456 eV  420.91 nm  f=0.4143  <S**2>=0.000
   284 -> 292        0.30827
   284 -> 293       -0.15816
   288 -> 292       -0.16581
   288 -> 293        0.43974
   289 -> 294       -0.27023
   290 -> 293       -0.12032
   291 -> 295       -0.12950
   291 -> 296       -0.15487

Excited State  23:      Singlet-B      3.0305 eV  409.12 nm  f=0.0000  <S**2>=0.000
   285 -> 292       -0.39302
   285 -> 293        0.56968

Excited State  24:      Singlet-A      3.0378 eV  408.13 nm  f=0.0618  <S**2>=0.000
   282 -> 292       -0.22051
   283 -> 292        0.63494
   291 -> 298       -0.10402
   291 -> 299       -0.14975

Excited State  25:      Singlet-A      3.0682 eV  404.09 nm  f=0.0003  <S**2>=0.000
   279 -> 292        0.11771
   282 -> 292       -0.35432
   283 -> 292       -0.13987
   287 -> 293        0.42469
   288 -> 294        0.17438
   290 -> 294       -0.14201
   291 -> 299       -0.21975

Excited State  26:      Singlet-A      3.1433 eV  394.44 nm  f=0.0048  <S**2>=0.000
   282 -> 292        0.33033
```

```
   283 -> 292        0.17237
   287 -> 292       -0.19183
   287 -> 293        0.40772
   288 -> 294        0.22472
   291 -> 298       -0.12692
   291 -> 299        0.20405

Excited State  27:      Singlet-A      3.1675 eV  391.43 nm  f=0.0122  <S**2>=0.000
   284 -> 294        0.11864
   285 -> 294        0.68277

Excited State  28:      Singlet-B      3.2248 eV  384.48 nm  f=0.0087  <S**2>=0.000
   287 -> 294        0.69511

Excited State  29:      Singlet-A      3.2831 eV  377.64 nm  f=0.0035  <S**2>=0.000
   283 -> 292        0.15036
   291 -> 298        0.66108
   291 -> 299        0.12609

Excited State  30:      Singlet-A      3.3059 eV  375.04 nm  f=0.0212  <S**2>=0.000
   284 -> 294       -0.12213
   287 -> 293       -0.32103
   288 -> 294        0.58774

Excited State  31:      Singlet-A      3.3849 eV  366.28 nm  f=0.4812  <S**2>=0.000
   277 -> 292       -0.17292
   279 -> 292       -0.11973
   281 -> 292       -0.32389
   282 -> 292       -0.36460
   291 -> 299        0.42596

Excited State  32:      Singlet-B      3.3870 eV  366.06 nm  f=0.0373  <S**2>=0.000
   284 -> 293       -0.16433
   290 -> 295        0.66501

Excited State  33:      Singlet-B      3.3997 eV  364.70 nm  f=0.0068  <S**2>=0.000
   262 -> 297        0.34233
   270 -> 297        0.11276
   284 -> 293        0.18280
   289 -> 297        0.54662

Excited State  34:      Singlet-A      3.4102 eV  363.57 nm  f=0.2965  <S**2>=0.000
   277 -> 292        0.26565
   279 -> 292       -0.13231
   281 -> 292        0.52345
   282 -> 292       -0.13777
```

291 -> 299 0.31658

Excited State 35: Singlet-B 3.4180 eV 362.74 nm f=0.1398 <S**2>=0.000
262 -> 297 -0.11004
284 -> 293 0.54005
286 -> 293 0.24592
288 -> 293 0.20505
289 -> 297 -0.18509
290 -> 295 0.16352

Excited State 36: Singlet-B 3.4351 eV 360.94 nm f=0.0014 <S**2>=0.000
278 -> 292 0.59989
280 -> 292 0.35710

Excited State 37: Singlet-A 3.4563 eV 358.72 nm f=0.0925 <S**2>=0.000
279 -> 292 0.26774
289 -> 295 0.28139
290 -> 297 0.48306
291 -> 297 0.23720
291 -> 299 0.12772

Excited State 38: Singlet-A 3.4638 eV 357.94 nm f=0.0501 <S**2>=0.000
279 -> 292 0.24620
289 -> 295 0.45765
290 -> 297 -0.37813
291 -> 297 -0.18361

Excited State 39: Singlet-A 3.4781 eV 356.48 nm f=0.2405 <S**2>=0.000
275 -> 292 -0.15881
279 -> 292 0.45912
279 -> 293 0.10926
289 -> 295 -0.39422
291 -> 299 0.21863

Excited State 40: Singlet-B 3.5252 eV 351.71 nm f=0.0158 <S**2>=0.000
284 -> 293 -0.27780
286 -> 293 0.63739

Excited State 41: Singlet-B 3.5467 eV 349.58 nm f=0.0128 <S**2>=0.000
274 -> 292 0.54465
276 -> 292 -0.18189
278 -> 292 -0.23184
280 -> 292 0.32872

Excited State 42: Singlet-A 3.5692 eV 347.37 nm f=0.0005 <S**2>=0.000
273 -> 292 0.46109

```
   275 -> 292       -0.26787
   277 -> 292        0.40167
   281 -> 292       -0.17041

Excited State  43:      Singlet-B      3.5862 eV  345.72 nm  f=0.0018  <S**2>=0.000
   274 -> 292       -0.37455
   276 -> 292        0.12634
   278 -> 292       -0.26804
   280 -> 292        0.48781
   280 -> 293        0.10513

Excited State  44:      Singlet-A      3.6122 eV  343.24 nm  f=0.0000  <S**2>=0.000
   273 -> 292       -0.33548
   275 -> 292        0.25932
   277 -> 292        0.46512
   281 -> 292       -0.25670

Excited State  45:      Singlet-B      3.6606 eV  338.70 nm  f=0.0581  <S**2>=0.000
   290 -> 296        0.68052

Excited State  46:      Singlet-A      3.6687 eV  337.95 nm  f=0.0063  <S**2>=0.000
   272 -> 292        0.69234

Excited State  47:      Singlet-B      3.6687 eV  337.95 nm  f=0.0013  <S**2>=0.000
   271 -> 292        0.68772

Excited State  48:      Singlet-A      3.6809 eV  336.83 nm  f=0.0045  <S**2>=0.000
   275 -> 292       -0.16814
   279 -> 292       -0.11234
   282 -> 293        0.11761
   284 -> 294        0.52836
   286 -> 294        0.27992
   288 -> 294        0.17716
   289 -> 295       -0.11951

Excited State  49:      Singlet-B      3.6897 eV  336.03 nm  f=0.0038  <S**2>=0.000
   274 -> 292        0.21509
   276 -> 292        0.65342
   276 -> 293        0.11351

Excited State  50:      Singlet-A      3.7000 eV  335.09 nm  f=0.0018  <S**2>=0.000
   273 -> 292        0.33522
   275 -> 292        0.50703
   275 -> 293        0.10885
   279 -> 292        0.19397
   282 -> 293       -0.10090
```

```
   284 -> 294        0.17960
   286 -> 294        0.11078

Excited State  51:      Singlet-A      3.7363 eV  331.83 nm  f=0.0010  <S**2>=0.000
   273 -> 292        0.20990
   275 -> 292        0.13112
   279 -> 292       -0.13133
   279 -> 293        0.19384
   282 -> 293        0.49893
   283 -> 293        0.28240

Excited State  52:      Singlet-A      3.7503 eV  330.60 nm  f=0.0060  <S**2>=0.000
   268 -> 292        0.68306

Excited State  53:      Singlet-A      3.7684 eV  329.01 nm  f=0.1988  <S**2>=0.000
   284 -> 294       -0.17301
   286 -> 294        0.33780
   291 -> 300        0.54268

Excited State  54:      Singlet-A      3.7752 eV  328.42 nm  f=0.0116  <S**2>=0.000
   284 -> 294       -0.26392
   286 -> 294        0.51038
   291 -> 300       -0.37671

Excited State  55:      Singlet-A      3.7984 eV  326.42 nm  f=0.0001  <S**2>=0.000
   289 -> 295       -0.12996
   289 -> 296        0.67142

Excited State  56:      Singlet-B      3.8085 eV  325.55 nm  f=0.0008  <S**2>=0.000
   265 -> 292       -0.22117
   269 -> 292       -0.21508
   291 -> 301        0.58528
   291 -> 303        0.17773

Excited State  57:      Singlet-B      3.8212 eV  324.47 nm  f=0.0000  <S**2>=0.000
   265 -> 292        0.52115
   266 -> 292        0.10534
   269 -> 292        0.26963
   291 -> 301        0.32291
   291 -> 305       -0.11482

Excited State  58:      Singlet-A      3.8365 eV  323.17 nm  f=0.1898  <S**2>=0.000
   270 -> 292        0.26608
   279 -> 293       -0.16626
   281 -> 293       -0.12112
   289 -> 296       -0.15010
```

290 -> 299 -0.13949
291 -> 302 0.45845
291 -> 306 0.25030

Excited State 59: Singlet-B 3.8557 eV 321.56 nm f=0.0149 <S**2>=0.000
265 -> 292 0.26137
269 -> 292 -0.16210
291 -> 301 -0.11332
291 -> 303 0.48069
291 -> 305 0.35052

Excited State 60: Singlet-A 3.8943 eV 318.37 nm f=0.0031 <S**2>=0.000
270 -> 292 -0.10905
281 -> 293 0.45195
283 -> 293 -0.21815
291 -> 302 0.20393
291 -> 304 0.37518

Table S2.3. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.7** using the M06 exchange correlation functional and bent geometry.

Excited State 1: Singlet-A' 1.2170 eV 1018.80 nm f=0.0000 <S**2>=0.000
282 -> 295 0.23407
282 -> 296 0.19443
283 -> 295 0.12692
283 -> 296 0.10592
284 -> 295 0.50255
284 -> 296 0.41944
284 <- 295 -0.17953
284 <- 296 -0.15009
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4801.57238638
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A" 1.2748 eV 972.61 nm f=0.3443 <S**2>=0.000
291 -> 292 0.70672

Excited State 3: Singlet-A" 1.3603 eV 911.42 nm f=0.0000 <S**2>=0.000
263 -> 295 -0.30506
263 -> 296 -0.25444
285 -> 295 -0.36011
285 -> 296 -0.30018
287 -> 295 0.13244
287 -> 296 0.11033
288 -> 295 -0.25688

```
   288 -> 296       -0.21388
   263 <- 295        0.11047
   285 <- 295        0.10789

Excited State   4:      Singlet-A'     1.4489 eV  855.69 nm  f=0.0001  <S**2>=0.000
   264 -> 295        0.21656
   264 -> 296        0.18106
   266 -> 295        0.16813
   266 -> 296        0.14018
   269 -> 295       -0.16811
   269 -> 296       -0.14012
   278 -> 295        0.10814
   286 -> 295        0.42996
   286 -> 296        0.35744
   286 <- 295       -0.12213
   286 <- 296       -0.10224

Excited State   5:      Singlet-A"     1.8750 eV  661.26 nm  f=0.0166  <S**2>=0.000
   289 -> 294       -0.11732
   290 -> 292        0.58788
   290 -> 293        0.11541
   291 -> 293        0.34713

Excited State   6:      Singlet-A"     1.9577 eV  633.31 nm  f=0.0001  <S**2>=0.000
   262 -> 295        0.51144
   262 -> 296        0.42726
   263 -> 295       -0.15527
   263 -> 296       -0.12878

Excited State   7:      Singlet-A"     1.9784 eV  626.69 nm  f=0.0659  <S**2>=0.000
   289 -> 294       -0.11253
   290 -> 292       -0.37198
   290 -> 293        0.11475
   291 -> 293        0.57051

Excited State   8:      Singlet-A'     2.0303 eV  610.68 nm  f=0.0007  <S**2>=0.000
   289 -> 292        0.58364
   289 -> 293        0.18871
   290 -> 294        0.14460
   291 -> 294        0.31229

Excited State   9:      Singlet-A'     2.1540 eV  575.61 nm  f=1.1491  <S**2>=0.000
   289 -> 292       -0.37518
   289 -> 293        0.12531
   290 -> 294        0.12891
   291 -> 294        0.56449
```

Excited State 10: Singlet-A" 2.4292 eV 510.39 nm f=0.0697 <S**2>=0.000
288 -> 292 0.11133
289 -> 294 -0.33916
290 -> 293 0.55553
291 -> 293 -0.20971

Excited State 11: Singlet-A' 2.4639 eV 503.20 nm f=0.5989 <S**2>=0.000
289 -> 292 -0.11186
289 -> 293 0.54292
290 -> 294 0.32396
291 -> 294 -0.26213

Excited State 12: Singlet-A" 2.6804 eV 462.56 nm f=0.0460 <S**2>=0.000
287 -> 292 0.42197
288 -> 292 0.52797

Excited State 13: Singlet-A" 2.7072 eV 457.98 nm f=0.0024 <S**2>=0.000
287 -> 292 0.10799
290 -> 295 0.28692
290 -> 296 0.23883
291 -> 295 0.49674
291 -> 296 0.29413

Excited State 14: Singlet-A" 2.7534 eV 450.29 nm f=0.0791 <S**2>=0.000
285 -> 292 0.13289
285 -> 293 -0.10002
287 -> 292 0.48927
288 -> 292 -0.33746
291 -> 295 0.11862
291 -> 296 -0.28346

Excited State 15: Singlet-A" 2.8311 eV 437.93 nm f=0.1744 <S**2>=0.000
287 -> 292 0.19946
288 -> 292 -0.21349
290 -> 293 0.12851
291 -> 295 -0.35182
291 -> 296 0.48979

Excited State 16: Singlet-A' 2.8440 eV 435.95 nm f=1.8597 <S**2>=0.000
282 -> 292 0.21724
284 -> 292 -0.13303
286 -> 292 -0.29111
289 -> 293 -0.31881
290 -> 294 0.46902

Excited State 17: Singlet-A" 2.8888 eV 429.18 nm f=1.7032 <S**2>=0.000
285 -> 292 -0.19347
288 -> 293 -0.14509
289 -> 294 0.53187
290 -> 293 0.34125

Excited State 18: Singlet-A' 2.9249 eV 423.90 nm f=0.0275 <S**2>=0.000
289 -> 295 0.52611
289 -> 296 0.42119
290 -> 294 -0.12291

Excited State 19: Singlet-A" 2.9302 eV 423.12 nm f=0.0943 <S**2>=0.000
285 -> 292 0.47994
285 -> 293 0.27402
287 -> 293 -0.13093
288 -> 293 0.28114
289 -> 294 0.23929
290 -> 293 0.15237

Excited State 20: Singlet-A" 3.0021 eV 413.00 nm f=0.2485 <S**2>=0.000
290 -> 297 -0.14846
291 -> 297 0.68223

Excited State 21: Singlet-A' 3.0099 eV 411.92 nm f=0.0584 <S**2>=0.000
282 -> 292 -0.18583
284 -> 292 0.13169
286 -> 292 0.47391
289 -> 293 -0.16956
289 -> 295 0.10255
290 -> 294 0.32788
291 -> 298 0.13996

Excited State 22: Singlet-A' 3.0767 eV 402.98 nm f=0.0014 <S**2>=0.000
282 -> 292 0.12486
282 -> 293 0.15271
283 -> 292 0.10586
283 -> 293 0.10131
284 -> 292 0.46125
284 -> 293 0.44772
286 -> 292 -0.10492

Excited State 23: Singlet-A' 3.1294 eV 396.19 nm f=0.0205 <S**2>=0.000
282 -> 292 -0.14413
283 -> 292 0.62526
284 -> 292 -0.12458
286 -> 292 -0.11921

291 -> 299 -0.13288

Excited State 24: Singlet-A' 3.2418 eV 382.45 nm f=0.0381 <S**2>=0.000
282 -> 292 0.35138
282 -> 293 0.10454
283 -> 292 0.21444
284 -> 292 -0.12612
285 -> 294 -0.13769
286 -> 292 0.22919
286 -> 293 0.35000
288 -> 294 -0.13848
291 -> 298 -0.16182

Excited State 25: Singlet-A" 3.2537 eV 381.06 nm f=0.0284 <S**2>=0.000
285 -> 292 0.43956
285 -> 293 -0.25164
287 -> 292 -0.11338
287 -> 293 0.14998
288 -> 292 0.18058
288 -> 293 -0.39869

Excited State 26: Singlet-A" 3.3445 eV 370.71 nm f=0.0001 <S**2>=0.000
290 -> 295 0.47763
290 -> 296 0.31945
291 -> 295 -0.28602
291 -> 296 -0.25999

Excited State 27: Singlet-A' 3.3759 eV 367.26 nm f=0.2690 <S**2>=0.000
285 -> 294 -0.10660
286 -> 292 -0.18715
286 -> 293 0.23072
288 -> 294 -0.21423
291 -> 298 0.53636
291 -> 299 0.10859

Excited State 28: Singlet-A' 3.4342 eV 361.03 nm f=0.2292 <S**2>=0.000
283 -> 292 0.10854
285 -> 294 0.12021
286 -> 292 0.16699
286 -> 293 -0.20421
288 -> 294 0.12552
290 -> 299 -0.11446
291 -> 298 0.13525
291 -> 299 0.57503

Excited State 29: Singlet-A" 3.4475 eV 359.64 nm f=0.0111 <S**2>=0.000

```
   286 -> 294        0.66400
   290 -> 296       -0.12216

Excited State  30:      Singlet-A"     3.4655 eV  357.77 nm  f=0.0002  <S**2>=0.000
   279 -> 292        0.17100
   285 -> 293        0.16472
   286 -> 294        0.12731
   288 -> 293       -0.11228
   290 -> 295       -0.35426
   290 -> 296        0.50027

Excited State  31:      Singlet-A'     3.4930 eV  354.96 nm  f=0.6343  <S**2>=0.000
   282 -> 292        0.30569
   284 -> 292       -0.26204
   284 -> 293        0.16249
   285 -> 294        0.13257
   286 -> 292        0.15646
   286 -> 293       -0.18216
   288 -> 294        0.16419
   291 -> 298        0.29367
   291 -> 299       -0.28352

Excited State  32:      Singlet-A"     3.5339 eV  350.84 nm  f=0.0169  <S**2>=0.000
   279 -> 292        0.33170
   285 -> 293        0.41607
   288 -> 293       -0.32624
   290 -> 295        0.15277
   290 -> 296       -0.20886

Excited State  33:      Singlet-A'     3.5514 eV  349.11 nm  f=0.0319  <S**2>=0.000
   284 -> 292        0.13070
   284 -> 293       -0.12097
   285 -> 294        0.20641
   286 -> 293        0.39321
   287 -> 294       -0.15505
   288 -> 294        0.46610

Excited State  34:      Singlet-A"     3.5563 eV  348.63 nm  f=0.0001  <S**2>=0.000
   282 -> 294        0.22539
   283 -> 294        0.15234
   284 -> 294        0.63586

Excited State  35:      Singlet-A'     3.5634 eV  347.94 nm  f=0.0112  <S**2>=0.000
   281 -> 292        0.27758
   282 -> 292       -0.30719
   282 -> 293        0.10605
```

```
   284 -> 292       -0.30716
   284 -> 293        0.35607
   286 -> 293        0.11586
   289 -> 296        0.12579

Excited State  36:      Singlet-A'     3.5826 eV  346.07 nm  f=0.0536  <S**2>=0.000
   274 -> 292       -0.18396
   277 -> 292        0.18492
   281 -> 292        0.52216
   282 -> 292        0.11366
   284 -> 292        0.15809
   284 -> 293       -0.21274
   286 -> 293       -0.10898

Excited State  37:      Singlet-A"     3.5829 eV  346.04 nm  f=0.0305  <S**2>=0.000
   279 -> 292        0.57064
   285 -> 293       -0.28698
   288 -> 293        0.24336

Excited State  38:      Singlet-A'     3.6036 eV  344.06 nm  f=0.0178  <S**2>=0.000
   277 -> 292       -0.12179
   281 -> 292       -0.15790
   285 -> 294        0.13581
   289 -> 295       -0.38811
   289 -> 296        0.48381

Excited State  39:      Singlet-A'     3.6632 eV  338.46 nm  f=0.0165  <S**2>=0.000
   274 -> 292       -0.22277
   277 -> 292       -0.27385
   278 -> 292        0.50565
   278 -> 293        0.11739
   282 -> 292       -0.12637
   282 -> 293       -0.12100
   289 -> 295        0.10042
   289 -> 296       -0.11177

Excited State  40:      Singlet-A"     3.6995 eV  335.14 nm  f=0.0179  <S**2>=0.000
   275 -> 292        0.51372
   276 -> 292       -0.22103
   279 -> 292       -0.13077
   280 -> 292        0.38586
   280 -> 293        0.11354

Excited State  41:      Singlet-A"     3.7430 eV  331.24 nm  f=0.0000  <S**2>=0.000
   275 -> 292       -0.36459
   276 -> 292        0.14611
```

```
   280 -> 292        0.52653
   280 -> 293        0.19586

Excited State  42:      Singlet-A'     3.7550 eV  330.18 nm  f=0.0276  <S**2>=0.000
   271 -> 292        0.27204
   271 -> 293        0.13103
   274 -> 292        0.15100
   277 -> 292        0.33343
   278 -> 293        0.10308
   282 -> 293       -0.16411
   285 -> 294        0.36133
   288 -> 294       -0.20585

Excited State  43:      Singlet-A"     3.7822 eV  327.81 nm  f=0.0163  <S**2>=0.000
   285 -> 293        0.15471
   287 -> 293        0.66030
   288 -> 293        0.14782

Excited State  44:      Singlet-A'     3.7957 eV  326.64 nm  f=0.0192  <S**2>=0.000
   271 -> 292       -0.21301
   271 -> 293       -0.11093
   277 -> 292       -0.25925
   278 -> 292       -0.12337
   278 -> 293       -0.11763
   282 -> 293        0.10338
   285 -> 294        0.42547
   288 -> 294       -0.26543

Excited State  45:      Singlet-A'     3.8177 eV  324.76 nm  f=0.0113  <S**2>=0.000
   273 -> 292        0.68387

Excited State  46:      Singlet-A"     3.8178 eV  324.75 nm  f=0.0001  <S**2>=0.000
   272 -> 292        0.69021

Excited State  47:      Singlet-A'     3.8451 eV  322.45 nm  f=0.0085  <S**2>=0.000
   274 -> 292        0.50785
   274 -> 293        0.11905
   277 -> 292       -0.26374
   278 -> 293        0.10917
   281 -> 292        0.26191
   281 -> 293        0.14751

Excited State  48:      Singlet-A"     3.8518 eV  321.88 nm  f=0.0258  <S**2>=0.000
   290 -> 297        0.66212
   291 -> 297        0.15410
```

Excited State 49: Singlet-A" 3.8550 eV 321.62 nm f=0.0000 <S**2>=0.000
268 -> 292 0.68633
268 -> 293 -0.10229

Excited State 50: Singlet-A' 3.8809 eV 319.47 nm f=0.6399 <S**2>=0.000
277 -> 292 0.12191
278 -> 292 0.19795
290 -> 298 -0.19828
291 -> 300 0.57407

Excited State 51: Singlet-A" 3.9163 eV 316.59 nm f=0.0032 <S**2>=0.000
275 -> 292 0.25670
276 -> 292 0.60949
276 -> 293 0.18302

Excited State 52: Singlet-A' 3.9345 eV 315.12 nm f=0.0341 <S**2>=0.000
267 -> 292 0.13002
271 -> 292 -0.23206
271 -> 293 -0.22223
274 -> 292 0.22778
277 -> 292 0.25404
277 -> 293 0.13181
278 -> 292 0.35308
281 -> 293 0.15164
282 -> 293 0.21530

Excited State 53: Singlet-A' 3.9463 eV 314.18 nm f=0.0039 <S**2>=0.000
266 -> 292 -0.23671
267 -> 292 0.62507

Excited State 54: Singlet-A" 3.9702 eV 312.29 nm f=0.0001 <S**2>=0.000
289 -> 298 -0.18352
291 -> 301 0.63523
291 -> 306 -0.13825

Excited State 55: Singlet-A' 3.9936 eV 310.46 nm f=0.0041 <S**2>=0.000
271 -> 292 -0.14322
282 -> 293 -0.12859
285 -> 294 0.15370
287 -> 294 0.62305
288 -> 294 0.13833

Excited State 56: Singlet-A' 4.0049 eV 309.59 nm f=0.0028 <S**2>=0.000
271 -> 292 0.43322
278 -> 293 -0.14632
282 -> 293 0.40627

```
   284 -> 293       -0.14305
   287 -> 294        0.19934

Excited State  57:      Singlet-A"     4.0256 eV  307.99 nm  f=0.0085  <S**2>=0.000
   270 -> 292        0.31070
   280 -> 293        0.13873
   291 -> 302       -0.37984
   291 -> 304       -0.10355
   291 -> 306        0.39532
   291 -> 310       -0.14021

Excited State  58:      Singlet-A'     4.0372 eV  307.10 nm  f=0.0050  <S**2>=0.000
   271 -> 292        0.16518
   278 -> 293       -0.11758
   281 -> 292       -0.10074
   281 -> 293        0.38557
   290 -> 298        0.34468
   291 -> 300        0.20747
   291 -> 303        0.19506
   291 -> 305        0.11801
   291 -> 311       -0.10509

Excited State  59:      Singlet-A"     4.0385 eV  307.01 nm  f=0.0321  <S**2>=0.000
   270 -> 292       -0.13127
   280 -> 292        0.13404
   280 -> 293       -0.35800
   289 -> 298        0.44838
   289 -> 299       -0.10917
   291 -> 301        0.18736
   291 -> 302       -0.14184
   291 -> 306        0.11881

Excited State  60:      Singlet-A'     4.0552 eV  305.74 nm  f=0.0062  <S**2>=0.000
   271 -> 292        0.10453
   274 -> 292       -0.10275
   280 -> 294       -0.10109
   281 -> 292       -0.10571
   281 -> 293        0.41173
   289 -> 297       -0.39816
   290 -> 298       -0.23713
   291 -> 303       -0.12528
```

Table S2.4. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.7** using the M06 exchange correlation functional and twisted geometry.

```
Excited State   1:      Singlet-B      1.2901 eV  961.04 nm  f=0.3551  <S**2>=0.000
    291 -> 292        0.70654
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4801.57278616
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:      Singlet-A      1.5660 eV  791.71 nm  f=0.0000  <S**2>=0.000
    284 -> 297        0.72662
    284 <- 297       -0.21119

 Excited State   3:      Singlet-A      1.7000 eV  729.30 nm  f=0.0004  <S**2>=0.000
    263 -> 297        0.28563
    265 -> 297        0.26180
    285 -> 297        0.41506
    287 -> 297       -0.19318
    288 -> 297        0.38706
    285 <- 297       -0.10369

 Excited State   4:      Singlet-B      1.7776 eV  697.50 nm  f=0.0001  <S**2>=0.000
    264 -> 297        0.26549
    267 -> 297        0.19926
    270 -> 297        0.24386
    278 -> 297        0.12685
    286 -> 297        0.56361
    286 <- 297       -0.13437

 Excited State   5:      Singlet-B      1.8820 eV  658.80 nm  f=0.0265  <S**2>=0.000
    289 -> 294       -0.13412
    290 -> 292        0.52140
    290 -> 293        0.13589
    291 -> 293       -0.43017

 Excited State   6:      Singlet-B      1.9836 eV  625.06 nm  f=0.0609  <S**2>=0.000
    290 -> 292        0.45965
    291 -> 293        0.51197

 Excited State   7:      Singlet-A      2.0501 eV  604.77 nm  f=0.0000  <S**2>=0.000
    289 -> 292        0.56357
    289 -> 293        0.20884
    290 -> 294        0.15894
    291 -> 294       -0.32897

 Excited State   8:      Singlet-B      2.0794 eV  596.26 nm  f=0.0003  <S**2>=0.000
    262 -> 297       -0.52096
```

```
   264 -> 297        0.15059
   270 -> 297       -0.23780
   273 -> 297        0.18809
   278 -> 297        0.13003
   289 -> 297        0.25296

Excited State   9:      Singlet-A      2.1836 eV  567.80 nm  f=1.2568  <S**2>=0.000
   289 -> 292        0.39906
   289 -> 293       -0.11242
   290 -> 294       -0.12329
   291 -> 294        0.55185

Excited State  10:      Singlet-B      2.4211 eV  512.10 nm  f=0.0983  <S**2>=0.000
   288 -> 292       -0.11237
   289 -> 294       -0.32104
   290 -> 293        0.56765
   291 -> 293        0.20481

Excited State  11:      Singlet-A      2.4689 eV  502.18 nm  f=0.5291  <S**2>=0.000
   289 -> 292       -0.12974
   289 -> 293        0.54457
   290 -> 294        0.30975
   291 -> 294        0.26663

Excited State  12:      Singlet-B      2.6901 eV  460.88 nm  f=0.0817  <S**2>=0.000
   287 -> 292        0.46197
   288 -> 292        0.50065

Excited State  13:      Singlet-B      2.7578 eV  449.58 nm  f=0.0660  <S**2>=0.000
   285 -> 293       -0.15860
   287 -> 292        0.47933
   288 -> 292       -0.37356
   288 -> 293       -0.19043
   291 -> 295       -0.21508

Excited State  14:      Singlet-B      2.8444 eV  435.88 nm  f=0.0303  <S**2>=0.000
   285 -> 292       -0.21423
   285 -> 293       -0.13573
   288 -> 292       -0.10215
   288 -> 293       -0.17592
   290 -> 293       -0.14233
   291 -> 295        0.58267

Excited State  15:      Singlet-A      2.8534 eV  434.51 nm  f=1.8154  <S**2>=0.000
   282 -> 292       -0.26050
   286 -> 292       -0.30680
```

```
   289 -> 293       -0.30932
   290 -> 294        0.46657

Excited State  16:      Singlet-B      2.9009 eV  427.41 nm  f=0.7892  <S**2>=0.000
   285 -> 292        0.42121
   285 -> 293        0.15155
   287 -> 292        0.11590
   287 -> 293       -0.12455
   288 -> 292       -0.13246
   288 -> 293        0.26070
   289 -> 294        0.24802
   290 -> 293        0.10788
   291 -> 295        0.30614

Excited State  17:      Singlet-B      2.9247 eV  423.92 nm  f=0.9630  <S**2>=0.000
   285 -> 292       -0.24327
   285 -> 293       -0.12094
   288 -> 293       -0.13395
   289 -> 294        0.53234
   290 -> 293        0.32743

Excited State  18:      Singlet-B      2.9755 eV  416.68 nm  f=0.0073  <S**2>=0.000
   284 -> 292        0.48445
   284 -> 293        0.50500

Excited State  19:      Singlet-A      2.9989 eV  413.43 nm  f=0.0014  <S**2>=0.000
   282 -> 292        0.16616
   286 -> 292        0.49093
   286 -> 293        0.14352
   289 -> 293       -0.17442
   290 -> 294        0.35458
   291 -> 299        0.10609

Excited State  20:      Singlet-B      3.0131 eV  411.49 nm  f=0.2199  <S**2>=0.000
   290 -> 296        0.14445
   291 -> 296        0.68382

Excited State  21:      Singlet-A      3.0867 eV  401.68 nm  f=0.0385  <S**2>=0.000
   290 -> 297       -0.39079
   291 -> 297        0.57054

Excited State  22:      Singlet-A      3.1287 eV  396.28 nm  f=0.0258  <S**2>=0.000
   282 -> 292       -0.25596
   283 -> 292        0.57503
   286 -> 292        0.11971
   286 -> 293        0.12335
```

291 -> 299 -0.17228

Excited State 23: Singlet-A 3.1889 eV 388.79 nm f=0.0079 <S**2>=0.000
282 -> 292 -0.31872
283 -> 292 -0.35120
285 -> 294 0.11166
286 -> 292 0.14271
286 -> 293 0.38815
288 -> 294 0.13251
291 -> 298 0.10391

Excited State 24: Singlet-B 3.2283 eV 384.05 nm f=0.0250 <S**2>=0.000
285 -> 292 0.43753
285 -> 293 -0.20450
287 -> 292 -0.13663
287 -> 293 0.14968
288 -> 292 0.22915
288 -> 293 -0.39496

Excited State 25: Singlet-A 3.3768 eV 367.16 nm f=0.1704 <S**2>=0.000
282 -> 292 -0.12071
283 -> 292 -0.11234
285 -> 294 -0.12106
286 -> 292 0.28438
286 -> 293 -0.29846
288 -> 294 -0.24528
291 -> 298 0.41359

Excited State 26: Singlet-B 3.4105 eV 363.53 nm f=0.0095 <S**2>=0.000
286 -> 294 0.67352
289 -> 297 -0.10964

Excited State 27: Singlet-B 3.4309 eV 361.38 nm f=0.0018 <S**2>=0.000
262 -> 297 0.23033
286 -> 294 0.11162
289 -> 297 0.64082

Excited State 28: Singlet-A 3.4328 eV 361.18 nm f=0.0539 <S**2>=0.000
283 -> 292 0.10546
286 -> 292 -0.14009
286 -> 293 0.16263
290 -> 299 0.11835
291 -> 298 0.44157
291 -> 299 0.44459

Excited State 29: Singlet-A 3.4659 eV 357.72 nm f=0.0284 <S**2>=0.000

```
   284 -> 294        0.68001
   288 -> 294       -0.14152

Excited State  30:      Singlet-B      3.4711 eV  357.19 nm  f=0.0007  <S**2>=0.000
   284 -> 292        0.50404
   284 -> 293       -0.47154
   285 -> 293       -0.10569

Excited State  31:      Singlet-A      3.5023 eV  354.01 nm  f=0.3388  <S**2>=0.000
   282 -> 292        0.11956
   284 -> 294        0.14568
   285 -> 294        0.25815
   286 -> 293       -0.25903
   287 -> 294       -0.17448
   288 -> 294        0.46117
   291 -> 298        0.16040
   291 -> 299       -0.19744

Excited State  32:      Singlet-A      3.5067 eV  353.56 nm  f=0.7168  <S**2>=0.000
   282 -> 292       -0.37806
   286 -> 292        0.12701
   286 -> 293       -0.29354
   288 -> 294        0.13392
   291 -> 298       -0.20440
   291 -> 299        0.39595

Excited State  33:      Singlet-B      3.5109 eV  353.14 nm  f=0.0712  <S**2>=0.000
   285 -> 293       -0.19413
   288 -> 293        0.13400
   290 -> 295        0.63239

Excited State  34:      Singlet-B      3.5665 eV  347.64 nm  f=0.0548  <S**2>=0.000
   284 -> 293       -0.11491
   285 -> 293        0.50687
   288 -> 293       -0.35426
   290 -> 295        0.24913

Excited State  35:      Singlet-A      3.5779 eV  346.52 nm  f=0.0002  <S**2>=0.000
   277 -> 292        0.33637
   281 -> 292        0.58331
   281 -> 293        0.10310

Excited State  36:      Singlet-B      3.6018 eV  344.22 nm  f=0.0018  <S**2>=0.000
   279 -> 292        0.58843
   280 -> 292        0.36462
```

Excited State 37: Singlet-A 3.6371 eV 340.88 nm f=0.0504 <S**2>=0.000
273 -> 292 0.10718
273 -> 293 0.13851
275 -> 292 -0.22107
277 -> 292 0.10965
278 -> 292 0.34365
278 -> 293 0.14362
282 -> 293 0.19014
285 -> 294 -0.13869
289 -> 295 0.39231

Excited State 38: Singlet-A 3.6601 eV 338.74 nm f=0.0187 <S**2>=0.000
273 -> 293 -0.12607
275 -> 292 0.18767
278 -> 292 -0.30346
278 -> 293 -0.14208
289 -> 295 0.53143

Excited State 39: Singlet-A 3.7178 eV 333.48 nm f=0.0030 <S**2>=0.000
290 -> 297 0.56347
291 -> 297 0.38924

Excited State 40: Singlet-B 3.7246 eV 332.88 nm f=0.0141 <S**2>=0.000
274 -> 292 0.61781
276 -> 292 -0.16210
279 -> 292 -0.17499
280 -> 292 0.20978

Excited State 41: Singlet-A 3.7443 eV 331.13 nm f=0.0004 <S**2>=0.000
273 -> 292 0.41832
273 -> 293 0.13233
275 -> 292 0.40023
277 -> 292 -0.27983
278 -> 293 0.11444
282 -> 293 0.12640

Excited State 42: Singlet-B 3.7570 eV 330.01 nm f=0.0164 <S**2>=0.000
285 -> 293 0.18238
287 -> 293 0.65071
288 -> 293 0.14885

Excited State 43: Singlet-B 3.7867 eV 327.42 nm f=0.0030 <S**2>=0.000
269 -> 292 -0.10590
274 -> 292 -0.24505
279 -> 292 -0.30070
280 -> 292 0.49372

```
   280 -> 293        0.22134
   285 -> 293        0.11001

Excited State  44:      Singlet-A      3.8021 eV  326.09 nm  f=0.0011  <S**2>=0.000
   273 -> 292        0.18140
   275 -> 292        0.18837
   277 -> 292        0.46240
   277 -> 293        0.18266
   278 -> 292       -0.14498
   281 -> 292       -0.28396
   281 -> 293       -0.19918

Excited State  45:      Singlet-B      3.8212 eV  324.46 nm  f=0.0000  <S**2>=0.000
   271 -> 292        0.69019

Excited State  46:      Singlet-A      3.8215 eV  324.44 nm  f=0.0086  <S**2>=0.000
   272 -> 292        0.68220

Excited State  47:      Singlet-A      3.8274 eV  323.94 nm  f=0.0424  <S**2>=0.000
   285 -> 294        0.52588
   287 -> 294       -0.11548
   288 -> 294       -0.31579
   289 -> 295        0.14020

Excited State  48:      Singlet-A      3.8585 eV  321.32 nm  f=0.0008  <S**2>=0.000
   267 -> 292       -0.12299
   268 -> 292        0.66002
   268 -> 293       -0.10593

Excited State  49:      Singlet-B      3.8754 eV  319.93 nm  f=0.0211  <S**2>=0.000
   290 -> 296        0.66114
   291 -> 296       -0.14997

Excited State  50:      Singlet-B      3.9046 eV  317.53 nm  f=0.0058  <S**2>=0.000
   266 -> 292        0.11465
   269 -> 292        0.17050
   274 -> 292        0.14140
   276 -> 292        0.60606
   276 -> 293        0.20133

Excited State  51:      Singlet-A      3.9054 eV  317.47 nm  f=0.0120  <S**2>=0.000
   273 -> 292       -0.15529
   273 -> 293       -0.18912
   275 -> 292        0.36393
   275 -> 293        0.19344
   277 -> 292        0.10629
```

```
   278 -> 292       0.43134
   281 -> 293      -0.10398
   282 -> 293      -0.16294

Excited State  52:      Singlet-A      3.9094 eV  317.14 nm  f=0.2494  <S**2>=0.000
   270 -> 292       0.18005
   270 -> 293       0.11969
   273 -> 292      -0.15425
   278 -> 292      -0.11369
   282 -> 293       0.35370
   283 -> 293       0.10351
   290 -> 298       0.19690
   290 -> 299      -0.13805
   291 -> 300       0.33911
   291 -> 302      -0.11660

Excited State  53:      Singlet-B      3.9396 eV  314.71 nm  f=0.0003  <S**2>=0.000
   265 -> 292      -0.20496
   266 -> 292       0.57195
   269 -> 292       0.22116
   276 -> 292      -0.16987

Excited State  54:      Singlet-A      3.9508 eV  313.82 nm  f=0.1431  <S**2>=0.000
   273 -> 292       0.33981
   275 -> 292      -0.17396
   278 -> 293      -0.18051
   281 -> 293      -0.14952
   282 -> 293      -0.30323
   283 -> 293      -0.10535
   290 -> 298       0.12089
   291 -> 300       0.34697

Excited State  55:      Singlet-A      3.9948 eV  310.36 nm  f=0.0062  <S**2>=0.000
   270 -> 292      -0.12377
   273 -> 292      -0.12330
   278 -> 293       0.11188
   285 -> 294      -0.10883
   287 -> 294      -0.29698
   291 -> 300       0.39521
   291 -> 302       0.34998
   291 -> 306       0.10957
   291 -> 310      -0.10114

Excited State  56:      Singlet-B      4.0098 eV  309.20 nm  f=0.0023  <S**2>=0.000
   266 -> 292       0.13206
   269 -> 292      -0.24763
```

291 -> 301 0.48881
291 -> 303 -0.32397

Excited State 57: Singlet-A 4.0101 eV 309.18 nm f=0.0006 <S**2>=0.000
281 -> 293 0.13377
285 -> 294 0.17467
287 -> 294 0.56187
288 -> 294 0.14034
290 -> 298 -0.10303
291 -> 300 0.12104
291 -> 302 0.22163

Excited State 58: Singlet-B 4.0293 eV 307.71 nm f=0.0004 <S**2>=0.000
266 -> 292 -0.12368
269 -> 292 0.30526
280 -> 293 0.12819
291 -> 301 0.45398
291 -> 303 0.28246
291 -> 305 -0.16315

Excited State 59: Singlet-A 4.0338 eV 307.36 nm f=0.0121 <S**2>=0.000
277 -> 292 0.15515
278 -> 293 -0.18342
281 -> 292 -0.17672
281 -> 293 0.58744

Excited State 60: Singlet-B 4.0564 eV 305.65 nm f=0.0699 <S**2>=0.000
266 -> 292 0.10449
269 -> 292 -0.30027
280 -> 292 0.11010
280 -> 293 -0.32744
291 -> 303 0.44362
291 -> 305 -0.10858

Table S2.5. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.2** using the B3LYP exchange correlation functional and bent geometry.

Excited State 1: Singlet-A' 1.7537 eV 707.00 nm f=0.0001 <S**2>=0.000
239 -> 251 -0.10790
241 -> 251 0.69862
241 <- 251 -0.15203
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4338.93952600
Copying the excited state density for this state as the 1-particle RhoCI density.

```
Excited State   2:      Singlet-A"     1.8646 eV  664.93 nm  f=0.0000  <S**2>=0.000
   223 -> 251        0.30938
   225 -> 251        0.13614
   240 -> 251        0.29200
   244 -> 251        0.53715

Excited State   3:      Singlet-A'     1.9362 eV  640.34 nm  f=0.0000  <S**2>=0.000
   224 -> 251        0.15505
   226 -> 251        0.31056
   243 -> 251        0.59993

Excited State   4:      Singlet-A'     2.0745 eV  597.65 nm  f=0.5248  <S**2>=0.000
   245 -> 248       -0.23300
   246 -> 247        0.64661
   246 -> 250        0.12707

Excited State   5:      Singlet-A"     2.1041 eV  589.24 nm  f=0.0373  <S**2>=0.000
   245 -> 247        0.32465
   245 -> 250        0.16298
   246 -> 248        0.59607
   246 -> 249        0.10035

Excited State   6:      Singlet-A'     2.3290 eV  532.36 nm  f=0.8656  <S**2>=0.000
   245 -> 248        0.58932
   246 -> 247        0.26870
   246 -> 250       -0.25774

Excited State   7:      Singlet-A"     2.3456 eV  528.59 nm  f=0.1714  <S**2>=0.000
   245 -> 247        0.55547
   246 -> 248       -0.34526
   246 -> 249        0.26000

Excited State   8:      Singlet-A"     2.5158 eV  492.82 nm  f=0.1144  <S**2>=0.000
   245 -> 247       -0.28758
   245 -> 250        0.27179
   246 -> 249        0.58002

Excited State   9:      Singlet-A"     2.5909 eV  478.53 nm  f=0.0000  <S**2>=0.000
   212 -> 251        0.10789
   222 -> 251        0.64337
   246 -> 251        0.24173

Excited State  10:      Singlet-A'     2.6022 eV  476.47 nm  f=0.0639  <S**2>=0.000
   245 -> 248       -0.25522
   245 -> 249        0.51475
   246 -> 250       -0.39519
```

Excited State 11: Singlet-A" 2.7716 eV 447.34 nm f=0.0171 <S**2>=0.000
240 -> 248 0.14716
244 -> 248 0.57723
244 -> 249 0.23574
245 -> 250 0.13751
246 -> 251 -0.21600

Excited State 12: Singlet-A" 2.7925 eV 443.99 nm f=0.0051 <S**2>=0.000
222 -> 251 -0.23943
244 -> 248 0.18175
246 -> 251 0.61596

Excited State 13: Singlet-A' 2.8000 eV 442.80 nm f=0.0151 <S**2>=0.000
245 -> 251 0.68549

Excited State 14: Singlet-A' 2.8311 eV 437.94 nm f=1.2199 <S**2>=0.000
244 -> 247 -0.23291
245 -> 248 0.13288
245 -> 249 0.39901
246 -> 250 0.47745

Excited State 15: Singlet-A' 2.8826 eV 430.11 nm f=0.0006 <S**2>=0.000
241 -> 248 0.63579
241 -> 249 0.27380
243 -> 248 -0.10354

Excited State 16: Singlet-A" 2.9176 eV 424.95 nm f=1.0576 <S**2>=0.000
240 -> 248 -0.11085
244 -> 248 -0.12953
245 -> 250 0.59803
246 -> 248 -0.14130
246 -> 249 -0.27197

Excited State 17: Singlet-A' 2.9726 eV 417.09 nm f=0.2092 <S**2>=0.000
243 -> 248 0.24426
244 -> 247 0.56433
244 -> 250 0.14327
245 -> 249 0.20651
246 -> 250 0.14983

Excited State 18: Singlet-A" 3.0418 eV 407.60 nm f=0.0060 <S**2>=0.000
241 -> 247 -0.10283
243 -> 247 0.61132
243 -> 250 0.30645

```
Excited State  19:      Singlet-A"     3.0654 eV  404.47 nm  f=0.0077  <S**2>=0.000
    241 -> 247        0.58570
    241 -> 250        0.36545
    243 -> 247        0.11958

Excited State  20:      Singlet-A'     3.0872 eV  401.61 nm  f=0.2351  <S**2>=0.000
    240 -> 247       -0.17641
    242 -> 247        0.53799
    243 -> 248       -0.30774
    243 -> 249       -0.12845
    244 -> 247        0.12372
    244 -> 250       -0.12856

Excited State  21:      Singlet-A'     3.1582 eV  392.58 nm  f=0.0009  <S**2>=0.000
    240 -> 247        0.13004
    242 -> 247        0.40636
    243 -> 248        0.42624
    243 -> 249        0.16241
    244 -> 247       -0.26880

Excited State  22:      Singlet-A'     3.2237 eV  384.60 nm  f=0.0000  <S**2>=0.000
    227 -> 248       -0.16116
    227 -> 249        0.14846
    230 -> 247        0.62661
    230 -> 250       -0.19394
    231 -> 247       -0.10100

Excited State  23:      Singlet-A'     3.2332 eV  383.47 nm  f=0.1000  <S**2>=0.000
    240 -> 247        0.61648
    243 -> 248       -0.24775

Excited State  24:      Singlet-A"     3.2487 eV  381.64 nm  f=0.0213  <S**2>=0.000
    240 -> 248        0.51365
    242 -> 248       -0.21840
    244 -> 248       -0.24700
    244 -> 249        0.21202
    246 -> 252       -0.25121

Excited State  25:      Singlet-A"     3.3316 eV  372.14 nm  f=0.0136  <S**2>=0.000
    240 -> 248        0.19116
    242 -> 248        0.57430
    242 -> 249       -0.23415
    246 -> 252       -0.22151

Excited State  26:      Singlet-A"     3.3553 eV  369.52 nm  f=0.0198  <S**2>=0.000
    240 -> 248        0.16751
```

```
   242 -> 248        0.16740
   244 -> 248       -0.14634
   244 -> 249        0.24060
   246 -> 252        0.57362

Excited State  27:      Singlet-A"     3.3803 eV  366.78 nm  f=0.0002  <S**2>=0.000
   227 -> 247        0.53480
   227 -> 250       -0.17645
   230 -> 248       -0.31089
   230 -> 249        0.25803

Excited State  28:      Singlet-A"     3.3994 eV  364.73 nm  f=0.1315  <S**2>=0.000
   240 -> 248       -0.33710
   244 -> 248       -0.11302
   244 -> 249        0.56627
   246 -> 252       -0.17598

Excited State  29:      Singlet-A'     3.4732 eV  356.98 nm  f=0.0113  <S**2>=0.000
   240 -> 247       -0.13964
   243 -> 248       -0.16184
   244 -> 247       -0.12728
   244 -> 250        0.61515
   245 -> 252        0.19297

Excited State  30:      Singlet-A"     3.4981 eV  354.43 nm  f=0.0102  <S**2>=0.000
   233 -> 247       -0.12804
   239 -> 247       -0.20142
   240 -> 249        0.10983
   242 -> 248       -0.13412
   243 -> 247       -0.26032
   243 -> 250        0.54708

Excited State  31:      Singlet-A'     3.5159 eV  352.64 nm  f=0.1733  <S**2>=0.000
   243 -> 249        0.25016
   244 -> 250       -0.20022
   245 -> 252        0.60342

Excited State  32:      Singlet-A'     3.5320 eV  351.04 nm  f=0.3419  <S**2>=0.000
   239 -> 248       -0.13961
   240 -> 247       -0.13483
   243 -> 248       -0.17215
   243 -> 249        0.56710
   245 -> 252       -0.26237

Excited State  33:      Singlet-A"     3.5861 eV  345.74 nm  f=0.0015  <S**2>=0.000
   239 -> 247       -0.16518
```

```
   241 -> 247       -0.34805
   241 -> 250        0.52836
   243 -> 247        0.12242
   243 -> 250       -0.18188

Excited State  34:      Singlet-A'     3.6101 eV  343.44 nm  f=0.0138  <S**2>=0.000
   241 -> 248       -0.27319
   241 -> 249        0.62521
   241 -> 252       -0.11230
   243 -> 249       -0.11618

Excited State  35:      Singlet-A"     3.6321 eV  341.35 nm  f=0.0619  <S**2>=0.000
   239 -> 247       -0.21348
   240 -> 249        0.51754
   241 -> 247        0.12267
   241 -> 250       -0.20089
   242 -> 249       -0.22002
   243 -> 247        0.11051
   243 -> 250       -0.15683

Excited State  36:      Singlet-A'     3.6721 eV  337.64 nm  f=0.0079  <S**2>=0.000
   229 -> 248       -0.10076
   235 -> 248       -0.12251
   239 -> 248        0.61311
   239 -> 249        0.17715
   243 -> 249        0.12128

Excited State  37:      Singlet-A"     3.6795 eV  336.95 nm  f=0.0366  <S**2>=0.000
   233 -> 247        0.13569
   239 -> 247        0.47031
   240 -> 249        0.38972
   241 -> 250        0.14362
   242 -> 248        0.12155
   243 -> 250        0.12461

Excited State  38:      Singlet-A"     3.7226 eV  333.05 nm  f=0.0008  <S**2>=0.000
   239 -> 247       -0.24206
   240 -> 249        0.16229
   242 -> 248        0.21478
   242 -> 249        0.58746

Excited State  39:      Singlet-A'     3.7501 eV  330.61 nm  f=0.0440  <S**2>=0.000
   236 -> 247        0.26573
   240 -> 250        0.54166
   242 -> 250       -0.20313
   246 -> 253       -0.24116
```

Excited State 40: Singlet-A" 3.7524 eV 330.41 nm f=0.0011 <S**2>=0.000
232 -> 247 0.10159
235 -> 247 0.17568
238 -> 247 0.63568
238 -> 250 0.11481
239 -> 247 -0.11605

Excited State 41: Singlet-A' 3.7582 eV 329.90 nm f=0.0026 <S**2>=0.000
235 -> 248 0.11006
236 -> 247 -0.18883
238 -> 248 0.59219
238 -> 249 0.13162
246 -> 253 -0.25706

Excited State 42: Singlet-A" 3.7933 eV 326.85 nm f=0.0186 <S**2>=0.000
236 -> 248 0.15907
237 -> 248 0.62967
237 -> 249 0.21821

Excited State 43: Singlet-A' 3.7956 eV 326.65 nm f=0.0085 <S**2>=0.000
236 -> 247 0.47654
237 -> 247 0.32629
237 -> 250 0.10590
238 -> 248 0.21725
240 -> 250 -0.15636
246 -> 253 0.20110

Excited State 44: Singlet-A' 3.8104 eV 325.38 nm f=0.0623 <S**2>=0.000
236 -> 247 -0.26702
237 -> 247 0.14405
238 -> 248 0.13282
239 -> 248 0.10335
240 -> 250 0.27421
242 -> 250 -0.13351
246 -> 253 0.49958

Excited State 45: Singlet-A" 3.8327 eV 323.49 nm f=0.0006 <S**2>=0.000
232 -> 247 0.17358
235 -> 247 -0.24619
236 -> 248 0.56581
237 -> 248 -0.16265
238 -> 247 0.11329

Excited State 46: Singlet-A' 3.8359 eV 323.22 nm f=0.0983 <S**2>=0.000
233 -> 248 -0.14612

235 -> 248 -0.12966
236 -> 247 -0.19366
237 -> 247 0.53624
237 -> 250 0.14996
238 -> 248 -0.13534
246 -> 253 -0.20733

Excited State 47: Singlet-A" 3.8523 eV 321.85 nm f=0.0150 <S**2>=0.000
229 -> 247 0.22318
232 -> 247 -0.26753
233 -> 247 0.29903
235 -> 247 0.28712
236 -> 248 0.32928
239 -> 247 -0.17047
239 -> 250 -0.16025
242 -> 249 -0.13662

Excited State 48: Singlet-A' 3.8599 eV 321.21 nm f=0.0134 <S**2>=0.000
229 -> 248 -0.10885
233 -> 248 -0.11202
240 -> 250 0.23533
242 -> 247 0.13979
242 -> 250 0.55559

Excited State 49: Singlet-A' 3.8945 eV 318.36 nm f=0.2626 <S**2>=0.000
228 -> 248 -0.11733
231 -> 247 0.32559
233 -> 248 0.19654
234 -> 247 -0.13130
235 -> 248 0.41643
236 -> 247 -0.12736
238 -> 248 -0.10345
239 -> 248 0.10834
239 -> 249 -0.11162
242 -> 250 0.22156

Excited State 50: Singlet-A" 3.9137 eV 316.79 nm f=0.0104 <S**2>=0.000
229 -> 247 -0.28484
233 -> 247 -0.23642
234 -> 248 -0.14772
235 -> 247 0.46137
235 -> 250 0.10587
236 -> 248 0.11190
239 -> 250 0.15916
245 -> 253 0.17379

Excited State 51: Singlet-A" 3.9292 eV 315.55 nm f=0.0000 <S**2>=0.000
227 -> 247 0.39113
230 -> 248 0.48427
230 -> 249 -0.24933
245 -> 253 0.12895

Excited State 52: Singlet-A" 3.9362 eV 314.99 nm f=0.0028 <S**2>=0.000
230 -> 248 -0.10322
234 -> 248 0.21329
245 -> 253 0.61713

Excited State 53: Singlet-A' 3.9397 eV 314.71 nm f=0.2012 <S**2>=0.000
229 -> 248 0.17453
231 -> 247 -0.34301
232 -> 248 0.18897
233 -> 248 0.36151
234 -> 247 0.26790
237 -> 247 0.15707
239 -> 249 -0.13037

Excited State 54: Singlet-A' 3.9447 eV 314.31 nm f=0.0443 <S**2>=0.000
231 -> 247 -0.31681
233 -> 248 -0.25152
235 -> 248 0.47299
239 -> 249 0.17618

Excited State 55: Singlet-A" 3.9730 eV 312.07 nm f=0.0206 <S**2>=0.000
231 -> 248 -0.20774
232 -> 247 0.53141
233 -> 247 0.26292
235 -> 247 0.19870
238 -> 247 -0.12922

Excited State 56: Singlet-A" 3.9780 eV 311.67 nm f=0.0011 <S**2>=0.000
229 -> 247 -0.15600
231 -> 248 -0.19553
232 -> 247 -0.13545
233 -> 247 -0.11112
234 -> 248 0.54997
234 -> 249 0.15416
245 -> 253 -0.20664

Excited State 57: Singlet-A' 3.9863 eV 311.03 nm f=0.1246 <S**2>=0.000
229 -> 248 0.14495
232 -> 248 0.56485
234 -> 247 -0.29489

234 -> 250 -0.10426
235 -> 248 -0.10005

Excited State 58: Singlet-A' 4.0130 eV 308.96 nm f=0.2799 <S**2>=0.000
228 -> 248 0.11608
229 -> 248 -0.30312
231 -> 247 0.28675
232 -> 248 0.25854
233 -> 248 0.12292
233 -> 249 0.13894
234 -> 247 0.36029
234 -> 250 0.11442
239 -> 249 0.16234

Excited State 59: Singlet-A" 4.0131 eV 308.95 nm f=0.0001 <S**2>=0.000
229 -> 247 -0.14348
230 -> 248 0.10003
231 -> 248 0.57895
233 -> 247 0.18873
233 -> 250 0.10799
234 -> 248 0.21244
234 -> 249 0.11766

Excited State 60: Singlet-A' 4.0344 eV 307.32 nm f=0.0206 <S**2>=0.000
229 -> 248 0.31027
231 -> 247 0.19192
233 -> 248 -0.35482
233 -> 249 -0.16412
234 -> 247 0.38114
239 -> 249 -0.14595

Table S2.6. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.2** using the B3LYP exchange correlation functional and twisted geometry.

Excited State 1: Singlet-A 2.0391 eV 608.04 nm f=0.0019 <S**2>=0.000
242 -> 252 0.69588
242 <- 252 -0.13014
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4338.93212113
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.0910 eV 592.95 nm f=0.5007 <S**2>=0.000
245 -> 248 -0.25358
246 -> 247 0.63759
246 -> 250 -0.13465

Excited State 3: Singlet-B 2.1076 eV 588.27 nm f=0.0559 <S**2>=0.000
245 -> 247 0.30460
245 -> 250 -0.16772
246 -> 248 0.60702

Excited State 4: Singlet-A 2.1597 eV 574.08 nm f=0.0096 <S**2>=0.000
223 -> 252 0.25883
225 -> 252 0.19115
240 -> 252 0.24554
244 -> 252 0.56130

Excited State 5: Singlet-B 2.2235 eV 557.60 nm f=0.0014 <S**2>=0.000
224 -> 252 0.16800
226 -> 252 0.28409
243 -> 252 0.60797

Excited State 6: Singlet-A 2.3400 eV 529.86 nm f=0.8953 <S**2>=0.000
245 -> 248 0.57656
246 -> 247 0.28605
246 -> 250 0.26104

Excited State 7: Singlet-B 2.3770 eV 521.60 nm f=0.1533 <S**2>=0.000
245 -> 247 0.56392
246 -> 248 -0.32201
246 -> 249 0.26745

Excited State 8: Singlet-B 2.5346 eV 489.17 nm f=0.1028 <S**2>=0.000
245 -> 247 -0.28932
245 -> 250 -0.26107
246 -> 249 0.58133

Excited State 9: Singlet-B 2.6122 eV 474.63 nm f=0.0081 <S**2>=0.000
222 -> 252 -0.49773
228 -> 252 -0.15481
230 -> 252 0.14417
232 -> 252 -0.10628
245 -> 252 0.39266

Excited State 10: Singlet-A 2.6358 eV 470.39 nm f=0.1282 <S**2>=0.000
245 -> 248 -0.25493
245 -> 249 0.51572
246 -> 250 0.39443

Excited State 11: Singlet-B 2.7163 eV 456.45 nm f=0.0019 <S**2>=0.000
240 -> 248 0.13390

```
   244 -> 248       0.63105
   244 -> 249       0.23490

Excited State  12:      Singlet-B      2.7710 eV  447.43 nm  f=0.0011  <S**2>=0.000
   242 -> 248       0.65309
   242 -> 249       0.25317

Excited State  13:      Singlet-A      2.8429 eV  436.12 nm  f=1.0277  <S**2>=0.000
   243 -> 248       0.10242
   244 -> 247      -0.28183
   244 -> 250       0.10711
   245 -> 248      -0.13071
   245 -> 249      -0.37902
   246 -> 250       0.45777

Excited State  14:      Singlet-A      2.9458 eV  420.88 nm  f=0.2768  <S**2>=0.000
   242 -> 247       0.10220
   243 -> 248      -0.32367
   244 -> 247       0.48010
   244 -> 250      -0.15722
   245 -> 249      -0.23100
   246 -> 250       0.17641

Excited State  15:      Singlet-B      2.9461 eV  420.84 nm  f=0.9548  <S**2>=0.000
   245 -> 250       0.60657
   246 -> 248       0.14842
   246 -> 249       0.26218

Excited State  16:      Singlet-A      2.9769 eV  416.49 nm  f=0.0363  <S**2>=0.000
   242 -> 247       0.57706
   242 -> 250      -0.36994

Excited State  17:      Singlet-B      3.0091 eV  412.04 nm  f=0.0231  <S**2>=0.000
   243 -> 247       0.61570
   243 -> 250      -0.31713

Excited State  18:      Singlet-A      3.0593 eV  405.27 nm  f=0.0929  <S**2>=0.000
   240 -> 247      -0.10612
   241 -> 247       0.27916
   243 -> 248       0.47051
   243 -> 249       0.17103
   244 -> 247       0.32973
   246 -> 252       0.14111

Excited State  19:      Singlet-A      3.1158 eV  397.93 nm  f=0.1041  <S**2>=0.000
   240 -> 247      -0.12239
```

```
   241 -> 247        0.55837
   243 -> 248       -0.18137
   244 -> 247       -0.13599
   246 -> 252       -0.29673

Excited State  20:      Singlet-A      3.1529 eV  393.24 nm  f=0.0023  <S**2>=0.000
   241 -> 247        0.22692
   243 -> 248       -0.18652
   244 -> 247       -0.13800
   246 -> 252        0.60787

Excited State  21:      Singlet-B      3.2234 eV  384.64 nm  f=0.0000  <S**2>=0.000
   227 -> 248       -0.15216
   227 -> 249        0.15577
   229 -> 247        0.63311
   229 -> 250        0.19118

Excited State  22:      Singlet-A      3.2507 eV  381.41 nm  f=0.0518  <S**2>=0.000
   240 -> 247        0.61088
   241 -> 247        0.15056
   243 -> 248        0.14693
   244 -> 250       -0.15882

Excited State  23:      Singlet-B      3.2796 eV  378.05 nm  f=0.0306  <S**2>=0.000
   240 -> 248        0.48519
   241 -> 248       -0.24178
   244 -> 248       -0.21976
   244 -> 249        0.27687
   246 -> 251        0.22275

Excited State  24:      Singlet-B      3.3338 eV  371.90 nm  f=0.0064  <S**2>=0.000
   240 -> 248        0.21961
   241 -> 248        0.58169
   241 -> 249       -0.25089
   246 -> 251        0.14679

Excited State  25:      Singlet-B      3.3717 eV  367.72 nm  f=0.0015  <S**2>=0.000
   240 -> 248       -0.11705
   244 -> 248       -0.15262
   244 -> 249        0.48275
   246 -> 251       -0.44675

Excited State  26:      Singlet-A      3.3818 eV  366.62 nm  f=0.0000  <S**2>=0.000
   227 -> 247        0.53875
   227 -> 250        0.17339
   229 -> 248       -0.29763
```

```
   229 -> 249        0.27291

Excited State  27:      Singlet-B      3.3859 eV  366.18 nm  f=0.0004  <S**2>=0.000
   222 -> 252        0.35784
   245 -> 252        0.56711

Excited State  28:      Singlet-B      3.4080 eV  363.80 nm  f=0.1822  <S**2>=0.000
   240 -> 248       -0.37880
   243 -> 250        0.10657
   244 -> 249        0.32988
   245 -> 252       -0.11360
   246 -> 251        0.43022

Excited State  29:      Singlet-A      3.4457 eV  359.82 nm  f=0.0342  <S**2>=0.000
   240 -> 247        0.17962
   243 -> 248       -0.10534
   244 -> 247        0.15898
   244 -> 250        0.63287

Excited State  30:      Singlet-B      3.4733 eV  356.97 nm  f=0.0041  <S**2>=0.000
   239 -> 247        0.15962
   241 -> 248       -0.13283
   243 -> 247        0.28397
   243 -> 250        0.55736
   246 -> 251       -0.11985

Excited State  31:      Singlet-A      3.5047 eV  353.76 nm  f=0.1833  <S**2>=0.000
   242 -> 247        0.30939
   242 -> 250        0.46760
   243 -> 248       -0.14199
   243 -> 249        0.37599

Excited State  32:      Singlet-A      3.5119 eV  353.04 nm  f=0.2554  <S**2>=0.000
   240 -> 247        0.13517
   242 -> 247       -0.22165
   242 -> 250       -0.35362
   243 -> 248       -0.14860
   243 -> 249        0.49586
   245 -> 251        0.10733

Excited State  33:      Singlet-B      3.5345 eV  350.79 nm  f=0.0007  <S**2>=0.000
   242 -> 248       -0.24827
   242 -> 249        0.64997
   242 -> 251       -0.11410

Excited State  34:      Singlet-A      3.5600 eV  348.27 nm  f=0.0003  <S**2>=0.000
```

245 -> 251 0.67097

Excited State 35: Singlet-A 3.6237 eV 342.15 nm f=0.0013 <S**2>=0.000
230 -> 248 0.14725
238 -> 248 -0.10920
239 -> 248 0.61415
239 -> 249 0.17991
243 -> 249 0.11773

Excited State 36: Singlet-B 3.6247 eV 342.05 nm f=0.0169 <S**2>=0.000
232 -> 247 0.14521
233 -> 247 -0.12446
238 -> 247 -0.13150
239 -> 247 0.45268
240 -> 249 0.27723
241 -> 248 -0.14093
241 -> 249 -0.21286
243 -> 247 -0.15277
243 -> 250 -0.20868

Excited State 37: Singlet-B 3.6975 eV 335.32 nm f=0.0686 <S**2>=0.000
239 -> 247 -0.34077
240 -> 249 0.57749

Excited State 38: Singlet-B 3.7059 eV 334.56 nm f=0.0092 <S**2>=0.000
239 -> 247 0.22806
240 -> 249 0.21445
241 -> 248 0.22907
241 -> 249 0.57380

Excited State 39: Singlet-A 3.7368 eV 331.79 nm f=0.0005 <S**2>=0.000
235 -> 248 0.12049
236 -> 247 -0.22599
238 -> 248 0.61591
238 -> 249 0.13137
239 -> 248 0.11464

Excited State 40: Singlet-B 3.7414 eV 331.38 nm f=0.0025 <S**2>=0.000
233 -> 247 0.13286
235 -> 247 0.22052
236 -> 248 -0.16674
238 -> 247 0.58620
239 -> 247 0.10703
241 -> 249 -0.13685

Excited State 41: Singlet-A 3.7875 eV 327.35 nm f=0.0009 <S**2>=0.000

```
   235 -> 248       -0.10381
   236 -> 247        0.50831
   237 -> 247        0.37599
   238 -> 248        0.22996

Excited State  42:      Singlet-B      3.7937 eV  326.82 nm  f=0.0046  <S**2>=0.000
   236 -> 248        0.30540
   237 -> 248        0.57554
   237 -> 249        0.14377
   238 -> 247        0.16926

Excited State  43:      Singlet-A      3.8066 eV  325.70 nm  f=0.0403  <S**2>=0.000
   237 -> 247        0.10222
   240 -> 250        0.57772
   241 -> 250       -0.21617
   246 -> 253        0.27162

Excited State  44:      Singlet-B      3.8322 eV  323.53 nm  f=0.0093  <S**2>=0.000
   230 -> 247        0.12302
   232 -> 247       -0.11833
   233 -> 247        0.13642
   236 -> 248        0.55239
   237 -> 248       -0.28420
   237 -> 249       -0.13228

Excited State  45:      Singlet-B      3.8423 eV  322.68 nm  f=0.0034  <S**2>=0.000
   230 -> 247       -0.16439
   232 -> 247        0.48927
   233 -> 247       -0.17963
   235 -> 247        0.14390
   236 -> 248        0.20308
   238 -> 247        0.14032
   239 -> 247       -0.14973
   239 -> 250        0.16287
   241 -> 249        0.13877

Excited State  46:      Singlet-A      3.8480 eV  322.21 nm  f=0.5495  <S**2>=0.000
   228 -> 249       -0.12212
   230 -> 248        0.27925
   232 -> 248       -0.30460
   233 -> 248        0.26332
   239 -> 248       -0.13832
   239 -> 249        0.17143
   241 -> 250        0.30952
   243 -> 249       -0.10311
   246 -> 253        0.11260
```

Excited State 47: Singlet-A 3.8618 eV 321.06 nm f=0.0067 <S**2>=0.000

233 -> 248	-0.16807
235 -> 248	-0.24222
236 -> 247	-0.26678
237 -> 247	0.24235
237 -> 250	-0.10754
240 -> 250	-0.12359
241 -> 250	0.20233
246 -> 253	0.40796

Excited State 48: Singlet-A 3.8788 eV 319.64 nm f=0.0190 <S**2>=0.000

232 -> 248	0.10945
235 -> 248	0.39725
236 -> 247	0.19539
237 -> 247	-0.12199
240 -> 250	-0.18500
246 -> 253	0.42526

Excited State 49: Singlet-A 3.8840 eV 319.22 nm f=0.3332 <S**2>=0.000

228 -> 248	0.17157
230 -> 248	-0.16476
232 -> 248	0.12604
235 -> 248	0.20519
240 -> 250	0.23975
241 -> 250	0.49603
246 -> 253	-0.13831

Excited State 50: Singlet-A 3.8917 eV 318.59 nm f=0.0015 <S**2>=0.000

231 -> 247	0.33666
232 -> 248	-0.17523
234 -> 247	-0.15924
235 -> 248	0.36358
236 -> 247	-0.18218
237 -> 247	0.33810

Excited State 51: Singlet-B 3.9024 eV 317.71 nm f=0.0006 <S**2>=0.000

230 -> 247	-0.22288
231 -> 248	0.13940
232 -> 247	-0.26799
234 -> 248	-0.25725
235 -> 247	0.48346
235 -> 250	-0.11047
238 -> 247	-0.10835
239 -> 250	0.11151

Excited State 52: Singlet-A 3.9317 eV 315.34 nm f=0.0001 <S**2>=0.000
227 -> 247 0.37779
229 -> 248 0.48452
229 -> 249 -0.26048
231 -> 247 -0.10616
237 -> 247 0.12064

Excited State 53: Singlet-A 3.9352 eV 315.06 nm f=0.0001 <S**2>=0.000
227 -> 247 0.12580
229 -> 248 0.13193
230 -> 248 -0.19867
231 -> 247 0.30714
232 -> 248 -0.24060
233 -> 248 -0.26980
234 -> 247 -0.21637
236 -> 247 0.14973
237 -> 247 -0.29688

Excited State 54: Singlet-B 3.9421 eV 314.51 nm f=0.0024 <S**2>=0.000
230 -> 247 0.15538
231 -> 248 -0.19462
232 -> 247 0.14444
233 -> 247 0.31250
234 -> 248 0.36062
235 -> 247 0.32261
238 -> 247 -0.19025

Excited State 55: Singlet-A 3.9495 eV 313.93 nm f=0.0100 <S**2>=0.000
230 -> 248 -0.22441
231 -> 247 0.32563
232 -> 248 0.23517
233 -> 248 0.43730
233 -> 249 0.12933
235 -> 248 -0.17018

Excited State 56: Singlet-B 3.9496 eV 313.91 nm f=0.0009 <S**2>=0.000
230 -> 247 -0.35771
232 -> 247 -0.25299
233 -> 247 -0.18882
234 -> 248 0.45812
234 -> 249 0.13312

Excited State 57: Singlet-A 3.9717 eV 312.17 nm f=0.0326 <S**2>=0.000
230 -> 248 0.40005
231 -> 247 0.19276
232 -> 248 0.41337

233 -> 248 -0.11278
234 -> 247 -0.28947

Excited State 58: Singlet-B 3.9867 eV 311.00 nm f=0.0071 <S**2>=0.000
231 -> 248 0.60760
232 -> 247 0.13550
233 -> 247 0.20910
234 -> 248 0.12926
245 -> 253 -0.14335

Excited State 59: Singlet-A 4.0200 eV 308.42 nm f=0.0050 <S**2>=0.000
230 -> 248 0.11781
231 -> 247 0.30904
233 -> 248 -0.20248
234 -> 247 0.54784
234 -> 250 -0.13092

Excited State 60: Singlet-B 4.0213 eV 308.32 nm f=0.0171 <S**2>=0.000
230 -> 247 0.26495
231 -> 248 0.22298
233 -> 247 -0.18975
245 -> 253 0.54982

Table S2.7. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.2** using the M06 exchange correlation functional and bent geometry.

Excited State 1: Singlet-A' 1.2128 eV 1022.33 nm f=0.0000 <S**2>=0.000
237 -> 251 0.20871
240 -> 251 0.68986
240 -> 252 0.17822
240 <- 251 -0.24776
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4336.75850204
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A" 1.3698 eV 905.14 nm f=0.0000 <S**2>=0.000
223 -> 251 0.39466
223 -> 252 0.10193
241 -> 251 0.42214
241 -> 252 0.10883
243 -> 251 -0.10082
244 -> 251 0.39208
244 -> 252 0.10087
223 <- 251 -0.14241
241 <- 251 -0.12634

```
   244 <- 251       -0.11267

Excited State   3:      Singlet-A'     1.4453 eV  857.86 nm  f=0.0001  <S**2>=0.000
   224 -> 251        0.33863
   226 -> 251        0.24455
   242 -> 251        0.56248
   242 -> 252        0.14441
   224 <- 251       -0.11733
   242 <- 251       -0.16090

Excited State   4:      Singlet-A"     1.9600 eV  632.58 nm  f=0.0000  <S**2>=0.000
   212 -> 251        0.10510
   222 -> 251        0.65426
   222 -> 252        0.16933
   223 -> 251       -0.17237
   222 <- 251       -0.11003

Excited State   5:      Singlet-A"     2.0934 eV  592.27 nm  f=0.0637  <S**2>=0.000
   245 -> 247        0.27384
   245 -> 250        0.19504
   246 -> 248        0.60605
   246 -> 249        0.12474

Excited State   6:      Singlet-A'     2.1155 eV  586.08 nm  f=0.2975  <S**2>=0.000
   245 -> 248       -0.33758
   245 -> 249       -0.11283
   246 -> 247        0.56455
   246 -> 250        0.21815

Excited State   7:      Singlet-A'     2.4186 eV  512.63 nm  f=1.5636  <S**2>=0.000
   244 -> 247       -0.10122
   245 -> 248        0.52182
   246 -> 247        0.40127
   246 -> 250       -0.19802

Excited State   8:      Singlet-A"     2.5054 eV  494.88 nm  f=0.2540  <S**2>=0.000
   245 -> 247        0.47014
   245 -> 250        0.12451
   246 -> 248       -0.32781
   246 -> 249        0.37643

Excited State   9:      Singlet-A"     2.6702 eV  464.33 nm  f=0.3598  <S**2>=0.000
   245 -> 247       -0.44150
   245 -> 250        0.14472
   246 -> 249        0.51847
```

Excited State 10: Singlet-A' 2.7516 eV 450.60 nm f=0.2633 <S**2>=0.000
245 -> 248 0.31336
245 -> 249 -0.38556
246 -> 250 0.47597

Excited State 11: Singlet-A" 2.8778 eV 430.82 nm f=0.0000 <S**2>=0.000
246 -> 251 0.67540
246 -> 252 0.16109

Excited State 12: Singlet-A' 2.9204 eV 424.55 nm f=0.0005 <S**2>=0.000
245 -> 251 0.67122
245 -> 252 0.16884

Excited State 13: Singlet-A' 2.9444 eV 421.09 nm f=0.7760 <S**2>=0.000
244 -> 247 -0.11932
245 -> 249 0.53345
246 -> 250 0.42344

Excited State 14: Singlet-A" 2.9450 eV 420.99 nm f=0.0595 <S**2>=0.000
241 -> 248 0.29413
241 -> 249 0.12850
244 -> 248 0.51777
244 -> 249 0.18280
245 -> 250 0.23303
246 -> 249 -0.11207

Excited State 15: Singlet-A" 3.0114 eV 411.71 nm f=0.8187 <S**2>=0.000
241 -> 248 -0.15588
244 -> 248 -0.18984
245 -> 250 0.59831
246 -> 248 -0.12412
246 -> 249 -0.20972

Excited State 16: Singlet-A' 3.1625 eV 392.04 nm f=0.0518 <S**2>=0.000
242 -> 248 0.19122
243 -> 247 0.26420
243 -> 250 -0.12969
244 -> 247 0.55662
245 -> 249 0.14491

Excited State 17: Singlet-A' 3.1697 eV 391.15 nm f=0.0010 <S**2>=0.000
237 -> 248 0.11939
240 -> 248 0.64049
240 -> 249 0.23226

Excited State 18: Singlet-A' 3.2268 eV 384.24 nm f=0.2992 <S**2>=0.000

```
   241 -> 247       -0.12364
   241 -> 250       -0.11196
   242 -> 248       -0.32337
   243 -> 247        0.52060
   243 -> 250       -0.12078
   244 -> 247       -0.12234
   244 -> 250       -0.17007

Excited State  19:      Singlet-A"     3.2731 eV  378.80 nm  f=0.0036  <S**2>=0.000
   242 -> 247        0.57385
   242 -> 250        0.33918
   244 -> 248       -0.13896

Excited State  20:      Singlet-A'     3.3065 eV  374.97 nm  f=0.0000  <S**2>=0.000
   227 -> 248       -0.15883
   227 -> 249        0.18895
   229 -> 247        0.59494
   229 -> 250       -0.25928

Excited State  21:      Singlet-A'     3.3249 eV  372.90 nm  f=0.0058  <S**2>=0.000
   241 -> 247        0.31968
   242 -> 248        0.38620
   242 -> 249        0.17557
   243 -> 247        0.29421
   244 -> 247       -0.27294

Excited State  22:      Singlet-A"     3.3666 eV  368.28 nm  f=0.0262  <S**2>=0.000
   240 -> 247        0.12768
   241 -> 248        0.48006
   242 -> 247       -0.11829
   242 -> 250       -0.14198
   243 -> 248       -0.15848
   244 -> 248       -0.34891
   244 -> 249        0.16020

Excited State  23:      Singlet-A"     3.4040 eV  364.24 nm  f=0.0000  <S**2>=0.000
   240 -> 247        0.54236
   240 -> 250        0.40246
   241 -> 248       -0.12000

Excited State  24:      Singlet-A"     3.4500 eV  359.38 nm  f=0.0009  <S**2>=0.000
   241 -> 248        0.23245
   243 -> 248        0.50793
   243 -> 249       -0.37590

Excited State  25:      Singlet-A'     3.4519 eV  359.17 nm  f=0.0446  <S**2>=0.000
```

```
   241 -> 247        0.51211
   241 -> 250        0.13936
   242 -> 248       -0.36340
   244 -> 247        0.13860
   244 -> 250        0.17980

Excited State  26:      Singlet-A"     3.4553 eV  358.83 nm  f=0.0000  <S**2>=0.000
   227 -> 247        0.50470
   227 -> 250       -0.23018
   229 -> 248       -0.27347
   229 -> 249        0.30154

Excited State  27:      Singlet-A"     3.5195 eV  352.28 nm  f=0.0261  <S**2>=0.000
   246 -> 251       -0.15566
   246 -> 252        0.65291

Excited State  28:      Singlet-A"     3.6500 eV  339.68 nm  f=0.0666  <S**2>=0.000
   233 -> 247       -0.14569
   237 -> 247       -0.18309
   241 -> 248       -0.18084
   241 -> 249       -0.17994
   242 -> 250       -0.17161
   243 -> 248        0.16931
   244 -> 249        0.51863

Excited State  29:      Singlet-A"     3.7389 eV  331.61 nm  f=0.0641  <S**2>=0.000
   232 -> 247       -0.12024
   233 -> 247        0.23661
   237 -> 247        0.27999
   239 -> 247       -0.16236
   242 -> 247       -0.16681
   242 -> 250        0.27903
   243 -> 248       -0.14003
   244 -> 248       -0.12405
   244 -> 249        0.35909

Excited State  30:      Singlet-A'     3.7449 eV  331.08 nm  f=0.0822  <S**2>=0.000
   237 -> 248       -0.15757
   239 -> 248        0.13678
   242 -> 249       -0.13036
   244 -> 247       -0.10831
   244 -> 250        0.32363
   245 -> 249        0.10124
   245 -> 251       -0.12711
   245 -> 252        0.49291
   246 -> 253       -0.13230
```

Excited State 31: Singlet-A' 3.7520 eV 330.45 nm f=0.3601 <S**2>=0.000
230 -> 248 -0.12584
237 -> 248 0.41720
239 -> 248 -0.13251
240 -> 248 -0.10491
241 -> 247 -0.20192
242 -> 248 -0.11366
242 -> 249 0.27300
244 -> 250 0.23985

Excited State 32: Singlet-A' 3.7774 eV 328.23 nm f=0.3877 <S**2>=0.000
241 -> 247 -0.11661
242 -> 249 -0.20220
244 -> 247 -0.11897
244 -> 250 0.45949
245 -> 252 -0.40269

Excited State 33: Singlet-A' 3.8408 eV 322.81 nm f=0.3809 <S**2>=0.000
228 -> 248 0.17702
230 -> 248 0.20568
233 -> 248 0.21484
236 -> 247 -0.10079
237 -> 248 -0.27279
237 -> 249 -0.20416
240 -> 249 0.10599
241 -> 250 -0.13315
242 -> 249 0.32006
244 -> 250 0.10429
245 -> 252 -0.12504
246 -> 253 -0.16672

Excited State 34: Singlet-A' 3.8790 eV 319.63 nm f=0.0007 <S**2>=0.000
237 -> 248 0.17348
239 -> 248 0.59731
239 -> 249 0.12107
246 -> 253 -0.18493

Excited State 35: Singlet-A" 3.8917 eV 318.59 nm f=0.0384 <S**2>=0.000
238 -> 248 0.50678
238 -> 249 0.16196
241 -> 248 0.11414
241 -> 249 -0.36543

Excited State 36: Singlet-A" 3.8974 eV 318.12 nm f=0.0000 <S**2>=0.000
239 -> 247 -0.10790

```
   242 -> 250        0.10326
   243 -> 248        0.37992
   243 -> 249        0.51045
   243 -> 252        0.12763

Excited State  37:      Singlet-A'     3.9063 eV  317.39 nm  f=0.0277  <S**2>=0.000
   236 -> 247       -0.12924
   239 -> 248        0.17427
   241 -> 250       -0.12220
   246 -> 253        0.60872

Excited State  38:      Singlet-A"     3.9106 eV  317.05 nm  f=0.0000  <S**2>=0.000
   236 -> 248        0.20849
   238 -> 248        0.37875
   238 -> 249        0.14238
   241 -> 248       -0.10379
   241 -> 249        0.46828

Excited State  39:      Singlet-A"     3.9341 eV  315.15 nm  f=0.0067  <S**2>=0.000
   232 -> 247       -0.12711
   236 -> 248       -0.15616
   239 -> 247        0.56687
   239 -> 250        0.15866
   241 -> 249        0.18958
   242 -> 250        0.12748

Excited State  40:      Singlet-A'     3.9650 eV  312.69 nm  f=0.0851  <S**2>=0.000
   236 -> 247        0.38380
   238 -> 247        0.16064
   241 -> 247       -0.13933
   241 -> 250        0.42260
   242 -> 249        0.14788
   243 -> 250       -0.10622
   246 -> 253        0.11080

Excited State  41:      Singlet-A"     3.9671 eV  312.53 nm  f=0.0012  <S**2>=0.000
   235 -> 247        0.14006
   236 -> 248       -0.13729
   237 -> 247        0.43886
   237 -> 250        0.20109
   240 -> 247       -0.11786
   242 -> 247        0.24578
   242 -> 250       -0.34833

Excited State  42:      Singlet-A"     3.9725 eV  312.10 nm  f=0.0020  <S**2>=0.000
   236 -> 248        0.61183
```

237 -> 247 0.13028
238 -> 248 -0.11923
239 -> 247 0.18100
241 -> 249 -0.11820

Excited State 43: Singlet-A' 3.9884 eV 310.86 nm f=0.0193 <S**2>=0.000
232 -> 248 0.12218
233 -> 248 0.12788
236 -> 247 0.29481
237 -> 248 0.14811
238 -> 247 0.37102
238 -> 250 0.16593
241 -> 250 -0.33191
243 -> 250 0.13137

Excited State 44: Singlet-A' 4.0282 eV 307.79 nm f=0.0027 <S**2>=0.000
232 -> 248 -0.21805
233 -> 248 -0.10280
236 -> 247 0.35996
238 -> 247 -0.30266
238 -> 250 -0.15605
239 -> 248 0.12226
241 -> 250 -0.12242
242 -> 249 0.10954
243 -> 247 0.11245
243 -> 250 0.28171

Excited State 45: Singlet-A' 4.0441 eV 306.58 nm f=0.0124 <S**2>=0.000
230 -> 248 0.12336
232 -> 249 0.10072
233 -> 248 0.18918
236 -> 247 -0.16723
241 -> 250 0.28029
242 -> 249 -0.23264
243 -> 247 0.19953
243 -> 250 0.40810

Excited State 46: Singlet-A" 4.0492 eV 306.19 nm f=0.0790 <S**2>=0.000
230 -> 247 0.25344
232 -> 247 -0.31509
233 -> 247 0.31992
237 -> 247 -0.11855
237 -> 250 -0.19196
242 -> 247 0.17486
242 -> 250 -0.25389
243 -> 249 0.18348

Excited State 47: Singlet-A' 4.0651 eV 304.99 nm f=0.0046 <S**2>=0.000
231 -> 247 0.16686
233 -> 248 -0.16759
234 -> 247 -0.12366
235 -> 248 0.51576
235 -> 249 0.10446
237 -> 248 -0.15096
238 -> 247 0.25438

Excited State 48: Singlet-A" 4.0731 eV 304.40 nm f=0.0000 <S**2>=0.000
234 -> 248 0.20445
235 -> 247 -0.12906
245 -> 253 0.61277
245 -> 254 0.12292

Excited State 49: Singlet-A" 4.0863 eV 303.41 nm f=0.0020 <S**2>=0.000
231 -> 248 0.15623
233 -> 247 -0.14609
234 -> 248 -0.38758
234 -> 249 -0.10294
235 -> 247 0.40384
235 -> 250 0.11692
237 -> 250 -0.10120
245 -> 253 0.25737

Excited State 50: Singlet-A' 4.0889 eV 303.22 nm f=0.1190 <S**2>=0.000
228 -> 248 0.15104
230 -> 248 0.10001
233 -> 248 0.19332
235 -> 248 0.28499
236 -> 247 0.14931
238 -> 247 -0.14136
240 -> 248 -0.14694
240 -> 249 0.35768
242 -> 249 -0.22284
243 -> 250 -0.21566

Excited State 51: Singlet-A' 4.1160 eV 301.23 nm f=0.0031 <S**2>=0.000
230 -> 248 -0.13325
231 -> 247 -0.18096
232 -> 248 -0.35264
233 -> 248 -0.15780
235 -> 248 -0.14941
237 -> 248 -0.14848
238 -> 247 0.20664

240 -> 248 -0.11399
240 -> 249 0.38505

Excited State 52: Singlet-A' 4.1256 eV 300.52 nm f=0.0065 <S**2>=0.000
230 -> 248 -0.26106
231 -> 247 -0.33349
232 -> 248 -0.18512
233 -> 248 0.33980
235 -> 248 0.13069
237 -> 248 -0.11617
240 -> 249 -0.25730

Excited State 53: Singlet-A" 4.1312 eV 300.12 nm f=0.0015 <S**2>=0.000
233 -> 247 -0.11114
234 -> 248 0.12930
237 -> 247 -0.12068
240 -> 247 -0.38605
240 -> 250 0.53247

Excited State 54: Singlet-A" 4.1339 eV 299.92 nm f=0.0175 <S**2>=0.000
230 -> 247 0.26377
233 -> 247 -0.15880
233 -> 250 -0.13891
234 -> 248 0.41531
234 -> 249 0.12160
235 -> 247 0.33886
236 -> 248 0.10529
237 -> 250 -0.10505
239 -> 247 -0.11394

Excited State 55: Singlet-A" 4.1503 eV 298.74 nm f=0.0022 <S**2>=0.000
231 -> 248 0.63987
234 -> 248 0.13650

Excited State 56: Singlet-A' 4.1530 eV 298.54 nm f=0.0534 <S**2>=0.000
230 -> 248 -0.17363
231 -> 247 0.43765
232 -> 248 -0.23412
233 -> 248 0.20419
234 -> 247 -0.28901
234 -> 250 -0.10122
235 -> 248 -0.15570
241 -> 250 -0.11265

Excited State 57: Singlet-A' 4.1602 eV 298.02 nm f=0.2821 <S**2>=0.000
228 -> 248 -0.23303

230 -> 248 -0.27395
232 -> 248 0.34855
233 -> 249 0.15810
237 -> 248 -0.14166
237 -> 249 0.15988
240 -> 249 0.22693
242 -> 249 0.13602
243 -> 250 0.19366

Excited State 58: Singlet-A" 4.1876 eV 296.08 nm f=0.0062 <S**2>=0.000
230 -> 247 0.15764
232 -> 247 0.48789
232 -> 250 0.14238
233 -> 247 0.30439
233 -> 250 0.15059
235 -> 247 0.14073
239 -> 250 0.12575

Excited State 59: Singlet-A" 4.1988 eV 295.29 nm f=0.0005 <S**2>=0.000
227 -> 247 0.38913
227 -> 250 -0.11430
229 -> 248 0.45731
229 -> 249 -0.32010

Excited State 60: Singlet-A' 4.2459 eV 292.01 nm f=0.0066 <S**2>=0.000
231 -> 247 0.26681
233 -> 248 0.16650
234 -> 247 0.54716
234 -> 250 0.21245
235 -> 248 0.10831

Table S2.8. TDDFT-predicted energies, oscillator strengths, and expansion coefficients for **2.2** using the M06 exchange correlation functional and twisted geometry.

Excited State 1: Singlet-A 1.5530 eV 798.35 nm f=0.0000 <S**2>=0.000
240 -> 252 0.72183
241 -> 252 0.10938
240 <- 252 -0.21157
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) = -4336.74906635
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 1.6993 eV 729.61 nm f=0.0001 <S**2>=0.000
223 -> 252 0.39419
241 -> 252 0.37165

```
   244 -> 252       0.46424
   223 <- 252      -0.12094
   244 <- 252      -0.11128

Excited State   3:      Singlet-B      1.7669 eV  701.72 nm  f=0.0001  <S**2>=0.000
   224 -> 252       0.31947
   226 -> 252       0.24877
   242 -> 252       0.58230
   242 <- 252      -0.14001

Excited State   4:      Singlet-B      2.0742 eV  597.75 nm  f=0.0084  <S**2>=0.000
   222 -> 252      -0.51363
   226 -> 252      -0.12086
   228 -> 252       0.21575
   230 -> 252       0.16646
   245 -> 252       0.23455
   246 -> 248       0.21741

Excited State   5:      Singlet-B      2.0936 eV  592.21 nm  f=0.0741  <S**2>=0.000
   222 -> 252       0.20281
   245 -> 247       0.24228
   245 -> 250      -0.17537
   246 -> 248       0.57360
   246 -> 249       0.10693

Excited State   6:      Singlet-A      2.1282 eV  582.59 nm  f=0.2589  <S**2>=0.000
   245 -> 248      -0.36538
   245 -> 249      -0.10508
   246 -> 247       0.54539
   246 -> 250      -0.22667

Excited State   7:      Singlet-A      2.4256 eV  511.16 nm  f=1.6349  <S**2>=0.000
   245 -> 248       0.50981
   246 -> 247       0.42645
   246 -> 250       0.17998

Excited State   8:      Singlet-B      2.5390 eV  488.31 nm  f=0.2417  <S**2>=0.000
   245 -> 247       0.47970
   245 -> 250      -0.12550
   246 -> 248      -0.31375
   246 -> 249       0.37568

Excited State   9:      Singlet-B      2.6947 eV  460.11 nm  f=0.3151  <S**2>=0.000
   245 -> 247      -0.43784
   245 -> 250      -0.14061
   246 -> 249       0.52261
```

Excited State 10: Singlet-A 2.7812 eV 445.79 nm f=0.3597 <S**2>=0.000
245 -> 248 -0.30375
245 -> 249 0.36339
246 -> 250 0.50017

Excited State 11: Singlet-B 2.8879 eV 429.32 nm f=0.0010 <S**2>=0.000
241 -> 248 0.25965
241 -> 249 0.10588
244 -> 248 0.58909
244 -> 249 0.19052

Excited State 12: Singlet-A 2.9652 eV 418.13 nm f=0.5698 <S**2>=0.000
244 -> 247 0.12259
245 -> 249 0.54802
246 -> 250 -0.39733

Excited State 13: Singlet-B 3.0284 eV 409.40 nm f=0.7892 <S**2>=0.000
245 -> 250 0.63088
246 -> 248 0.13172
246 -> 249 0.22492

Excited State 14: Singlet-B 3.0575 eV 405.51 nm f=0.0061 <S**2>=0.000
240 -> 248 0.64956
240 -> 249 0.21536
241 -> 248 0.14824

Excited State 15: Singlet-A 3.1474 eV 393.92 nm f=0.0086 <S**2>=0.000
241 -> 250 -0.10322
242 -> 248 -0.39932
243 -> 247 0.10353
244 -> 247 0.47443
244 -> 250 -0.17012
245 -> 249 -0.15581

Excited State 16: Singlet-A 3.2005 eV 387.39 nm f=0.2549 <S**2>=0.000
241 -> 247 -0.13606
242 -> 248 0.30351
242 -> 249 0.10666
243 -> 247 0.52503
243 -> 250 0.15141
244 -> 247 0.17752
246 -> 252 0.11120

Excited State 17: Singlet-A 3.2433 eV 382.28 nm f=0.0423 <S**2>=0.000
243 -> 247 -0.16974

```
   244 -> 247        0.10250
   246 -> 252        0.65888

Excited State  18:      Singlet-B      3.2435 eV  382.26 nm  f=0.0023  <S**2>=0.000
   242 -> 247        0.57799
   242 -> 250       -0.36624

Excited State  19:      Singlet-A      3.3018 eV  375.51 nm  f=0.0066  <S**2>=0.000
   240 -> 247       -0.19767
   240 -> 250        0.17864
   241 -> 247       -0.19995
   242 -> 248        0.31651
   242 -> 249        0.13428
   243 -> 247       -0.31343
   244 -> 247        0.33146
   246 -> 252       -0.16840

Excited State  20:      Singlet-B      3.3061 eV  375.02 nm  f=0.0000  <S**2>=0.000
   227 -> 248       -0.14952
   227 -> 249        0.19473
   229 -> 247        0.59767
   229 -> 250        0.25393

Excited State  21:      Singlet-A      3.3215 eV  373.28 nm  f=0.0024  <S**2>=0.000
   240 -> 247        0.50859
   240 -> 250       -0.38204
   242 -> 248        0.16610
   243 -> 247       -0.12402
   244 -> 247        0.16122

Excited State  22:      Singlet-B      3.3941 eV  365.30 nm  f=0.0345  <S**2>=0.000
   240 -> 248       -0.10574
   241 -> 248        0.45128
   242 -> 250       -0.11537
   243 -> 248       -0.26118
   243 -> 249        0.15677
   244 -> 248       -0.28404
   244 -> 249        0.16854
   245 -> 252       -0.13755

Excited State  23:      Singlet-B      3.4143 eV  363.13 nm  f=0.0139  <S**2>=0.000
   222 -> 252        0.23122
   245 -> 252        0.63698

Excited State  24:      Singlet-A      3.4268 eV  361.81 nm  f=0.0177  <S**2>=0.000
   240 -> 247       -0.11042
```

```
   241 -> 247        0.55994
   241 -> 250       -0.11394
   242 -> 248        0.23630
   244 -> 250       -0.22677

Excited State  25:      Singlet-A      3.4567 eV  358.68 nm  f=0.0001  <S**2>=0.000
   227 -> 247        0.51007
   227 -> 250        0.22671
   229 -> 248       -0.25927
   229 -> 249        0.31150

Excited State  26:      Singlet-B      3.4579 eV  358.55 nm  f=0.0093  <S**2>=0.000
   241 -> 248        0.34413
   243 -> 248        0.45227
   243 -> 249       -0.36352
   244 -> 248       -0.11176

Excited State  27:      Singlet-B      3.5557 eV  348.69 nm  f=0.0349  <S**2>=0.000
   246 -> 249        0.10025
   246 -> 251        0.67204

Excited State  28:      Singlet-B      3.6618 eV  338.59 nm  f=0.0462  <S**2>=0.000
   232 -> 247       -0.14350
   233 -> 247        0.10859
   238 -> 247        0.21355
   239 -> 247       -0.16953
   241 -> 248       -0.18854
   241 -> 249       -0.18575
   242 -> 250       -0.20714
   243 -> 248        0.20138
   244 -> 249        0.44028

Excited State  29:      Singlet-A      3.7185 eV  333.42 nm  f=0.0853  <S**2>=0.000
   230 -> 248        0.23989
   230 -> 249        0.12299
   238 -> 248       -0.38061
   239 -> 248        0.41247
   241 -> 247       -0.14888
   242 -> 249       -0.14416

Excited State  30:      Singlet-B      3.7358 eV  331.89 nm  f=0.0580  <S**2>=0.000
   232 -> 247        0.15096
   233 -> 247       -0.12940
   238 -> 247       -0.23307
   239 -> 247        0.17871
   242 -> 247        0.16506
```

```
   242 -> 250        0.24806
   243 -> 248       -0.11876
   244 -> 248       -0.13105
   244 -> 249        0.45048

Excited State  31:      Singlet-A      3.7590 eV  329.83 nm  f=0.3888  <S**2>=0.000
   238 -> 248       -0.12464
   241 -> 247        0.12332
   242 -> 249       -0.22752
   244 -> 247        0.19546
   244 -> 250        0.51156
   245 -> 251        0.21608

Excited State  32:      Singlet-A      3.7952 eV  326.68 nm  f=0.5737  <S**2>=0.000
   230 -> 248        0.14444
   232 -> 248       -0.12604
   238 -> 249       -0.12571
   242 -> 248       -0.10967
   242 -> 249        0.30562
   245 -> 251        0.50804
   246 -> 253        0.12988

Excited State  33:      Singlet-A      3.8236 eV  324.26 nm  f=0.2897  <S**2>=0.000
   228 -> 248       -0.13228
   230 -> 248       -0.19661
   232 -> 248        0.15020
   238 -> 249        0.12726
   241 -> 247       -0.19303
   242 -> 249       -0.24676
   244 -> 250       -0.31779
   245 -> 251        0.37322

Excited State  34:      Singlet-A      3.8550 eV  321.62 nm  f=0.0051  <S**2>=0.000
   236 -> 247       -0.12097
   238 -> 248        0.44419
   239 -> 248        0.47527
   239 -> 249        0.11986

Excited State  35:      Singlet-B      3.8762 eV  319.86 nm  f=0.0007  <S**2>=0.000
   239 -> 247        0.14104
   242 -> 247        0.11071
   242 -> 250        0.14900
   243 -> 248        0.37572
   243 -> 249        0.50467
   243 -> 251        0.12237
```

Excited State 36: Singlet-B 3.9013 eV 317.80 nm f=0.0286 <S**2>=0.000
237 -> 248 0.56848
237 -> 249 0.14861
241 -> 249 -0.28846

Excited State 37: Singlet-B 3.9099 eV 317.10 nm f=0.0135 <S**2>=0.000
235 -> 247 -0.15630
236 -> 248 0.40653
237 -> 248 0.21210
238 -> 247 -0.19301
239 -> 247 -0.23718
241 -> 249 0.33210

Excited State 38: Singlet-B 3.9286 eV 315.59 nm f=0.0163 <S**2>=0.000
235 -> 247 0.11169
237 -> 248 0.17430
238 -> 247 0.20978
239 -> 247 0.35154
239 -> 250 -0.15990
241 -> 249 0.41276
242 -> 250 -0.14788

Excited State 39: Singlet-B 3.9484 eV 314.01 nm f=0.0012 <S**2>=0.000
238 -> 247 0.36320
238 -> 250 -0.14408
239 -> 247 -0.27223
239 -> 250 0.12087
241 -> 249 0.18176
242 -> 247 0.24907
242 -> 250 0.34086

Excited State 40: Singlet-A 3.9526 eV 313.68 nm f=0.0001 <S**2>=0.000
233 -> 248 -0.14488
235 -> 248 -0.28134
236 -> 247 0.23901
237 -> 247 0.27354
237 -> 250 -0.11300
246 -> 253 0.45645

Excited State 41: Singlet-A 3.9620 eV 312.93 nm f=0.0066 <S**2>=0.000
235 -> 248 0.25997
236 -> 247 -0.28403
237 -> 247 -0.22675
241 -> 250 0.15746
246 -> 253 0.45872

Excited State 42: Singlet-B 3.9680 eV 312.46 nm f=0.0030 <S**2>=0.000

233 -> 247	0.11553
236 -> 248	0.52872
237 -> 248	-0.13047
238 -> 247	0.23295
239 -> 247	0.21299
241 -> 249	-0.12466
242 -> 250	0.11379

Excited State 43: Singlet-A 3.9848 eV 311.14 nm f=0.0138 <S**2>=0.000

228 -> 248	-0.13652
230 -> 248	-0.15356
233 -> 248	-0.13067
236 -> 247	-0.10209
238 -> 248	-0.24428
241 -> 250	0.38604
242 -> 249	0.26693
243 -> 250	-0.17232
246 -> 253	-0.15858

Excited State 44: Singlet-A 4.0064 eV 309.47 nm f=0.0053 <S**2>=0.000

228 -> 248	0.10517
233 -> 248	0.16895
235 -> 248	0.32804
236 -> 247	0.35595
236 -> 250	-0.10611
237 -> 247	0.17024
241 -> 250	0.31707
242 -> 249	-0.10902
243 -> 250	-0.13389

Excited State 45: Singlet-A 4.0214 eV 308.31 nm f=0.1159 <S**2>=0.000

228 -> 248	-0.19492
230 -> 248	-0.20662
232 -> 248	0.14919
235 -> 248	0.30932
236 -> 247	0.22639
238 -> 248	-0.11064
239 -> 248	0.12154
241 -> 250	-0.28898
242 -> 249	0.27731

Excited State 46: Singlet-B 4.0361 eV 307.19 nm f=0.0317 <S**2>=0.000

228 -> 247	0.11096
230 -> 247	-0.25535
232 -> 247	0.38705

```
   233 -> 247       -0.13626
   234 -> 248       -0.10765
   235 -> 247        0.19582
   238 -> 247        0.14709
   238 -> 250       -0.19913
   239 -> 250        0.13019
   242 -> 247       -0.13675
   242 -> 250       -0.20451
   243 -> 249        0.16343

Excited State  47:      Singlet-A      4.0491 eV  306.20 nm  f=0.0029  <S**2>=0.000
   228 -> 248       -0.12161
   240 -> 247        0.36195
   240 -> 250        0.45887
   243 -> 247       -0.12461
   243 -> 250        0.29308

Excited State  48:      Singlet-B      4.0520 eV  305.98 nm  f=0.0001  <S**2>=0.000
   240 -> 248       -0.21004
   240 -> 249        0.64756
   240 -> 251       -0.15056

Excited State  49:      Singlet-A      4.0569 eV  305.61 nm  f=0.0001  <S**2>=0.000
   228 -> 248       -0.14994
   232 -> 248       -0.12321
   240 -> 247       -0.20233
   240 -> 250       -0.30444
   241 -> 250        0.21194
   243 -> 247       -0.18914
   243 -> 250        0.41891

Excited State  50:      Singlet-B      4.0639 eV  305.09 nm  f=0.0001  <S**2>=0.000
   231 -> 248       -0.18694
   232 -> 247        0.21932
   234 -> 248        0.53755
   234 -> 249        0.14030
   235 -> 247       -0.25473
   235 -> 250        0.11544

Excited State  51:      Singlet-A      4.0665 eV  304.89 nm  f=0.0002  <S**2>=0.000
   231 -> 247       -0.13269
   232 -> 248        0.29362
   233 -> 248        0.44259
   233 -> 249        0.11139
   234 -> 247        0.15119
   235 -> 248       -0.25451
```

```
   236 -> 247        0.14027
   237 -> 247       -0.16766

Excited State  52:      Singlet-A      4.0955 eV  302.74 nm  f=0.0169  <S**2>=0.000
   230 -> 248       -0.30469
   231 -> 247        0.32143
   232 -> 248       -0.27666
   233 -> 248        0.30909
   236 -> 247       -0.15800
   237 -> 247        0.19562
   243 -> 250       -0.10808

Excited State  53:      Singlet-B      4.1144 eV  301.34 nm  f=0.0016  <S**2>=0.000
   228 -> 247        0.12370
   230 -> 247       -0.18456
   231 -> 248        0.32973
   232 -> 247       -0.18477
   233 -> 247        0.11952
   233 -> 250       -0.12917
   234 -> 248        0.32947
   234 -> 249        0.11230
   235 -> 247        0.32049
   239 -> 250        0.11245

Excited State  54:      Singlet-A      4.1169 eV  301.16 nm  f=0.0390  <S**2>=0.000
   230 -> 248        0.20089
   232 -> 248        0.37296
   233 -> 248        0.12862
   236 -> 247       -0.25923
   237 -> 247        0.39919
   237 -> 250       -0.17036

Excited State  55:      Singlet-B      4.1303 eV  300.18 nm  f=0.0090  <S**2>=0.000
   230 -> 247       -0.11968
   231 -> 248        0.51215
   233 -> 247       -0.15088
   235 -> 247       -0.31077
   235 -> 250        0.11971
   238 -> 247        0.14414

Excited State  56:      Singlet-B      4.1484 eV  298.88 nm  f=0.0265  <S**2>=0.000
   230 -> 247       -0.16731
   232 -> 247       -0.25051
   233 -> 247       -0.20817
   245 -> 253        0.54623
```

Excited State 57: Singlet-A 4.1587 eV 298.13 nm f=0.0009 <S**2>=0.000

230 -> 248	0.13622
231 -> 247	0.50395
232 -> 248	0.20088
234 -> 247	-0.27830
237 -> 247	-0.16273
237 -> 250	0.10921
241 -> 250	0.10274

Excited State 58: Singlet-B 4.1645 eV 297.71 nm f=0.0181 <S**2>=0.000

230 -> 247	0.29496
231 -> 248	0.23697
232 -> 247	0.33065
233 -> 247	0.22828
245 -> 253	0.37416

Excited State 59: Singlet-B 4.2004 eV 295.17 nm f=0.2211 <S**2>=0.000

228 -> 247	0.52627
228 -> 250	-0.16265
230 -> 247	0.10561
230 -> 250	-0.15167
232 -> 250	0.16098
235 -> 247	-0.18606
238 -> 250	-0.12198

Excited State 60: Singlet-A 4.2017 eV 295.08 nm f=0.0003 <S**2>=0.000

227 -> 247	0.39286
227 -> 250	0.11222
229 -> 248	0.46081
229 -> 249	-0.33923

Table S2.9. Optimized geometry for **2.7** using the B3LYP exchange correlation functional and bent geometry.

N	0.31041	-4.29222	1.93713
N	-0.45498	-6.09387	0.
N	0.5871	-2.30886	0.
N	0.31041	-4.29222	-1.93713
C	0.16106	-5.3937	2.76508
C	0.81365	-3.30195	2.74225
C	-0.84228	-6.84101	1.09486
C	-0.84228	-6.84101	-1.09486
C	0.65232	-1.49411	1.11595
C	0.65232	-1.49411	-1.11595
C	0.16106	-5.3937	-2.76508

C	0.81365	-3.30195	-2.74225
C	0.67087	-5.10347	4.07605
C	1.08398	-3.81139	4.06131
C	-1.56266	-8.00877	0.67949
C	-1.56266	-8.00877	-0.67949
C	0.53985	-0.09188	0.7171
C	0.53985	-0.09188	-0.7171
C	0.67087	-5.10347	-4.07605
C	1.08398	-3.81139	-4.06131
H	0.7012	-5.80173	-4.89791
H	1.51527	-3.2441	-4.87102
H	1.51527	-3.2441	4.87102
H	0.7012	-5.80173	4.89791
H	-2.00007	-8.73752	1.34377
H	-2.00007	-8.73752	-1.34377
C	0.90499	-1.94726	2.40252
C	-0.47676	-6.57529	2.41639
C	-0.47676	-6.57529	-2.41639
C	0.90499	-1.94726	-2.40252
C	-0.76688	-7.59039	3.47342
C	-0.14031	-8.84407	3.4554
C	-1.67132	-7.30798	4.50608
C	-0.40727	-9.78761	4.44525
H	0.56798	-9.07444	2.66665
C	-1.94513	-8.25446	5.49169
H	-2.16992	-6.34477	4.52862
C	-1.31227	-9.49639	5.46533
H	0.09378	-10.74987	4.41992
H	-2.65429	-8.02099	6.27922
H	-1.52278	-10.23243	6.23434
C	-0.76688	-7.59039	-3.47342
C	-1.67132	-7.30798	-4.50608
C	-0.14031	-8.84407	-3.4554
C	-1.94513	-8.25446	-5.49169
H	-2.16992	-6.34477	-4.52862
C	-0.40727	-9.78761	-4.44525
H	0.56798	-9.07444	-2.66665
C	-1.31227	-9.49639	-5.46533
H	-2.65429	-8.02099	-6.27922
H	0.09378	-10.74987	-4.41992
H	-1.52278	-10.23243	-6.23434
C	1.29336	-0.9901	-3.48625
C	2.56302	-0.39907	-3.48294
C	0.4118	-0.6824	-4.53002
C	2.93918	0.48541	-4.49135
H	3.25752	-0.63452	-2.68317

C	0.78416	0.20702	-5.53706
H	-0.57474	-1.13383	-4.54512
C	2.04884	0.79465	-5.5196
H	3.92771	0.93268	-4.47454
H	0.08654	0.43868	-6.3354
H	2.34021	1.48565	-6.30378
C	1.29336	-0.9901	3.48625
C	2.56302	-0.39907	3.48294
C	0.4118	-0.6824	4.53002
C	2.93918	0.48541	4.49135
H	3.25752	-0.63452	2.68317
C	0.78416	0.20702	5.53706
H	-0.57474	-1.13383	4.54512
C	2.04884	0.79465	5.5196
H	3.92771	0.93268	4.47454
H	0.08654	0.43868	6.3354
H	2.34021	1.48565	6.30378
C	0.37062	1.07242	-1.42335
C	0.37062	1.07242	1.42335
C	0.2045	2.30423	0.72463
C	0.2045	2.30423	-0.72463
C	0.03222	3.50999	1.39957
C	0.03222	3.50999	-1.39957
C	-0.14147	4.73261	-0.72565
C	-0.14147	4.73261	0.72565
C	-0.31525	5.95767	-1.43523
C	-0.31525	5.95767	1.43523
C	-0.49107	7.18017	-0.72495
C	-0.49107	7.18017	0.72495
C	-0.66769	8.40549	-1.39924
C	-0.66769	8.40549	1.39924
C	-0.84055	9.60656	-0.72365
C	-0.84055	9.60656	0.72365
C	-1.02006	10.85247	-1.40987
C	-1.02006	10.85247	1.40987
C	-1.18765	12.01453	-0.71533
H	-1.32268	12.95178	-1.24495
C	-1.18765	12.01453	0.71533
H	-1.01976	10.85247	-2.49553
H	-1.32268	12.95178	1.24495
H	-1.01976	10.85247	2.49553
H	-0.66906	8.40739	2.48373
H	0.03378	3.50724	2.48352
H	0.34102	1.0899	2.50339
H	0.34102	1.0899	-2.50339
H	0.03378	3.50724	-2.48352

H	-0.66906	8.40739	-2.48373
C	-0.31315	5.95819	-2.84787
C	-0.31315	5.95819	2.84787
C	-0.31094	5.95855	-4.06215
C	-0.31094	5.95855	4.06215
C	-0.30879	5.96065	-5.48287
C	-0.14605	4.75983	-6.20231
C	-0.46983	7.16425	-6.19792
C	-0.14584	4.76852	-7.59204
H	-0.02067	3.82834	-5.66162
C	-0.46783	7.16176	-7.58758
H	-0.59523	8.09345	-5.65338
C	-0.30637	5.96654	-8.28988
H	-0.02049	3.83703	-8.13396
H	-0.5929	8.09561	-8.12543
H	-0.30571	5.96867	-9.37463
C	-0.30879	5.96065	5.48287
C	-0.14605	4.75983	6.20231
C	-0.46983	7.16425	6.19792
C	-0.14584	4.76852	7.59204
H	-0.02067	3.82834	5.66162
C	-0.46783	7.16176	7.58758
H	-0.59523	8.09345	5.65338
C	-0.30637	5.96654	8.28988
H	-0.02049	3.83703	8.13396
H	-0.5929	8.09561	8.12543
H	-0.30571	5.96867	9.37463
Ni	0.19042	-4.24723	0.

Table S2.10. Optimized geometry for **2.7** using the B3LYP exchange correlation functional and twisted geometry.

N	-1.02575	1.61207	4.27802
N	0.	0.	6.20254
N	0.	0.	2.3236
N	1.02575	-1.61207	4.27802
C	-1.15293	2.52259	5.31056
C	-1.82387	2.06706	3.26626
C	-0.24254	1.07252	7.03344
C	0.24254	-1.07252	7.03344
C	-0.94198	0.61161	1.52027
C	0.94198	-0.61161	1.52027
C	1.15293	-2.52259	5.31056
C	1.82387	-2.06706	3.26626
C	-2.02862	3.59096	4.90991

C	-2.48703	3.28245	3.66879
C	-0.12171	0.66978	8.40549
C	0.12171	-0.66978	8.40549
C	-0.63511	0.33937	0.11385
C	0.63511	-0.33937	0.11385
C	2.02862	-3.59096	4.90991
C	2.48703	-3.28245	3.66879
H	2.29931	-4.43556	5.52479
H	3.18919	-3.83878	3.06836
H	-3.18919	3.83878	3.06836
H	-2.29931	4.43556	5.52479
H	-0.24479	1.31776	9.25905
H	0.24479	-1.31776	9.25905
C	-1.88848	1.52531	1.97228
C	-0.70963	2.32442	6.61302
C	0.70963	-2.32442	6.61302
C	1.88848	-1.52531	1.97228
C	-0.86385	3.43504	7.60276
C	0.	4.53638	7.55288
C	-1.87135	3.41432	8.576
C	-0.1336	5.58713	8.45923
H	0.78353	4.56527	6.80277
C	-2.0074	4.46621	9.48006
H	-2.55812	2.57542	8.61628
C	-1.13743	5.55464	9.42572
H	0.5475	6.43046	8.40889
H	-2.79674	4.43642	10.22419
H	-1.24334	6.37304	10.13028
C	0.86385	-3.43504	7.60276
C	0.	-4.53638	7.55288
C	1.87135	-3.41432	8.576
C	0.1336	-5.58713	8.45923
H	-0.78353	-4.56527	6.80277
C	2.0074	-4.46621	9.48006
H	2.55812	-2.57542	8.61628
C	1.13743	-5.55464	9.42572
H	-0.5475	-6.43046	8.40889
H	2.79674	-4.43642	10.22419
H	1.24334	-6.37304	10.13028
C	2.94054	-2.06905	1.05608
C	4.12393	-1.34978	0.85216
C	2.78079	-3.30066	0.40845
C	5.12182	-1.84484	0.01354
H	4.26065	-0.39626	1.35192
C	3.77692	-3.79714	-0.43
H	1.86626	-3.86571	0.5552

C	4.9502	-3.06964	-0.63062
H	6.03371	-1.27513	-0.13286
H	3.63621	-4.75121	-0.9274
H	5.72728	-3.45777	-1.28098
C	-2.94054	2.06905	1.05608
C	-2.78079	3.30066	0.40845
C	-4.12393	1.34978	0.85216
C	-3.77692	3.79714	-0.43
H	-1.86626	3.86571	0.5552
C	-5.12182	1.84484	0.01354
H	-4.26065	0.39626	1.35192
C	-4.9502	3.06964	-0.63062
H	-3.63621	4.75121	-0.9274
H	-6.03371	1.27513	-0.13286
H	-5.72728	3.45777	-1.28098
C	1.27597	-0.62775	-1.06468
C	-1.27597	0.62775	-1.06468
C	-0.65657	0.30493	-2.30865
C	0.65657	-0.30493	-2.30865
C	-1.27504	0.57695	-3.52579
C	1.27504	-0.57695	-3.52579
C	0.66363	-0.2935	-4.76126
C	-0.66363	0.2935	-4.76126
C	1.31598	-0.57261	-5.9984
C	-1.31598	0.57261	-5.9984
C	0.66551	-0.28759	-7.23379
C	-0.66551	0.28759	-7.23379
C	1.28555	-0.55278	-8.47164
C	-1.28555	0.55278	-8.47164
C	0.66507	-0.28554	-9.68528
C	-0.66507	0.28554	-9.68528
C	1.29572	-0.55598	-10.944
C	-1.29572	0.55598	-10.944
C	0.65763	-0.28205	-12.1182
H	1.14435	-0.49065	-13.06516
C	-0.65763	0.28205	-12.1182
H	2.29353	-0.98387	-10.94405
H	-1.14435	0.49065	-13.06516
H	-2.29353	0.98387	-10.94405
H	-2.28174	0.98054	-8.4739
H	-2.26035	1.02876	-3.52285
H	-2.24782	1.09708	-1.08934
H	2.24782	-1.09708	-1.08934
H	2.26035	-1.02876	-3.52285
H	2.28174	-0.98054	-8.4739
C	2.61406	-1.12981	-5.99941

C	-2.61406	1.12981	-5.99941
C	-3.73247	1.60279	-6.00361
C	3.73247	-1.60279	-6.00361
C	5.04274	-2.15173	-6.00773
C	5.67252	-2.49596	-7.22032
C	5.73636	-2.35946	-4.79896
C	6.95555	-3.03002	-7.21858
H	5.14647	-2.34079	-8.1555
C	7.01932	-2.89351	-4.80841
H	5.26032	-2.09751	-3.86091
C	7.63377	-3.23078	-6.01537
H	7.42883	-3.2906	-8.15928
H	7.54271	-3.04639	-3.87051
H	8.63528	-3.64726	-6.01832
C	-5.04274	2.15173	-6.00773
C	-5.73636	2.35946	-4.79896
C	-5.67252	2.49596	-7.22032
C	-7.01932	2.89351	-4.80841
H	-5.26032	2.09751	-3.86091
C	-6.95555	3.03002	-7.21858
H	-5.14647	2.34079	-8.1555
C	-7.63377	3.23078	-6.01537
H	-7.54271	3.04639	-3.87051
H	-7.42883	3.2906	-8.15928
H	-8.63528	3.64726	-6.01832
Ni	0.	0.	4.27109

Table S2.11. Optimized geometry for **2.7** using the M06 exchange correlation functional and bent geometry.

N	0.31041	-4.29222	1.93713
N	-0.45498	-6.09387	0.
N	0.5871	-2.30886	0.
N	0.31041	-4.29222	-1.93713
C	0.16106	-5.3937	2.76508
C	0.81365	-3.30195	2.74225
C	-0.84228	-6.84101	1.09486
C	-0.84228	-6.84101	-1.09486
C	0.65232	-1.49411	1.11595
C	0.65232	-1.49411	-1.11595
C	0.16106	-5.3937	-2.76508
C	0.81365	-3.30195	-2.74225
C	0.67087	-5.10347	4.07605
C	1.08398	-3.81139	4.06131
C	-1.56266	-8.00877	0.67949

C	-1.56266	-8.00877	-0.67949
C	0.53985	-0.09188	0.7171
C	0.53985	-0.09188	-0.7171
C	0.67087	-5.10347	-4.07605
C	1.08398	-3.81139	-4.06131
H	0.7012	-5.80173	-4.89791
H	1.51527	-3.2441	-4.87102
H	1.51527	-3.2441	4.87102
H	0.7012	-5.80173	4.89791
H	-2.00007	-8.73752	1.34377
H	-2.00007	-8.73752	-1.34377
C	0.90499	-1.94726	2.40252
C	-0.47676	-6.57529	2.41639
C	-0.47676	-6.57529	-2.41639
C	0.90499	-1.94726	-2.40252
C	-0.76688	-7.59039	3.47342
C	-0.14031	-8.84407	3.4554
C	-1.67132	-7.30798	4.50608
C	-0.40727	-9.78761	4.44525
H	0.56798	-9.07444	2.66665
C	-1.94513	-8.25446	5.49169
H	-2.16992	-6.34477	4.52862
C	-1.31227	-9.49639	5.46533
H	0.09378	-10.74987	4.41992
H	-2.65429	-8.02099	6.27922
H	-1.52278	-10.23243	6.23434
C	-0.76688	-7.59039	-3.47342
C	-1.67132	-7.30798	-4.50608
C	-0.14031	-8.84407	-3.4554
C	-1.94513	-8.25446	-5.49169
H	-2.16992	-6.34477	-4.52862
C	-0.40727	-9.78761	-4.44525
H	0.56798	-9.07444	-2.66665
C	-1.31227	-9.49639	-5.46533
H	-2.65429	-8.02099	-6.27922
H	0.09378	-10.74987	-4.41992
H	-1.52278	-10.23243	-6.23434
C	1.29336	-0.9901	-3.48625
C	2.56302	-0.39907	-3.48294
C	0.4118	-0.6824	-4.53002
C	2.93918	0.48541	-4.49135
H	3.25752	-0.63452	-2.68317
C	0.78416	0.20702	-5.53706
H	-0.57474	-1.13383	-4.54512
C	2.04884	0.79465	-5.5196
H	3.92771	0.93268	-4.47454

H	0.08654	0.43868	-6.3354
H	2.34021	1.48565	-6.30378
C	1.29336	-0.9901	3.48625
C	2.56302	-0.39907	3.48294
C	0.4118	-0.6824	4.53002
C	2.93918	0.48541	4.49135
H	3.25752	-0.63452	2.68317
C	0.78416	0.20702	5.53706
H	-0.57474	-1.13383	4.54512
C	2.04884	0.79465	5.5196
H	3.92771	0.93268	4.47454
H	0.08654	0.43868	6.3354
H	2.34021	1.48565	6.30378
C	0.37062	1.07242	-1.42335
C	0.37062	1.07242	1.42335
C	0.2045	2.30423	0.72463
C	0.2045	2.30423	-0.72463
C	0.03222	3.50999	1.39957
C	0.03222	3.50999	-1.39957
C	-0.14147	4.73261	-0.72565
C	-0.14147	4.73261	0.72565
C	-0.31525	5.95767	-1.43523
C	-0.31525	5.95767	1.43523
C	-0.49107	7.18017	-0.72495
C	-0.49107	7.18017	0.72495
C	-0.66769	8.40549	-1.39924
C	-0.66769	8.40549	1.39924
C	-0.84055	9.60656	-0.72365
C	-0.84055	9.60656	0.72365
C	-1.02006	10.85247	-1.40987
C	-1.02006	10.85247	1.40987
C	-1.18765	12.01453	-0.71533
H	-1.32268	12.95178	-1.24495
C	-1.18765	12.01453	0.71533
H	-1.01976	10.85247	-2.49553
H	-1.32268	12.95178	1.24495
H	-1.01976	10.85247	2.49553
H	-0.66906	8.40739	2.48373
H	0.03378	3.50724	2.48352
H	0.34102	1.0899	2.50339
H	0.34102	1.0899	-2.50339
H	0.03378	3.50724	-2.48352
H	-0.66906	8.40739	-2.48373
C	-0.31315	5.95819	-2.84787
C	-0.31315	5.95819	2.84787
C	-0.31094	5.95855	-4.06215

C	-0.31094	5.95855	4.06215
C	-0.30879	5.96065	-5.48287
C	-0.14605	4.75983	-6.20231
C	-0.46983	7.16425	-6.19792
C	-0.14584	4.76852	-7.59204
H	-0.02067	3.82834	-5.66162
C	-0.46783	7.16176	-7.58758
H	-0.59523	8.09345	-5.65338
C	-0.30637	5.96654	-8.28988
H	-0.02049	3.83703	-8.13396
H	-0.5929	8.09561	-8.12543
H	-0.30571	5.96867	-9.37463
C	-0.30879	5.96065	5.48287
C	-0.14605	4.75983	6.20231
C	-0.46983	7.16425	6.19792
C	-0.14584	4.76852	7.59204
H	-0.02067	3.82834	5.66162
C	-0.46783	7.16176	7.58758
H	-0.59523	8.09345	5.65338
C	-0.30637	5.96654	8.28988
H	-0.02049	3.83703	8.13396
H	-0.5929	8.09561	8.12543
H	-0.30571	5.96867	9.37463
Ni	0.19042	-4.24723	0.

Table S2.12. Optimized geometry for **2.7** using the M06 exchange correlation functional and twisted geometry.

N	-1.02575	1.61207	4.27802
N	0.	0.	6.20254
N	0.	0.	2.3236
N	1.02575	-1.61207	4.27802
C	-1.15293	2.52259	5.31056
C	-1.82387	2.06706	3.26626
C	-0.24254	1.07252	7.03344
C	0.24254	-1.07252	7.03344
C	-0.94198	0.61161	1.52027
C	0.94198	-0.61161	1.52027
C	1.15293	-2.52259	5.31056
C	1.82387	-2.06706	3.26626
C	-2.02862	3.59096	4.90991
C	-2.48703	3.28245	3.66879
C	-0.12171	0.66978	8.40549
C	0.12171	-0.66978	8.40549
C	-0.63511	0.33937	0.11385

C	0.63511	-0.33937	0.11385
C	2.02862	-3.59096	4.90991
C	2.48703	-3.28245	3.66879
H	2.29931	-4.43556	5.52479
H	3.18919	-3.83878	3.06836
H	-3.18919	3.83878	3.06836
H	-2.29931	4.43556	5.52479
H	-0.24479	1.31776	9.25905
H	0.24479	-1.31776	9.25905
C	-1.88848	1.52531	1.97228
C	-0.70963	2.32442	6.61302
C	0.70963	-2.32442	6.61302
C	1.88848	-1.52531	1.97228
C	-0.86385	3.43504	7.60276
C	0.	4.53638	7.55288
C	-1.87135	3.41432	8.576
C	-0.1336	5.58713	8.45923
H	0.78353	4.56527	6.80277
C	-2.0074	4.46621	9.48006
H	-2.55812	2.57542	8.61628
C	-1.13743	5.55464	9.42572
H	0.5475	6.43046	8.40889
H	-2.79674	4.43642	10.22419
H	-1.24334	6.37304	10.13028
C	0.86385	-3.43504	7.60276
C	0.	-4.53638	7.55288
C	1.87135	-3.41432	8.576
C	0.1336	-5.58713	8.45923
H	-0.78353	-4.56527	6.80277
C	2.0074	-4.46621	9.48006
H	2.55812	-2.57542	8.61628
C	1.13743	-5.55464	9.42572
H	-0.5475	-6.43046	8.40889
H	2.79674	-4.43642	10.22419
H	1.24334	-6.37304	10.13028
C	2.94054	-2.06905	1.05608
C	4.12393	-1.34978	0.85216
C	2.78079	-3.30066	0.40845
C	5.12182	-1.84484	0.01354
H	4.26065	-0.39626	1.35192
C	3.77692	-3.79714	-0.43
H	1.86626	-3.86571	0.5552
C	4.9502	-3.06964	-0.63062
H	6.03371	-1.27513	-0.13286
H	3.63621	-4.75121	-0.9274
H	5.72728	-3.45777	-1.28098

C	-2.94054	2.06905	1.05608
C	-2.78079	3.30066	0.40845
C	-4.12393	1.34978	0.85216
C	-3.77692	3.79714	-0.43
H	-1.86626	3.86571	0.5552
C	-5.12182	1.84484	0.01354
H	-4.26065	0.39626	1.35192
C	-4.9502	3.06964	-0.63062
H	-3.63621	4.75121	-0.9274
H	-6.03371	1.27513	-0.13286
H	-5.72728	3.45777	-1.28098
C	1.27597	-0.62775	-1.06468
C	-1.27597	0.62775	-1.06468
C	-0.65657	0.30493	-2.30865
C	0.65657	-0.30493	-2.30865
C	-1.27504	0.57695	-3.52579
C	1.27504	-0.57695	-3.52579
C	0.66363	-0.2935	-4.76126
C	-0.66363	0.2935	-4.76126
C	1.31598	-0.57261	-5.9984
C	-1.31598	0.57261	-5.9984
C	0.66551	-0.28759	-7.23379
C	-0.66551	0.28759	-7.23379
C	1.28555	-0.55278	-8.47164
C	-1.28555	0.55278	-8.47164
C	0.66507	-0.28554	-9.68528
C	-0.66507	0.28554	-9.68528
C	1.29572	-0.55598	-10.944
C	-1.29572	0.55598	-10.944
C	0.65763	-0.28205	-12.1182
H	1.14435	-0.49065	-13.06516
C	-0.65763	0.28205	-12.1182
H	2.29353	-0.98387	-10.94405
H	-1.14435	0.49065	-13.06516
H	-2.29353	0.98387	-10.94405
H	-2.28174	0.98054	-8.4739
H	-2.26035	1.02876	-3.52285
H	-2.24782	1.09708	-1.08934
H	2.24782	-1.09708	-1.08934
H	2.26035	-1.02876	-3.52285
H	2.28174	-0.98054	-8.4739
C	2.61406	-1.12981	-5.99941
C	-2.61406	1.12981	-5.99941
C	-3.73247	1.60279	-6.00361
C	3.73247	-1.60279	-6.00361
C	5.04274	-2.15173	-6.00773

C	5.67252	-2.49596	-7.22032
C	5.73636	-2.35946	-4.79896
C	6.95555	-3.03002	-7.21858
H	5.14647	-2.34079	-8.1555
C	7.01932	-2.89351	-4.80841
H	5.26032	-2.09751	-3.86091
C	7.63377	-3.23078	-6.01537
H	7.42883	-3.2906	-8.15928
H	7.54271	-3.04639	-3.87051
H	8.63528	-3.64726	-6.01832
C	-5.04274	2.15173	-6.00773
C	-5.73636	2.35946	-4.79896
C	-5.67252	2.49596	-7.22032
C	-7.01932	2.89351	-4.80841
H	-5.26032	2.09751	-3.86091
C	-6.95555	3.03002	-7.21858
H	-5.14647	2.34079	-8.1555
C	-7.63377	3.23078	-6.01537
H	-7.54271	3.04639	-3.87051
H	-7.42883	3.2906	-8.15928
H	-8.63528	3.64726	-6.01832
Ni	0.	0.	4.27109

Table S2.13. Optimized geometry for **2.2** using the B3LYP exchange correlation functional and bent geometry.

N	0.29651	-3.20134	1.93791
N	-0.45115	-5.01004	0.
N	0.56682	-1.22089	0.
N	0.29651	-3.20134	-1.93791
C	0.15213	-4.30072	2.76572
C	0.79066	-2.20553	2.74526
C	-0.83303	-5.75938	1.09504
C	-0.83303	-5.75938	-1.09504
C	0.62152	-0.40451	1.11413
C	0.62152	-0.40451	-1.11413
C	0.15213	-4.30072	-2.76572
C	0.79066	-2.20553	-2.74526
C	0.65483	-4.00664	4.07925
C	1.0592	-2.7122	4.06567
C	-1.54458	-6.93467	0.6789
C	-1.54458	-6.93467	-0.6789
C	0.50046	0.99276	0.71123
C	0.50046	0.99276	-0.71123
C	0.65483	-4.00664	-4.07925

C	1.0592	-2.7122	-4.06567
H	0.68682	-4.70446	-4.90127
H	1.48377	-2.1416	-4.87619
H	1.48377	-2.1416	4.87619
H	0.68682	-4.70446	4.90127
H	-1.9774	-7.66566	1.34364
H	-1.9774	-7.66566	-1.34364
C	0.87358	-0.8527	2.40447
C	-0.47537	-5.48975	2.41618
C	-0.47537	-5.48975	-2.41618
C	0.87358	-0.8527	-2.40447
C	-0.76253	-6.50417	3.47462
C	-0.1249	-7.7523	3.46374
C	-1.67504	-6.22624	4.50142
C	-0.38959	-8.6953	4.45474
H	0.59019	-7.97875	2.68
C	-1.94619	-7.17218	5.48816
H	-2.1821	-5.26735	4.51848
C	-1.30273	-8.40881	5.46881
H	0.11971	-9.65332	4.43499
H	-2.66164	-6.94251	6.27107
H	-1.5113	-9.14438	6.23876
C	-0.76253	-6.50417	-3.47462
C	-1.67504	-6.22624	-4.50142
C	-0.1249	-7.7523	-3.46374
C	-1.94619	-7.17218	-5.48816
H	-2.1821	-5.26735	-4.51848
C	-0.38959	-8.6953	-4.45474
H	0.59019	-7.97875	-2.68
C	-1.30273	-8.40881	-5.46881
H	-2.66164	-6.94251	-6.27107
H	0.11971	-9.65332	-4.43499
H	-1.5113	-9.14438	-6.23876
C	1.25819	0.1112	-3.48281
C	2.52239	0.71332	-3.47022
C	0.37674	0.41823	-4.52713
C	2.89336	1.6087	-4.47109
H	3.21674	0.47792	-2.6703
C	0.74365	1.31999	-5.52483
H	-0.60588	-0.04136	-4.54827
C	2.00279	1.91864	-5.49865
H	3.87776	2.06466	-4.44787
H	0.04541	1.55466	-6.32162
H	2.28919	2.61991	-6.27545
C	1.25819	0.1112	3.48281
C	2.52239	0.71332	3.47022

C	0.37674	0.41823	4.52713
C	2.89336	1.6087	4.47109
H	3.21674	0.47792	2.6703
C	0.74365	1.31999	5.52483
H	-0.60588	-0.04136	4.54827
C	2.00279	1.91864	5.49865
H	3.87776	2.06466	4.44787
H	0.04541	1.55466	6.32162
H	2.28919	2.61991	6.27545
C	0.32061	2.16734	-1.41994
C	0.32061	2.16734	1.41994
C	0.14094	3.37879	0.71914
C	0.14094	3.37879	-0.71914
C	-0.05582	4.60655	1.39841
C	-0.05582	4.60655	-1.39841
C	-0.24569	5.78797	-0.71668
C	-0.24569	5.78797	0.71668
C	-0.44986	7.04076	-1.49091
C	-0.44986	7.04076	1.49091
C	-0.66005	8.29393	-0.71454
C	-0.66005	8.29393	0.71454
C	-0.85876	9.47564	-1.39751
C	-0.85876	9.47564	1.39751
C	-1.06429	10.69775	-0.71677
C	-1.06429	10.69775	0.71677
C	-1.27029	11.92182	-1.40538
C	-1.27029	11.92182	1.40538
C	-1.46677	13.08993	-0.7081
H	-1.62342	14.02109	-1.24193
C	-1.46677	13.08993	0.7081
H	-1.27022	11.92127	-2.4906
H	-1.62342	14.02109	1.24193
H	-1.27022	11.92127	2.4906
H	-0.856	9.45631	2.48167
H	-0.05849	4.62484	2.4826
H	0.29246	2.18586	2.49978
H	0.29246	2.18586	-2.49978
H	-0.05849	4.62484	-2.4826
H	-0.856	9.45631	-2.48167
O	-0.44702	7.0439	-2.71616
O	-0.44702	7.0439	2.71616
Ni	0.18048	-3.15928	0.

Table S2.14. Optimized geometry for **2.2** using the B3LYP exchange correlation functional and twisted geometry.

N	-1.01653	1.61886	3.18548
N	0.	0.	5.11021
N	0.	0.	1.23188
N	1.01653	-1.61886	3.18548
C	-1.14592	2.5249	4.2188
C	-1.8131	2.0794	2.17202
C	-0.23937	1.07308	5.94107
C	0.23937	-1.07308	5.94107
C	-0.93371	0.62101	0.42775
C	0.93371	-0.62101	0.42775
C	1.14592	-2.5249	4.2188
C	1.8131	-2.0794	2.17202
C	-2.02079	3.59571	3.82144
C	-2.47679	3.29303	2.57854
C	-0.11856	0.66954	7.31467
C	0.11856	-0.66954	7.31467
C	-0.6229	0.34897	-0.97515
C	0.6229	-0.34897	-0.97515
C	2.02079	-3.59571	3.82144
C	2.47679	-3.29303	2.57854
H	2.29163	-4.43748	4.43985
H	3.17841	-3.85123	1.97946
H	-3.17841	3.85123	1.97946
H	-2.29163	4.43748	4.43985
H	-0.23784	1.31856	8.16784
H	0.23784	-1.31856	8.16784
C	-1.87493	1.54416	0.87747
C	-0.70254	2.32527	5.52289
C	0.70254	-2.32527	5.52289
C	1.87493	-1.54416	0.87747
C	-0.85653	3.43556	6.51299
C	0.	4.54241	6.4572
C	-1.85788	3.40868	7.49249
C	-0.13444	5.59218	7.36451
H	0.77856	4.57621	5.70216
C	-1.99469	4.45969	8.39736
H	-2.53939	2.56576	7.53715
C	-1.13183	5.55338	8.33747
H	0.54114	6.43965	7.30995
H	-2.77909	4.42509	9.14645
H	-1.23815	6.37115	9.04267
C	0.85653	-3.43556	6.51299
C	0.	-4.54241	6.4572
C	1.85788	-3.40868	7.49249

C	0.13444	-5.59218	7.36451
H	-0.77856	-4.57621	5.70216
C	1.99469	-4.45969	8.39736
H	2.53939	-2.56576	7.53715
C	1.13183	-5.55338	8.33747
H	-0.54114	-6.43965	7.30995
H	2.77909	-4.42509	9.14645
H	1.23815	-6.37115	9.04267
C	2.91672	-2.09573	-0.04551
C	4.09296	-1.37364	-0.2787
C	2.74867	-3.33358	-0.67874
C	5.07385	-1.87094	-1.13574
H	4.23613	-0.41532	0.20992
C	3.72834	-3.83151	-1.53569
H	1.8397	-3.90126	-0.5092
C	4.89266	-3.1	-1.76868
H	5.97923	-1.29803	-1.30748
H	3.58017	-4.78928	-2.02374
H	5.65453	-3.48634	-2.43762
C	-2.91672	2.09573	-0.04551
C	-2.74867	3.33358	-0.67874
C	-4.09296	1.37364	-0.2787
C	-3.72834	3.83151	-1.53569
H	-1.8397	3.90126	-0.5092
C	-5.07385	1.87094	-1.13574
H	-4.23613	0.41532	0.20992
C	-4.89266	3.1	-1.76868
H	-3.58017	4.78928	-2.02374
H	-5.97923	1.29803	-1.30748
H	-5.65453	3.48634	-2.43762
C	1.25677	-0.65679	-2.16574
C	-1.25677	0.65679	-2.16574
C	-0.64211	0.32171	-3.39143
C	0.64211	-0.32171	-3.39143
C	-1.25529	0.61609	-4.63396
C	1.25529	-0.61609	-4.63396
C	0.6446	-0.31281	-5.83078
C	-0.6446	0.31281	-5.83078
C	1.34424	-0.64432	-7.1002
C	-1.34424	0.64432	-7.1002
C	0.64486	-0.30776	-8.37099
C	-0.64486	0.30776	-8.37099
C	1.26178	-0.60077	-9.56927
C	-1.26178	0.60077	-9.56927
C	0.64735	-0.30776	-10.80856
C	-0.64735	0.30776	-10.80856

C	1.26946	-0.60288	-12.04984
C	-1.26946	0.60288	-12.04984
C	0.63963	-0.30375	-13.2344
H	1.12186	-0.53275	-14.17863
C	-0.63963	0.30375	-13.2344
H	2.2499	-1.06813	-12.04942
H	-1.12186	0.53275	-14.17863
H	-2.2499	1.06813	-12.04942
H	-2.24057	1.06703	-9.54979
H	-2.22823	1.0945	-4.65231
H	-2.21791	1.14667	-2.19245
H	2.21791	-1.14667	-2.19245
H	2.22823	-1.0945	-4.65231
H	2.24057	-1.06703	-9.54979
O	2.44997	-1.17203	-7.10263
O	-2.44997	1.17203	-7.10263
Ni	0.	0.	3.17935

Table S2.15. Optimized geometry for **2.2** using the M06 exchange correlation functional and bent geometry.

N	0.29651	-3.20134	1.93791
N	-0.45115	-5.01004	0.
N	0.56682	-1.22089	0.
N	0.29651	-3.20134	-1.93791
C	0.15213	-4.30072	2.76572
C	0.79066	-2.20553	2.74526
C	-0.83303	-5.75938	1.09504
C	-0.83303	-5.75938	-1.09504
C	0.62152	-0.40451	1.11413
C	0.62152	-0.40451	-1.11413
C	0.15213	-4.30072	-2.76572
C	0.79066	-2.20553	-2.74526
C	0.65483	-4.00664	4.07925
C	1.0592	-2.7122	4.06567
C	-1.54458	-6.93467	0.6789
C	-1.54458	-6.93467	-0.6789
C	0.50046	0.99276	0.71123
C	0.50046	0.99276	-0.71123
C	0.65483	-4.00664	-4.07925
C	1.0592	-2.7122	-4.06567
H	0.68682	-4.70446	-4.90127
H	1.48377	-2.1416	-4.87619
H	1.48377	-2.1416	4.87619
H	0.68682	-4.70446	4.90127

H	-1.9774	-7.66566	1.34364
H	-1.9774	-7.66566	-1.34364
C	0.87358	-0.8527	2.40447
C	-0.47537	-5.48975	2.41618
C	-0.47537	-5.48975	-2.41618
C	0.87358	-0.8527	-2.40447
C	-0.76253	-6.50417	3.47462
C	-0.1249	-7.7523	3.46374
C	-1.67504	-6.22624	4.50142
C	-0.38959	-8.6953	4.45474
H	0.59019	-7.97875	2.68
C	-1.94619	-7.17218	5.48816
H	-2.1821	-5.26735	4.51848
C	-1.30273	-8.40881	5.46881
H	0.11971	-9.65332	4.43499
H	-2.66164	-6.94251	6.27107
H	-1.5113	-9.14438	6.23876
C	-0.76253	-6.50417	-3.47462
C	-1.67504	-6.22624	-4.50142
C	-0.1249	-7.7523	-3.46374
C	-1.94619	-7.17218	-5.48816
H	-2.1821	-5.26735	-4.51848
C	-0.38959	-8.6953	-4.45474
H	0.59019	-7.97875	-2.68
C	-1.30273	-8.40881	-5.46881
H	-2.66164	-6.94251	-6.27107
H	0.11971	-9.65332	-4.43499
H	-1.5113	-9.14438	-6.23876
C	1.25819	0.1112	-3.48281
C	2.52239	0.71332	-3.47022
C	0.37674	0.41823	-4.52713
C	2.89336	1.6087	-4.47109
H	3.21674	0.47792	-2.6703
C	0.74365	1.31999	-5.52483
H	-0.60588	-0.04136	-4.54827
C	2.00279	1.91864	-5.49865
H	3.87776	2.06466	-4.44787
H	0.04541	1.55466	-6.32162
H	2.28919	2.61991	-6.27545
C	1.25819	0.1112	3.48281
C	2.52239	0.71332	3.47022
C	0.37674	0.41823	4.52713
C	2.89336	1.6087	4.47109
H	3.21674	0.47792	2.6703
C	0.74365	1.31999	5.52483
H	-0.60588	-0.04136	4.54827

C	2.00279	1.91864	5.49865
H	3.87776	2.06466	4.44787
H	0.04541	1.55466	6.32162
H	2.28919	2.61991	6.27545
C	0.32061	2.16734	-1.41994
C	0.32061	2.16734	1.41994
C	0.14094	3.37879	0.71914
C	0.14094	3.37879	-0.71914
C	-0.05582	4.60655	1.39841
C	-0.05582	4.60655	-1.39841
C	-0.24569	5.78797	-0.71668
C	-0.24569	5.78797	0.71668
C	-0.44986	7.04076	-1.49091
C	-0.44986	7.04076	1.49091
C	-0.66005	8.29393	-0.71454
C	-0.66005	8.29393	0.71454
C	-0.85876	9.47564	-1.39751
C	-0.85876	9.47564	1.39751
C	-1.06429	10.69775	-0.71677
C	-1.06429	10.69775	0.71677
C	-1.27029	11.92182	-1.40538
C	-1.27029	11.92182	1.40538
C	-1.46677	13.08993	-0.7081
H	-1.62342	14.02109	-1.24193
C	-1.46677	13.08993	0.7081
H	-1.27022	11.92127	-2.4906
H	-1.62342	14.02109	1.24193
H	-1.27022	11.92127	2.4906
H	-0.856	9.45631	2.48167
H	-0.05849	4.62484	2.4826
H	0.29246	2.18586	2.49978
H	0.29246	2.18586	-2.49978
H	-0.05849	4.62484	-2.4826
H	-0.856	9.45631	-2.48167
O	-0.44702	7.0439	-2.71616
O	-0.44702	7.0439	2.71616
Ni	0.18048	-3.15928	0.

Table S2.16. Optimized geometry for **2.2** using the M06 exchange correlation functional and twisted geometry.

N	-1.01653	1.61886	3.18548
N	0.	0.	5.11021
N	0.	0.	1.23188
N	1.01653	-1.61886	3.18548

C	-1.14592	2.5249	4.2188
C	-1.8131	2.0794	2.17202
C	-0.23937	1.07308	5.94107
C	0.23937	-1.07308	5.94107
C	-0.93371	0.62101	0.42775
C	0.93371	-0.62101	0.42775
C	1.14592	-2.5249	4.2188
C	1.8131	-2.0794	2.17202
C	-2.02079	3.59571	3.82144
C	-2.47679	3.29303	2.57854
C	-0.11856	0.66954	7.31467
C	0.11856	-0.66954	7.31467
C	-0.6229	0.34897	-0.97515
C	0.6229	-0.34897	-0.97515
C	2.02079	-3.59571	3.82144
C	2.47679	-3.29303	2.57854
H	2.29163	-4.43748	4.43985
H	3.17841	-3.85123	1.97946
H	-3.17841	3.85123	1.97946
H	-2.29163	4.43748	4.43985
H	-0.23784	1.31856	8.16784
H	0.23784	-1.31856	8.16784
C	-1.87493	1.54416	0.87747
C	-0.70254	2.32527	5.52289
C	0.70254	-2.32527	5.52289
C	1.87493	-1.54416	0.87747
C	-0.85653	3.43556	6.51299
C	0.	4.54241	6.4572
C	-1.85788	3.40868	7.49249
C	-0.13444	5.59218	7.36451
H	0.77856	4.57621	5.70216
C	-1.99469	4.45969	8.39736
H	-2.53939	2.56576	7.53715
C	-1.13183	5.55338	8.33747
H	0.54114	6.43965	7.30995
H	-2.77909	4.42509	9.14645
H	-1.23815	6.37115	9.04267
C	0.85653	-3.43556	6.51299
C	0.	-4.54241	6.4572
C	1.85788	-3.40868	7.49249
C	0.13444	-5.59218	7.36451
H	-0.77856	-4.57621	5.70216
C	1.99469	-4.45969	8.39736
H	2.53939	-2.56576	7.53715
C	1.13183	-5.55338	8.33747
H	-0.54114	-6.43965	7.30995

H	2.77909	-4.42509	9.14645
H	1.23815	-6.37115	9.04267
C	2.91672	-2.09573	-0.04551
C	4.09296	-1.37364	-0.2787
C	2.74867	-3.33358	-0.67874
C	5.07385	-1.87094	-1.13574
H	4.23613	-0.41532	0.20992
C	3.72834	-3.83151	-1.53569
H	1.8397	-3.90126	-0.5092
C	4.89266	-3.1	-1.76868
H	5.97923	-1.29803	-1.30748
H	3.58017	-4.78928	-2.02374
H	5.65453	-3.48634	-2.43762
C	-2.91672	2.09573	-0.04551
C	-2.74867	3.33358	-0.67874
C	-4.09296	1.37364	-0.2787
C	-3.72834	3.83151	-1.53569
H	-1.8397	3.90126	-0.5092
C	-5.07385	1.87094	-1.13574
H	-4.23613	0.41532	0.20992
C	-4.89266	3.1	-1.76868
H	-3.58017	4.78928	-2.02374
H	-5.97923	1.29803	-1.30748
H	-5.65453	3.48634	-2.43762
C	1.25677	-0.65679	-2.16574
C	-1.25677	0.65679	-2.16574
C	-0.64211	0.32171	-3.39143
C	0.64211	-0.32171	-3.39143
C	-1.25529	0.61609	-4.63396
C	1.25529	-0.61609	-4.63396
C	0.6446	-0.31281	-5.83078
C	-0.6446	0.31281	-5.83078
C	1.34424	-0.64432	-7.1002
C	-1.34424	0.64432	-7.1002
C	0.64486	-0.30776	-8.37099
C	-0.64486	0.30776	-8.37099
C	1.26178	-0.60077	-9.56927
C	-1.26178	0.60077	-9.56927
C	0.64735	-0.30776	-10.80856
C	-0.64735	0.30776	-10.80856
C	1.26946	-0.60288	-12.04984
C	-1.26946	0.60288	-12.04984
C	0.63963	-0.30375	-13.2344
H	1.12186	-0.53275	-14.17863
C	-0.63963	0.30375	-13.2344
H	2.2499	-1.06813	-12.04942

H	-1.12186	0.53275	-14.17863
H	-2.2499	1.06813	-12.04942
H	-2.24057	1.06703	-9.54979
H	-2.22823	1.0945	-4.65231
H	-2.21791	1.14667	-2.19245
H	2.21791	-1.14667	-2.19245
H	2.22823	-1.0945	-4.65231
H	2.24057	-1.06703	-9.54979
O	2.44997	-1.17203	-7.10263
O	-2.44997	1.17203	-7.10263
Ni	0.	0.	3.17935

Chapter 3 Supporting Information:

Full Citation for Gaussian 09:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, **2009**.

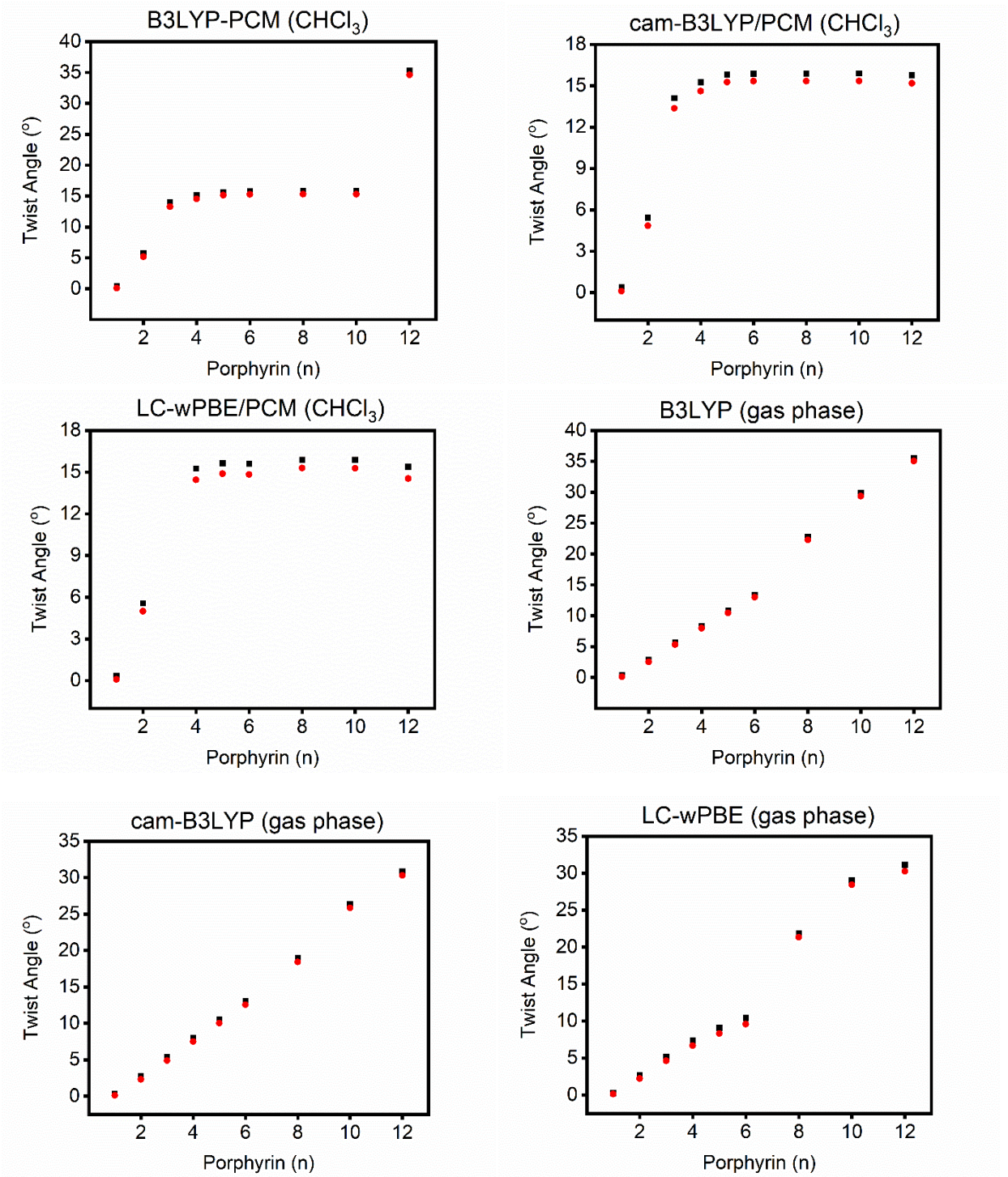


Figure S3.1. α (black)- and β (red)-twist angle vs. number of porphyrin subunits in chain for three comparative exchange correlation functionals modelled with (PCM) and without (gas phase) solvent effects.

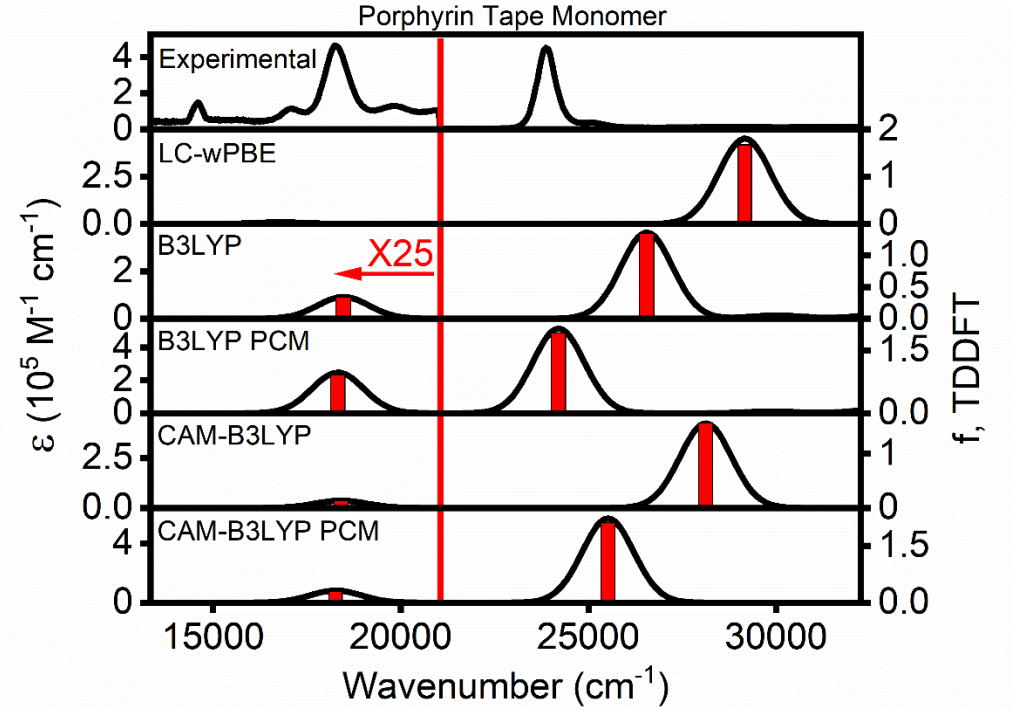


Figure S3.2. TDDFT-predicted UV-vis spectrum of **1.1** showing the exchange correlation functional comparison.

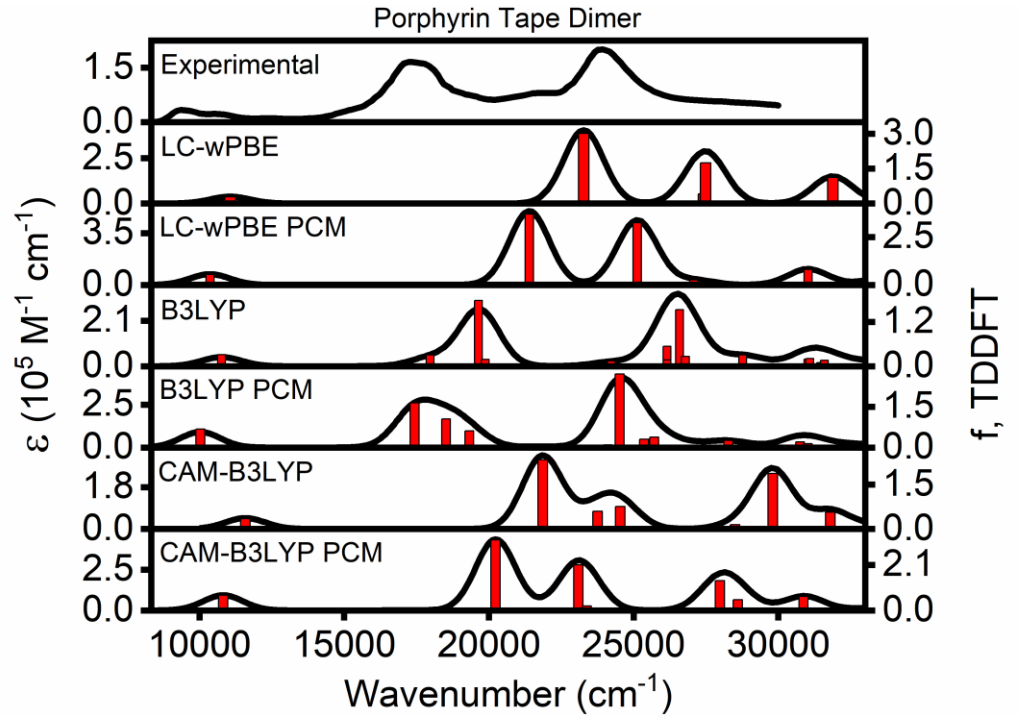


Figure S3.3. TDDFT-predicted UV-vis spectrum of **3.2** showing the exchange correlation functional comparison.

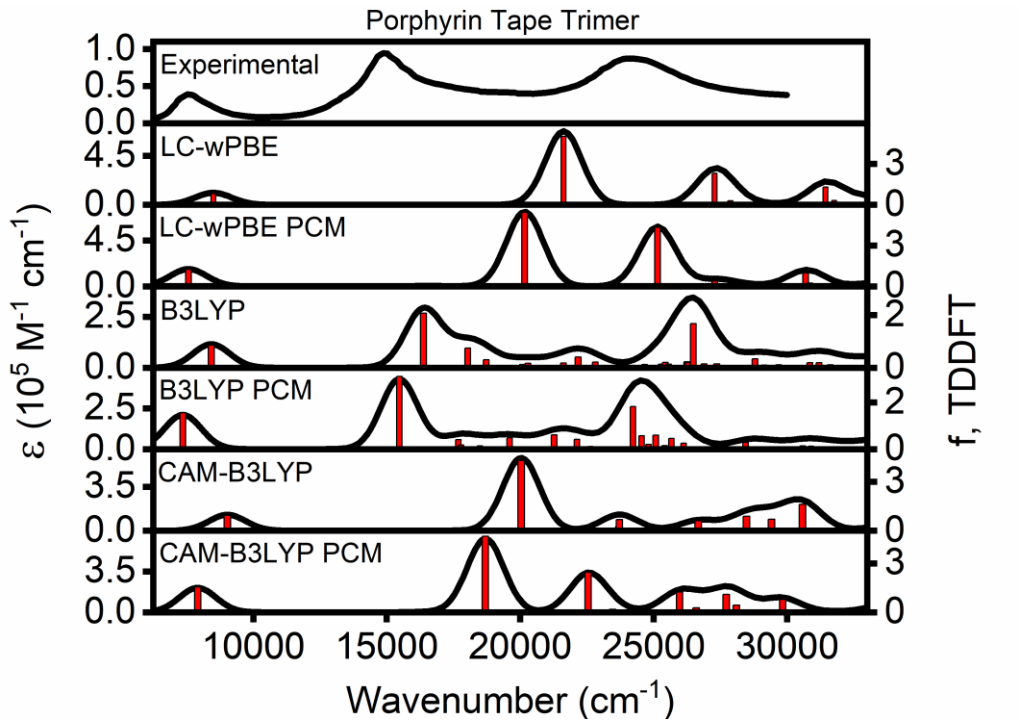


Figure S3.4. TDDFT-predicted UV-vis spectrum of **3.3** showing the exchange correlation functional comparison.

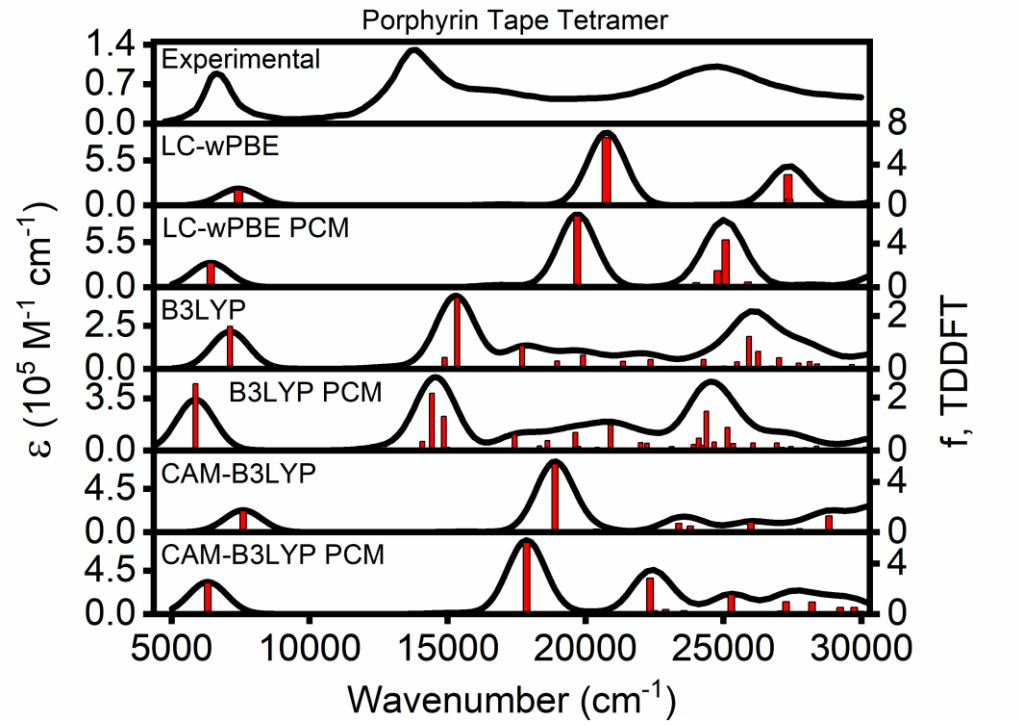


Figure S3.5. TDDFT-predicted UV-vis spectrum of **3.4** showing the exchange correlation functional comparison.

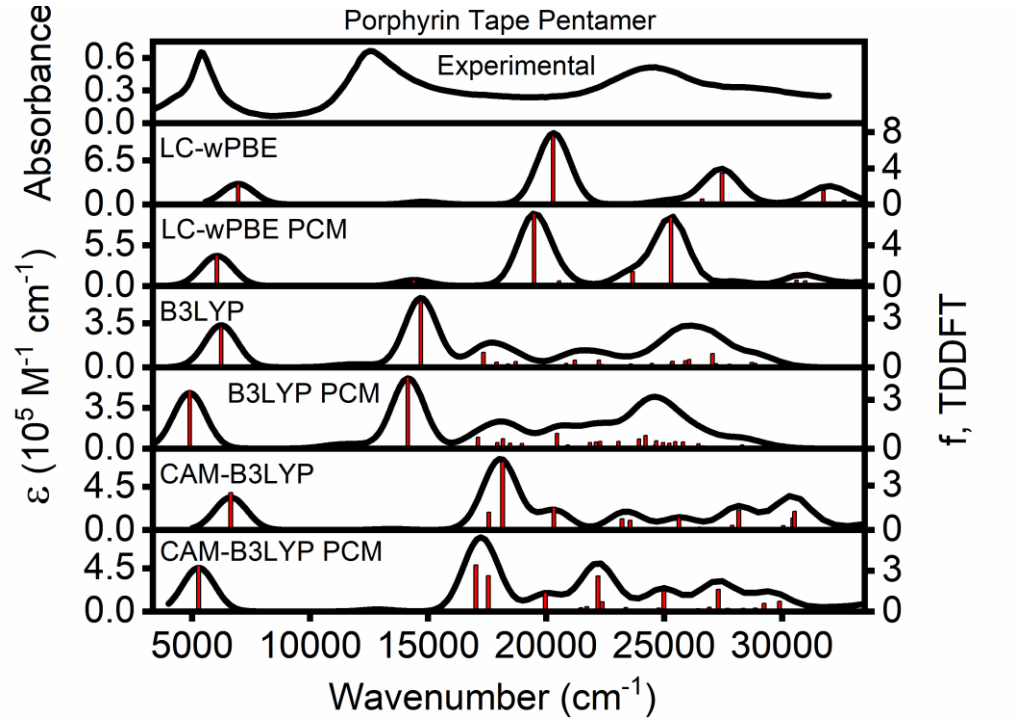


Figure S3.6. TDDFT-predicted UV-vis spectrum of **3.5** showing the exchange correlation functional comparison.

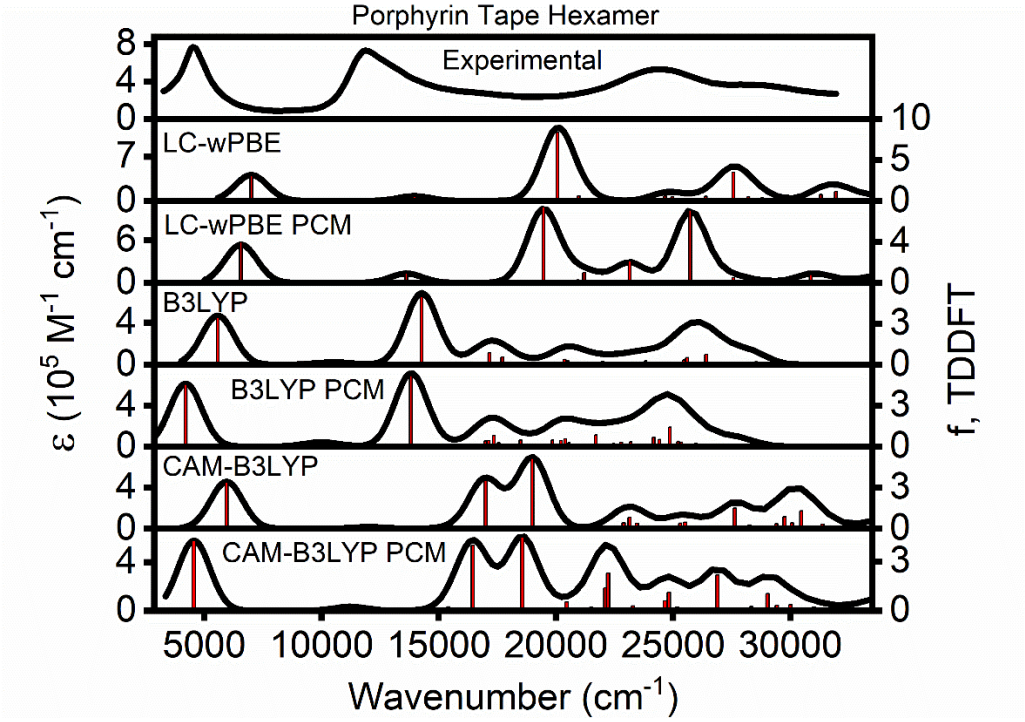


Figure S3.7. TDDFT-predicted UV-vis spectrum of **3.6** showing the exchange correlation functional comparison.

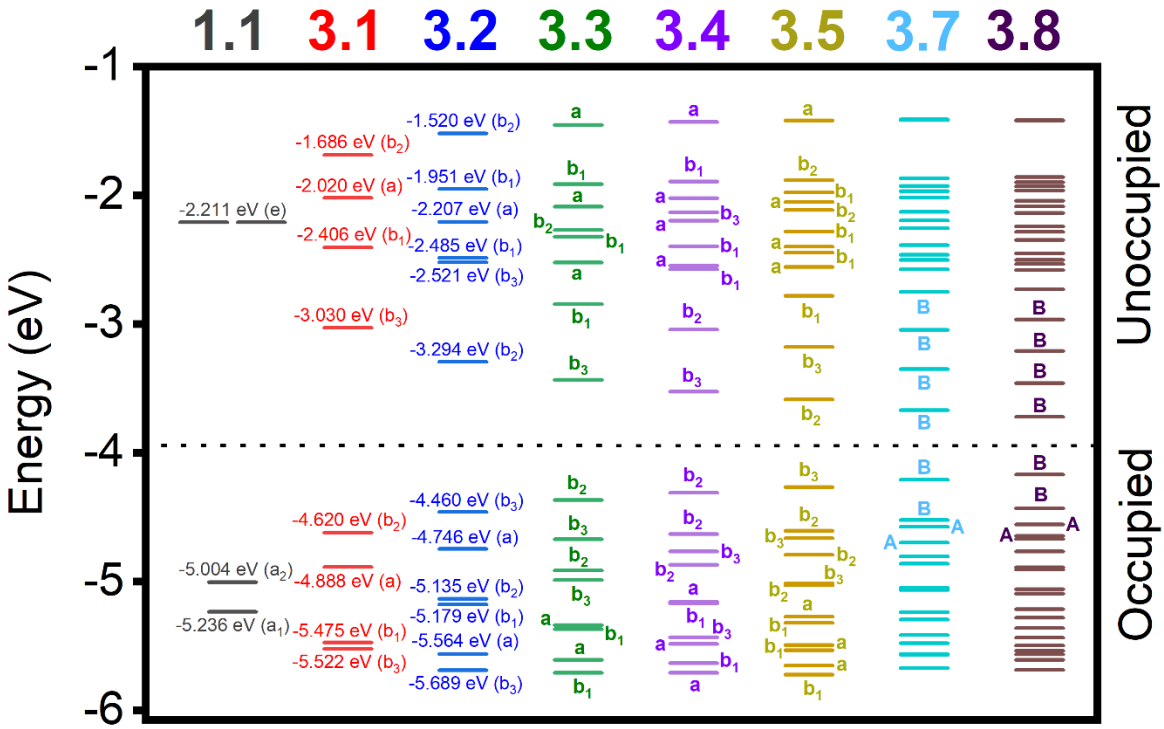


Figure S3.8. DFT-predicted energy level diagram for porphyrin tapes **1** and **3.1**-**3.8** (the 12-mer energy levels are not included due to program limitations associated with the large file size).

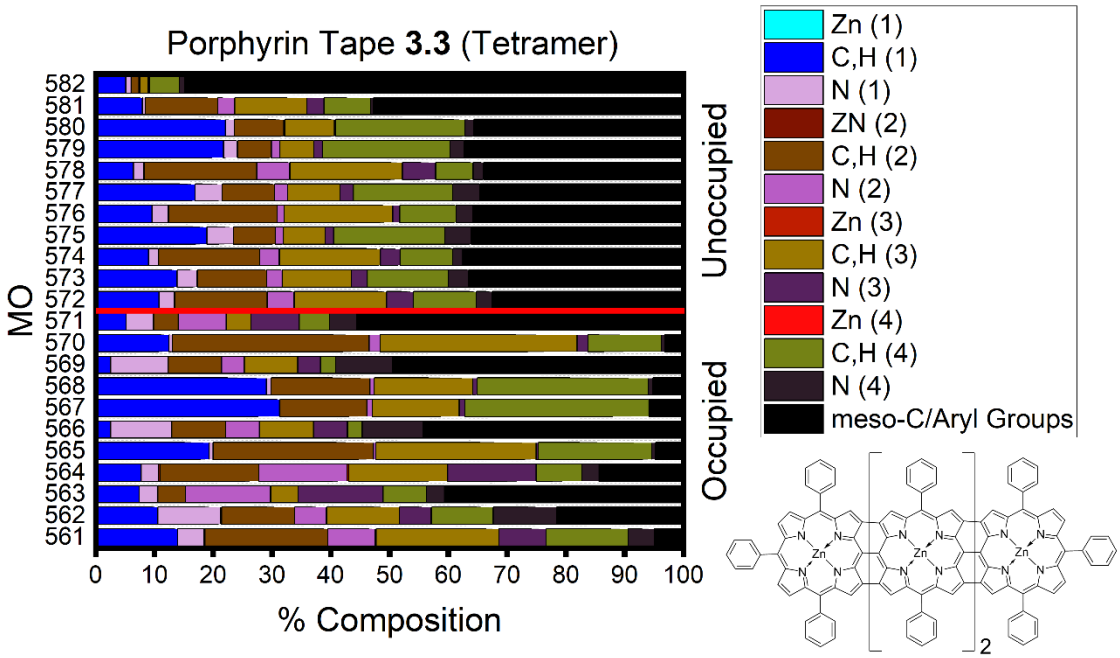


Figure S3.9. Molecular orbital percent composition diagram for tetramer **3.3**.

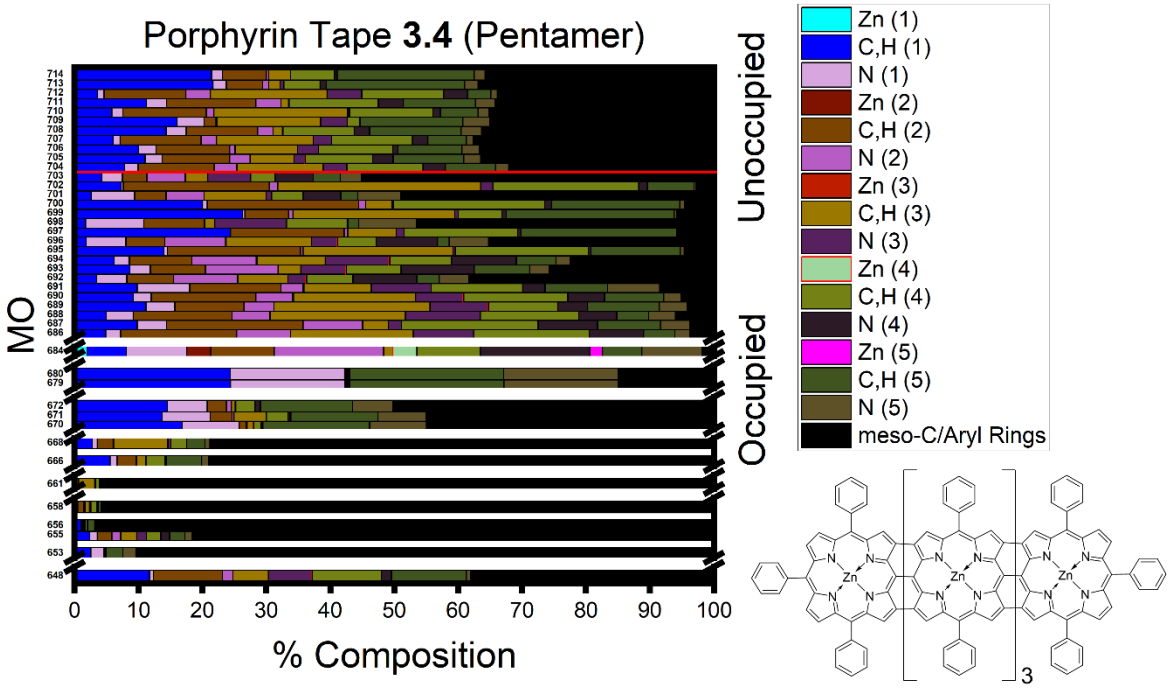


Figure S3.10. Molecular orbital percent composition diagram for pentamer **3.4**.

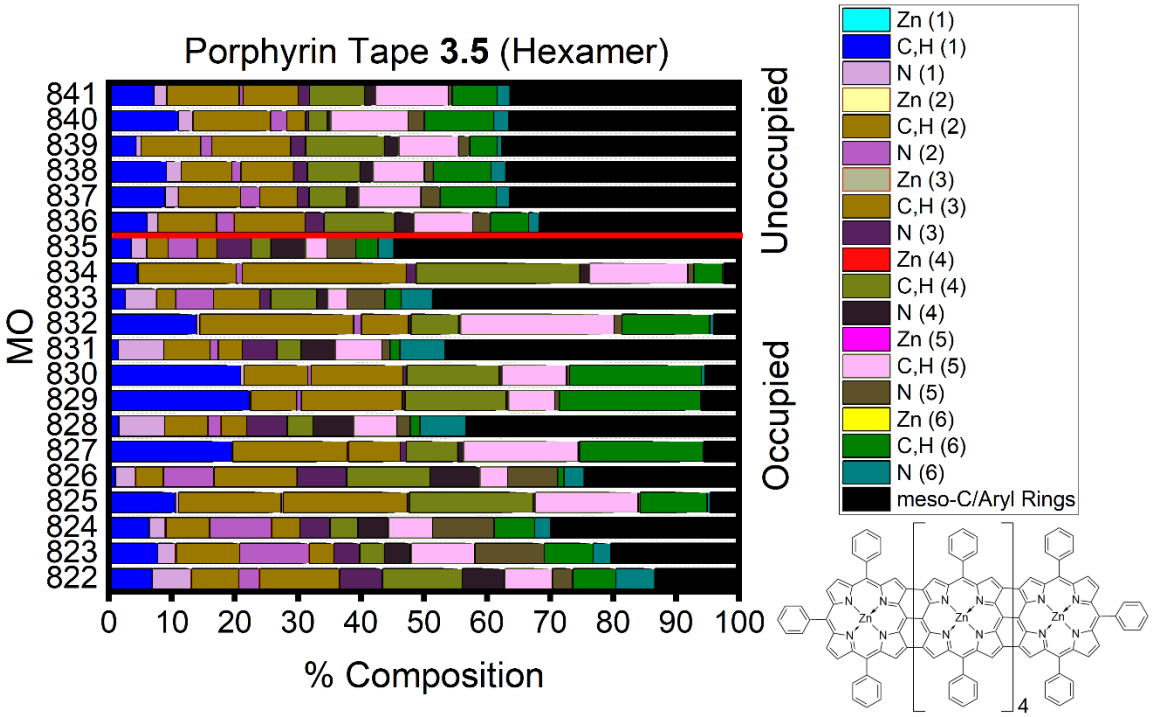


Figure S3.11. Molecular orbital percent composition diagram for hexamer **3.5**.

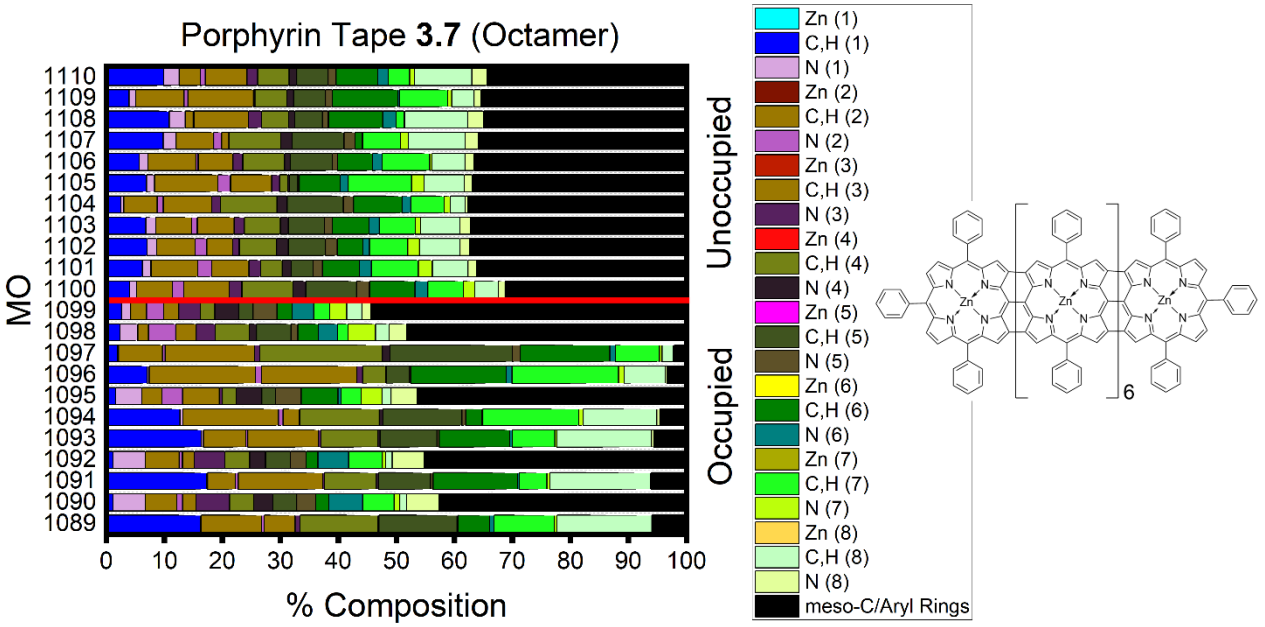


Figure S3.12. Molecular orbital percent composition diagram for octamer **3.7**.

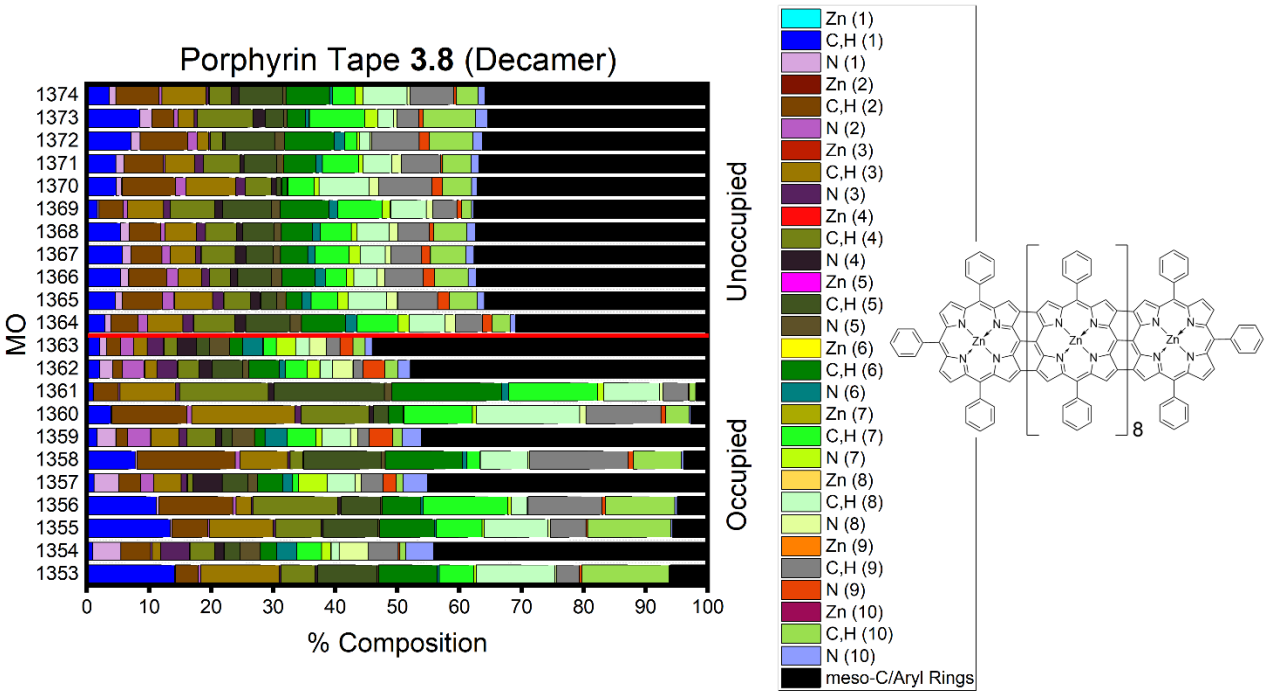


Figure S3.13. Molecular orbital percent composition diagram for decamer **3.8**.

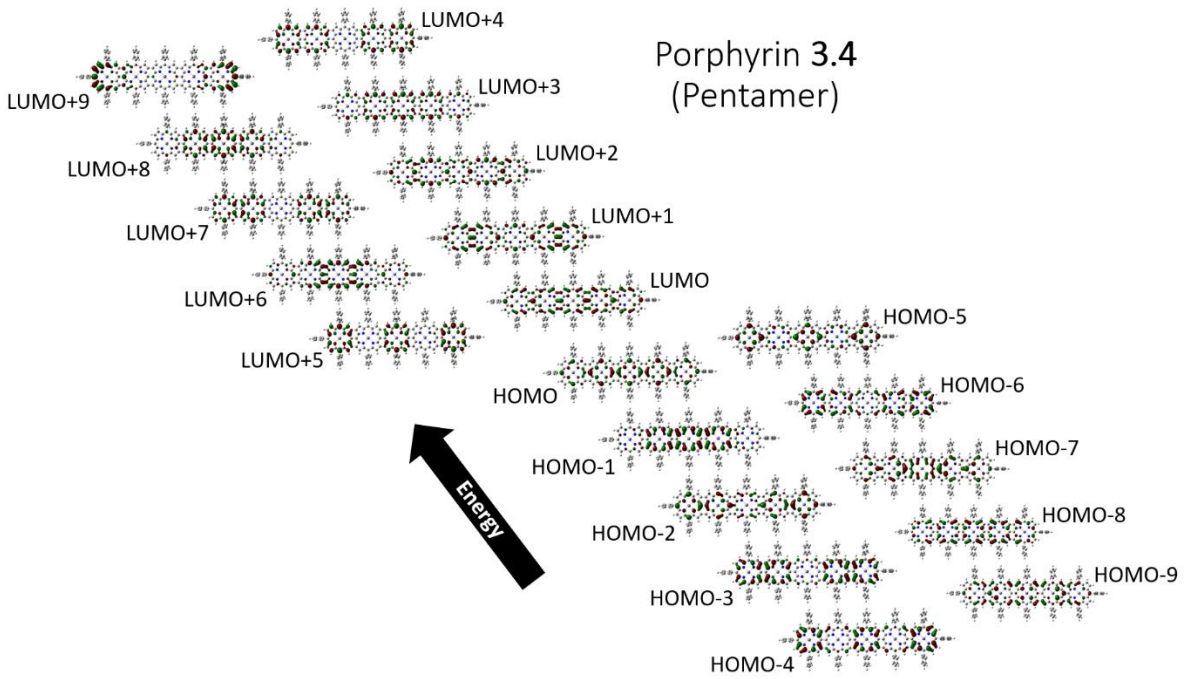


Figure S3.14. Selected DFT-predicted molecular orbitals for porphyrin tape **3.4**.

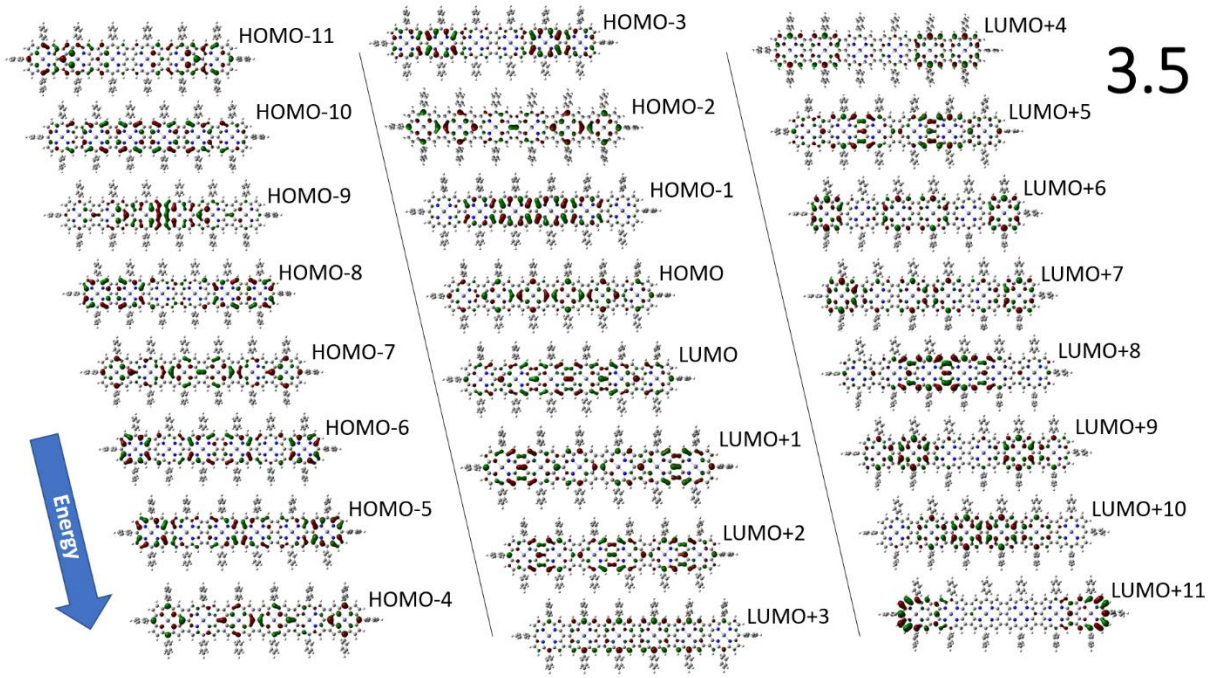
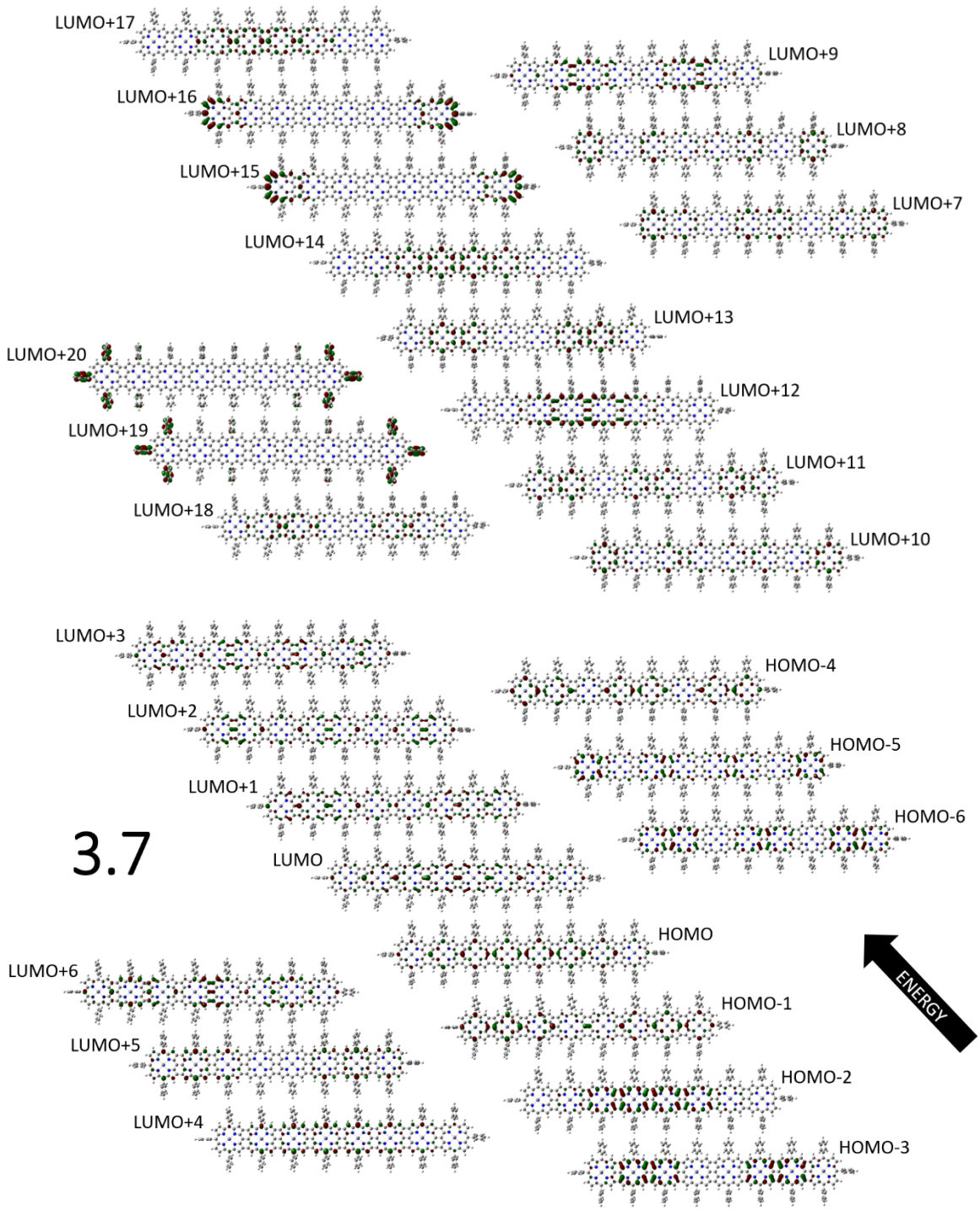


Figure S3.15. Selected DFT-predicted molecular orbitals for porphyrin tape **3.5**.


LUMO+17
LUMO+9
LUMO+16
LUMO+8
LUMO+15
LUMO+7
LUMO+14
LUMO+13
LUMO+20
LUMO+12
LUMO+19
LUMO+11
LUMO+18
LUMO+10
LUMO+3
HOMO-4
LUMO+2
HOMO-5
LUMO+1
HOMO-6
3.7
LUMO
HOMO
LUMO+6
HOMO-1
ENERGY
LUMO+5
HOMO-2
LUMO+4
HOMO-3

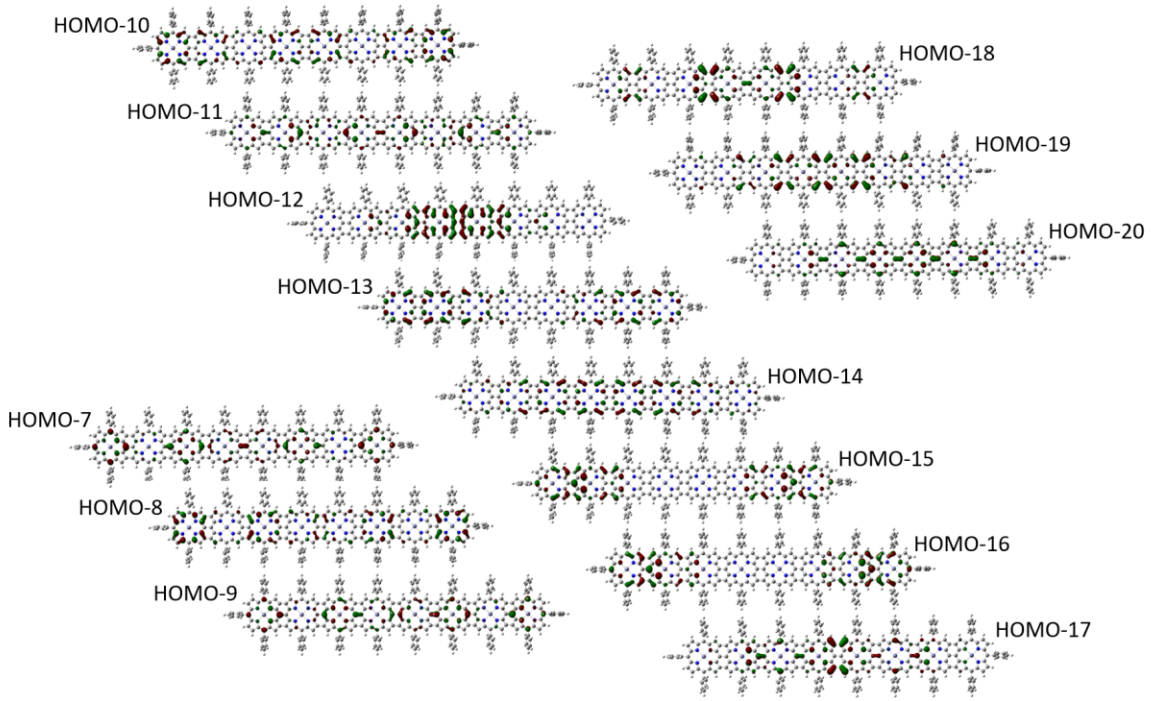
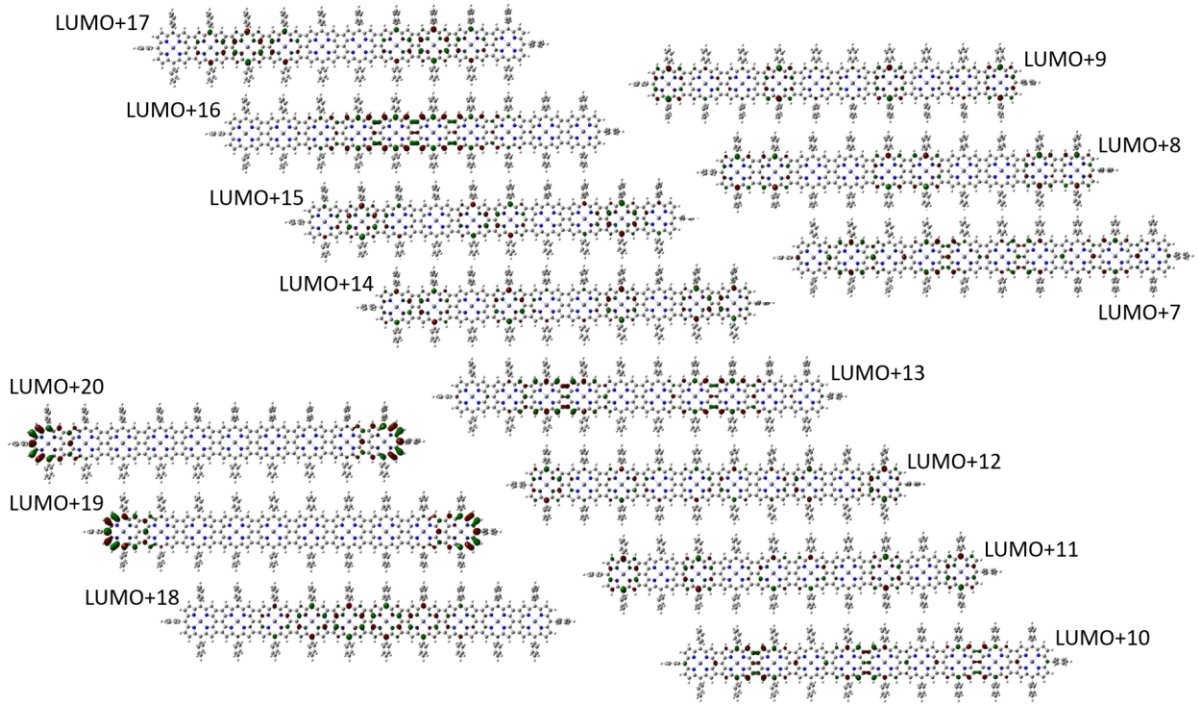


Figure S3.16. Selected DFT-predicted molecular orbitals for porphyrin tape **3.7**.



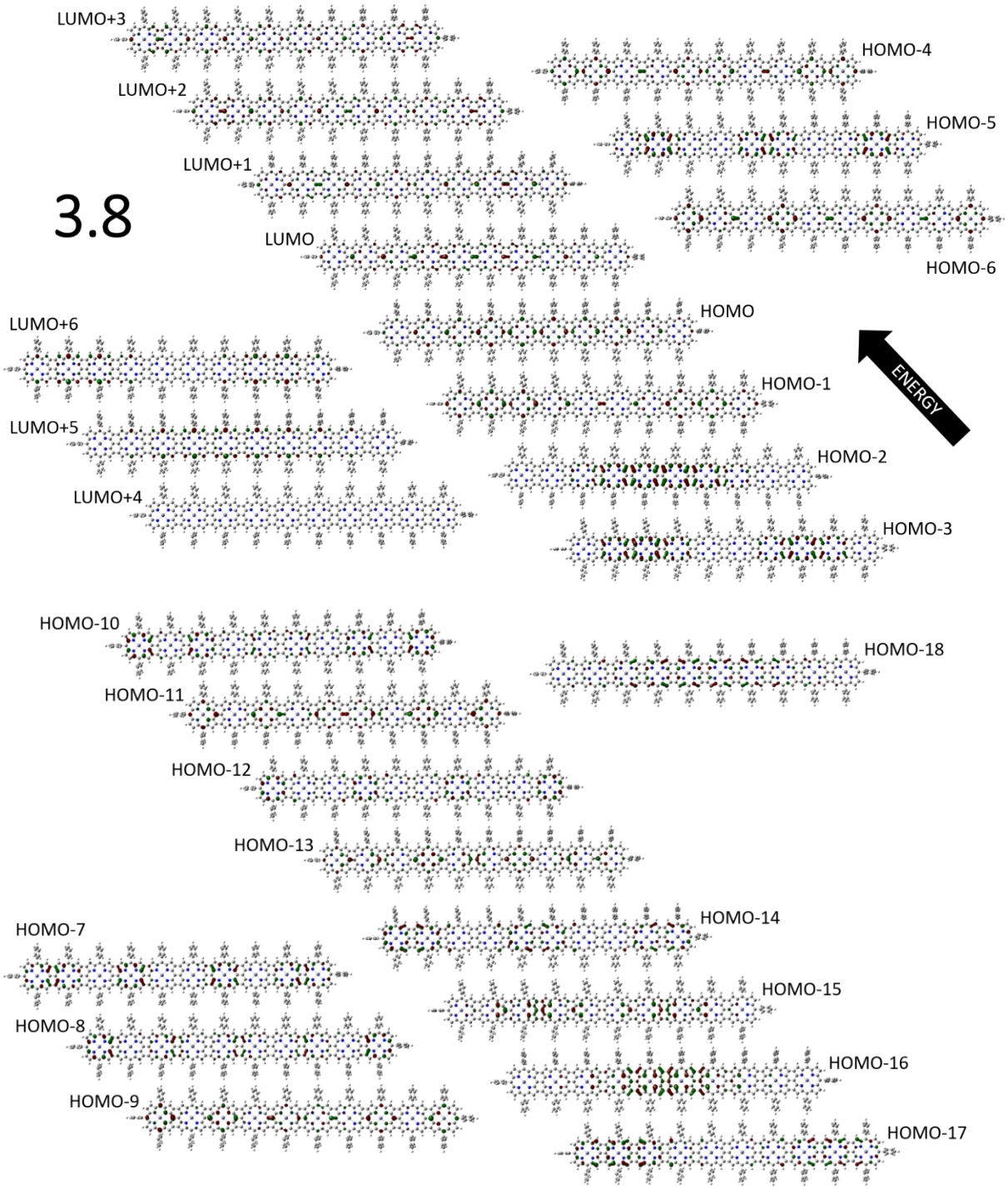
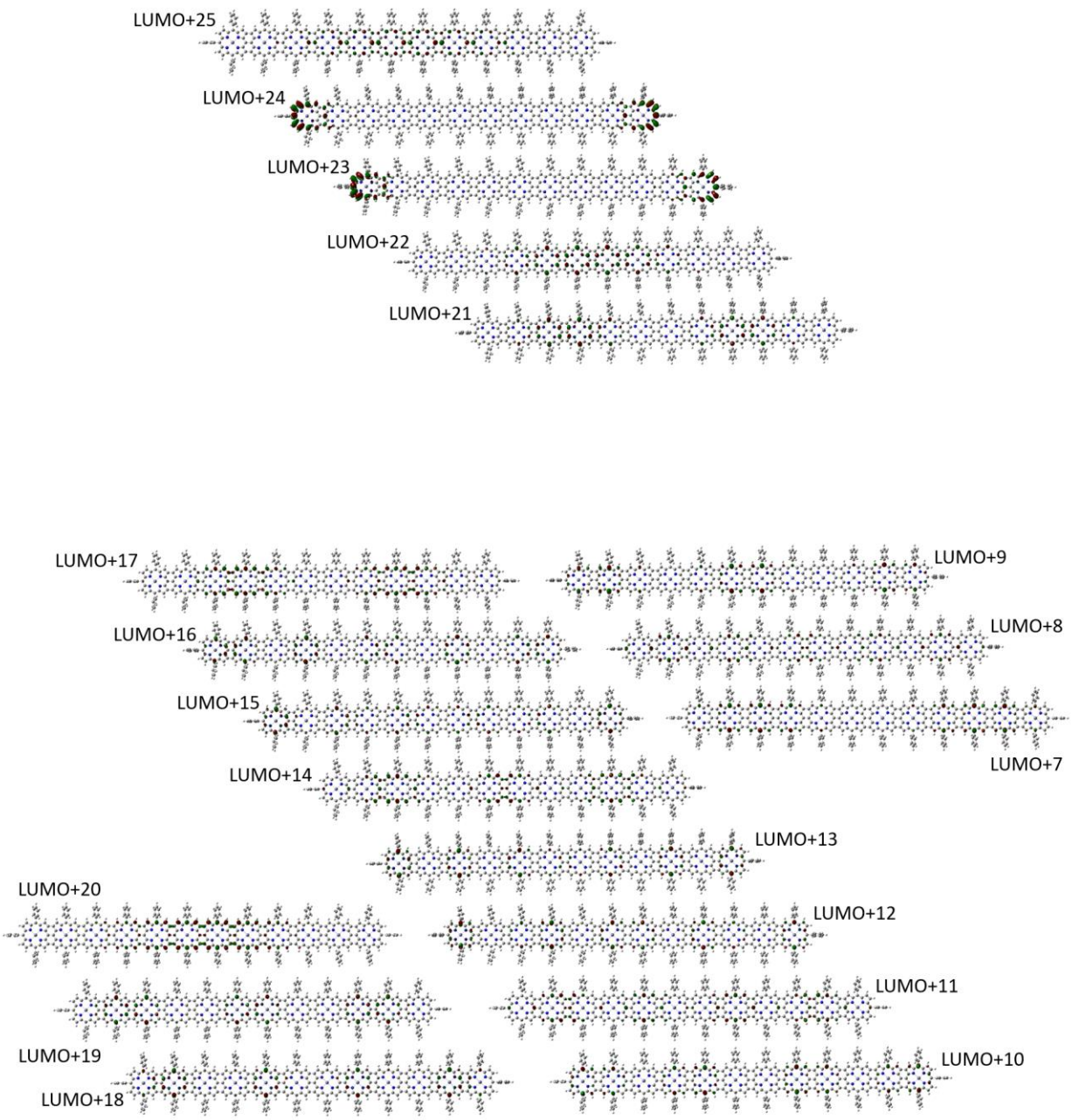
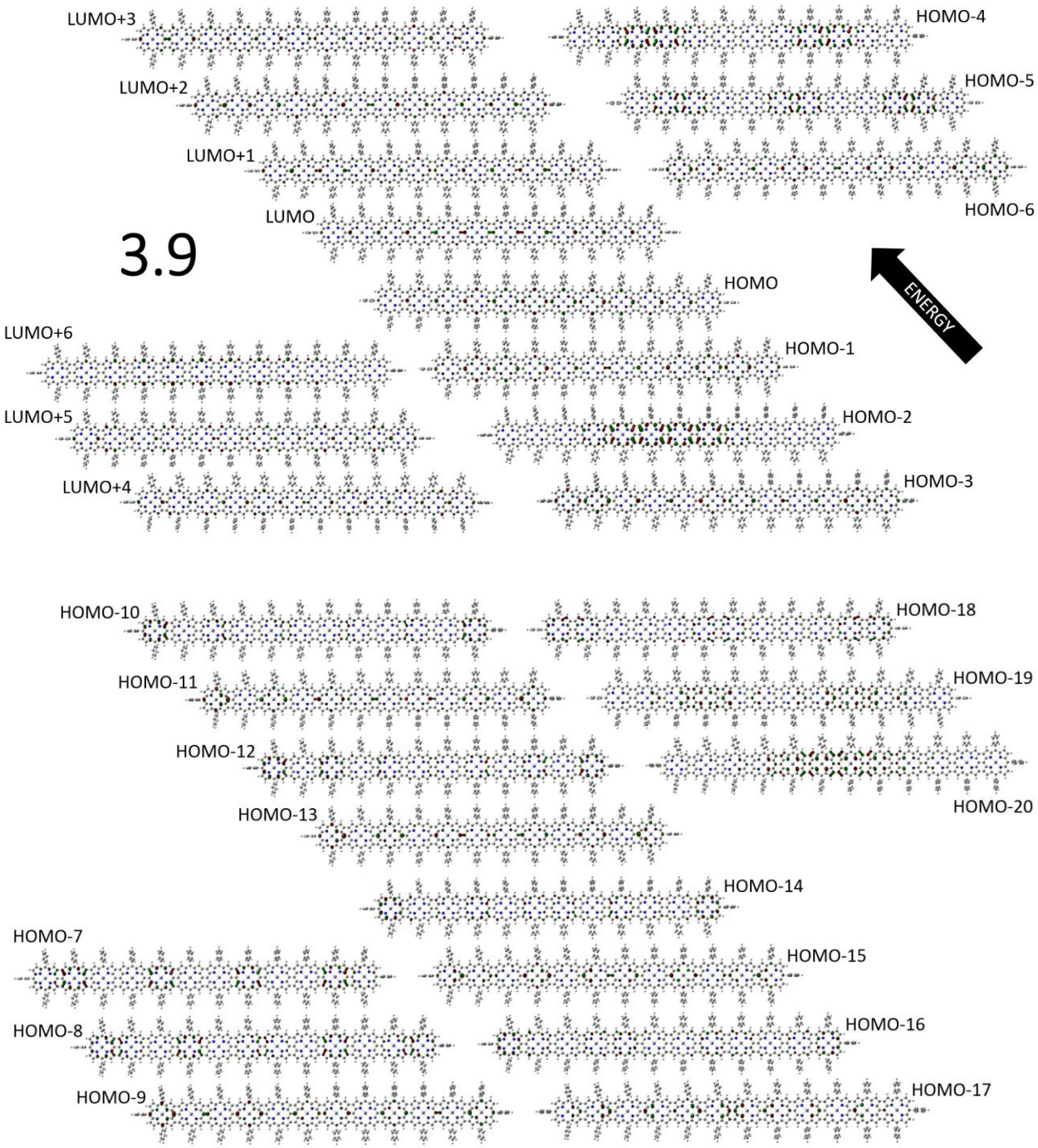


Figure S3.17. Selected DFT-predicted molecular orbitals for porphyrin tape **3.8**.


LUMO+25
LUMO+24
LUMO+23
LUMO+22
LUMO+21
LUMO+17
LUMO+9
LUMO+16
LUMO+8
LUMO+15
LUMO+7
LUMO+14
LUMO+13
LUMO+20
LUMO+12
LUMO+11
LUMO+19
LUMO+10
LUMO+18


LUMO+3
HOMO-4
LUMO+2
HOMO-5
LUMO+1
HOMO-6
LUMO
3.9
HOMO
ENERGY
LUMO+6
HOMO-1
LUMO+5
HOMO-2
LUMO+4
HOMO-3
HOMO-10
HOMO-18
HOMO-11
HOMO-19
HOMO-12
HOMO-20
HOMO-13
HOMO-14
HOMO-7
HOMO-15
HOMO-8
HOMO-16
HOMO-9
HOMO-17

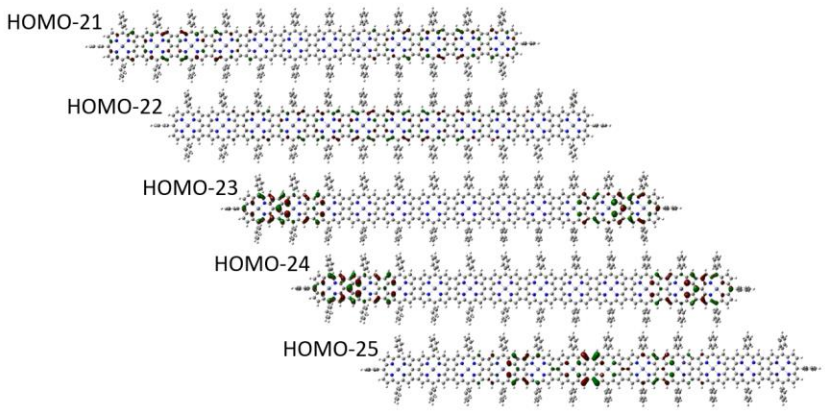


Figure S3.18. Selected DFT-predicted molecular orbitals for porphyrin tape **3.9**.

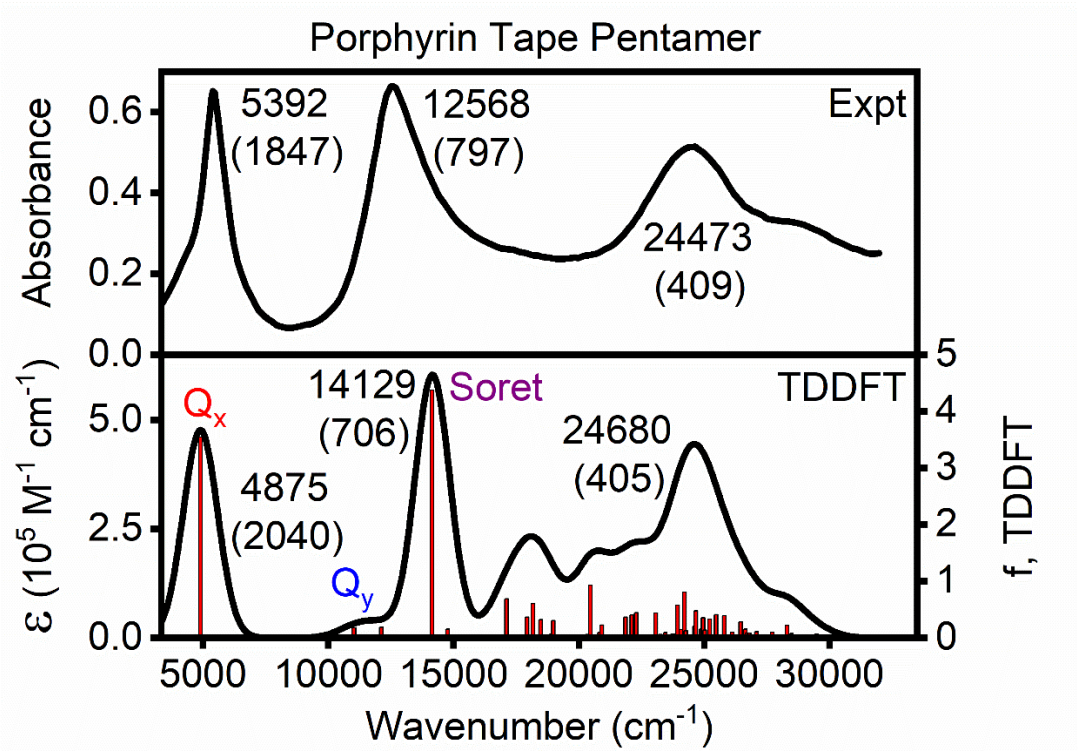


Figure S3.19. Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of pentamer **3.4**.

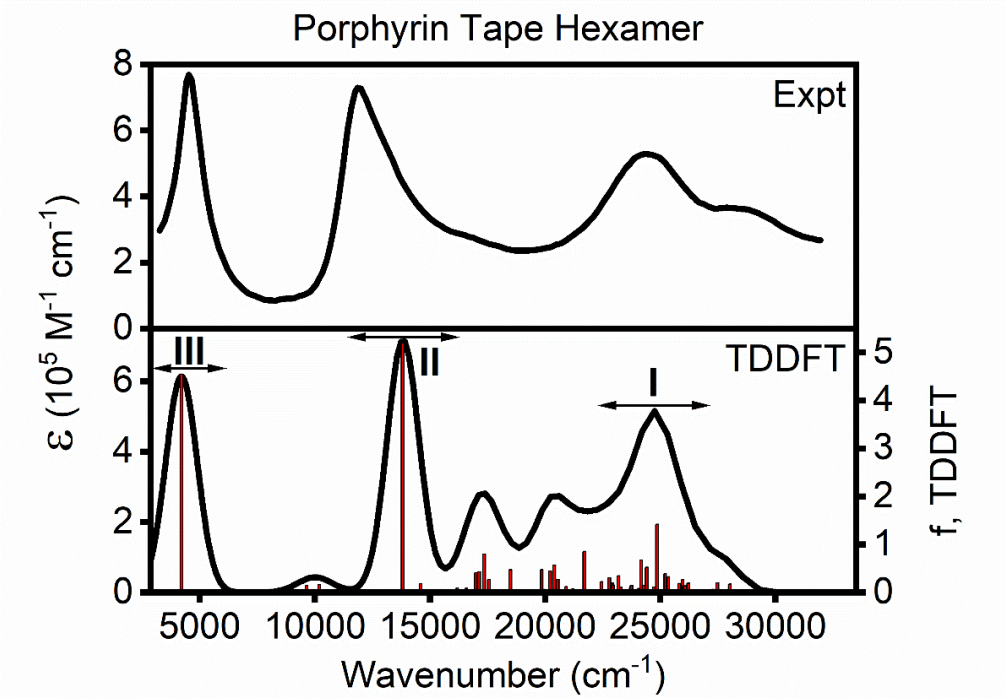


Figure S3.20. Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of hexamer **3.5**.

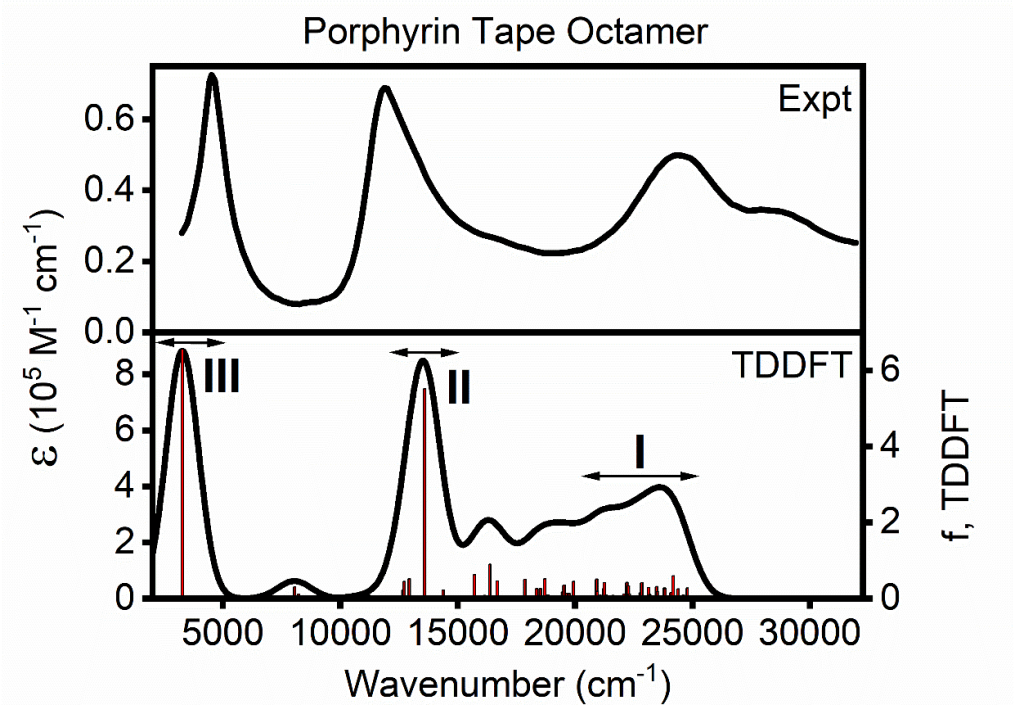


Figure S3.21. Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of octamer **3.7**.

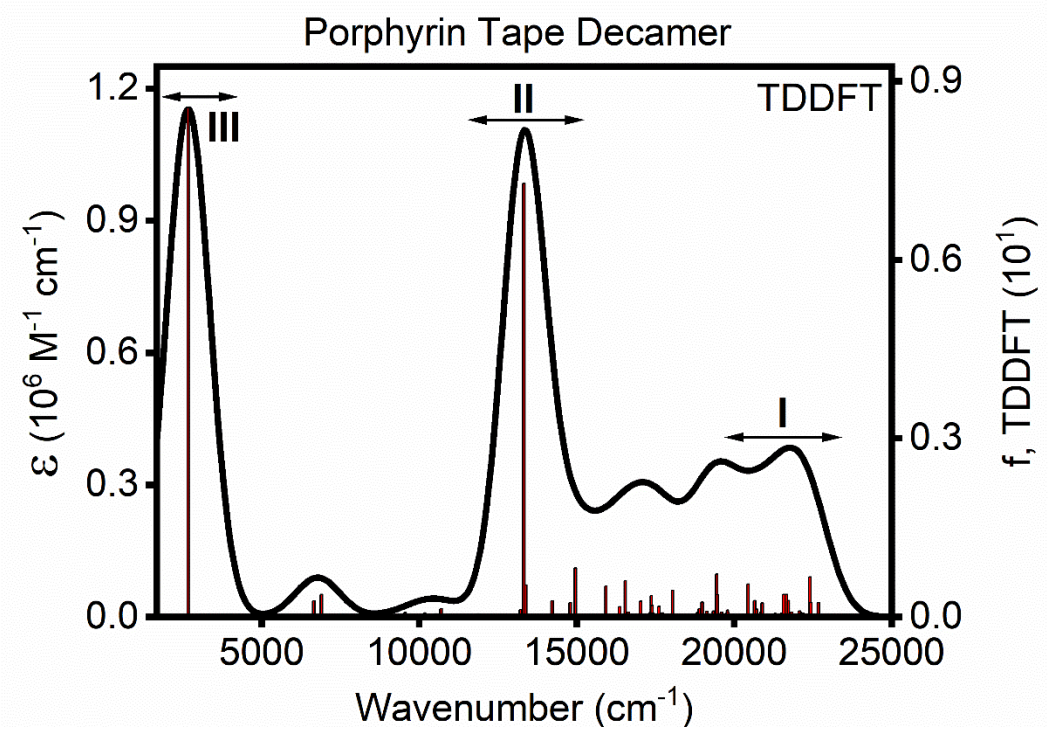


Figure S3.22. TDDFT-predicted (bottom) UV-vis spectrum of decamer **3.8**.

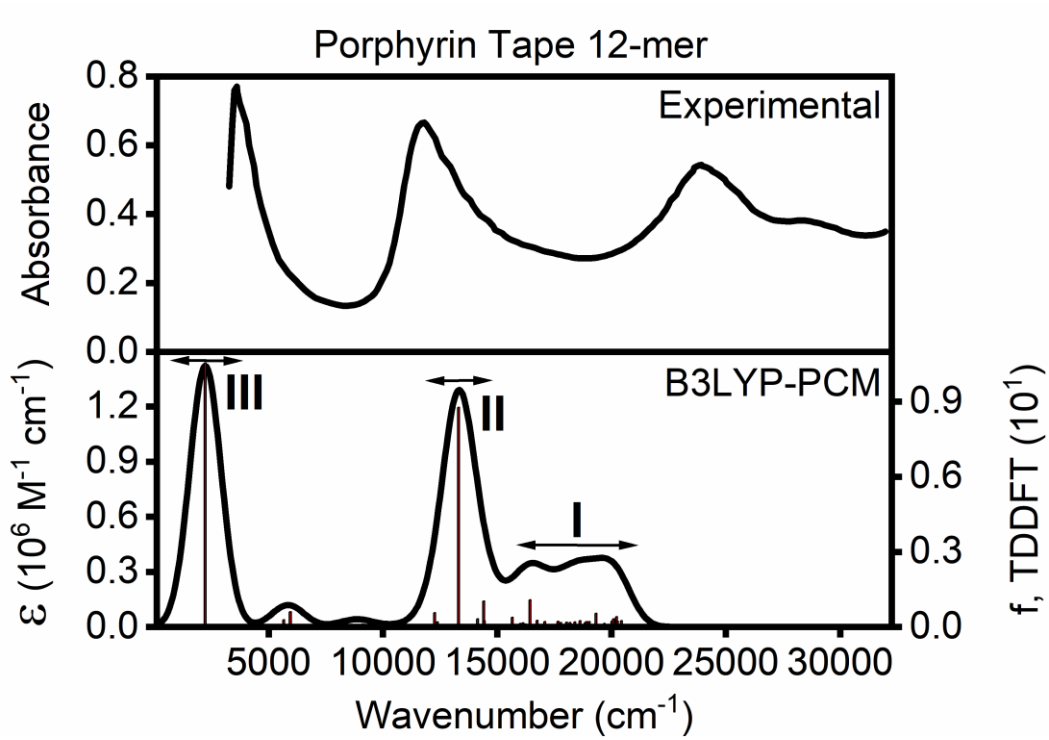


Figure S3.23. Experimental (top) and TDDFT-predicted (bottom) UV-vis spectrum of dodecamer **3.9**.

Table S3.1. TDDFT-predicted energies and compositions Q- and Soret-band assignments. [a]

Cmpd.	*Excited State*	*Assignment*	*λ/nm*	*E, cm^{-1}*	*f*	*Single-electron excitation contributions*
1.1	1,2	Q	546	18324	0.0368	H→L/L+1 (64%), H-1→L/L+1 (36%)
	3,4	Soret	413	24205	1.9080	H-1→L/L+1 (64%), H→L/L+1 (36%)
3.1	1	Q_1	997	10034	0.6740	H→L (94%), H-1→L+1 (5%)
	4	Q_2	620	16138	0.0174	H-2→L (65%), H→L+2 (33%)
	6	Soret-1	574	17434	1.6390	H-1→L+1 (91%), H-4→L (4%), H→L (4%)
	7	CT	540	18523	1.0460	H-4→L (93%), H-1→L+1 (3%), H→L (3%)
	8	Soret-type	517	19325	0.6133	H→L+2 (58%), H-2→L (27%), H-1→L+3 (11%), H-3→L+1 (4%)
	18	Soret-2	408	24518	2.7060	H-1→L+3 (59%), H-3→L+1 (24%), H→L+2 (8%), H-2→L (6%)
	22	CT	394	25362	0.3028	H→L+4 (37%), H-5→L+1 (33%), H-2→L+2 (26%), H-12→L (2%)
	23	CT	389	25715	0.3771	H-5→L+1 (58%), H→L+4 (29%), H-12→L (9%)
	42	Soret-type	354	28276	0.2657	H-3→L+3 (85%), H-2→L+2 (5%), H-18→L (2%)
	49	CT	325	30752	0.1397	H-25→L (62%), H-11→L+1 (29%), H-10→L+2 (3%)
	50	CT	325	30753	0.2023	H-13→L+1 (80%), H-14→L+2 (7%), H-15→L+1 (4%), H-12→L+2 (2%)
	53	CT	322	31014	0.1444	H-11→L+1 (56%), H-25→L (30%), H-10→L+2 (4%)
3.2	1	Q_1	1358	7363	1.5580	H→L (97%), H-1→L+2 (2%)
	6	Q-type	747	13388	0.0037	H→L+2 (96%)
	8	Q_2	649	15400	0.0645	H-4→L (76%), H→L+4 (20%), H-2→L+3 (2%)
	9	Soret-1	646	15475	3.1210	H-1→L+2 (90%), H-5→L (6%), H→L (3%)
	13	CT	565	17689	0.4068	H-7→L (66%), H-2→L+1 (22%), H-1→L+4 (4%), H-3→L+3 (2%)
	14	Q-type	562	17789	0.1775	H→L+4 (46%), H-3→L+1 (35%), H-4→L (16%)
	16	Q-type	541	18486	0.1366	H-2→L+1 (54%), H-7→L (30%), H-1→L+4 (7%), H-5→L (4%), H-3→L+3 (3%)
	21	Soret-type	510	19602	0.4884	H-3→L+1 (33%), H→L+4 (27%), H-9→L (25%), H-2→L+3 (7%), H-5→L+2 (4%)
	25	Soret-type	470	21275	0.6094	H-2→L+3 (69%), H-1→L+5 (13%), H-3→L+1 (8%), H-4→L (3%)
	30	Soret-type	452	22133	0.4242	H-3→L+3 (48%), H-4→L+2 (45%)
	31	CT	442	22616	0.1127	H-6→L+1 (92%), H→L+5 (2%)

	40	Soret-2	413	24226	1.8210	H-1→L+5 (46%), H-8→L+1 (16%), H-5→L+2 (11%), H-7→L+2 (10%), H-2→L+3 (5%)
	41	Soret-type	407	24548	0.5675	H-4→L+2 (28%), H→L+5 (22%), H-3→L+3 (13%), H-1→L+4 (9%), H-2→L+1 (7%), H-5→L (5%), H-30→L (4%), H-24→L (3%)
	46	CT	403	24810	0.2079	H-7→L+2 (45%), H-16→L (24%), H-6→L+3 (15%), H-5→L+2 (6%), H-1→L+5 (4%), H-8→L+1 (2%)
	48	CT	399	25082	0.5987	H-8→L+1 (68%), H-6→L+3 (9%), H-1→L+5 (8%), H-2→L+3 (4%), H-5→L+4 (3%), H-5→L+2 (2%)
	54	CT	394	25408	0.1447	H-9→L+2 (64%), H-21→L (25%), H-8→L+3 (3%), H-23→L (2%), H-19→L (2%)
	56	CT	390	25665	0.4594	H-6→L+3 (50%), H-7→L+2 (24%), H-8→L+1 (9)%, H-7→L+4 (6%), H-5→L+4 (3%), H-1→L+5 (3%)
	60	Soret-type	383	26128	0.2541	H-4→L+4 (80%), H-9→L+2 (5%), H-8→L+3 (4%)
	85	Soret-type	352	28446	0.2923	H-2→L+6 (86%), H-11→L+1 (3%), H-5→L+5 (2%), H-4→L+4 (2%)
	100	CT	327	30586	0.1371	H-37→L (64%), H-16→L+2 (15%), H-5→L+5 (4%), H-17→L+3 (4%), H-6→L+6 (3%)
	104	CT	324	30890	0.1301	H-19→L+2 (46%), H-21→L+2 (14%), H-18→L+3 (9%), H-20→L+3 (9%), H-13→L+1 (5%), H-12→L+2 (4%), H-11→L+3 (3%)
3.3	1	Q_1	1703	5871	2.5360	H→L (98%)
	10	Q-type	710	14091	0.3410	H→L+4 (38%), H-2→L+1 (34%), H-5→L (9%), H-7→L (7%), H-1→L+2 (6%), H-3→L+3 (2%)
	13	Soret-1	693	14439	2.1570	H-1→L+2 (43%), H→L+4 (39%), H-2→L+1 (14%)
	14	Soret-type	672	14872	1.2940	H-1→L+2 (45%), H-2→L+1 (39%), H→L+4 (12%)
	15	Q_2	666	15006	0.1087	H-6→L (81%), H→L+6 (14%), H-2→L+5 (2%)
	24	CT	573	17438	0.6096	H-11→L (94%), H-9→L+1 (3%)
	30	Soret-type	537	18623	0.3683	H-4→L+1 (29%), H-12→L (28%), H→L+6 (27%), H-3→L+4 (9%)
	35	Soret-type	509	19632	0.6761	H-3→L+3 (83%), H-2→L+1 (2%), H→L+8 (2%), H-1→L+2 (2%)
	44	Soret-type	478	20916	0.9720	H-2→L+5 (66%), H-3→L+4 (12%), H-1→L+7 (4%), H-4→L+1 (4%), H-10→L+1 (3%), H-6→L (2%)
	51	CT	455	22000	0.2914	H-9→L+1 (40%), H→L+8 (38%), H-5→L+4 (7%), H-7→L+4 (2%)

	52	Soret-type	450	22226	0.2735	H-5→L+3 (63%), H-10→L+1 (16%), H-1→L+7 (5%), H-2→L+5 (4%)
	68	CT	418	23926	0.2222	H-24→L (48%), H-4→L+5 (19%), H-6→L+3 (5%), H-5→L+4 (5%), H→L+8 (4%), H-26→L (3%), H-7→L+4 (2%), H-28→L (2%)
	71	Soret-type	415	24106	0.4672	H→L
	75	Soret-2	410	24385	1.4850	H-1→L+7 (30%), H-6→L+4 (14%), H-5→L+6 (13%), H-8→L+2 (11%), H-7→L+3 (10%), H-2→L+5 (4%)
	81	CT	405	24668	0.3100	H-9→L+2 (36%), H-6→L+4 (27%), H-8→L+2 (10%), H-7→L+3 (8%), H-5→L+6 (7%), H-1→L+7 (4%)
	89	CT	398	25144	0.8709	H-7→L+3 (43%), H-9→L+2 (24%), H-6→L+4 (12%), H-1→L+7 (8%), H-8→L+5 (3%)
	92	CT	394	25354	0.2540	H-13→L+2 (71%), H-7→L+4 (12%), H-12→L+3 (9%)
	107	Soret-type	384	26072	0.2753	H-2→L+7 (63%), H-42→L (12%), H-6→L+3 (4%), H-32→L (3%), H-4→L+5 (3%)
	121	Soret-type	371	26936	0.2849	H-6→L+6 (45%), H-12→L+3 (23%), H-10→L+5 (14%), H-13→L+5 (5%), H-13→L+2 (4%)
3.4	1	Q_1	2041	4899	3.5380	H→L (99%)
	17	Soret-1	707	14141	4.3760	H-1→L+3 (91%), H-3→LUMO+4 (4%)
	20	Q_2	678	14758	0.1508	H-8→LUMO (83.5%), HOMO→L+8 (10.2%)
	35	CT	584	17113	0.6864	H-15→L (88%), H-12→L+1 (5%), H-5→L+2 (2%)
	44	Soret-type	550	18177	0.6039	H-3→L+4 (57%), H-5→L+2 (11%), H-1→L+8 (5%), H-2→L+6 (4%), H-1→L+3 (3%), H-9→L+1 (3%), H-4→L+5 (3%), H-7→L+1 (3%), H-15→L (3%), H-4→L+3 (2%)
	63	Soret-type	489	20468	0.9282	H-2→L+7 (46%), H-3→L+6 (22%), H-13→L+1 (13%), H-5→L+8 (3%), H-4→L+2 (2%)
	81	CT	452	22117	0.4041	H-16→L+1 (41%), H-5→L+5 (33%), H-13→L+1 (5%), H-1→L+9 (4%), H-7→L+4 (3%), H-24→L (2%)
	82	Soret-type	449	22288	0.4433	H-4→L+5 (65%), H-8→L+3 (16%), H-6→L+4 (8%), H-6→L+7 (2%)
	96	CT	443	23075	0.4360	H-10→L+3 (52%), H-9→L+4 (14%), H-1→L+9 (8%), H-7→L+4 (6%), H-8→L+2 (4%), H-24→L (2%), H-12→L+4 (2%)
	107	Soret-type	418	23940	0.5761	H-5→L+8 (48%), H-1→L+9 (10%), H-6→L+6 (6%),

						H-8→L+2 (6%), H-7→L+7 (5%), H-3→L+10 (3%), H-2→L+7 (3%), H-7→L+4 (2%), H-9→L+4 (2%)
	113	Soret-2	413	24222	0.8048	H-1→L+9 (48%), H-6→L+6 (14%), H-11→L+3 (7%), H-7→L+4 (6%), H-5→L+8 (6%), H-8→L+2 (5%)
	123	CT	405	24671	0.4728	H-11→L+3 (50%), H-15→L+3 (18%), H-7→L+4 (4%), H-6→L+6 (4%), H-11→L+5 (3%), H-9→L+4 (3%), H-7→L+7 (3%), H-10→L+5 (2%), H-42→L (2%), H-14→L+2 (2%)
	150	CT	393	25473	0.4084	H-14→L+2 (67%), H-17→L+2 (11%), H-7→L+7 (3%), H-9→L+4 (3%), H-11→L+3 (2%)
3.5	1	Q_1	2378	4205	4.5470	H→L (99%)
	23	Soret-1	724	13815	5.2069	H-1→L+3 (88%), H-3→L+4 (6%)
	27	Q_2	685	14589	0.1823	H-10→L (85%), H→L+10 (8%), H-8→L+1 (2%)
	47	CT	589	16992	0.4099	H-18→L (74%), H-4→L+2 (9%), H-1→L+6 (7%), H-16→L+1 (4%), H-2→L+5 (2%)
	51	Soret-type	583	17142	0.4296	H-1→L+6 (63%), H-3→L+4 (12%), H-13→L (11%), H-18→L (5%)
	53	Soret-type	576	17359	0.7993	H-3→L+4 (64%), H-1→L+6 (14%), H-5→L+3 (8%), H-1→L+3 (6%)
	65	Soret-type	541	18492	0.4732	H-6→L+2 (61%), H→L+10 (21%), H-2→L+9 (5%), H-4→L+4 (3%), H-4→L+7 (2%)
	80	CT	504	19856	0.4737	H-15→L+1 (47%), H-2→L+9 (22%), H-5→L+5 (13%), H-10→L+2 (3%)
	86	CT	495	20219	0.4409	H-16→L+1 (52%), H-3→L+7 (11%), H-14→L+1 (6%), H-18→L (5%), H-25→L (4%), H-7→L+5 (3%), H-5→L+6 (3%), H-13→L+2 (2%)
	90	Soret-type	490	20403	0.5661	H-2→L+9 (33%), H-3→L+8 (24%), H-15→L+1 (19%), H-7→L+3 (4%), H-4→L+10 (2%)
	109	Soret-type	461	21700	0.8562	H-4→L+7 (67%), H-10→L+2 (3%), H-1→L+11 (3%), H-3→L+8 (2%), H-21→L+1 (2%), H-7→L+6 (2%)
	161	CT	414	24173	0.6758	H-1→L+11 (38%), H-6→L+8 (18%), H-14→L+3 (6%), H-12→L+3 (5%), H-9→L+4 (4%), H-3→L+12 (4%), H-17→L+2 (3%), H-8→L+5 (3%), H-12→L+6 (2%), H-4→L+7 (2%)
	169	CT	410	24416	0.5232	H-16→L+3 (17%), H-20→L+2 (12%), H-17→L+2 (7%),

						H-13→L+4 (7%), H-7→L+6 (7%), H-1→L+11 (6%), H-6→L+8 (6%), H-9→L+7 (5%), H-14→L+3 (4%), H-7→L+9 (4%), H-12→L+6 (4%), H-4→L+10 (3%), H-18→L+4 (2%)
	188	Soret-2	402	24862	1.4173	H-14→L+3 (32%), H-1→L+11 (14%), H-13→L+4 (11%), H-11→L+4 (10%), H-7→L+9 (6%), H-16→L+3 (5%)
3.7	1	Q_1	3055	3274	6.5580	H→L (99%)
	30	Soret-type	786	12719	0.4475	H-4→L+2 (49%), H-12→L (17%), H→L+6 (11%), H-1→L+3 (7%), H-7→L+1 (6%), H-2→L+4 (3%)
	33	Soret-type	773	12935	0.5184	H-1→L+3 (66%), H-4→L+2 (15%), H→L+6 (9%), H-2→L+4 (4%)
	37	Soret-1	736	13593	5.5077	H-2→L+4 (74%), H-3→L+5 (9%), H-4→L+2 (8%)
	44	Q_2	695	14384	0.2170	H-14→L (72%), H-6→L+2 (7%), H-8→L+1 (5%), H→L+14 (5%), H-13→L+1 (3%)
	62	Soret-type	636	15718	0.6282	H-2→L+7 (30%), H-3→L+5 (27%), H-17→L (8%), H-5→L+4 (7%), H-21→L (6%), H-11→L+1 (3%), H-16→L (2%), H→L+12 (2%)
	72	Soret-type	611	16368	0.9001	H-2→L+7 (41%), H-3→L+5 (24%), H-2→L+4 (11%), H-25→L (7%), H-5→L+4 (6%), H-3→L+8 (3%), H-7→L+3 (2%)
	78	CT	599	16694	0.4588	H-25→L (56%), H-9→L+2 (11%), H-23→L+1 (8%), H-21→L (7%), H-2→L+7 (6%), H-5→L+4 (5%)
	101	Soret-type	560	17868	0.4990	H-10→L+2 (60%), H→L+14 (22%), H-1→L+10 (6%)
	115	Soret-type	534	18712	0.5159	H-5→L+7 (39%), H-18→L+1 (29%), H-2→L+10 (4%), H-21→L (3%), H-3→L+8 (3%), H-3→L+5 (2%)
	147	Soret-type	502	19935	0.4488	H-1→L+13 (29%), H-14→L+2 (20%), H-5→L+9 (10%), H-3→L+12 (10%), H-7→L+7 (7%), H-11→L+4 (3%), H-9→L+5 (3%), H-24→L+1 (2%)
	171	Soret-type	478	20922	0.5058	H-4→L+11 (47%), H-13→L+3 (19%), H-7→L+13 (5%), H-14→L+2 (4%), H-10→L+6 (3%), H-1→L+13 (2%)
	178	Soret-type	471	21249	0.4190	H-13→L+3 (48%), H-4→L+11 (24%), H-4→L+14 (4%), H-22→L+2 (3%), H-14→L+2 (3%), H-10→L+6 (3%), H-3→L+12 (2%)
	208	Soret-type	450	22211	0.4272	H-7→L+10 (30%), H-43→L (14%), H-26→L+2 (11%), H-10→L+6 (8%), H-22→L+2 (5%), H-45→L (4%), H-4→L+14 (2%), H-9→L+8 (2%)
	227	Soret-type	438	22840	0.4189	H-9→L+8 (20%), H-8→L+9 (16%), H-15→L+4 (8%), H-10→L+6 (8%), H-11→L+7 (7%), H-16→L+5 (7%),

						H-7→L+10 (7%), H-6→L+12 (7%)
	277	Soret-2	414	24174	0.5980	H-2→L+15 (36%), H-15→L+4 (10%), H-3→L+16 (9%), H-67→L (6%), H-7→L+13 (5%), H-19→L+3 (5%)
3.8	1	Q_1	3748	2668	8.5540	H→L (98%), H-1→L+1 (2%)
	54	Soret-1	750	13325	7.2832	H-2→L+5 (64%), H-3→L+6 (12%), H-6→L+3 (4%)
	55	Soret-type	747	13390	0.5356	H→L+10 (36%), H-11→L+1 (34%), H-1→L+7 (12%), H-2→L+5 (5%), H-4→L+4 (5%)
	65	Q_2	703	14225	0.2703	H-18→L (84%), H-17→L+1 (5%), H→L+18 (4%), H-12→L+1 (2%)
	76	Soret-type	668	14963	0.8191	H-2→L+8 (29%), H-3→L+6 (27%), H-5→L+5 (14%), H-15→L+1 (7%), H-22→L (4%), H-19→L (4%)
	98	Soret-type	628	15930	0.5227	H-2→L+8 (48%), H-3→L+6 (19%), H-2→L+5 (15%), H-5→L+5 (9%), H-3→L+9 (4%)
	114	CT	604	16545	0.6096	H-32→L (67%), H-30→L+1 (10%), H-13→L+2 (6%), H-28→L (4%), H-3→L+6 (3%), H-28→L+2 (3%)
	156	Soret-type	554	18043	0.4439	H-12→L+3 (53%), H-24→L+1 (15%), H→L+18 (13%), H-10→L+4 (4%), H-14→L+2 (3%), H-10→L+2 (2%)
	206	Soret-type	514	19446	0.7194	H-8→L+7 (33%), H-1→L+17 (26%), H-36→L+1 (5%), H-4→L+12 (3%), H-37→L+1 (3%), H-18→L+2 (3%), H-4→L+18 (2%)
	241	Soret-2	489	20444	0.5550	H-27→L+2 (31%), H-4→L+15 (30%), H-17→L+3 (6%), H-6→L+11 (4%)
	326	Soret-type	446	22404	0.6740	H-9→L+12 (33%), H-11→L+11 (10%), H-6→L+14 (9%), H-15→L+8 (5%), H-13→L+9 (5%), H-10→L+10 (5%), H-18→L+4 (3%), H-24→L+3 (3%), H-6→L+17 (2%)
3.9	1	Q_1	4489	2228	10.550	H→L (98%), H-1→L+1 (2%)
	9	Soret-type	1681	5948	0.6014	H-1→L+1 (58%), H→L+2 (23%), H-3→L (16%)
	57	Soret-type	816	12259	0.5659	H-6→L+3 (47%), H-1→L+5 (35%), H-9→L+2 (6%), H→L+8 (3%)
	73	Soret-1	752	13306	8.7710	H-2→L+6 (63%), H-4→L+7 (15%), H-5→L+9 (5%), H-2→L+9 (5%)
	91	Q_2	707	14138	0.3177	H-22→L (83%), H-21→L+1 (6%), H→L+22 (3%)
	94	Soret-type	694	14414	1.028	H-2→L+9 (25%), H-4→L+7 (22%), H-5→L+6 (17%), H-13→L+2 (17%), H-15→L+1 (3%), H-7→L+7 (2%)
	156	CT	608	16438	1.080	H-40→L (64%), H-38→L+1 (13%), H-35→L (6%), H-35→L+2 (3%)

284	Soret-2	518	19319	0.5391	H-10→L+8 (25%), H-1→L+21 (20%), H-21→L+3 (10.5%), H-8→L+11 (7%), H-2→L+1 (5%)
331	Soret-type	494	20224	0.4124	H-3→L+19 (26%), H-18→L+4 (20%), H-36→L+2 (19%), H-6→L+15 (7%), H-31→L+2 (3%), H-6→L+21 (2%)

[a] For compounds **3.1** and **3.2**, only excited states with $f \geq 0.1$ are listed; for compound **3.3**, only excited states with $f \geq 0.2$ are listed; for compounds **3.4**-**3.9**, only excited states with $f \geq 0.4$ are listed; for all compounds, the additional excited states of lower than threshold intensities that are discussed specifically in the text (i.e. Q_2) are also listed. For a complete description of the TDDFT-predicted excited states, see Supporting Information tables below.

Table S3.2. Optimized coordinates for **1.1**.

```
Zn 0.0000000000 0.0000000000 0.0000000000
N 0.0000000000 2.0509880000 0.0000000000
N 2.0509880000 0.0000000000 0.0000000000
N -2.0509880000 0.0000000000 0.0000000000
N 0.0000000000 -2.0509880000 0.0000000000
C 1.1038440000 2.8705470000 0.0045110000
C -1.1038440000 2.8705470000 -0.0045110000
C 2.8705470000 1.1038440000 -0.0045110000
C 2.8705470000 -1.1038440000 0.0045110000
C -2.8705470000 1.1038440000 0.0045110000
C -2.8705470000 -1.1038440000 -0.0045110000
C 1.1038440000 -2.8705470000 -0.0045110000
C -1.1038440000 -2.8705470000 0.0045110000
C 2.4478980000 2.4478980000 0.0000000000
C 0.6806860000 4.2542560000 -0.0023390000
C -0.6806860000 4.2542560000 0.0023390000
C 4.2542560000 0.6806860000 0.0023390000
C 2.4478980000 -2.4478980000 0.0000000000
C 4.2542560000 -0.6806860000 -0.0023390000
C -2.4478980000 2.4478980000 0.0000000000
C -4.2542560000 0.6806860000 -0.0023390000
C -4.2542560000 -0.6806860000 0.0023390000
C 0.6806860000 -4.2542560000 0.0023390000
C -2.4478980000 -2.4478980000 0.0000000000
C -0.6806860000 -4.2542560000 -0.0023390000
H 5.1101940000 1.3396930000 0.0076810000
H 5.1101940000 -1.3396930000 -0.0076810000
H 1.3396930000 5.1101940000 -0.0076810000
H -1.3396930000 5.1101940000 0.0076810000
H -5.1101940000 1.3396930000 -0.0076810000
H -5.1101940000 -1.3396930000 0.0076810000
H -1.3396930000 -5.1101940000 -0.0076810000
H 1.3396930000 -5.1101940000 0.0076810000
C -3.5086390000 3.5086390000 0.0000000000
C -4.2879200000 3.7445890000 1.1439740000
C -3.7445890000 4.2879200000 -1.1439740000
C -5.2754600000 4.7318790000 1.1445680000
H -4.1122760000 3.1523820000 2.0378680000
C -4.7318790000 5.2754600000 -1.1445680000
H -3.1523820000 4.1122760000 -2.0378680000
C -5.5005180000 5.5005180000 0.0000000000
H -4.9020900000 5.8659580000 -2.0409240000
C 3.5086390000 3.5086390000 0.0000000000
C 3.7445890000 4.2879200000 1.1439740000
C 4.2879200000 3.7445890000 -1.1439740000
C 4.7318790000 5.2754600000 1.1445680000
H 3.1523820000 4.1122760000 2.0378680000
C 5.2754600000 4.7318790000 -1.1445680000
H 4.1122760000 3.1523820000 -2.0378680000
C 5.5005180000 5.5005180000 0.0000000000
H 4.9020900000 5.8659580000 2.0409240000
H 5.8659580000 4.9020900000 -2.0409240000
C -3.5086390000 -3.5086390000 0.0000000000
C -4.2879200000 -3.7445890000 -1.1439740000
C -3.7445890000 -4.2879200000 1.1439740000
C -5.2754600000 -4.7318790000 -1.1445680000
H -4.1122760000 -3.1523820000 -2.0378680000
C -4.7318790000 -5.2754600000 1.1445680000
H -3.1523820000 -4.1122760000 2.0378680000
C -5.5005180000 -5.5005180000 0.0000000000
H -5.8659580000 -4.9020900000 -2.0409240000
```

```
H -4.9020900000 -5.8659580000 2.0409240000
C 3.5086390000 -3.5086390000 0.0000000000
C 3.7445890000 -4.2879200000 -1.1439740000
C 4.2879200000 -3.7445890000 1.1439740000
C 4.7318790000 -5.2754600000 -1.1445680000
H 3.1523820000 -4.1122760000 -2.0378680000
C 5.2754600000 -4.7318790000 1.1445680000
H 4.1122760000 -3.1523820000 2.0378680000
C 5.5005180000 -5.5005180000 0.0000000000
H 4.9020900000 -5.8659580000 -2.0409240000
H 5.8659580000 -4.9020900000 2.0409240000
H -5.8659580000 4.9020900000 2.0409240000
H 6.2688820000 6.2688820000 0.0000000000
H -6.2688820000 6.2688820000 0.0000000000
H -6.2688820000 -6.2688820000 0.0000000000
H 6.2688820000 -6.2688820000 0.0000000000
```

Table S3.3. Optimized coordinates for **3.1**.

```
C -0.1143410000 2.5269970000 7.7012460000
C -0.0627620000 1.2509230000 7.0236920000
N -0.0607050000 1.4532420000 5.6634080000
Zn 0.0000000000 0.0000000000 4.2210860000
N 0.0661100000 -1.4440330000 2.7707160000
C 0.0284950000 -1.2378130000 1.4217280000
C 0.0000000000 0.0000000000 0.7415400000
C -0.0284950000 1.2378130000 1.4217280000
N -0.0661100000 1.4440330000 2.7707160000
C -0.0890930000 2.8112100000 2.9582530000
C -0.1190610000 3.4631090000 4.2058990000
C -0.1080090000 2.8113950000 5.4603540000
C -0.1539160000 3.4889670000 6.7367420000
H -0.2065610000 4.5586850000 6.8770060000
C -0.0530240000 3.4811860000 1.6794480000
C -0.0217250000 2.5012890000 0.7188170000
C 0.0217250000 2.5012890000 -0.7188170000
C 0.0284950000 1.2378130000 -1.4217280000
N 0.0661100000 1.4440330000 -2.7707160000
Zn 0.0000000000 0.0000000000 -4.2210860000
N -0.0607050000 -1.4532420000 -5.6634080000
C -0.0627620000 -1.2509230000 -7.0236920000
C 0.0000000000 0.0000000000 -7.6728600000
C 0.0627620000 1.2509230000 -7.0236920000
N 0.0607050000 1.4532420000 -5.6634080000
C 0.1080090000 2.8113950000 -5.4603540000
C 0.1190610000 3.4631090000 -4.2058990000
C 0.0890930000 2.8112100000 -2.9582530000
C 0.0530240000 3.4811860000 -1.6794480000
H 0.0466060000 4.5511970000 -1.5316480000
C 0.1539160000 3.4889670000 -6.7367420000
C 0.1143410000 2.5269970000 -7.7012460000
H 0.1205900000 2.6685080000 -8.7721180000
H 0.2065610000 4.5586850000 -6.8770060000
C -0.1143410000 -2.5269970000 -7.7012460000
C -0.1539160000 -3.4889670000 -6.7367420000
C -0.1080090000 -2.8113950000 -5.4603540000
C -0.1190610000 -3.4631090000 -4.2058990000
C -0.0890930000 -2.8112100000 -2.9582530000
N -0.0661100000 -1.4440330000 -2.7707160000
```

C -0.0284950000 -1.2378130000 -1.4217280000
C -0.0217250000 -2.5012890000 -0.7188170000
C 0.0217250000 -2.5012890000 0.7188170000
C 0.0530240000 -3.4811860000 1.6794480000
C 0.0890930000 -2.8112100000 2.9582530000
C 0.1190610000 -3.4631090000 4.2058990000
C 0.1080090000 -2.8113950000 5.4603540000
N 0.0607050000 -1.4532420000 5.6634080000
C 0.0627620000 -1.2509230000 7.0236920000
C 0.1143410000 -2.5269970000 7.7012460000
C 0.1539160000 -3.4889670000 6.7367420000
H 0.2065610000 -4.5586850000 6.8770060000
C 0.0000000000 0.0000000000 7.6728600000
H 0.0466060000 -4.5511970000 1.5316480000
C -0.0530240000 -3.4811860000 -1.6794480000
H -0.0466060000 -4.5511970000 -1.5316480000
C 0.0000000000 0.0000000000 -0.7415400000
H -0.2065610000 -4.5586850000 -6.8770060000
H -0.1205900000 -2.6685080000 -8.7721180000
H -0.0466060000 4.5511970000 1.5316480000
H 0.1205900000 -2.6685080000 8.7721180000
H -0.1205900000 2.6685080000 8.7721180000
C 0.1631010000 4.9611570000 -4.2034820000
C -0.9354740000 5.7139450000 -4.6496350000
C 1.3047280000 5.6436940000 -3.7525630000
C -0.8939000000 7.1095010000 -4.6449650000
H -1.8278520000 5.1990370000 -4.9944890000
C 1.3474920000 7.0393330000 -3.7490270000
H 2.1638320000 5.0736460000 -3.4100530000
C 0.2481180000 7.7767190000 -4.1951050000
H -1.7559330000 7.6745890000 -4.9893680000
H 2.2416510000 7.5493090000 -3.4005700000
H 0.2808610000 8.8628200000 -4.1919820000
C -0.1631010000 4.9611570000 4.2034820000
C 0.9354740000 5.7139450000 4.6496350000
C -1.3047280000 5.6436940000 3.7525630000
C 0.8939000000 7.1095010000 4.6449650000
H 1.8278520000 5.1990370000 4.9944890000
C -1.3474920000 7.0393330000 3.7490270000
H -2.1638320000 5.0736460000 3.4100530000
C -0.2481180000 7.7767190000 4.1951050000
H 1.7559330000 7.6745890000 4.9893680000
H -2.2416510000 7.5493090000 3.4005700000
H -0.2808610000 8.8628200000 4.1919820000
C 0.1631010000 -4.9611570000 4.2034820000
C -0.9354740000 -5.7139450000 4.6496350000
C 1.3047280000 -5.6436940000 3.7525630000
C -0.8939000000 -7.1095010000 4.6449650000
H -1.8278520000 -5.1990370000 4.9944890000
C 1.3474920000 -7.0393330000 3.7490270000
H 2.1638320000 -5.0736460000 3.4100530000
C 0.2481180000 -7.7767190000 4.1951050000
H -1.7559330000 -7.6745890000 4.9893680000
H 2.2416510000 -7.5493090000 3.4005700000
H 0.2808610000 -8.8628200000 4.1919820000
C -0.1631010000 -4.9611570000 -4.2034820000
C 0.9354740000 -5.7139450000 -4.6496350000
C -1.3047280000 -5.6436940000 -3.7525630000
C 0.8939000000 -7.1095010000 -4.6449650000
H 1.8278520000 -5.1990370000 -4.9944890000
C -1.3474920000 -7.0393330000 -3.7490270000
H -2.1638320000 -5.0736460000 -3.4100530000
C -0.2481180000 -7.7767190000 -4.1951050000

```
H 1.7559330000 -7.6745890000 -4.9893680000
H -2.2416510000 -7.5493090000 -3.4005700000
H -0.2808610000 -8.8628200000 -4.1919820000
C 0.0000000000 0.0000000000 -9.1723590000
C 1.1561890000 0.3466450000 -9.8899790000
C -1.1561890000 -0.3466450000 -9.8899790000
C 1.1566960000 0.3463030000 -11.2863120000
H 2.0593440000 0.6114180000 -9.3471180000
C -1.1566960000 -0.3463030000 -11.2863120000
H -2.0593440000 -0.6114180000 -9.3471180000
C 0.0000000000 0.0000000000 -11.9889110000
H 2.0624680000 0.6133980000 -11.8241690000
H -2.0624680000 -0.6133980000 -11.8241690000
H 0.0000000000 0.0000000000 -13.0755090000
C 0.0000000000 0.0000000000 9.1723590000
C -1.1561890000 0.3466450000 9.8899790000
C 1.1561890000 -0.3466450000 9.8899790000
C -1.1566960000 0.3463030000 11.2863120000
H -2.0593440000 0.6114180000 9.3471180000
C 1.1566960000 -0.3463030000 11.2863120000
H 2.0593440000 -0.6114180000 9.3471180000
C 0.0000000000 0.0000000000 11.9889110000
H -2.0624680000 0.6133980000 11.8241690000
H 2.0624680000 -0.6133980000 11.8241690000
H 0.0000000000 0.0000000000 13.0755090000
```

Table S3.4. Optimized coordinates for **3.2**.

```
C -0.2929400000 2.5118230000 11.9077600000
C -0.1523990000 1.2431860000 11.2298530000
N -0.1623590000 1.4452580000 9.8692170000
Zn 0.0000000000 0.0000000000 8.4271250000
N -0.1620930000 1.4363150000 6.9780880000
C -0.1035950000 1.2349240000 5.6298870000
C 0.0000000000 0.0000000000 4.9485030000
C 0.1035950000 -1.2349240000 5.6298870000
N 0.1620930000 -1.4363150000 6.9780880000
C 0.2681050000 -2.8006470000 7.1658630000
C 0.3462230000 -3.4481640000 8.4126510000
C 0.2994560000 -2.7971160000 9.6674560000
N 0.1623590000 -1.4452580000 9.8692170000
C 0.1523990000 -1.2431860000 11.2298530000
C 0.0000000000 0.0000000000 11.8788620000
C 0.2929400000 -2.5118230000 11.9077600000
C 0.3948980000 -3.4695400000 10.9432910000
H 0.5202700000 -4.5331450000 11.0836210000
C 0.2624820000 -3.4727770000 5.8881810000
C 0.1661990000 -2.4973550000 4.9270650000
C 0.1099300000 -2.5005830000 3.4905050000
C 0.0344800000 -1.2407300000 2.7896050000
N -0.0058620000 -1.4485990000 1.4414870000
Zn 0.0000000000 0.0000000000 0.0000000000
N -0.0058620000 1.4485990000 -1.4414870000
C 0.0344800000 1.2407300000 -2.7896050000
C 0.0000000000 0.0000000000 -3.4698210000
C -0.0344800000 -1.2407300000 -2.7896050000
N 0.0058620000 -1.4485990000 -1.4414870000
C -0.0292000000 -2.8156520000 -1.2520790000
C 0.0000000000 -3.4682050000 0.0000000000
```

C 0.0292000000 -2.8156520000 1.2520790000
C 0.1137850000 -3.4821210000 2.5279400000
H 0.1726660000 -4.5503910000 2.6762920000
C -0.1137850000 -3.4821210000 -2.5279400000
C -0.1099300000 -2.5005830000 -3.4905050000
C -0.1661990000 -2.4973550000 -4.9270650000
C -0.1035950000 -1.2349240000 -5.6298870000
N -0.1620930000 -1.4363150000 -6.9780880000
Zn 0.0000000000 0.0000000000 -8.4271250000
N 0.1623590000 1.4452580000 -9.8692170000
C 0.1523990000 1.2431860000 -11.2298530000
C 0.0000000000 0.0000000000 -11.8788620000
C -0.1523990000 -1.2431860000 -11.2298530000
N -0.1623590000 -1.4452580000 -9.8692170000
C -0.2994560000 -2.7971160000 -9.6674560000
C -0.3462230000 -3.4481640000 -8.4126510000
C -0.2681050000 -2.8006470000 -7.1658630000
C -0.2624820000 -3.4727770000 -5.8881810000
H -0.3183170000 -4.5414080000 -5.7411120000
C -0.3948980000 -3.4695400000 -10.9432910000
C -0.2929400000 -2.5118230000 -11.9077600000
H -0.3111330000 -2.6519700000 -12.9786520000
H -0.5202700000 -4.5331450000 -11.0836210000
C 0.2929400000 2.5118230000 -11.9077600000
C 0.3948980000 3.4695400000 -10.9432910000
C 0.2994560000 2.7971160000 -9.6674560000
C 0.3462230000 3.4481640000 -8.4126510000
C 0.2681050000 2.8006470000 -7.1658630000
N 0.1620930000 1.4363150000 -6.9780880000
C 0.1035950000 1.2349240000 -5.6298870000
C 0.1661990000 2.4973550000 -4.9270650000
C 0.1099300000 2.5005830000 -3.4905050000
C 0.1137850000 3.4821210000 -2.5279400000
C 0.0292000000 2.8156520000 -1.2520790000
C 0.0000000000 3.4682050000 0.0000000000
C -0.0292000000 2.8156520000 1.2520790000
N 0.0058620000 1.4485990000 1.4414870000
C -0.0344800000 1.2407300000 2.7896050000
C -0.1099300000 2.5005830000 3.4905050000
C -0.1661990000 2.4973550000 4.9270650000
C -0.2624820000 3.4727770000 5.8881810000
C -0.2681050000 2.8006470000 7.1658630000
C -0.3462230000 3.4481640000 8.4126510000
C -0.2994560000 2.7971160000 9.6674560000
C -0.3948980000 3.4695400000 10.9432910000
H -0.5202700000 4.5331450000 11.0836210000
H -0.3183170000 4.5414080000 5.7411120000
C -0.1137850000 3.4821210000 2.5279400000
H -0.1726660000 4.5503910000 2.6762920000
C 0.0000000000 0.0000000000 3.4698210000
H 0.1726660000 4.5503910000 -2.6762920000
C 0.2624820000 3.4727770000 -5.8881810000
H 0.3183170000 4.5414080000 -5.7411120000
C 0.0000000000 0.0000000000 -4.9485030000
H 0.5202700000 4.5331450000 -11.0836210000
H 0.3111330000 2.6519700000 -12.9786520000
H -0.1726660000 -4.5503910000 -2.6762920000
H 0.3183170000 -4.5414080000 5.7411120000
H -0.3111330000 2.6519700000 12.9786520000
H 0.3111330000 -2.6519700000 12.9786520000
C 0.0000000000 4.9655020000 0.0000000000
C 1.0931460000 5.6835270000 0.5127170000
C -1.0931460000 5.6835270000 -0.5127170000

C 1.0939390000 7.0795790000 0.5111880000
H 1.9484110000 5.1409500000 0.9053910000
C -1.0939390000 7.0795790000 -0.5111880000
H -1.9484110000 5.1409500000 -0.9053910000
C 0.0000000000 7.7821340000 0.0000000000
H 1.9515140000 7.6173150000 0.9066070000
H -1.9515140000 7.6173150000 -0.9066070000
H 0.0000000000 8.8687210000 0.0000000000
C 0.4842690000 4.9402750000 -8.4109820000
C -0.5605230000 5.7597250000 -8.8688390000
C 1.6617430000 5.5504410000 -7.9486320000
C -0.4318090000 7.1498990000 -8.8641640000
H -1.4799060000 5.3013780000 -9.2224070000
C 1.7916730000 6.9406680000 -7.9454740000
H 2.4799600000 4.9282020000 -7.5970450000
C 0.7451210000 7.7448400000 -8.4029840000
H -1.2533430000 7.7674190000 -9.2173860000
H 2.7124080000 7.3940750000 -7.5881940000
H 0.8456910000 8.8267630000 -8.4000060000
C -0.4842690000 -4.9402750000 -8.4109820000
C 0.5605230000 -5.7597250000 -8.8688390000
C -1.6617430000 -5.5504410000 -7.9486320000
C 0.4318090000 -7.1498990000 -8.8641640000
H 1.4799060000 -5.3013780000 -9.2224070000
C -1.7916730000 -6.9406680000 -7.9454740000
H -2.4799600000 -4.9282020000 -7.5970450000
C -0.7451210000 -7.7448400000 -8.4029840000
H 1.2533430000 -7.7674190000 -9.2173860000
H -2.7124080000 -7.3940750000 -7.5881940000
H -0.8456910000 -8.8267630000 -8.4000060000
C 0.0000000000 -4.9655020000 0.0000000000
C -1.0931460000 -5.6835270000 0.5127170000
C 1.0931460000 -5.6835270000 -0.5127170000
C -1.0939390000 -7.0795790000 0.5111880000
H -1.9484110000 -5.1409500000 0.9053910000
C 1.0939390000 -7.0795790000 -0.5111880000
H 1.9484110000 -5.1409500000 -0.9053910000
C 0.0000000000 -7.7821340000 0.0000000000
H -1.9515140000 -7.6173150000 0.9066070000
H 1.9515140000 -7.6173150000 -0.9066070000
H 0.0000000000 -8.8687210000 0.0000000000
C 0.4842690000 -4.9402750000 8.4109820000
C -0.5605230000 -5.7597250000 8.8688390000
C 1.6617430000 -5.5504410000 7.9486320000
C -0.4318090000 -7.1498990000 8.8641640000
H -1.4799060000 -5.3013780000 9.2224070000
C 1.7916730000 -6.9406680000 7.9454740000
H 2.4799600000 -4.9282020000 7.5970450000
C 0.7451210000 -7.7448400000 8.4029840000
H -1.2533430000 -7.7674190000 9.2173860000
H 2.7124080000 -7.3940750000 7.5881940000
H 0.8456910000 -8.8267630000 8.4000060000
C -0.4842690000 4.9402750000 8.4109820000
C 0.5605230000 5.7597250000 8.8688390000
C -1.6617430000 5.5504410000 7.9486320000
C 0.4318090000 7.1498990000 8.8641640000
H 1.4799060000 5.3013780000 9.2224070000
C -1.7916730000 6.9406680000 7.9454740000
H -2.4799600000 4.9282020000 7.5970450000
C -0.7451210000 7.7448400000 8.4029840000
H 1.2533430000 7.7674190000 9.2173860000
H -2.7124080000 7.3940750000 7.5881940000
H -0.8456910000 8.8267630000 8.4000060000

```
C 0.0000000000 0.0000000000 -13.3782430000
C 1.1787370000 0.2603400000 -14.0956240000
C -1.1787370000 -0.2603400000 -14.0956240000
C 1.1791870000 0.2597320000 -15.4919420000
H 2.0989840000 0.4576950000 -13.5527820000
C -1.1791870000 -0.2597320000 -15.4919420000
H -2.0989840000 -0.4576950000 -13.5527820000
C 0.0000000000 0.0000000000 -16.1944930000
H 2.1022300000 0.4590130000 -16.0298070000
H -2.1022300000 -0.4590130000 -16.0298070000
H 0.0000000000 0.0000000000 -17.2810820000
C 0.0000000000 0.0000000000 13.3782430000
C -1.1787370000 0.2603400000 14.0956240000
C 1.1787370000 -0.2603400000 14.0956240000
C -1.1791870000 0.2597320000 15.4919420000
H -2.0989840000 0.4576950000 13.5527820000
C 1.1791870000 -0.2597320000 15.4919420000
H 2.0989840000 -0.4576950000 13.5527820000
C 0.0000000000 0.0000000000 16.1944930000
H -2.1022300000 0.4590130000 16.0298070000
H 2.1022300000 -0.4590130000 16.0298070000
H 0.0000000000 0.0000000000 17.2810820000
```

Table S3.5. Optimized coordinates for **3.3**.

```
Zn 0.0000000000 0.0000000000 12.6376340000
N -0.1875500000 1.4324580000 11.1885000000
C -0.1362330000 1.2319170000 9.8401650000
C 0.0000000000 0.0000000000 9.1580100000
C 0.1362330000 -1.2319170000 9.8401650000
N 0.1875500000 -1.4324580000 11.1885000000
C 0.3271080000 -2.7941450000 11.3765160000
C 0.4072130000 -3.4408240000 12.6231380000
C 0.3387710000 -2.7920350000 13.8784630000
N 0.1800310000 -1.4427570000 14.0802260000
C 0.1648710000 -1.2415500000 15.4410210000
C 0.0000000000 0.0000000000 16.0901160000
C -0.1648710000 1.2415500000 15.4410210000
N -0.1800310000 1.4427570000 14.0802260000
C -0.3387710000 2.7920350000 13.8784630000
C -0.4072130000 3.4408240000 12.6231380000
C -0.3271080000 2.7941450000 11.3765160000
C -0.3533170000 3.4649220000 10.0985130000
C -0.2413810000 2.4914220000 9.1371860000
C -0.2014730000 2.4949080000 7.7004030000
C -0.0843570000 1.2388560000 6.9995650000
N -0.0644060000 1.4471060000 5.6510610000
Zn 0.0000000000 0.0000000000 4.2076170000
N -0.0823070000 1.4463300000 2.7659890000
C -0.0337360000 1.2423040000 1.4186320000
C 0.0000000000 0.0000000000 0.7367810000
C 0.0337360000 -1.2423040000 1.4186320000
N 0.0823070000 -1.4463300000 2.7659890000
C 0.1167330000 -2.8145060000 2.9564800000
C 0.1683160000 -3.4638040000 4.2084780000
C 0.1568450000 -2.8113920000 5.4617700000
N 0.0644060000 -1.4471060000 5.6510610000
C 0.0843570000 -1.2388560000 6.9995650000
C 0.0000000000 0.0000000000 7.6803620000
```

C 0.2014730000 -2.4949080000 7.7004030000
C 0.2413810000 -2.4914220000 9.1371860000
C 0.3533170000 -3.4649220000 10.0985130000
H 0.4391330000 -4.5315310000 9.9513310000
C 0.2547470000 -3.4750120000 6.7372760000
H 0.3548130000 -4.5401360000 6.8859100000
C 0.0720850000 -3.4850010000 1.6814620000
C 0.0271750000 -2.5049520000 0.7178890000
C -0.0271750000 -2.5049520000 -0.7178890000
C -0.0337360000 -1.2423040000 -1.4186320000
N -0.0823070000 -1.4463300000 -2.7659890000
Zn 0.0000000000 0.0000000000 -4.2076170000
N 0.0644060000 1.4471060000 -5.6510610000
C 0.0843570000 1.2388560000 -6.9995650000
C 0.0000000000 0.0000000000 -7.6803620000
C -0.0843570000 -1.2388560000 -6.9995650000
N -0.0644060000 -1.4471060000 -5.6510610000
C -0.1568450000 -2.8113920000 -5.4617700000
C -0.1683160000 -3.4638040000 -4.2084780000
C -0.1167330000 -2.8145060000 -2.9564800000
C -0.0720850000 -3.4850010000 -1.6814620000
H -0.0692510000 -4.5549370000 -1.5336350000
C -0.2547470000 -3.4750120000 -6.7372760000
C -0.2014730000 -2.4949080000 -7.7004030000
C -0.2413810000 -2.4914220000 -9.1371860000
C -0.1362330000 -1.2319170000 -9.8401650000
N -0.1875500000 -1.4324580000 -11.1885000000
Zn 0.0000000000 0.0000000000 -12.6376340000
N 0.1800310000 1.4427570000 -14.0802260000
C 0.1648710000 1.2415500000 -15.4410210000
C 0.0000000000 0.0000000000 -16.0901160000
C -0.1648710000 -1.2415500000 -15.4410210000
N -0.1800310000 -1.4427570000 -14.0802260000
C -0.3387710000 -2.7920350000 -13.8784630000
C -0.4072130000 -3.4408240000 -12.6231380000
C -0.3271080000 -2.7941450000 -11.3765160000
C -0.3533170000 -3.4649220000 -10.0985130000
H -0.4391330000 -4.5315310000 -9.9513310000
C -0.4383270000 -3.4641070000 -15.1539560000
C -0.3197820000 -2.5084560000 -16.1187060000
H -0.3365520000 -2.6489620000 -17.1895610000
H -0.5781010000 -4.5259510000 -15.2939840000
C 0.3197820000 2.5084560000 -16.1187060000
C 0.4383270000 3.4641070000 -15.1539560000
C 0.3387710000 2.7920350000 -13.8784630000
C 0.4072130000 3.4408240000 -12.6231380000
C 0.3271080000 2.7941450000 -11.3765160000
N 0.1875500000 1.4324580000 -11.1885000000
C 0.1362330000 1.2319170000 -9.8401650000
C 0.2413810000 2.4914220000 -9.1371860000
C 0.2014730000 2.4949080000 -7.7004030000
C 0.2547470000 3.4750120000 -6.7372760000
C 0.1568450000 2.8113920000 -5.4617700000
C 0.1683160000 3.4638040000 -4.2084780000
C 0.1167330000 2.8145060000 -2.9564800000
N 0.0823070000 1.4463300000 -2.7659890000
C 0.0337360000 1.2423040000 -1.4186320000
C 0.0271750000 2.5049520000 -0.7178890000
C -0.0271750000 2.5049520000 0.7178890000
C -0.0720850000 3.4850010000 1.6814620000
C -0.1167330000 2.8145060000 2.9564800000
C -0.1683160000 3.4638040000 4.2084780000
C -0.1568450000 2.8113920000 5.4617700000

C -0.2547470000 3.4750120000 6.7372760000
H -0.3548130000 4.5401360000 6.8859100000
H -0.0692510000 4.5549370000 1.5336350000
C 0.0720850000 3.4850010000 -1.6814620000
H 0.0692510000 4.5549370000 -1.5336350000
C 0.0000000000 0.0000000000 -0.7367810000
H 0.3548130000 4.5401360000 -6.8859100000
C 0.3533170000 3.4649220000 -10.0985130000
H 0.4391330000 4.5315310000 -9.9513310000
C 0.0000000000 0.0000000000 -9.1580100000
H 0.5781010000 4.5259510000 -15.2939840000
H 0.3365520000 2.6489620000 -17.1895610000
H -0.3548130000 -4.5401360000 -6.8859100000
H 0.0692510000 -4.5549370000 1.5336350000
H -0.4391330000 4.5315310000 9.9513310000
C -0.4383270000 3.4641070000 15.1539560000
C -0.3197820000 2.5084560000 16.1187060000
C 0.3197820000 -2.5084560000 16.1187060000
C 0.4383270000 -3.4641070000 15.1539560000
H 0.5781010000 -4.5259510000 15.2939840000
H -0.5781010000 4.5259510000 15.2939840000
H -0.3365520000 2.6489620000 17.1895610000
H 0.3365520000 -2.6489620000 17.1895610000
C 0.5751040000 4.9299560000 -12.6220300000
C -0.4597470000 5.7702120000 -13.0643100000
C 1.7710570000 5.5160050000 -12.1764050000
C -0.3033990000 7.1575580000 -13.0605390000
H -1.3929750000 5.3304780000 -13.4050370000
C 1.9285480000 6.9033960000 -12.1742110000
H 2.5817240000 4.8772800000 -11.8370900000
C 0.8916520000 7.7285720000 -12.6160200000
H -1.1174880000 7.7915950000 -13.4015100000
H 2.8631340000 7.3381390000 -11.8299420000
H 1.0137190000 8.8082790000 -12.6137850000
C 0.2391200000 4.9595300000 -4.2090180000
C -0.8251510000 5.7286990000 -4.7079300000
C 1.3717180000 5.6242200000 -3.7104380000
C -0.7593910000 7.1231990000 -4.7066990000
H -1.7101590000 5.2275800000 -5.0896300000
C 1.4390060000 7.0186680000 -3.7125180000
H 2.2049030000 5.0413260000 -3.3282500000
C 0.3733080000 7.7726370000 -4.2098580000
H -1.5953900000 7.7012980000 -5.0911900000
H 2.3261640000 7.5148020000 -3.3281660000
H 0.4250690000 8.8579840000 -4.2102130000
C -0.2391200000 4.9595300000 4.2090180000
C 0.8251510000 5.7286990000 4.7079300000
C -1.3717180000 5.6242200000 3.7104380000
C 0.7593910000 7.1231990000 4.7066990000
H 1.7101590000 5.2275800000 5.0896300000
C -1.4390060000 7.0186680000 3.7125180000
H -2.2049030000 5.0413260000 3.3282500000
C -0.3733080000 7.7726370000 4.2098580000
H 1.5953900000 7.7012980000 5.0911900000
H -2.3261640000 7.5148020000 3.3281660000
H -0.4250690000 8.8579840000 4.2102130000
C -0.5751040000 4.9299560000 12.6220300000
C 0.4597470000 5.7702120000 13.0643100000
C -1.7710570000 5.5160050000 12.1764050000
C 0.3033990000 7.1575580000 13.0605390000
H 1.3929750000 5.3304780000 13.4050370000
C -1.9285480000 6.9033960000 12.1742110000
H -2.5817240000 4.8772800000 11.8370900000

C -0.8916520000 7.7285720000 12.6160200000
H 1.1174880000 7.7915950000 13.4015100000
H -2.8631340000 7.3381390000 11.8299420000
H -1.0137190000 8.8082790000 12.6137850000
C 0.5751040000 -4.9299560000 12.6220300000
C -0.4597470000 -5.7702120000 13.0643100000
C 1.7710570000 -5.5160050000 12.1764050000
C -0.3033990000 -7.1575580000 13.0605390000
H -1.3929750000 -5.3304780000 13.4050370000
C 1.9285480000 -6.9033960000 12.1742110000
H 2.5817240000 -4.8772800000 11.8370900000
C 0.8916520000 -7.7285720000 12.6160200000
H -1.1174880000 -7.7915950000 13.4015100000
H 2.8631340000 -7.3381390000 11.8299420000
H 1.0137190000 -8.8082790000 12.6137850000
C 0.0000000000 0.0000000000 17.5894040000
C 1.1809710000 -0.2502450000 18.3067230000
C -1.1809710000 0.2502450000 18.3067230000
C 1.1814050000 -0.2495030000 19.7030230000
H 2.1028840000 -0.4396630000 17.7639000000
C -1.1814050000 0.2495030000 19.7030230000
H -2.1028840000 0.4396630000 17.7639000000
C 0.0000000000 0.0000000000 20.4055510000
H 2.1061400000 -0.4407470000 20.2408830000
H -2.1061400000 0.4407470000 20.2408830000
H 0.0000000000 0.0000000000 21.4921340000
C 0.2391200000 -4.9595300000 4.2090180000
C -0.8251510000 -5.7286990000 4.7079300000
C 1.3717180000 -5.6242200000 3.7104380000
C -0.7593910000 -7.1231990000 4.7066990000
H -1.7101590000 -5.2275800000 5.0896300000
C 1.4390060000 -7.0186680000 3.7125180000
H 2.2049030000 -5.0413260000 3.3282500000
C 0.3733080000 -7.7726370000 4.2098580000
H -1.5953900000 -7.7012980000 5.0911900000
H 2.3261640000 -7.5148020000 3.3281660000
H 0.4250690000 -8.8579840000 4.2102130000
C -0.2391200000 -4.9595300000 -4.2090180000
C 0.8251510000 -5.7286990000 -4.7079300000
C -1.3717180000 -5.6242200000 -3.7104380000
C 0.7593910000 -7.1231990000 -4.7066990000
H 1.7101590000 -5.2275800000 -5.0896300000
C -1.4390060000 -7.0186680000 -3.7125180000
H -2.2049030000 -5.0413260000 -3.3282500000
C -0.3733080000 -7.7726370000 -4.2098580000
H 1.5953900000 -7.7012980000 -5.0911900000
H -2.3261640000 -7.5148020000 -3.3281660000
H -0.4250690000 -8.8579840000 -4.2102130000
C -0.5751040000 -4.9299560000 -12.6220300000
C 0.4597470000 -5.7702120000 -13.0643100000
C -1.7710570000 -5.5160050000 -12.1764050000
C 0.3033990000 -7.1575580000 -13.0605390000
H 1.3929750000 -5.3304780000 -13.4050370000
C -1.9285480000 -6.9033960000 -12.1742110000
H -2.5817240000 -4.8772800000 -11.8370900000
C -0.8916520000 -7.7285720000 -12.6160200000
H 1.1174880000 -7.7915950000 -13.4015100000
H -2.8631340000 -7.3381390000 -11.8299420000
H -1.0137190000 -8.8082790000 -12.6137850000
C 0.0000000000 0.0000000000 -17.5894040000
C 1.1809710000 0.2502450000 -18.3067230000
C -1.1809710000 -0.2502450000 -18.3067230000
C 1.1814050000 0.2495030000 -19.7030230000

```
H 2.1028840000 0.4396630000 -17.7639000000
C -1.1814050000 -0.2495030000 -19.7030230000
H -2.1028840000 -0.4396630000 -17.7639000000
C 0.0000000000 0.0000000000 -20.4055510000
H 2.1061400000 0.4407470000 -20.2408830000
H -2.1061400000 -0.4407470000 -20.2408830000
H 0.0000000000 0.0000000000 -21.4921340000
```

Table S3.6. Optimized coordinates for **3.4**.

```
Zn 0.0000000000 0.0000000000 8.4147170000
N -0.1561400000 1.4400870000 6.9745820000
C -0.0989140000 1.2391220000 5.6273250000
C 0.0000000000 0.0000000000 4.9448420000
C 0.0989140000 -1.2391220000 5.6273250000
N 0.1561400000 -1.4400870000 6.9745820000
C 0.2523230000 -2.8058590000 7.1648190000
C 0.3210110000 -3.4530840000 8.4164710000
C 0.2702620000 -2.8027260000 9.6700310000
N 0.1273810000 -1.4426900000 9.8587480000
C 0.1271570000 -1.2353540000 11.2076660000
C 0.0000000000 0.0000000000 11.8888250000
C -0.1271570000 1.2353540000 11.2076660000
N -0.1273810000 1.4426900000 9.8587480000
C -0.2702620000 2.8027260000 9.6700310000
C -0.3210110000 3.4530840000 8.4164710000
C -0.2523230000 2.8058590000 7.1648190000
C -0.2438260000 3.4773890000 5.8899020000
C -0.1550200000 2.5003390000 4.9262700000
C -0.1015880000 2.5028600000 3.4907320000
C -0.0307430000 1.2428070000 2.7903880000
N 0.0086020000 1.4484720000 1.4430890000
Zn 0.0000000000 0.0000000000 0.0000000000
N -0.0086020000 1.4484720000 -1.4430890000
C 0.0307430000 1.2428070000 -2.7903880000
C 0.0000000000 0.0000000000 -3.4729400000
C -0.0307430000 -1.2428070000 -2.7903880000
N 0.0086020000 -1.4484720000 -1.4430890000
C -0.0249620000 -2.8167310000 -1.2528110000
C 0.0000000000 -3.4678070000 0.0000000000
C 0.0249620000 -2.8167310000 1.2528110000
N -0.0086020000 -1.4484720000 1.4430890000
C 0.0307430000 -1.2428070000 2.7903880000
C 0.0000000000 0.0000000000 3.4729400000
C 0.1015880000 -2.5028600000 3.4907320000
C 0.1550200000 -2.5003390000 4.9262700000
C 0.2438260000 -3.4773890000 5.8899020000
H 0.2912530000 -4.5462700000 5.7421320000
C 0.1053000000 -3.4842170000 2.5266650000
H 0.1621570000 -4.5526140000 2.6744650000
C -0.1053000000 -3.4842170000 -2.5266650000
C -0.1015880000 -2.5028600000 -3.4907320000
C -0.1550200000 -2.5003390000 -4.9262700000
C -0.0989140000 -1.2391220000 -5.6273250000
N -0.1561400000 -1.4400870000 -6.9745820000
Zn 0.0000000000 0.0000000000 -8.4147170000
N 0.1273810000 1.4426900000 -9.8587480000
C 0.1271570000 1.2353540000 -11.2076660000
C 0.0000000000 0.0000000000 -11.8888250000
C -0.1271570000 -1.2353540000 -11.2076660000
N -0.1273810000 -1.4426900000 -9.8587480000
```

C -0.2702620000 -2.8027260000 -9.6700310000
C -0.3210110000 -3.4530840000 -8.4164710000
C -0.2523230000 -2.8058590000 -7.1648190000
C -0.2438260000 -3.4773890000 -5.8899020000
H -0.2912530000 -4.5462700000 -5.7421320000
C -0.3766900000 -3.4640100000 -10.9455870000
C -0.2786180000 -2.4873140000 -11.9087760000
C -0.3012850000 -2.4848670000 -13.3457490000
C -0.1608450000 -1.2288930000 -14.0487630000
N -0.2030180000 -1.4296260000 -15.3972230000
Zn 0.0000000000 0.0000000000 -16.8467810000
N 0.1894690000 1.4412060000 -18.2894750000
C 0.1705870000 1.2407300000 -19.6503510000
C 0.0000000000 0.0000000000 -20.2995090000
C -0.1705870000 -1.2407300000 -19.6503510000
N -0.1894690000 -1.4412060000 -18.2894750000
C -0.3619610000 -2.7886410000 -18.0875500000
C -0.4472570000 -3.4351600000 -16.8319280000
C -0.3682600000 -2.7886290000 -15.5854280000
C -0.4225600000 -3.4571250000 -14.3071640000
H -0.5318810000 -4.5215570000 -14.1598590000
C -0.4624660000 -3.4608250000 -19.3628200000
C -0.3331190000 -2.5067410000 -20.3278000000
H -0.3482100000 -2.6476410000 -21.3986240000
H -0.6106400000 -4.5215730000 -19.5025380000
C 0.3331190000 2.5067410000 -20.3278000000
C 0.4624660000 3.4608250000 -19.3628200000
C 0.3619610000 2.7886410000 -18.0875500000
C 0.4472570000 3.4351600000 -16.8319280000
C 0.3682600000 2.7886290000 -15.5854280000
N 0.2030180000 1.4296260000 -15.3972230000
C 0.1608450000 1.2288930000 -14.0487630000
C 0.3012850000 2.4848670000 -13.3457490000
C 0.2786180000 2.4873140000 -11.9087760000
C 0.3766900000 3.4640100000 -10.9455870000
C 0.2702620000 2.8027260000 -9.6700310000
C 0.3210110000 3.4530840000 -8.4164710000
C 0.2523230000 2.8058590000 -7.1648190000
N 0.1561400000 1.4400870000 -6.9745820000
C 0.0989140000 1.2391220000 -5.6273250000
C 0.1550200000 2.5003390000 -4.9262700000
C 0.1015880000 2.5028600000 -3.4907320000
C 0.1053000000 3.4842170000 -2.5266650000
C 0.0249620000 2.8167310000 -1.2528110000
C 0.0000000000 3.4678070000 0.0000000000
C -0.0249620000 2.8167310000 1.2528110000
C -0.1053000000 3.4842170000 2.5266650000
H -0.1621570000 4.5526140000 2.6744650000
H 0.1621570000 4.5526140000 -2.6744650000
C 0.2438260000 3.4773890000 -5.8899020000
H 0.2912530000 4.5462700000 -5.7421320000
C 0.0000000000 0.0000000000 -4.9448420000
H 0.5126310000 4.5250860000 -11.0945600000
C 0.4225600000 3.4571250000 -14.3071640000
H 0.5318810000 4.5215570000 -14.1598590000
C 0.0000000000 0.0000000000 -13.3660870000
H 0.6106400000 4.5215730000 -19.5025380000
H 0.3482100000 2.6476410000 -21.3986240000
H -0.5126310000 -4.5250860000 -11.0945600000
H -0.1621570000 -4.5526140000 -2.6744650000
H -0.2912530000 4.5462700000 5.7421320000
C -0.3766900000 3.4640100000 10.9455870000
C -0.2786180000 2.4873140000 11.9087760000

C -0.3012850000 2.4848670000 13.3457490000
C -0.1608450000 1.2288930000 14.0487630000
N -0.2030180000 1.4296260000 15.3972230000
Zn 0.0000000000 0.0000000000 16.8467810000
N -0.1894690000 1.4412060000 18.2894750000
C -0.1705870000 1.2407300000 19.6503510000
C -0.3331190000 2.5067410000 20.3278000000
C 0.0000000000 0.0000000000 20.2995090000
C 0.1705870000 -1.2407300000 19.6503510000
N 0.1894690000 -1.4412060000 18.2894750000
C 0.3619610000 -2.7886410000 18.0875500000
C 0.4472570000 -3.4351600000 16.8319280000
C 0.3682600000 -2.7886290000 15.5854280000
N 0.2030180000 -1.4296260000 15.3972230000
C 0.1608450000 -1.2288930000 14.0487630000
C 0.0000000000 0.0000000000 13.3660870000
C 0.3012850000 -2.4848670000 13.3457490000
C 0.2786180000 -2.4873140000 11.9087760000
C 0.3766900000 -3.4640100000 10.9455870000
H 0.5126310000 -4.5250860000 11.0945600000
C 0.4225600000 -3.4571250000 14.3071640000
H 0.5318810000 -4.5215570000 14.1598590000
C 0.4624660000 -3.4608250000 19.3628200000
C 0.3331190000 -2.5067410000 20.3278000000
H 0.6106400000 -4.5215730000 19.5025380000
C -0.4624660000 3.4608250000 19.3628200000
C -0.3619610000 2.7886410000 18.0875500000
C -0.4472570000 3.4351600000 16.8319280000
C -0.3682600000 2.7886290000 15.5854280000
C -0.4225600000 3.4571250000 14.3071640000
H -0.5318810000 4.5215570000 14.1598590000
H -0.6106400000 4.5215730000 19.5025380000
H -0.5126310000 4.5250860000 11.0945600000
H -0.3482100000 2.6476410000 21.3986240000
H 0.3482100000 -2.6476410000 21.3986240000
C 0.6362130000 4.9218950000 -16.8312900000
C -0.3931080000 5.7768730000 -17.2577680000
C 1.8466460000 5.4904620000 -16.4026460000
C -0.2173020000 7.1619090000 -17.2549470000
H -1.3371470000 5.3505530000 -17.5855480000
C 2.0235270000 6.8755330000 -16.4013900000
H 2.6531280000 4.8400400000 -16.0757840000
C 0.9919580000 7.7156160000 -16.8272850000
H -1.0272400000 7.8076720000 -17.5835590000
H 2.9689860000 7.2967980000 -16.0703110000
H 1.1291540000 8.7935030000 -16.8257960000
C 0.4534100000 4.9446410000 -8.4168440000
C -0.5843980000 5.7576590000 -8.9017010000
C 1.6184250000 5.5611690000 -7.9313800000
C -0.4612230000 7.1482550000 -8.8997020000
H -1.4939660000 5.2940550000 -9.2729410000
C 1.7429950000 6.9516850000 -7.9326750000
H 2.4313930000 4.9438290000 -7.5598850000
C 0.7032670000 7.7496800000 -8.4160610000
H -1.2773760000 7.7609030000 -9.2731640000
H 2.6543960000 7.4102430000 -7.5585350000
H 0.7996690000 8.8319710000 -8.4158010000
C 0.0000000000 4.9650550000 0.0000000000
C 1.0954840000 5.6826860000 0.5080940000
C -1.0954840000 5.6826860000 -0.5080940000
C 1.0963470000 7.0787090000 0.5061280000
H 1.9522640000 5.1400430000 0.8972610000
C -1.0963470000 7.0787090000 -0.5061280000

H -1.9522640000 5.1400430000 -0.8972610000
C 0.0000000000 7.7811750000 0.0000000000
H 1.9557260000 7.6164540000 0.8975480000
H -1.9557260000 7.6164540000 -0.8975480000
H 0.0000000000 8.8677550000 0.0000000000
C -0.4534100000 4.9446410000 8.4168440000
C 0.5843980000 5.7576590000 8.9017010000
C -1.6184250000 5.5611690000 7.9313800000
C 0.4612230000 7.1482550000 8.8997020000
H 1.4939660000 5.2940550000 9.2729410000
C -1.7429950000 6.9516850000 7.9326750000
H -2.4313930000 4.9438290000 7.5598850000
C -0.7032670000 7.7496800000 8.4160610000
H 1.2773760000 7.7609030000 9.2731640000
H -2.6543960000 7.4102430000 7.5585350000
H -0.7996690000 8.8319710000 8.4158010000
C 0.0000000000 0.0000000000 -21.7987840000
C -1.1821190000 -0.2449390000 -22.5160310000
C 1.1821190000 0.2449390000 -22.5160310000
C -1.1825430000 -0.2441170000 -23.9123260000
H -2.1048710000 -0.4302130000 -21.9732150000
C 1.1825430000 0.2441170000 -23.9123260000
H 2.1048710000 0.4302130000 -21.9732150000
C 0.0000000000 0.0000000000 -24.6148280000
H -2.1081310000 -0.4311360000 -24.4501940000
H 2.1081310000 0.4311360000 -24.4501940000
H 0.0000000000 0.0000000000 -25.7014090000
C -0.6362130000 -4.9218950000 -16.8312900000
C 0.3931080000 -5.7768730000 -17.2577680000
C -1.8466460000 -5.4904620000 -16.4026460000
C 0.2173020000 -7.1619090000 -17.2549470000
H 1.3371470000 -5.3505530000 -17.5855480000
C -2.0235270000 -6.8755330000 -16.4013900000
H -2.6531280000 -4.8400400000 -16.0757840000
C -0.9919580000 -7.7156160000 -16.8272850000
H 1.0272400000 -7.8076720000 -17.5835590000
H -2.9689860000 -7.2967980000 -16.0703110000
H -1.1291540000 -8.7935030000 -16.8257960000
C 0.0000000000 -4.9650550000 0.0000000000
C -1.0954840000 -5.6826860000 0.5080940000
C 1.0954840000 -5.6826860000 -0.5080940000
C -1.0963470000 -7.0787090000 0.5061280000
H -1.9522640000 -5.1400430000 0.8972610000
C 1.0963470000 -7.0787090000 -0.5061280000
H 1.9522640000 -5.1400430000 -0.8972610000
C 0.0000000000 -7.7811750000 0.0000000000
H -1.9557260000 -7.6164540000 0.8975480000
H 1.9557260000 -7.6164540000 -0.8975480000
H 0.0000000000 -8.8677550000 0.0000000000
C -0.4534100000 -4.9446410000 -8.4168440000
C 0.5843980000 -5.7576590000 -8.9017010000
C -1.6184250000 -5.5611690000 -7.9313800000
C 0.4612230000 -7.1482550000 -8.8997020000
H 1.4939660000 -5.2940550000 -9.2729410000
C -1.7429950000 -6.9516850000 -7.9326750000
H -2.4313930000 -4.9438290000 -7.5598850000
C -0.7032670000 -7.7496800000 -8.4160610000
H 1.2773760000 -7.7609030000 -9.2731640000
H -2.6543960000 -7.4102430000 -7.5585350000
H -0.7996690000 -8.8319710000 -8.4158010000
C 0.4534100000 -4.9446410000 8.4168440000
C -0.5843980000 -5.7576590000 8.9017010000
C 1.6184250000 -5.5611690000 7.9313800000

```
C -0.4612230000 -7.1482550000 8.8997020000
H -1.4939660000 -5.2940550000 9.2729410000
C 1.7429950000 -6.9516850000 7.9326750000
H 2.4313930000 -4.9438290000 7.5598850000
C 0.7032670000 -7.7496800000 8.4160610000
H -1.2773760000 -7.7609030000 9.2731640000
H 2.6543960000 -7.4102430000 7.5585350000
H 0.7996690000 -8.8319710000 8.4158010000
C 0.0000000000 0.0000000000 21.7987840000
C -1.1821190000 0.2449390000 22.5160310000
C 1.1821190000 -0.2449390000 22.5160310000
C -1.1825430000 0.2441170000 23.9123260000
H -2.1048710000 0.4302130000 21.9732150000
C 1.1825430000 -0.2441170000 23.9123260000
H 2.1048710000 -0.4302130000 21.9732150000
C 0.0000000000 0.0000000000 24.6148280000
H -2.1081310000 0.4311360000 24.4501940000
H 2.1081310000 -0.4311360000 24.4501940000
H 0.0000000000 0.0000000000 25.7014090000
C -0.6362130000 4.9218950000 16.8312900000
C 0.3931080000 5.7768730000 17.2577680000
C -1.8466460000 5.4904620000 16.4026460000
C 0.2173020000 7.1619090000 17.2549470000
H 1.3371470000 5.3505530000 17.5855480000
C -2.0235270000 6.8755330000 16.4013900000
H -2.6531280000 4.8400400000 16.0757840000
C -0.9919580000 7.7156160000 16.8272850000
H 1.0272400000 7.8076720000 17.5835590000
H -2.9689860000 7.2967980000 16.0703110000
H -1.1291540000 8.7935030000 16.8257960000
C 0.6362130000 -4.9218950000 16.8312900000
C -0.3931080000 -5.7768730000 17.2577680000
C 1.8466460000 -5.4904620000 16.4026460000
C -0.2173020000 -7.1619090000 17.2549470000
H -1.3371470000 -5.3505530000 17.5855480000
C 2.0235270000 -6.8755330000 16.4013900000
H 2.6531280000 -4.8400400000 16.0757840000
C 0.9919580000 -7.7156160000 16.8272850000
H -1.0272400000 -7.8076720000 17.5835590000
H 2.9689860000 -7.2967980000 16.0703110000
H 1.1291540000 -8.7935030000 16.8257960000
```

Table S3.7. Optimized coordinates for **3.5**.

Zn	0.	0.	4.20613
N	-0.04967	1.44269	2.76761
C	-0.02171	1.24065	1.4186
C	0.	0.	0.73525
C	0.02171	-1.24065	1.4186
N	0.04967	-1.44269	2.76761
C	0.06465	-2.8126	2.95567
C	0.08495	-3.46364	4.20618
C	0.07342	-2.81205	5.45718
N	0.02111	-1.44344	5.64508
C	0.03932	-1.24004	6.99437
C	0.	0.	7.67735
C	-0.03932	1.24004	6.99437
N	-0.02111	1.44344	5.64508
C	-0.07342	2.81205	5.45718

C	-0.08495	3.46364	4.20618
C	-0.06465	2.8126	2.95567
C	-0.03348	3.48144	1.68175
C	-0.0151	2.50121	0.71786
C	0.0151	2.50121	-0.71786
C	0.02171	1.24065	-1.4186
N	0.04967	1.44269	-2.76761
Zn	0.	0.	-4.20613
N	0.02111	1.44344	-5.64508
C	0.03932	1.24004	-6.99437
C	0.	0.	-7.67735
C	-0.03932	-1.24004	-6.99437
N	-0.02111	-1.44344	-5.64508
C	-0.07342	-2.81205	-5.45718
C	-0.08495	-3.46364	-4.20618
C	-0.06465	-2.8126	-2.95567
N	-0.04967	-1.44269	-2.76761
C	-0.02171	-1.24065	-1.4186
C	0.	0.	-0.73525
C	-0.0151	-2.50121	-0.71786
C	0.0151	-2.50121	0.71786
C	0.03348	-3.48144	1.68175
H	0.01901	-4.55138	1.5356
C	-0.03348	-3.48144	-1.68175
H	-0.01901	-4.55138	-1.5356
C	-0.13765	-3.4786	-6.73092
C	-0.10804	-2.49864	-7.69488
C	-0.13823	-2.49753	-9.13075
C	-0.08266	-1.23771	-9.8319
N	-0.12005	-1.43854	-11.18084
Zn	0.	0.	-12.61787
N	0.09161	1.44076	-14.05696
C	0.09919	1.23528	-15.40712
C	0.	0.	-16.08834
C	-0.09919	-1.23528	-15.40712
N	-0.09161	-1.44076	-14.05696
C	-0.21027	-2.80399	-13.86998
C	-0.25388	-3.45551	-12.61858
C	-0.20225	-2.80619	-11.36903
C	-0.20445	-3.47552	-10.09411
H	-0.24268	-4.54489	-9.94789
C	-0.3061	-3.46627	-15.14469
C	-0.22849	-2.48864	-16.10779
C	-0.25706	-2.48627	-17.54456
C	-0.14048	-1.2291	-18.24757
N	-0.18414	-1.42868	-19.59717
Zn	0.	0.	-21.04218
N	0.17324	1.43904	-22.4817
C	0.15744	1.24023	-23.84368
C	0.	0.	-24.49375
C	-0.15744	-1.24023	-23.84368
N	-0.17324	-1.43904	-22.4817
C	-0.33081	-2.78957	-22.28115
C	-0.40412	-3.43841	-21.02785
C	-0.32887	-2.79073	-19.78321
C	-0.36686	-3.45934	-18.50555
H	-0.45703	-4.52575	-18.3602
C	-0.42583	-3.4618	-23.55535
C	-0.30712	-2.50689	-24.52007
H	-0.32021	-2.6464	-25.59101
H	-0.56421	-4.52402	-23.69314
C	0.30712	2.50689	-24.52007
C	0.42583	3.4618	-23.55535

C	0.33081	2.78957	-22.28115
C	0.40412	3.43841	-21.02785
C	0.32887	2.79073	-19.78321
N	0.18414	1.42868	-19.59717
C	0.14048	1.2291	-18.24757
C	0.25706	2.48627	-17.54456
C	0.22849	2.48864	-16.10779
C	0.3061	3.46627	-15.14469
C	0.21027	2.80399	-13.86998
C	0.25388	3.45551	-12.61858
C	0.20225	2.80619	-11.36903
N	0.12005	1.43854	-11.18084
C	0.08266	1.23771	-9.8319
C	0.13823	2.49753	-9.13075
C	0.10804	2.49864	-7.69488
C	0.13765	3.4786	-6.73092
C	0.07342	2.81205	-5.45718
C	0.08495	3.46364	-4.20618
C	0.06465	2.8126	-2.95567
C	0.03348	3.48144	-1.68175
H	0.01901	4.55138	-1.5356
H	0.20467	4.54655	-6.87701
C	0.20445	3.47552	-10.09411
H	0.24268	4.54489	-9.94789
C	0.	0.	-9.14891
H	0.42442	4.52974	-15.29112
C	0.36686	3.45934	-18.50555
H	0.45703	4.52575	-18.3602
C	0.	0.	-17.5651
H	0.56421	4.52402	-23.69314
H	0.32021	2.6464	-25.59101
H	-0.42442	-4.52974	-15.29112
H	-0.20467	-4.54655	-6.87701
H	-0.01901	4.55138	1.5356
C	-0.13765	3.4786	6.73092
C	-0.10804	2.49864	7.69488
C	-0.13823	2.49753	9.13075
C	-0.08266	1.23771	9.8319
N	-0.12005	1.43854	11.18084
Zn	0.	0.	12.61787
N	-0.09161	1.44076	14.05696
C	-0.09919	1.23528	15.40712
C	-0.22849	2.48864	16.10779
C	-0.25706	2.48627	17.54456
C	-0.14048	1.2291	18.24757
N	-0.18414	1.42868	19.59717
Zn	0.	0.	21.04218
N	0.18414	-1.42868	19.59717
C	0.14048	-1.2291	18.24757
C	0.	0.	17.5651
C	0.	0.	16.08834
C	0.09919	-1.23528	15.40712
N	0.09161	-1.44076	14.05696
C	0.21027	-2.80399	13.86998
C	0.25388	-3.45551	12.61858
C	0.20225	-2.80619	11.36903
N	0.12005	-1.43854	11.18084
C	0.08266	-1.23771	9.8319
C	0.	0.	9.14891
C	0.13823	-2.49753	9.13075
C	0.10804	-2.49864	7.69488
C	0.13765	-3.4786	6.73092
H	0.20467	-4.54655	6.87701

C	0.20445	-3.47552	10.09411
H	0.24268	-4.54489	9.94789
C	0.3061	-3.46627	15.14469
C	0.22849	-2.48864	16.10779
C	0.25706	-2.48627	17.54456
C	0.36686	-3.45934	18.50555
C	0.32887	-2.79073	19.78321
C	0.40412	-3.43841	21.02785
C	0.33081	-2.78957	22.28115
N	0.17324	-1.43904	22.4817
C	0.15744	-1.24023	23.84368
C	0.	0.	24.49375
C	-0.15744	1.24023	23.84368
N	-0.17324	1.43904	22.4817
C	-0.33081	2.78957	22.28115
C	-0.40412	3.43841	21.02785
C	-0.32887	2.79073	19.78321
C	-0.36686	3.45934	18.50555
H	-0.45703	4.52575	18.3602
C	-0.42583	3.4618	23.55535
C	-0.30712	2.50689	24.52007
H	-0.32021	2.6464	25.59101
H	-0.56421	4.52402	23.69314
C	0.30712	-2.50689	24.52007
C	0.42583	-3.4618	23.55535
H	0.56421	-4.52402	23.69314
H	0.32021	-2.6464	25.59101
H	0.45703	-4.52575	18.3602
H	0.42442	-4.52974	15.29112
C	-0.3061	3.46627	15.14469
C	-0.21027	2.80399	13.86998
C	-0.25388	3.45551	12.61858
C	-0.20225	2.80619	11.36903
C	-0.20445	3.47552	10.09411
H	-0.24268	4.54489	9.94789
H	-0.42442	4.52974	15.29112
H	-0.20467	4.54655	6.87701
C	0.	0.	-25.99265
C	1.17933	0.25514	-26.71018
C	-1.17933	-0.25514	-26.71018
C	1.17973	0.25468	-28.10601
H	2.09964	0.44828	-26.16599
C	-1.17973	-0.25468	-28.10601
H	-2.09964	-0.44828	-26.16599
C	0.	0.	-28.80837
H	2.1037	0.44981	-28.64405
H	-2.1037	-0.44981	-28.64405
H	0.	0.	-29.89507
C	0.	0.	25.99265
C	-1.17933	0.25514	26.71018
C	1.17933	-0.25514	26.71018
C	-1.17973	0.25468	28.10601
H	-2.09964	0.44828	26.16599
C	1.17973	-0.25468	28.10601
H	2.09964	-0.44828	26.16599
C	0.	0.	28.80837
H	-2.1037	0.44981	28.64405
H	2.1037	-0.44981	28.64405
H	0.	0.	29.89507
C	0.57351	-4.92708	21.02685
C	-0.46448	-5.76879	21.45747
C	1.77398	-5.51166	20.59294
C	-0.30679	-7.15553	21.45393

H	-1.40091	-5.3288	21.78893
C	1.9326	-6.89846	20.59046
H	2.58646	-4.87053	20.26265
C	0.89259	-7.72483	21.02081
H	-1.12372	-7.79092	21.78592
H	2.87106	-7.33213	20.25508
H	1.01566	-8.80455	21.01851
C	0.36344	-4.9487	12.61974
C	-0.69189	-5.7453	13.09256
C	1.52378	-5.58357	12.14822
C	-0.5904	-7.13722	13.09229
H	-1.59745	-5.26591	13.45341
C	1.62638	-6.97544	12.15063
H	2.34965	-4.97776	11.78635
C	0.56936	-7.75676	12.622
H	-1.42024	-7.73715	13.45656
H	2.5348	-7.44845	11.78695
H	0.6488	-8.84057	12.6228
C	0.12176	-4.96039	4.20644
C	1.2495	-5.65045	3.73342
C	-0.9706	-5.70495	4.67989
C	1.28452	-7.04563	3.73534
H	2.10339	-5.08521	3.37096
C	-0.93678	-7.10015	4.67875
H	-1.85131	-5.18229	5.04207
C	0.1912	-7.77497	4.20724
H	2.16866	-7.56197	3.37078
H	-1.79442	-7.65927	5.04354
H	0.21799	-8.86136	4.20754
C	-0.12176	-4.96039	-4.20644
C	0.9706	-5.70495	-4.67989
C	-1.2495	-5.65045	-3.73342
C	0.93678	-7.10015	-4.67875
H	1.85131	-5.18229	-5.04207
C	-1.28452	-7.04563	-3.73534
H	-2.10339	-5.08521	-3.37096
C	-0.1912	-7.77497	-4.20724
H	1.79442	-7.65927	-5.04354
H	-2.16866	-7.56197	-3.37078
H	-0.21799	-8.86136	-4.20754
C	-0.36344	-4.9487	-12.61974
C	0.69189	-5.7453	-13.09256
C	-1.52378	-5.58357	-12.14822
C	0.5904	-7.13722	-13.09229
H	1.59745	-5.26591	-13.45341
C	-1.62638	-6.97544	-12.15063
H	-2.34965	-4.97776	-11.78635
C	-0.56936	-7.75676	-12.622
H	1.42024	-7.73715	-13.45656
H	-2.5348	-7.44845	-11.78695
H	-0.6488	-8.84057	-12.6228
C	-0.57351	-4.92708	-21.02685
C	0.46448	-5.76879	-21.45747
C	-1.77398	-5.51166	-20.59294
C	0.30679	-7.15553	-21.45393
H	1.40091	-5.3288	-21.78893
C	-1.9326	-6.89846	-20.59046
H	-2.58646	-4.87053	-20.26265
C	-0.89259	-7.72483	-21.02081
H	1.12372	-7.79092	-21.78592
H	-2.87106	-7.33213	-20.25508
H	-1.01566	-8.80455	-21.01851
C	0.57351	4.92708	-21.02685

C	-0.46448	5.76879	-21.45747
C	1.77398	5.51166	-20.59294
C	-0.30679	7.15553	-21.45393
H	-1.40091	5.3288	-21.78893
C	1.9326	6.89846	-20.59046
H	2.58646	4.87053	-20.26265
C	0.89259	7.72483	-21.02081
H	-1.12372	7.79092	-21.78592
H	2.87106	7.33213	-20.25508
H	1.01566	8.80455	-21.01851
C	-0.57351	4.92708	21.02685
C	0.46448	5.76879	21.45747
C	-1.77398	5.51166	20.59294
C	0.30679	7.15553	21.45393
H	1.40091	5.3288	21.78893
C	-1.9326	6.89846	20.59046
H	-2.58646	4.87053	20.26265
C	-0.89259	7.72483	21.02081
H	1.12372	7.79092	21.78592
H	-2.87106	7.33213	20.25508
H	-1.01566	8.80455	21.01851
C	-0.36344	4.9487	12.61974
C	0.69189	5.7453	13.09256
C	-1.52378	5.58357	12.14822
C	0.5904	7.13722	13.09229
H	1.59745	5.26591	13.45341
C	-1.62638	6.97544	12.15063
H	-2.34965	4.97776	11.78635
C	-0.56936	7.75676	12.622
H	1.42024	7.73715	13.45656
H	-2.5348	7.44845	11.78695
H	-0.6488	8.84057	12.6228
C	-0.12176	4.96039	4.20644
C	-1.2495	5.65045	3.73342
C	0.9706	5.70495	4.67989
C	-1.28452	7.04563	3.73534
H	-2.10339	5.08521	3.37096
C	0.93678	7.10015	4.67875
H	1.85131	5.18229	5.04207
C	-0.1912	7.77497	4.20724
H	-2.16866	7.56197	3.37078
H	1.79442	7.65927	5.04354
H	-0.21799	8.86136	4.20754
C	0.12176	4.96039	-4.20644
C	-0.9706	5.70495	-4.67989
C	1.2495	5.65045	-3.73342
C	-0.93678	7.10015	-4.67875
H	-1.85131	5.18229	-5.04207
C	1.28452	7.04563	-3.73534
H	2.10339	5.08521	-3.37096
C	0.1912	7.77497	-4.20724
H	-1.79442	7.65927	-5.04354
H	2.16866	7.56197	-3.37078
H	0.21799	8.86136	-4.20754
C	0.36344	4.9487	-12.61974
C	-0.69189	5.7453	-13.09256
C	1.52378	5.58357	-12.14822
C	-0.5904	7.13722	-13.09229
H	-1.59745	5.26591	-13.45341
C	1.62638	6.97544	-12.15063
H	2.34965	4.97776	-11.78635
C	0.56936	7.75676	-12.622
H	-1.42024	7.73715	-13.45656

H	2.5348	7.44845	-11.78695
H	0.6488	8.84057	-12.6228

Table S3.8. Optimized coordinates for **3.6**.

```
Zn 0.0000000000 0.0000000000 4.2081980000
N -0.0806790000 1.4463700000 2.7650440000
C -0.0330720000 1.2433590000 1.4180990000
C 0.0000000000 0.0000000000 0.7349280000
C 0.0330720000 -1.2433590000 1.4180990000
N 0.0806790000 -1.4463700000 2.7650440000
C 0.1132500000 -2.8150790000 2.9556750000
C 0.1618250000 -3.4638860000 4.2084870000
C 0.1499370000 -2.8129910000 5.4619470000
N 0.0609600000 -1.4471850000 5.6522160000
C 0.0807690000 -1.2409080000 6.9997790000
C 0.0000000000 0.0000000000 7.6827680000
C -0.0807690000 1.2409080000 6.9997790000
N -0.0609600000 1.4471850000 5.6522160000
C -0.1499370000 2.8129910000 5.4619470000
C -0.1618250000 3.4638860000 4.2084870000
C -0.1132500000 2.8150790000 2.9556750000
C -0.0692760000 3.4857830000 1.6819920000
C -0.0262970000 2.5054200000 0.7176470000
C 0.0262970000 2.5054200000 -0.7176470000
C 0.0330720000 1.2433590000 -1.4180990000
N 0.0806790000 1.4463700000 -2.7650440000
Zn 0.0000000000 0.0000000000 -4.2081980000
N 0.0609600000 1.4471850000 -5.6522160000
C 0.0807690000 1.2409080000 -6.9997790000
C 0.0000000000 0.0000000000 -7.6827680000
C -0.0807690000 -1.2409080000 -6.9997790000
N -0.0609600000 -1.4471850000 -5.6522160000
C -0.1499370000 -2.8129910000 -5.4619470000
C -0.1618250000 -3.4638860000 -4.2084870000
C -0.1132500000 -2.8150790000 -2.9556750000
N -0.0806790000 -1.4463700000 -2.7650440000
C -0.0330720000 -1.2433590000 -1.4180990000
C 0.0000000000 0.0000000000 -0.7349280000
C -0.0262970000 -2.5054200000 -0.7176470000
C 0.0262970000 -2.5054200000 0.7176470000
C 0.0692760000 -3.4857830000 1.6819920000
H 0.0653540000 -4.5556980000 1.5342750000
C -0.0692760000 -3.4857830000 -1.6819920000
H -0.0653540000 -4.5556980000 -1.5342750000
C -0.2445120000 -3.4775960000 -6.7358400000
C -0.1931980000 -2.4975780000 -7.7002140000
C -0.2317570000 -2.4945110000 -9.1359780000
C -0.1325760000 -1.2360220000 -9.8371740000
N -0.1834380000 -1.4361100000 -11.1846360000
Zn 0.0000000000 0.0000000000 -12.6255300000
N 0.1520340000 1.4400570000 -14.0689250000
C 0.1428580000 1.2337100000 -15.4179760000
C 0.0000000000 0.0000000000 -16.0993180000
C -0.1428580000 -1.2337100000 -15.4179760000
N -0.1520340000 -1.4400570000 -14.0689250000
C -0.3163260000 -2.7976340000 -13.8802490000
C -0.3882440000 -3.4456330000 -12.6264260000
C -0.3152010000 -2.7992090000 -11.3749550000
```

C -0.3380520000 -3.4696020000 -10.0997880000
H -0.4166240000 -4.5366120000 -9.9518620000
C -0.4245190000 -3.4584510000 -15.1556750000
C -0.3072360000 -2.4839320000 -16.1190290000
C -0.3224740000 -2.4822650000 -17.5560430000
C -0.1693540000 -1.2277870000 -18.2590990000
N -0.2077780000 -1.4287410000 -19.6075230000
Zn 0.0000000000 0.0000000000 -21.0572040000
N 0.1921150000 1.4407570000 -22.4999420000
C 0.1718070000 1.2405730000 -23.8608540000
C 0.0000000000 0.0000000000 -24.5100220000
C -0.1718070000 -1.2405730000 -23.8608540000
N -0.1921150000 -1.4407570000 -22.4999420000
C -0.3685360000 -2.7875950000 -22.2979680000
C -0.4596510000 -3.4332940000 -21.0422080000
C -0.3816520000 -2.7867560000 -19.7958050000
C -0.4462840000 -3.4541840000 -18.5174610000
H -0.5635860000 -4.5177550000 -18.3701080000
C -0.4686040000 -3.4599600000 -23.5731190000
C -0.3359080000 -2.5063960000 -24.5382000000
H -0.3500450000 -2.6475180000 -25.6090030000
H -0.6189210000 -4.5204230000 -23.7127060000
C 0.3359080000 2.5063960000 -24.5382000000
C 0.4686040000 3.4599600000 -23.5731190000
C 0.3685360000 2.7875950000 -22.2979680000
C 0.4596510000 3.4332940000 -21.0422080000
C 0.3816520000 2.7867560000 -19.7958050000
N 0.2077780000 1.4287410000 -19.6075230000
C 0.1693540000 1.2277870000 -18.2590990000
C 0.3224740000 2.4822650000 -17.5560430000
C 0.3072360000 2.4839320000 -16.1190290000
C 0.4245190000 3.4584510000 -15.1556750000
C 0.3163260000 2.7976340000 -13.8802490000
C 0.3882440000 3.4456330000 -12.6264260000
C 0.3152010000 2.7992090000 -11.3749550000
N 0.1834380000 1.4361100000 -11.1846360000
C 0.1325760000 1.2360220000 -9.8371740000
C 0.2317570000 2.4945110000 -9.1359780000
C 0.1931980000 2.4975780000 -7.7002140000
C 0.2445120000 3.4775960000 -6.7358400000
C 0.1499370000 2.8129910000 -5.4619470000
C 0.1618250000 3.4638860000 -4.2084870000
C 0.1132500000 2.8150790000 -2.9556750000
C 0.0692760000 3.4857830000 -1.6819920000
H 0.0653540000 4.5556980000 -1.5342750000
H 0.3416860000 4.5430120000 -6.8839850000
C 0.3380520000 3.4696020000 -10.0997880000
H 0.4166240000 4.5366120000 -9.9518620000
C 0.0000000000 0.0000000000 -9.1540350000
H 0.5749990000 4.5175720000 -15.3045870000
C 0.4462840000 3.4541840000 -18.5174610000
H 0.5635860000 4.5177550000 -18.3701080000
C 0.0000000000 0.0000000000 -17.5762680000
H 0.6189210000 4.5204230000 -23.7127060000
H 0.3500450000 2.6475180000 -25.6090030000
H -0.5749990000 -4.5175720000 -15.3045870000
H -0.3416860000 -4.5430120000 -6.8839850000
H -0.0653540000 4.5556980000 1.5342750000
C -0.2445120000 3.4775960000 6.7358400000
C -0.1931980000 2.4975780000 7.7002140000
C -0.2317570000 2.4945110000 9.1359780000
C -0.1325760000 1.2360220000 9.8371740000
N -0.1834380000 1.4361100000 11.1846360000

Zn 0.0000000000 0.0000000000 12.6255300000
N -0.1520340000 1.4400570000 14.0689250000
C -0.1428580000 1.2337100000 15.4179760000
C -0.3072360000 2.4839320000 16.1190290000
C -0.3224740000 2.4822650000 17.5560430000
C -0.1693540000 1.2277870000 18.2590990000
N -0.2077780000 1.4287410000 19.6075230000
Zn 0.0000000000 0.0000000000 21.0572040000
N 0.2077780000 -1.4287410000 19.6075230000
C 0.1693540000 -1.2277870000 18.2590990000
C 0.0000000000 0.0000000000 17.5762680000
C 0.0000000000 0.0000000000 16.0993180000
C 0.1428580000 -1.2337100000 15.4179760000
N 0.1520340000 -1.4400570000 14.0689250000
C 0.3163260000 -2.7976340000 13.8802490000
C 0.3882440000 -3.4456330000 12.6264260000
C 0.3152010000 -2.7992090000 11.3749550000
N 0.1834380000 -1.4361100000 11.1846360000
C 0.1325760000 -1.2360220000 9.8371740000
C 0.0000000000 0.0000000000 9.1540350000
C 0.2317570000 -2.4945110000 9.1359780000
C 0.1931980000 -2.4975780000 7.7002140000
C 0.2445120000 -3.4775960000 6.7358400000
H 0.3416860000 -4.5430120000 6.8839850000
C 0.3380520000 -3.4696020000 10.0997880000
H 0.4166240000 -4.5366120000 9.9518620000
C 0.4245190000 -3.4584510000 15.1556750000
C 0.3072360000 -2.4839320000 16.1190290000
C 0.3224740000 -2.4822650000 17.5560430000
C 0.4462840000 -3.4541840000 18.5174610000
C 0.3816520000 -2.7867560000 19.7958050000
C 0.4596510000 -3.4332940000 21.0422080000
C 0.3685360000 -2.7875950000 22.2979680000
N 0.1921150000 -1.4407570000 22.4999420000
C 0.1718070000 -1.2405730000 23.8608540000
C 0.0000000000 0.0000000000 24.5100220000
C -0.1718070000 1.2405730000 23.8608540000
N -0.1921150000 1.4407570000 22.4999420000
C -0.3685360000 2.7875950000 22.2979680000
C -0.4596510000 3.4332940000 21.0422080000
C -0.3816520000 2.7867560000 19.7958050000
C -0.4462840000 3.4541840000 18.5174610000
H -0.5635860000 4.5177550000 18.3701080000
C -0.4686040000 3.4599600000 23.5731190000
C -0.3359080000 2.5063960000 24.5382000000
H -0.3500450000 2.6475180000 25.6090030000
H -0.6189210000 4.5204230000 23.7127060000
C 0.3359080000 -2.5063960000 24.5382000000
C 0.4686040000 -3.4599600000 23.5731190000
H 0.6189210000 -4.5204230000 23.7127060000
H 0.3500450000 -2.6475180000 25.6090030000
H 0.5635860000 -4.5177550000 18.3701080000
H 0.5749990000 -4.5175720000 15.3045870000
C -0.4245190000 3.4584510000 15.1556750000
C -0.3163260000 2.7976340000 13.8802490000
C -0.3882440000 3.4456330000 12.6264260000
C -0.3152010000 2.7992090000 11.3749550000
C -0.3380520000 3.4696020000 10.0997880000
H -0.4166240000 4.5366120000 9.9518620000
H -0.5749990000 4.5175720000 15.3045870000
H -0.3416860000 4.5430120000 6.8839850000
C 0.0000000000 0.0000000000 -26.0092700000
C 1.1821850000 0.2447220000 -26.7264830000

C -1.1821850000 -0.2447220000 -26.7264830000
C 1.1826030000 0.2438490000 -28.1227730000
H 2.1049750000 0.4298050000 -26.1836750000
C -1.1826030000 -0.2438490000 -28.1227730000
H -2.1049750000 -0.4298050000 -26.1836750000
C 0.0000000000 0.0000000000 -28.8252630000
H 2.1082300000 0.4306410000 -28.6606450000
H -2.1082300000 -0.4306410000 -28.6606450000
H 0.0000000000 0.0000000000 -29.9118410000
C 0.0000000000 0.0000000000 26.0092700000
C -1.1821850000 0.2447220000 26.7264830000
C 1.1821850000 -0.2447220000 26.7264830000
C -1.1826030000 0.2438490000 28.1227730000
H -2.1049750000 0.4298050000 26.1836750000
C 1.1826030000 -0.2438490000 28.1227730000
H 2.1049750000 -0.4298050000 26.1836750000
C 0.0000000000 0.0000000000 28.8252630000
H -2.1082300000 0.4306410000 28.6606450000
H 2.1082300000 -0.4306410000 28.6606450000
H 0.0000000000 0.0000000000 29.9118410000
C 0.6552680000 -4.9192110000 21.0417960000
C -0.3726400000 -5.7788360000 21.4622070000
C 1.8705950000 -5.4821370000 20.6197030000
C -0.1906940000 -7.1630850000 21.4597510000
H -1.3203210000 -5.3568110000 21.7850060000
C 2.0535840000 -6.8664230000 20.6188210000
H 2.6759990000 -4.8279990000 20.2976280000
C 1.0233660000 -7.7112330000 21.0385770000
H -0.9995640000 -7.8125780000 21.7835990000
H 3.0027150000 -7.2833680000 20.2928280000
H 1.1653280000 -8.7885010000 21.0373750000
C 0.5514000000 -4.9342900000 12.6270450000
C -0.4761340000 -5.7687680000 13.0969070000
C 1.7353270000 -5.5261180000 12.1570590000
C -0.3245250000 -7.1565680000 13.0952880000
H -1.3999190000 -5.3242670000 13.4562440000
C 1.8881910000 -6.9138330000 12.1586180000
H 2.5404760000 -4.8918070000 11.7972840000
C 0.8584740000 -7.7334790000 12.6269560000
H -1.1329720000 -7.7862210000 13.4570420000
H 2.8137490000 -7.3532430000 11.7964490000
H 0.9769620000 -8.8135740000 12.6269280000
C 0.2295370000 -4.9597130000 4.2084510000
C 1.3617290000 -5.6262180000 3.7114820000
C -0.8373530000 -5.7266210000 4.7051040000
C 1.4261630000 -7.0207730000 3.7133150000
H 2.1967270000 -5.0448530000 3.3309910000
C -0.7745520000 -7.1212400000 4.7029580000
H -1.7218610000 -5.2237860000 5.0856160000
C 0.3578290000 -7.7727140000 4.2080870000
H 2.3130680000 -7.5185720000 3.3305740000
H -1.6125140000 -7.6977920000 5.0854530000
H 0.4073290000 -8.8581610000 4.2079800000
C -0.2295370000 -4.9597130000 -4.2084510000
C 0.8373530000 -5.7266210000 -4.7051040000
C -1.3617290000 -5.6262180000 -3.7114820000
C 0.7745520000 -7.1212400000 -4.7029580000
H 1.7218610000 -5.2237860000 -5.0856160000
C -1.4261630000 -7.0207730000 -3.7133150000
H -2.1967270000 -5.0448530000 -3.3309910000
C -0.3578290000 -7.7727140000 -4.2080870000
H 1.6125140000 -7.6977920000 -5.0854530000
H -2.3130680000 -7.5185720000 -3.3305740000

H -0.4073290000 -8.8581610000 -4.2079800000
C -0.5514000000 -4.9342900000 -12.6270450000
C 0.4761340000 -5.7687680000 -13.0969070000
C -1.7353270000 -5.5261180000 -12.1570590000
C 0.3245250000 -7.1565680000 -13.0952880000
H 1.3999190000 -5.3242670000 -13.4562440000
C -1.8881910000 -6.9138330000 -12.1586180000
H -2.5404760000 -4.8918070000 -11.7972840000
C -0.8584740000 -7.7334790000 -12.6269560000
H 1.1329720000 -7.7862210000 -13.4570420000
H -2.8137490000 -7.3532430000 -11.7964490000
H -0.9769620000 -8.8135740000 -12.6269280000
C -0.6552680000 -4.9192110000 -21.0417960000
C 0.3726400000 -5.7788360000 -21.4622070000
C -1.8705950000 -5.4821370000 -20.6197030000
C 0.1906940000 -7.1630850000 -21.4597510000
H 1.3203210000 -5.3568110000 -21.7850060000
C -2.0535840000 -6.8664230000 -20.6188210000
H -2.6759990000 -4.8279990000 -20.2976280000
C -1.0233660000 -7.7112330000 -21.0385770000
H 0.9995640000 -7.8125780000 -21.7835990000
H -3.0027150000 -7.2833680000 -20.2928280000
H -1.1653280000 -8.7885010000 -21.0373750000
C 0.6552680000 4.9192110000 -21.0417960000
C -0.3726400000 5.7788360000 -21.4622070000
C 1.8705950000 5.4821370000 -20.6197030000
C -0.1906940000 7.1630850000 -21.4597510000
H -1.3203210000 5.3568110000 -21.7850060000
C 2.0535840000 6.8664230000 -20.6188210000
H 2.6759990000 4.8279990000 -20.2976280000
C 1.0233660000 7.7112330000 -21.0385770000
H -0.9995640000 7.8125780000 -21.7835990000
H 3.0027150000 7.2833680000 -20.2928280000
H 1.1653280000 8.7885010000 -21.0373750000
C -0.6552680000 4.9192110000 21.0417960000
C 0.3726400000 5.7788360000 21.4622070000
C -1.8705950000 5.4821370000 20.6197030000
C 0.1906940000 7.1630850000 21.4597510000
H 1.3203210000 5.3568110000 21.7850060000
C -2.0535840000 6.8664230000 20.6188210000
H -2.6759990000 4.8279990000 20.2976280000
C -1.0233660000 7.7112330000 21.0385770000
H 0.9995640000 7.8125780000 21.7835990000
H -3.0027150000 7.2833680000 20.2928280000
H -1.1653280000 8.7885010000 21.0373750000
C -0.5514000000 4.9342900000 12.6270450000
C 0.4761340000 5.7687680000 13.0969070000
C -1.7353270000 5.5261180000 12.1570590000
C 0.3245250000 7.1565680000 13.0952880000
H 1.3999190000 5.3242670000 13.4562440000
C -1.8881910000 6.9138330000 12.1586180000
H -2.5404760000 4.8918070000 11.7972840000
C -0.8584740000 7.7334790000 12.6269560000
H 1.1329720000 7.7862210000 13.4570420000
H -2.8137490000 7.3532430000 11.7964490000
H -0.9769620000 8.8135740000 12.6269280000
C -0.2295370000 4.9597130000 4.2084510000
C -1.3617290000 5.6262180000 3.7114820000
C 0.8373530000 5.7266210000 4.7051040000
C -1.4261630000 7.0207730000 3.7133150000
H -2.1967270000 5.0448530000 3.3309910000
C 0.7745520000 7.1212400000 4.7029580000
H 1.7218610000 5.2237860000 5.0856160000

```
C -0.3578290000 7.7727140000 4.2080870000
H -2.3130680000 7.5185720000 3.3305740000
H 1.6125140000 7.6977920000 5.0854530000
H -0.4073290000 8.8581610000 4.2079800000
C 0.2295370000 4.9597130000 -4.2084510000
C -0.8373530000 5.7266210000 -4.7051040000
C 1.3617290000 5.6262180000 -3.7114820000
C -0.7745520000 7.1212400000 -4.7029580000
H -1.7218610000 5.2237860000 -5.0856160000
C 1.4261630000 7.0207730000 -3.7133150000
H 2.1967270000 5.0448530000 -3.3309910000
C 0.3578290000 7.7727140000 -4.2080870000
H -1.6125140000 7.6977920000 -5.0854530000
H 2.3130680000 7.5185720000 -3.3305740000
H 0.4073290000 8.8581610000 -4.2079800000
C 0.5514000000 4.9342900000 -12.6270450000
C -0.4761340000 5.7687680000 -13.0969070000
C 1.7353270000 5.5261180000 -12.1570590000
C -0.3245250000 7.1565680000 -13.0952880000
H -1.3999190000 5.3242670000 -13.4562440000
C 1.8881910000 6.9138330000 -12.1586180000
H 2.5404760000 4.8918070000 -11.7972840000
C 0.8584740000 7.7334790000 -12.6269560000
H -1.1329720000 7.7862210000 -13.4570420000
H 2.8137490000 7.3532430000 -11.7964490000
H 0.9769620000 8.8135740000 -12.6269280000
```

Table S3.9. Optimized coordinates for **3.7**.

```
Zn 0.0000000000 0.0000000000 12.6257730000
N 1.4362910000 0.1817660000 11.1833460000
C 1.2369970000 0.1312730000 9.8361470000
C 0.0000000000 0.0000000000 9.1519730000
C -1.2369970000 -0.1312730000 9.8361470000
N -1.4362910000 -0.1817660000 11.1833460000
C -2.7999610000 -0.3108150000 11.3737390000
C -3.4462480000 -0.3809520000 12.6261360000
C -2.7997320000 -0.3092490000 13.8798540000
N -1.4403070000 -0.1486110000 14.0695550000
C -1.2358270000 -0.1394700000 15.4176030000
C 0.0000000000 0.0000000000 16.1011400000
C 1.2358270000 0.1394700000 15.4176030000
N 1.4403070000 0.1486110000 14.0695550000
C 2.7997320000 0.3092490000 13.8798540000
C 3.4462480000 0.3809520000 12.6261360000
C 2.7999610000 0.3108150000 11.3737390000
C 3.4705990000 0.3330380000 10.0999040000
C 2.4950760000 0.2287000000 9.1353400000
C 2.4982680000 0.1907590000 7.6999700000
C 1.2417170000 0.0796700000 6.9995640000
N 1.4472150000 0.0597380000 5.6524870000
Zn 0.0000000000 0.0000000000 4.2081490000
N 1.4463980000 0.0804630000 2.7644070000
C 1.2440060000 0.0329320000 1.4177850000
C 0.0000000000 0.0000000000 0.7338010000
C -1.2440060000 -0.0329320000 1.4177850000
N -1.4463980000 -0.0804630000 2.7644070000
C -2.8155030000 -0.1124370000 2.9552020000
C -3.4639530000 -0.1600410000 4.2083970000
```

C -2.8136710000 -0.1478800000 5.4619650000
N -1.4472150000 -0.0597380000 5.6524870000
C -1.2417170000 -0.0796700000 6.9995640000
C 0.0000000000 0.0000000000 7.6835720000
C -2.4982680000 -0.1907590000 7.6999700000
C -2.4950760000 -0.2287000000 9.1353400000
C -3.4705990000 -0.3330380000 10.0999040000
H -4.5377430000 -0.4096700000 9.9521030000
C -3.4784460000 -0.2416110000 6.7352030000
H -4.5439090000 -0.3381170000 6.8833190000
C -3.4863000000 -0.0684960000 1.6822650000
C -2.5057780000 -0.0260380000 0.7174900000
C -2.5057780000 0.0260670000 -0.7174910000
C -1.2440050000 0.0329440000 -1.4177850000
N -1.4463970000 0.0804770000 -2.7644070000
Zn 0.0000000000 0.0000000000 -4.2081510000
N 1.4472150000 -0.0597520000 -5.6524870000
C 1.2417160000 -0.0796860000 -6.9995640000
C 0.0000000000 0.0000000000 -7.6835720000
C -1.2417160000 0.0796860000 -6.9995640000
N -1.4472150000 0.0597520000 -5.6524870000
C -2.8136690000 0.1479170000 -5.4619660000
C -3.4639510000 0.1600850000 -4.2083980000
C -2.8155020000 0.1124700000 -2.9552020000
C -3.4862990000 0.0685370000 -1.6822650000
H -4.5561990000 0.0641740000 -1.5345910000
C -3.4784420000 0.2416600000 -6.7352030000
C -2.4982650000 0.1907950000 -7.6999700000
C -2.4950720000 0.2287360000 -9.1353400000
C -1.2369950000 0.1312910000 -9.8361470000
N -1.4362880000 0.1817890000 -11.1833450000
Zn 0.0000000000 0.0000000000 -12.6257720000
N 1.4403060000 -0.1486220000 -14.0695550000
C 1.2358260000 -0.1394780000 -15.4176020000
C 0.0000000000 0.0000000000 -16.1011400000
C -1.2358260000 0.1394780000 -15.4176020000
N -1.4403060000 0.1486220000 -14.0695550000
C -2.7997290000 0.3092770000 -13.8798530000
C -3.4462430000 0.3809940000 -12.6261350000
C -2.7999570000 0.3108520000 -11.3737380000
C -3.4705940000 0.3330870000 -10.0999040000
H -4.5377370000 0.4097320000 -9.9521030000
C -3.4615310000 0.4143690000 -15.1538000000
C -2.4869420000 0.2993240000 -16.1183280000
H -4.5210890000 0.5619390000 -15.3022500000
C 2.4869420000 -0.2993240000 -16.1183280000
C 3.4615310000 -0.4143690000 -15.1538000000
C 2.7997290000 -0.3092770000 -13.8798530000
C 3.4462430000 -0.3809940000 -12.6261350000
C 2.7999570000 -0.3108520000 -11.3737380000
N 1.4362880000 -0.1817890000 -11.1833450000
C 1.2369950000 -0.1312910000 -9.8361470000
C 2.4950720000 -0.2287360000 -9.1353400000
C 2.4982650000 -0.1907950000 -7.6999700000
C 3.4784420000 -0.2416600000 -6.7352030000
C 2.8136690000 -0.1479170000 -5.4619660000
C 3.4639510000 -0.1600850000 -4.2083980000
C 2.8155020000 -0.1124700000 -2.9552020000
N 1.4463970000 -0.0804770000 -2.7644070000
C 1.2440050000 -0.0329440000 -1.4177850000
C 2.5057780000 -0.0260670000 -0.7174910000
C 2.5057780000 0.0260380000 0.7174900000
C 3.4863000000 0.0684960000 1.6822650000

C 2.8155030000 0.1124370000 2.9552020000
C 3.4639530000 0.1600410000 4.2083970000
C 2.8136710000 0.1478800000 5.4619650000
C 3.4784460000 0.2416110000 6.7352030000
H 4.5439090000 0.3381170000 6.8833190000
H 4.5562000000 0.0641220000 1.5345910000
C 3.4862990000 -0.0685370000 -1.6822650000
H 4.5561990000 -0.0641740000 -1.5345910000
C 0.0000000000 0.0000000000 -0.7338010000
H 4.5439040000 -0.3381810000 -6.8833190000
C 3.4705940000 -0.3330870000 -10.0999040000
H 4.5377370000 -0.4097320000 -9.9521030000
C 0.0000000000 0.0000000000 -9.1519720000
H 4.5210890000 -0.5619390000 -15.3022500000
H -4.5439040000 0.3381810000 -6.8833190000
H -4.5562000000 -0.0641220000 1.5345910000
H 4.5377430000 0.4096700000 9.9521030000
C 3.4615340000 0.4143450000 15.1538000000
C 2.4869430000 0.2993120000 16.1183280000
C 2.4855410000 0.3136750000 17.5543110000
C 1.2319030000 0.1661380000 18.2555860000
N 1.4323220000 0.2042540000 19.6031660000
Zn 0.0000000000 0.0000000000 21.0448300000
N 1.4380240000 0.1677050000 22.4879390000
C 1.2327300000 0.1518500000 23.8370390000
C 2.4817500000 0.3250180000 24.5378850000
C 2.4807390000 0.3350150000 25.9749190000
C 1.2271970000 0.1741970000 26.6780280000
N 1.4282520000 0.2102270000 28.0263560000
Zn 0.0000000000 0.0000000000 29.4761350000
N -1.4282520000 -0.2102270000 28.0263560000
C -1.2271970000 -0.1741970000 26.6780280000
C 0.0000000000 0.0000000000 25.9951100000
C 0.0000000000 0.0000000000 24.5185540000
C -1.2327300000 -0.1518500000 23.8370390000
N -1.4380240000 -0.1677050000 22.4879390000
C -2.7932860000 -0.3493520000 22.2990730000
C -3.4380940000 -0.4435070000 21.0449440000
C -2.7918300000 -0.3714660000 19.7936970000
N -1.4323220000 -0.2042540000 19.6031660000
C -1.2319030000 -0.1661380000 18.2555860000
C 0.0000000000 0.0000000000 17.5717580000
C -2.4855410000 -0.3136750000 17.5543110000
C -2.4869430000 -0.2993120000 16.1183280000
C -3.4615340000 -0.4143450000 15.1538000000
H -4.5210930000 -0.5619080000 15.3022500000
C -3.4590450000 -0.4327120000 18.5182450000
H -4.5231650000 -0.5434070000 18.3701100000
C -3.4542420000 -0.4572260000 23.5742640000
C -2.4817500000 -0.3250180000 24.5378850000
C -2.4807390000 -0.3350150000 25.9749190000
C -3.4524630000 -0.4601150000 26.9363350000
C -2.7857110000 -0.3891360000 28.2147330000
C -3.4322530000 -0.4663300000 29.4609950000
C -2.7870240000 -0.3718170000 30.7169260000
N -1.4405310000 -0.1935240000 30.9188950000
C -1.2405480000 -0.1722370000 32.2798470000
C 0.0000000000 0.0000000000 32.9290060000
C 1.2405480000 0.1722370000 32.2798470000
N 1.4405310000 0.1935240000 30.9188950000
C 2.7870240000 0.3718170000 30.7169260000
C 3.4322530000 0.4663300000 29.4609950000
C 2.7857110000 0.3891360000 28.2147330000

C 3.4524630000 0.4601150000 26.9363350000
H 4.5154960000 0.5821550000 26.7889730000
C 3.4595910000 0.4712200000 31.9919550000
C 2.5063080000 0.3367490000 32.9571180000
H 2.6476340000 0.3500810000 34.0278970000
H 4.5199400000 0.6223900000 32.1314550000
C -2.5063080000 -0.3367490000 32.9571180000
C -3.4595910000 -0.4712200000 31.9919550000
H -4.5199400000 -0.6223900000 32.1314550000
H -2.6476340000 -0.3500810000 34.0278970000
H -4.5154960000 -0.5821550000 26.7889730000
H -4.5118060000 -0.6185560000 23.7229330000
C 3.4542420000 0.4572260000 23.5742640000
C 2.7932860000 0.3493520000 22.2990730000
C 3.4380940000 0.4435070000 21.0449440000
C 2.7918300000 0.3714660000 19.7936970000
C 3.4590450000 0.4327120000 18.5182450000
H 4.5231650000 0.5434070000 18.3701100000
H 4.5118060000 0.6185560000 23.7229330000
H 4.5210930000 0.5619080000 15.3022500000
C 0.0000000000 0.0000000000 34.4282120000
C 0.2457170000 1.1820070000 35.1453910000
C -0.2457170000 -1.1820070000 35.1453910000
C 0.2447840000 1.1824180000 36.5416710000
H 0.4315400000 2.1046490000 34.6025960000
C -0.2447840000 -1.1824180000 36.5416710000
H -0.4315400000 -2.1046490000 34.6025960000
C 0.0000000000 0.0000000000 37.2441490000
H 0.4322860000 2.1078960000 37.0795430000
H -0.4322860000 -2.1078960000 37.0795430000
H 0.0000000000 0.0000000000 38.3307240000
C -4.9177060000 -0.6656410000 29.4607660000
C -5.7798810000 0.3617060000 29.8772400000
C -5.4774520000 -1.8838830000 29.0429410000
C -7.1636800000 0.1763660000 29.8750210000
H -5.3602530000 1.3115540000 30.1967840000
C -6.8612930000 -2.0702380000 29.0423280000
H -4.8212480000 -2.6888460000 28.7239780000
C -7.7087210000 -1.0405540000 29.4580840000
H -7.8152460000 0.9848030000 30.1957570000
H -7.2758320000 -3.0215530000 28.7196580000
H -8.7856370000 -1.1851420000 29.4570820000
C -4.9236330000 -0.6346250000 21.0461630000
C -5.7775960000 0.3862850000 21.4946570000
C -5.4923090000 -1.8384670000 20.5990410000
C -7.1623610000 0.2088390000 21.4942490000
H -5.3508490000 1.3249530000 21.8365840000
C -6.8769810000 -2.0170370000 20.6017640000
H -4.8424890000 -2.6385860000 20.2560770000
C -7.7163740000 -0.9937010000 21.0486100000
H -7.8075430000 1.0123190000 21.8393110000
H -7.2985440000 -2.9575470000 20.2573330000
H -8.7940760000 -1.1322600000 21.0495290000
C -4.9353070000 -0.5402040000 12.6259850000
C -5.5296870000 -1.7232740000 12.1571570000
C -5.7671590000 0.4903080000 13.0938330000
C -6.9177720000 -1.8725190000 12.1582650000
H -4.8972500000 -2.5305310000 11.7988600000
C -7.1553490000 0.3424020000 13.0911910000
H -5.3203860000 1.4132840000 13.4523460000
C -7.7349880000 -0.8398410000 12.6243560000
H -7.3593750000 -2.7975130000 11.7973470000
H -7.7831160000 1.1530640000 13.4512300000

H -8.8153880000 -0.9554840000 12.6237570000
C -4.9597670000 -0.2269160000 4.2082300000
C -5.6267160000 -1.3587800000 3.7111440000
C -5.7259750000 0.8404630000 4.7048720000
C -7.0212860000 -1.4224700000 3.7130690000
H -5.0457800000 -2.1940640000 3.3306680000
C -7.1206150000 0.7784690000 4.7024310000
H -5.2226570000 1.7246400000 5.0854670000
C -7.7726400000 -0.3536310000 4.2076490000
H -7.5195510000 -2.3091530000 3.3304440000
H -7.6967330000 1.6167930000 5.0847610000
H -8.8581100000 -0.4025310000 4.2074660000
C -4.9597640000 0.2269830000 -4.2082310000
C -5.7259880000 -0.8403840000 -4.7048740000
C -5.6266960000 1.3588560000 -3.7111440000
C -7.1206270000 -0.7783680000 -4.7024360000
H -5.2226830000 -1.7245680000 -5.0854700000
C -7.0212650000 1.4225680000 -3.7130700000
H -5.0457480000 2.1941310000 -3.3306660000
C -7.7726350000 0.3537410000 -4.2076520000
H -7.6967580000 -1.6166820000 -5.0847670000
H -7.5195160000 2.3092590000 -3.3304450000
H -8.8581040000 0.4026580000 -4.2074710000
C -4.9353010000 0.5402660000 -12.6259840000
C -5.7671670000 -0.4902340000 -13.0938320000
C -5.5296630000 1.7233460000 -12.1571580000
C -7.1553550000 -0.3423070000 -13.0911910000
H -5.3204080000 -1.4132170000 -13.4523440000
C -6.9177460000 1.8726110000 -12.1582660000
H -4.8972140000 2.5305930000 -11.7988600000
C -7.7349770000 0.8399440000 -12.6243560000
H -7.7831340000 -1.1529610000 -13.4512290000
H -7.3593350000 2.7976110000 -11.7973490000
H -8.8153760000 0.9556030000 -12.6237570000
C 4.9353010000 -0.5402660000 -12.6259840000
C 5.7671670000 0.4902340000 -13.0938320000
C 5.5296630000 -1.7233460000 -12.1571580000
C 7.1553550000 0.3423070000 -13.0911910000
H 5.3204080000 1.4132170000 -13.4523440000
C 6.9177460000 -1.8726110000 -12.1582660000
H 4.8972140000 -2.5305930000 -11.7988600000
C 7.7349770000 -0.8399440000 -12.6243560000
H 7.7831340000 1.1529610000 -13.4512290000
H 7.3593350000 -2.7976110000 -11.7973490000
H 8.8153760000 -0.9556030000 -12.6237570000
C 4.9177060000 0.6656410000 29.4607660000
C 5.7798810000 -0.3617060000 29.8772400000
C 5.4774520000 1.8838830000 29.0429410000
C 7.1636800000 -0.1763660000 29.8750210000
H 5.3602530000 -1.3115540000 30.1967840000
C 6.8612930000 2.0702380000 29.0423280000
H 4.8212480000 2.6888460000 28.7239780000
C 7.7087210000 1.0405540000 29.4580840000
H 7.8152460000 -0.9848030000 30.1957570000
H 7.2758320000 3.0215530000 28.7196580000
H 8.7856370000 1.1851420000 29.4570820000
C 4.9236330000 0.6346250000 21.0461630000
C 5.7775960000 -0.3862850000 21.4946570000
C 5.4923090000 1.8384670000 20.5990410000
C 7.1623610000 -0.2088390000 21.4942490000
H 5.3508490000 -1.3249530000 21.8365840000
C 6.8769810000 2.0170370000 20.6017640000
H 4.8424890000 2.6385860000 20.2560770000

C 7.7163740000 0.9937010000 21.0486100000
H 7.8075430000 -1.0123190000 21.8393110000
H 7.2985440000 2.9575470000 20.2573330000
H 8.7940760000 1.1322600000 21.0495290000
C 4.9353070000 0.5402040000 12.6259850000
C 5.5296870000 1.7232740000 12.1571570000
C 5.7671590000 -0.4903080000 13.0938330000
C 6.9177720000 1.8725190000 12.1582650000
H 4.8972500000 2.5305310000 11.7988600000
C 7.1553490000 -0.3424020000 13.0911910000
H 5.3203860000 -1.4132840000 13.4523460000
C 7.7349880000 0.8398410000 12.6243560000
H 7.3593750000 2.7975130000 11.7973470000
H 7.7831160000 -1.1530640000 13.4512300000
H 8.8153880000 0.9554840000 12.6237570000
C 4.9597670000 0.2269160000 4.2082300000
C 5.6267160000 1.3587800000 3.7111440000
C 5.7259750000 -0.8404630000 4.7048720000
C 7.0212860000 1.4224700000 3.7130690000
H 5.0457800000 2.1940640000 3.3306680000
C 7.1206150000 -0.7784690000 4.7024310000
H 5.2226570000 -1.7246400000 5.0854670000
C 7.7726400000 0.3536310000 4.2076490000
H 7.5195510000 2.3091530000 3.3304440000
H 7.6967330000 -1.6167930000 5.0847610000
H 8.8581100000 0.4025310000 4.2074660000
C 4.9597640000 -0.2269830000 -4.2082310000
C 5.7259880000 0.8403840000 -4.7048740000
C 5.6266960000 -1.3588560000 -3.7111440000
C 7.1206270000 0.7783680000 -4.7024360000
H 5.2226830000 1.7245680000 -5.0854700000
C 7.0212650000 -1.4225680000 -3.7130700000
H 5.0457480000 -2.1941310000 -3.3306660000
C 7.7726350000 -0.3537410000 -4.2076520000
H 7.6967580000 1.6166820000 -5.0847670000
H 7.5195160000 -2.3092590000 -3.3304450000
H 8.8581040000 -0.4026580000 -4.2074710000
C 2.5063170000 -0.3366890000 -32.9571180000
C 1.2405530000 -0.1722060000 -32.2798470000
N 1.4405350000 -0.1934880000 -30.9188950000
Zn 0.0000000000 0.0000000000 -29.4761350000
N 1.4282560000 -0.2101970000 -28.0263560000
C 1.2272010000 -0.1741720000 -26.6780280000
C 2.4807460000 -0.3349680000 -25.9749190000
C 2.4817550000 -0.3249790000 -24.5378850000
C 1.2327320000 -0.1518310000 -23.8370390000
N 1.4380260000 -0.1676850000 -22.4879380000
Zn 0.0000000000 0.0000000000 -21.0448300000
N -1.4380260000 0.1676850000 -22.4879380000
C -1.2327320000 0.1518310000 -23.8370390000
C 0.0000000000 0.0000000000 -24.5185540000
C 0.0000000000 0.0000000000 -25.9951100000
C -1.2272010000 0.1741720000 -26.6780280000
N -1.4282560000 0.2101970000 -28.0263560000
C -2.7857190000 0.3890780000 -28.2147330000
C -3.4322630000 0.4662560000 -29.4609950000
C -2.7870320000 0.3717520000 -30.7169260000
N -1.4405350000 0.1934880000 -30.9188950000
C -1.2405530000 0.1722060000 -32.2798470000
C 0.0000000000 0.0000000000 -32.9290070000
C -2.5063170000 0.3366890000 -32.9571180000
C -3.4596020000 0.4711370000 -31.9919540000
H -4.5199550000 0.6222840000 -32.1314540000

C -3.4524720000 0.4600470000 -26.9363350000
C -2.4807460000 0.3349680000 -25.9749190000
C -2.4817550000 0.3249790000 -24.5378850000
C -3.4542480000 0.4571790000 -23.5742640000
C -2.7932900000 0.3493210000 -22.2990730000
C -3.4380970000 0.4434800000 -21.0449430000
C -2.7918320000 0.3714510000 -19.7936970000
N -1.4323230000 0.2042500000 -19.6031660000
C -1.2319030000 0.1661370000 -18.2555860000
C 0.0000000000 0.0000000000 -17.5717580000
C 1.2319030000 -0.1661370000 -18.2555860000
N 1.4323230000 -0.2042500000 -19.6031660000
C 2.7918320000 -0.3714510000 -19.7936970000
C 3.4380970000 -0.4434800000 -21.0449430000
C 2.7932900000 -0.3493210000 -22.2990730000
C 3.4542480000 -0.4571790000 -23.5742640000
H 4.5118150000 -0.6184940000 -23.7229320000
C 3.4590460000 -0.4327050000 -18.5182450000
C 2.4855400000 -0.3136770000 -17.5543110000
H 4.5231660000 -0.5433980000 -18.3701100000
C -2.4855400000 0.3136770000 -17.5543110000
C -3.4590460000 0.4327050000 -18.5182450000
H -4.5231660000 0.5433980000 -18.3701100000
H -4.5118150000 0.6184940000 -23.7229320000
H -4.5155070000 0.5820670000 -26.7889730000
C 3.4524720000 -0.4600470000 -26.9363350000
C 2.7857190000 -0.3890780000 -28.2147330000
C 3.4322630000 -0.4662560000 -29.4609950000
C 2.7870320000 -0.3717520000 -30.7169260000
C 3.4596020000 -0.4711370000 -31.9919540000
H 4.5199550000 -0.6222840000 -32.1314540000
H 4.5155070000 -0.5820670000 -26.7889730000
C 0.0000000000 0.0000000000 -34.4282120000
C 0.2457520000 -1.1819990000 -35.1453910000
C -0.2457520000 1.1819990000 -35.1453910000
C 0.2448200000 -1.1824110000 -36.5416710000
H 0.4316030000 -2.1046370000 -34.6025960000
C -0.2448200000 1.1824110000 -36.5416710000
H -0.4316030000 2.1046370000 -34.6025960000
C 0.0000000000 0.0000000000 -37.2441490000
H 0.4323490000 -2.1078830000 -37.0795430000
H -0.4323490000 2.1078830000 -37.0795430000
H 0.0000000000 0.0000000000 -38.3307240000
C -4.9236380000 0.6345890000 -21.0461630000
C -5.4923190000 1.8384290000 -20.5990460000
C -5.7775960000 -0.3863280000 -21.4946510000
C -6.8769930000 2.0169920000 -20.6017680000
H -4.8425030000 2.6385530000 -20.2560850000
C -7.1623610000 -0.2088890000 -21.4942430000
H -5.3508430000 -1.3249950000 -21.8365740000
C -7.7163800000 0.9936500000 -21.0486090000
H -7.2985600000 2.9575020000 -20.2573410000
H -7.8075400000 -1.0123750000 -21.8393010000
H -8.7940830000 1.1322030000 -21.0495290000
C -4.9177200000 0.6655410000 -29.4607660000
C -5.4774850000 1.8837740000 -29.0429410000
C -5.7798770000 -0.3618210000 -29.8772380000
C -6.8613290000 2.0701060000 -29.0423280000
H -4.8212940000 2.6887480000 -28.7239780000
C -7.1636800000 -0.1765030000 -29.8750190000
H -5.3602340000 -1.3116620000 -30.1967820000
C -7.7087410000 1.0404080000 -29.4580830000
H -7.2758840000 3.0214150000 -28.7196580000

```
H -7.8152320000 -0.9849510000 -30.1957550000
H -8.7856590000 1.1849790000 -29.4570810000
C 4.9236380000 -0.6345890000 -21.0461630000
C 5.4923190000 -1.8384290000 -20.5990460000
C 5.7775960000 0.3863280000 -21.4946510000
C 6.8769930000 -2.0169920000 -20.6017680000
H 4.8425030000 -2.6385530000 -20.2560850000
C 7.1623610000 0.2088890000 -21.4942430000
H 5.3508430000 1.3249950000 -21.8365740000
C 7.7163800000 -0.9936500000 -21.0486090000
H 7.2985600000 -2.9575020000 -20.2573410000
H 7.8075400000 1.0123750000 -21.8393010000
H 8.7940830000 -1.1322030000 -21.0495290000
C 4.9177200000 -0.6655410000 -29.4607660000
C 5.4774850000 -1.8837740000 -29.0429410000
C 5.7798770000 0.3618210000 -29.8772380000
C 6.8613290000 -2.0701060000 -29.0423280000
H 4.8212940000 -2.6887480000 -28.7239780000
C 7.1636800000 0.1765030000 -29.8750190000
H 5.3602340000 1.3116620000 -30.1967820000
C 7.7087410000 -1.0404080000 -29.4580830000
H 7.2758840000 -3.0214150000 -28.7196580000
H 7.8152320000 0.9849510000 -30.1957550000
H 8.7856590000 -1.1849790000 -29.4570810000
H 2.6476420000 -0.3500180000 -34.0278970000
H -2.6476420000 0.3500180000 -34.0278970000
```

Table S3.10. Optimized coordinates for **3.8**.

```
Zn 0.0000000000 0.0000000000 21.0446950000
N 0.2029440000 -1.4325070000 19.6015650000
C 0.1650890000 -1.2328700000 18.2542180000
C 0.0000000000 0.0000000000 17.5693910000
C -0.1650890000 1.2328700000 18.2542180000
N -0.2029440000 1.4325070000 19.6015650000
C -0.3676320000 2.7926200000 19.7921240000
C -0.4368950000 3.4387900000 21.0443230000
C -0.3429390000 2.7954440000 22.2982720000
N -0.1648830000 1.4382390000 22.4881650000
C -0.1488740000 1.2348210000 23.8362380000
C 0.0000000000 0.0000000000 24.5199770000
C 0.1488740000 -1.2348210000 23.8362380000
N 0.1648830000 -1.4382390000 22.4881650000
C 0.3429390000 -2.7954440000 22.2982720000
C 0.4368950000 -3.4387900000 21.0443230000
C 0.3676320000 -2.7926200000 19.7921240000
C 0.4282340000 -3.4601050000 18.5180280000
C 0.3109420000 -2.4861440000 17.5533410000
C 0.2969320000 -2.4877410000 16.1177500000
C 0.1384040000 -1.2366410000 15.4170180000
N 0.1472630000 -1.4404100000 14.0694700000
Zn 0.0000000000 0.0000000000 12.6254160000
N 0.1812100000 -1.4363980000 11.1824480000
C 0.1308530000 -1.2375970000 9.8354830000
C 0.0000000000 0.0000000000 9.1506480000
C -0.1308530000 1.2375970000 9.8354830000
N -0.1812100000 1.4363980000 11.1824480000
C -0.3094250000 2.8004310000 11.3729580000
C -0.3786000000 3.4464970000 12.6258000000
```

C -0.3069470000 2.8005810000 13.8795010000
N -0.1472630000 1.4404100000 14.0694700000
C -0.1384040000 1.2366410000 15.4170180000
C 0.0000000000 0.0000000000 16.1015490000
C -0.2969320000 2.4877410000 16.1177500000
C -0.3109420000 2.4861440000 17.5533410000
C -0.4282340000 3.4601050000 18.5180280000
H -0.5371150000 4.5244050000 18.3699990000
C -0.4113160000 3.4625370000 15.1528730000
H -0.5581480000 4.5221880000 15.3012890000
C -0.3314260000 3.4711640000 10.0998450000
C -0.2277230000 2.4954400000 9.1348670000
C -0.1900290000 2.4986690000 7.6997570000
C -0.0793800000 1.2422300000 6.9994130000
N -0.0594030000 1.4472090000 5.6526490000
Zn 0.0000000000 0.0000000000 4.2080170000
N 0.0804530000 -1.4464050000 2.7639380000
C 0.0329090000 -1.2444670000 1.4175620000
C 0.0000000000 0.0000000000 0.7329920000
C -0.0329090000 1.2444670000 1.4175620000
N -0.0804530000 1.4464050000 2.7639380000
C -0.1122770000 2.8158150000 2.9548630000
C -0.1595760000 3.4639570000 4.2082840000
C -0.1473100000 2.8140720000 5.4619530000
C -0.2407310000 3.4789420000 6.7347050000
H -0.3370440000 4.5444190000 6.8827730000
C -0.0683930000 3.4866810000 1.6824520000
C -0.0260300000 2.5060610000 0.7173770000
C 0.0258660000 2.5060640000 -0.7173790000
C 0.0328170000 1.2444700000 -1.4175640000
N 0.0803430000 1.4464090000 -2.7639390000
Zn 0.0000000000 0.0000000000 -4.2080360000
N -0.0593100000 -1.4472140000 -5.6526500000
C -0.0793240000 -1.2422330000 -6.9994140000
C 0.0000000000 0.0000000000 -7.6840910000
C 0.0793240000 1.2422330000 -6.9994140000
N 0.0593100000 1.4472140000 -5.6526500000
C 0.1471620000 2.8140810000 -5.4619540000
C 0.1593680000 3.4639650000 -4.2082830000
C 0.1120910000 2.8158210000 -2.9548640000
C 0.0681710000 3.4866850000 -1.6824540000
H 0.0636390000 4.5565800000 -1.5348310000
C 0.2405740000 3.4789540000 -6.7347050000
C 0.1899350000 2.4986770000 -7.6997560000
H 0.3368410000 4.5444350000 -6.8827730000
C -0.1899350000 -2.4986770000 -7.6997560000
C -0.2405740000 -3.4789540000 -6.7347050000
C -0.1471620000 -2.8140810000 -5.4619540000
C -0.1593680000 -3.4639650000 -4.2082830000
C -0.1120910000 -2.8158210000 -2.9548640000
N -0.0803430000 -1.4464090000 -2.7639390000
C -0.0328170000 -1.2444700000 -1.4175640000
C -0.0258660000 -2.5060640000 -0.7173790000
C 0.0260300000 -2.5060610000 0.7173770000
C 0.0683930000 -3.4866810000 1.6824520000
C 0.1122770000 -2.8158150000 2.9548630000
C 0.1595760000 -3.4639570000 4.2082840000
C 0.1473100000 -2.8140720000 5.4619530000
N 0.0594030000 -1.4472090000 5.6526490000
C 0.0793800000 -1.2422300000 6.9994130000
C 0.1900290000 -2.4986690000 7.6997570000
C 0.2277230000 -2.4954400000 9.1348670000
C 0.3314260000 -3.4711640000 10.0998450000

C 0.3094250000 -2.8004310000 11.3729580000
C 0.3786000000 -3.4464970000 12.6258000000
C 0.3069470000 -2.8005810000 13.8795010000
C 0.4113160000 -3.4625370000 15.1528730000
H 0.5581480000 -4.5221880000 15.3012890000
H 0.4073980000 -4.5383470000 9.9520950000
C 0.2407310000 -3.4789420000 6.7347050000
H 0.3370440000 -4.5444190000 6.8827730000
C 0.0000000000 0.0000000000 7.6840910000
H 0.0639320000 -4.5565750000 1.5348280000
C -0.0681710000 -3.4866850000 -1.6824540000
H -0.0636390000 -4.5565800000 -1.5348310000
C 0.0000000000 0.0000000000 -0.7329930000
H -0.3368410000 -4.5444350000 -6.8827730000
H -0.0639320000 4.5565750000 1.5348280000
H -0.4073980000 4.5383470000 9.9520950000
H 0.5371150000 -4.5244050000 18.3699990000
C 0.4476490000 -3.4573670000 23.5719950000
C 0.3175530000 -2.4847700000 24.5367770000
C 0.3266350000 -2.4840000000 25.9727660000
C 0.1711600000 -1.2313160000 26.6740970000
N 0.2068950000 -1.4318410000 28.0215880000
Zn 0.0000000000 0.0000000000 29.4632970000
N 0.1695860000 -1.4377800000 30.9064700000
C 0.1528090000 -1.2326930000 32.2555750000
C 0.3270230000 -2.4815180000 32.9563450000
C 0.3363590000 -2.4806170000 34.3933630000
C 0.1746990000 -1.2271770000 35.0964920000
N 0.2104240000 -1.4281980000 36.4447620000
Zn 0.0000000000 0.0000000000 37.8945350000
N -0.2104240000 1.4281980000 36.4447620000
C -0.1746990000 1.2271770000 35.0964920000
C 0.0000000000 0.0000000000 34.4135250000
C 0.0000000000 0.0000000000 32.9371600000
C -0.1528090000 1.2326930000 32.2555750000
N -0.1695860000 1.4377800000 30.9064700000
C -0.3535310000 2.7926980000 30.7175850000
C -0.4510780000 3.4370120000 29.4633170000
C -0.3795250000 2.7907910000 28.2121820000
N -0.2068950000 1.4318410000 28.0215880000
C -0.1711600000 1.2313160000 26.6740970000
C 0.0000000000 0.0000000000 25.9901580000
C -0.3266350000 2.4840000000 25.9727660000
C -0.3175530000 2.4847700000 24.5367770000
C -0.4476490000 3.4573670000 23.5719950000
H -0.6061060000 4.5153940000 23.7202290000
C -0.4471980000 3.4573130000 26.9367080000
H -0.5628750000 4.5208920000 26.7885200000
C -0.4612330000 3.4537310000 31.9926460000
C -0.3270230000 2.4815180000 32.9563450000
C -0.3363590000 2.4806170000 34.3933630000
C -0.4615450000 3.4523240000 35.3547580000
C -0.3898780000 2.7856390000 36.6331750000
C -0.4669550000 3.4321620000 37.8793650000
C -0.3720630000 2.7869490000 39.1353950000
N -0.1935810000 1.4405330000 39.3373280000
C -0.1722320000 1.2405760000 40.6982980000
C 0.0000000000 0.0000000000 41.3474380000
C 0.1722320000 -1.2405760000 40.6982980000
N 0.1935810000 -1.4405330000 39.3373280000
C 0.3720630000 -2.7869490000 39.1353950000
C 0.4669550000 -3.4321620000 37.8793650000
C 0.3898780000 -2.7856390000 36.6331750000

C 0.4615450000 -3.4523240000 35.3547580000
H 0.5839950000 -4.5153050000 35.2073780000
C 0.4714030000 -3.4595590000 40.4103720000
C 0.3367490000 -2.5063050000 41.3755610000
H 0.3499510000 -2.6476790000 42.4463310000
H 0.6226640000 -4.5198910000 40.5498730000
C -0.3367490000 2.5063050000 41.3755610000
C -0.4714030000 3.4595590000 40.4103720000
H -0.6226640000 4.5198910000 40.5498730000
H -0.3499510000 2.6476790000 42.4463310000
H -0.5839950000 4.5153050000 35.2073780000
H -0.6239900000 4.5110810000 32.1412710000
C 0.4612330000 -3.4537310000 31.9926460000
C 0.3535310000 -2.7926980000 30.7175850000
C 0.4510780000 -3.4370120000 29.4633170000
C 0.3795250000 -2.7907910000 28.2121820000
C 0.4471980000 -3.4573130000 26.9367080000
H 0.5628750000 -4.5208920000 26.7885200000
H 0.6239900000 -4.5110810000 32.1412710000
H 0.6061060000 -4.5153940000 23.7202290000
C 0.0000000000 0.0000000000 42.8466220000
C 1.1819510000 -0.2460600000 43.5637780000
C -1.1819510000 0.2460600000 43.5637780000
C 1.1823560000 -0.2450990000 44.9600520000
H 2.1045450000 -0.4321310000 43.0209880000
C -1.1823560000 0.2450990000 44.9600520000
H -2.1045450000 0.4321310000 43.0209880000
C 0.0000000000 0.0000000000 45.6625230000
H 2.1077830000 -0.4328370000 45.4979240000
H -2.1077830000 0.4328370000 45.4979240000
H 0.0000000000 0.0000000000 46.7490950000
C -0.6667000000 4.9175350000 37.8792040000
C 0.3603900000 5.7799810000 38.2957470000
C -1.8851260000 5.4769110000 37.4614110000
C 0.1746280000 7.1637190000 38.2935710000
H 1.3103700000 5.3606380000 38.6152690000
C -2.0718980000 6.8606920000 37.4608840000
H -2.6898990000 4.8204780000 37.1424420000
C -1.0424620000 7.7084080000 37.8766670000
H 0.9828690000 7.8155120000 38.6143290000
H -3.0233420000 7.2749560000 37.1382490000
H -1.1873760000 8.7852770000 37.8757220000
C -0.6462730000 4.9220300000 29.4647260000
C 0.3737380000 5.7787910000 29.9098760000
C -1.8530660000 5.4872890000 29.0212960000
C 0.1925430000 7.1630680000 29.9097130000
H 1.3146050000 5.3546470000 30.2489910000
C -2.0353640000 6.8714770000 29.0243060000
H -2.6524990000 4.8352270000 28.6809970000
C -1.0128940000 7.7137210000 29.4677460000
H 0.9953460000 7.8104970000 30.2521250000
H -2.9780850000 7.2904240000 28.6827440000
H -1.1543600000 8.7910420000 29.4688730000
C -0.6241610000 4.9247900000 21.0447150000
C -1.8271250000 5.4960610000 20.5986380000
C 0.3996970000 5.7762040000 21.4912030000
C -2.0020910000 6.8811700000 20.6008120000
H -2.6293340000 4.8480800000 20.2571280000
C 0.2259240000 7.1614240000 21.4897080000
H 1.3375600000 5.3471700000 21.8323860000
C -0.9758400000 7.7181930000 21.0454480000
H -2.9420240000 7.3049330000 20.2575310000
H 1.0315920000 7.8047550000 21.8330970000

H -1.1115760000 8.7962520000 21.0457300000
C -0.5366650000 4.9356450000 12.6254560000
C -1.7192660000 5.5308020000 12.1564700000
C 0.4945650000 5.7665870000 13.0932930000
C -1.8674140000 6.9189880000 12.1576150000
H -2.5269860000 4.8989800000 11.7981690000
C 0.3478020000 7.1548880000 13.0903580000
H 1.4171070000 5.3190700000 13.4519480000
C -0.8340190000 7.7353960000 12.6235490000
H -2.7920870000 7.3613030000 11.7967680000
H 1.1589810000 7.7820390000 13.4502840000
H -0.9488010000 8.8158850000 12.6228570000
C -0.2262310000 4.9597570000 4.2080630000
C -1.3580280000 5.6267360000 3.7109050000
C 0.8413000000 5.7257160000 4.7047180000
C -1.4215420000 7.0213040000 3.7129220000
H -2.1933520000 5.0458960000 3.3303970000
C 0.7795250000 7.1203580000 4.7021040000
H 1.7253580000 5.2222640000 5.0853810000
C -0.3525380000 7.7724980000 4.2073920000
H -2.3081850000 7.5196880000 3.3303750000
H 1.6179540000 7.6963740000 5.0843380000
H -0.4012860000 8.8579710000 4.2071800000
C 0.2259320000 4.9597690000 -4.2080630000
C -0.8416410000 5.7256620000 -4.7047300000
C 1.3576810000 5.6268190000 -3.7108910000
C -0.7799540000 7.1203080000 -4.7021150000
H -1.7256640000 5.2221550000 -5.0854040000
C 1.4211080000 7.0213910000 -3.7129070000
H 2.1930360000 5.0460310000 -3.3303710000
C 0.3520630000 7.7725180000 -4.2073890000
H -1.6184140000 7.6962720000 -5.0843580000
H 2.3077150000 7.5198300000 -3.3303480000
H 0.4007430000 8.8579940000 -4.2071760000
C -0.2259320000 -4.9597690000 -4.2080630000
C 0.8416410000 -5.7256620000 -4.7047300000
C -1.3576810000 -5.6268190000 -3.7108910000
C 0.7799540000 -7.1203080000 -4.7021150000
H 1.7256640000 -5.2221550000 -5.0854040000
C -1.4211080000 -7.0213910000 -3.7129070000
H -2.1930360000 -5.0460310000 -3.3303710000
C -0.3520630000 -7.7725180000 -4.2073890000
H 1.6184140000 -7.6962720000 -5.0843580000
H -2.3077150000 -7.5198300000 -3.3303480000
H -0.4007430000 -8.8579940000 -4.2071760000
C 0.6667000000 -4.9175350000 37.8792040000
C -0.3603900000 -5.7799810000 38.2957470000
C 1.8851260000 -5.4769110000 37.4614110000
C -0.1746280000 -7.1637190000 38.2935710000
H -1.3103700000 -5.3606380000 38.6152690000
C 2.0718980000 -6.8606920000 37.4608840000
H 2.6898990000 -4.8204780000 37.1424420000
C 1.0424620000 -7.7084080000 37.8766670000
H -0.9828690000 -7.8155120000 38.6143290000
H 3.0233420000 -7.2749560000 37.1382490000
H 1.1873760000 -8.7852770000 37.8757220000
C 0.6462730000 -4.9220300000 29.4647260000
C -0.3737380000 -5.7787910000 29.9098760000
C 1.8530660000 -5.4872890000 29.0212960000
C -0.1925430000 -7.1630680000 29.9097130000
H -1.3146050000 -5.3546470000 30.2489910000
C 2.0353640000 -6.8714770000 29.0243060000
H 2.6524990000 -4.8352270000 28.6809970000

C 1.0128940000 -7.7137210000 29.4677460000
H -0.9953460000 -7.8104970000 30.2521250000
H 2.9780850000 -7.2904240000 28.6827440000
H 1.1543600000 -8.7910420000 29.4688730000
C 0.6241610000 -4.9247900000 21.0447150000
C 1.8271250000 -5.4960610000 20.5986380000
C -0.3996970000 -5.7762040000 21.4912030000
C 2.0020910000 -6.8811700000 20.6008120000
H 2.6293340000 -4.8480800000 20.2571280000
C -0.2259240000 -7.1614240000 21.4897080000
H -1.3375600000 -5.3471700000 21.8323860000
C 0.9758400000 -7.7181930000 21.0454480000
H 2.9420240000 -7.3049330000 20.2575310000
H -1.0315920000 -7.8047550000 21.8330970000
H 1.1115760000 -8.7962520000 21.0457300000
C 0.5366650000 -4.9356450000 12.6254560000
C 1.7192660000 -5.5308020000 12.1564700000
C -0.4945650000 -5.7665870000 13.0932930000
C 1.8674140000 -6.9189880000 12.1576150000
H 2.5269860000 -4.8989800000 11.7981690000
C -0.3478020000 -7.1548880000 13.0903580000
H -1.4171070000 -5.3190700000 13.4519480000
C 0.8340190000 -7.7353960000 12.6235490000
H 2.7920870000 -7.3613030000 11.7967680000
H -1.1589810000 -7.7820390000 13.4502840000
H 0.9488010000 -8.8158850000 12.6228570000
C 0.2262310000 -4.9597570000 4.2080630000
C 1.3580280000 -5.6267360000 3.7109050000
C -0.8413000000 -5.7257160000 4.7047180000
C 1.4215420000 -7.0213040000 3.7129220000
H 2.1933520000 -5.0458960000 3.3303970000
C -0.7795250000 -7.1203580000 4.7021040000
H -1.7253580000 -5.2222640000 5.0853810000
C 0.3525380000 -7.7724980000 4.2073920000
H 2.3081850000 -7.5196880000 3.3303750000
H -1.6179540000 -7.6963740000 5.0843380000
H 0.4012860000 -8.8579710000 4.2071800000
Zn 0.0000000000 0.0000000000 -29.4632990000
N -0.1696010000 -1.4377800000 -30.9064700000
C -0.1528340000 -1.2326910000 -32.2555750000
C 0.0000000000 0.0000000000 -32.9371590000
C 0.1528340000 1.2326910000 -32.2555750000
N 0.1696010000 1.4377800000 -30.9064700000
C 0.3536000000 2.7926920000 -30.7175860000
C 0.4511660000 3.4370030000 -29.4633170000
C 0.3796020000 2.7907820000 -28.2121820000
N 0.2069250000 1.4318360000 -28.0215890000
C 0.1711940000 1.2313110000 -26.6740980000
C 0.0000000000 0.0000000000 -25.9901600000
C -0.1711940000 -1.2313110000 -26.6740980000
N -0.2069250000 -1.4318360000 -28.0215890000
C -0.3796020000 -2.7907820000 -28.2121820000
C -0.4511660000 -3.4370030000 -29.4633170000
C -0.3536000000 -2.7926920000 -30.7175860000
C -0.4613280000 -3.4537200000 -31.9926470000
C -0.3270910000 -2.4815100000 -32.9563460000
C -0.3364200000 -2.4806080000 -34.3933630000
C -0.1747300000 -1.2271730000 -35.0964920000
N -0.2104560000 -1.4281940000 -36.4447630000
Zn 0.0000000000 0.0000000000 -37.8945340000
N -0.1935900000 -1.4405340000 -39.3373270000
C -0.1722500000 -1.2405740000 -40.6982980000
C 0.0000000000 0.0000000000 -41.3474390000

C 0.1722500000 1.2405740000 -40.6982980000
N 0.1935900000 1.4405340000 -39.3373270000
C 0.3721200000 2.7869430000 -39.1353950000
C 0.4670330000 3.4321530000 -37.8793650000
C 0.3899460000 2.7856300000 -36.6331750000
N 0.2104560000 1.4281940000 -36.4447630000
C 0.1747300000 1.2271730000 -35.0964920000
C 0.0000000000 0.0000000000 -34.4135250000
C 0.3364200000 2.4806080000 -34.3933630000
C 0.3270910000 2.4815100000 -32.9563460000
C 0.4613280000 3.4537200000 -31.9926470000
H 0.6241180000 4.5110630000 -32.1412730000
C 0.4616240000 3.4523130000 -35.3547580000
H 0.5840950000 4.5152910000 -35.2073810000
C 0.4715050000 3.4595460000 -40.4103710000
C 0.3368320000 2.5062920000 -41.3755600000
C -0.3368320000 -2.5062920000 -41.3755600000
C -0.4715050000 -3.4595460000 -40.4103710000
C -0.3721200000 -2.7869430000 -39.1353950000
C -0.4670330000 -3.4321530000 -37.8793650000
C -0.3899460000 -2.7856300000 -36.6331750000
C -0.4616240000 -3.4523130000 -35.3547580000
H -0.5840950000 -4.5152910000 -35.2073810000
H -0.6228070000 -4.5198730000 -40.5498640000
H 0.6228070000 4.5198730000 -40.5498640000
H -0.6241180000 -4.5110630000 -32.1412730000
C -0.4472960000 -3.4573020000 -26.9367070000
C -0.3267060000 -2.4839910000 -25.9727670000
C -0.3176220000 -2.4847600000 -24.5367780000
C -0.1489000000 -1.2348190000 -23.8362400000
N -0.1649190000 -1.4382340000 -22.4881660000
Zn 0.0000000000 0.0000000000 -21.0446990000
N -0.2029740000 -1.4325010000 -19.6015660000
C -0.1651080000 -1.2328670000 -18.2542200000
C -0.3109800000 -2.4861390000 -17.5533410000
C -0.2969510000 -2.4877370000 -16.1177510000
C -0.1383920000 -1.2366430000 -15.4170190000
N -0.1472210000 -1.4404140000 -14.0694720000
Zn 0.0000000000 0.0000000000 -12.6254140000
N 0.1472210000 1.4404140000 -14.0694720000
C 0.1383920000 1.2366430000 -15.4170190000
C 0.0000000000 0.0000000000 -16.1015500000
C 0.0000000000 0.0000000000 -17.5693920000
C 0.1651080000 1.2328670000 -18.2542200000
N 0.2029740000 1.4325010000 -19.6015660000
C 0.3677010000 2.7926110000 -19.7921240000
C 0.4369860000 3.4387770000 -21.0443230000
C 0.3430110000 2.7954360000 -22.2982740000
N 0.1649190000 1.4382340000 -22.4881660000
C 0.1489000000 1.2348190000 -23.8362400000
C 0.0000000000 0.0000000000 -24.5199800000
C 0.3176220000 2.4847600000 -24.5367780000
C 0.3267060000 2.4839910000 -25.9727670000
C 0.4472960000 3.4573020000 -26.9367070000
H 0.5629950000 4.5208770000 -26.7885190000
C 0.4477480000 3.4573530000 -23.5719960000
H 0.6062420000 4.5153740000 -23.7202310000
C 0.4282970000 3.4600960000 -18.5180290000
C 0.3109800000 2.4861390000 -17.5533410000
C 0.2969510000 2.4877370000 -16.1177510000
C 0.4113240000 3.4625340000 -15.1528740000
C 0.3069160000 2.8005850000 -13.8795020000
C 0.3785560000 3.4465020000 -12.6258000000

C 0.3093810000 2.8004360000 -11.3729580000
N 0.1811940000 1.4364000000 -11.1824470000
C 0.1308220000 1.2376010000 -9.8354820000
C 0.0000000000 0.0000000000 -9.1506480000
C -0.1308220000 -1.2376010000 -9.8354820000
N -0.1811940000 -1.4364000000 -11.1824470000
C -0.3093810000 -2.8004360000 -11.3729580000
C -0.3785560000 -3.4465020000 -12.6258000000
C -0.3069160000 -2.8005850000 -13.8795020000
C -0.4113240000 -3.4625340000 -15.1528740000
H -0.5581720000 -4.5221830000 -15.3012930000
C -0.3313320000 -3.4711710000 -10.0998450000
C -0.2276460000 -2.4954470000 -9.1348660000
H -0.4072660000 -4.5383580000 -9.9520940000
C 0.2276460000 2.4954470000 -9.1348660000
C 0.3313320000 3.4711710000 -10.0998450000
H 0.4072660000 4.5383580000 -9.9520940000
H 0.5581720000 4.5221830000 -15.3012930000
H 0.5371910000 4.5243940000 -18.3700020000
C -0.4282970000 -3.4600960000 -18.5180290000
C -0.3677010000 -2.7926110000 -19.7921240000
C -0.4369860000 -3.4387770000 -21.0443230000
C -0.3430110000 -2.7954360000 -22.2982740000
C -0.4477480000 -3.4573530000 -23.5719960000
H -0.6062420000 -4.5153740000 -23.7202310000
H -0.5371910000 -4.5243940000 -18.3700020000
H -0.5629950000 -4.5208770000 -26.7885190000
C 0.0000000000 0.0000000000 -42.8466230000
C -1.1819670000 -0.2459820000 -43.5637770000
C 1.1819670000 0.2459820000 -43.5637770000
C -1.1823720000 -0.2450210000 -44.9600520000
H -2.1045730000 -0.4319940000 -43.0209870000
C 1.1823720000 0.2450210000 -44.9600520000
H 2.1045730000 0.4319940000 -43.0209870000
C 0.0000000000 0.0000000000 -45.6625220000
H -2.1078100000 -0.4327010000 -45.4979250000
H 2.1078100000 0.4327010000 -45.4979250000
H 0.0000000000 0.0000000000 -46.7490940000
C 0.5366020000 4.9356510000 -12.6254550000
C 1.7191760000 5.5308220000 -12.1564160000
C -0.4946150000 5.7665820000 -13.0933390000
C 1.8673100000 6.9190100000 -12.1575590000
H 2.5268870000 4.8990100000 -11.7980780000
C -0.3478660000 7.1548850000 -13.0904020000
H -1.4171380000 5.3190560000 -13.4520320000
C 0.8339280000 7.7354060000 -12.6235420000
H 2.7919630000 7.3613360000 -11.7966730000
H -1.1590360000 7.7820270000 -13.4503640000
H 0.9486980000 8.8158960000 -12.6228480000
C 0.6242890000 4.9247730000 -21.0447130000
C 1.8272710000 5.4960080000 -20.5986350000
C -0.3995460000 5.7762170000 -21.4911950000
C 2.0022760000 6.8811120000 -20.6008060000
H 2.6294620000 4.8480040000 -20.2571290000
C -0.2257330000 7.1614330000 -21.4896960000
H -1.3374220000 5.3472110000 -21.8323760000
C 0.9760470000 7.7181660000 -21.0454370000
H 2.9422210000 7.3048480000 -20.2575250000
H -1.0313840000 7.8047870000 -21.8330800000
H 1.1118140000 8.7962210000 -21.0457160000
C 0.6463890000 4.9220170000 -29.4647290000
C -0.3735940000 5.7787950000 -29.9099090000
C 1.8531840000 5.4872560000 -29.0212750000

C -0.1923720000 7.1630690000 -29.9097500000
H -1.3144620000 5.3546690000 -30.2490420000
C 2.0355090000 6.8714400000 -29.0242890000
H 2.6525970000 4.8351800000 -28.6809540000
C 1.0130650000 7.7137010000 -29.4677570000
H -0.9951550000 7.8105110000 -30.2521830000
H 2.9782300000 7.2903700000 -28.6827090000
H 1.1545510000 8.7910200000 -29.4688880000
C 0.6668180000 4.9175200000 -37.8792010000
C -0.3602330000 5.7799970000 -38.2957740000
C 1.8852510000 5.4768590000 -37.4613730000
C -0.1744280000 7.1637290000 -38.2935950000
H -1.3102170000 5.3606820000 -38.6153240000
C 2.0720650000 6.8606340000 -37.4608420000
H 2.6899920000 4.8204020000 -37.1423790000
C 1.0426670000 7.7083810000 -37.8766570000
H -0.9826400000 7.8155460000 -38.6143760000
H 3.0235120000 7.2748700000 -37.1381810000
H 1.1876130000 8.7852460000 -37.8757090000
C -0.5366020000 -4.9356510000 -12.6254550000
C -1.7191760000 -5.5308220000 -12.1564160000
C 0.4946150000 -5.7665820000 -13.0933390000
C -1.8673100000 -6.9190100000 -12.1575590000
H -2.5268870000 -4.8990100000 -11.7980780000
C 0.3478660000 -7.1548850000 -13.0904020000
H 1.4171380000 -5.3190560000 -13.4520320000
C -0.8339280000 -7.7354060000 -12.6235420000
H -2.7919630000 -7.3613360000 -11.7966730000
H 1.1590360000 -7.7820270000 -13.4503640000
H -0.9486980000 -8.8158960000 -12.6228480000
C -0.6242890000 -4.9247730000 -21.0447130000
C -1.8272710000 -5.4960080000 -20.5986350000
C 0.3995460000 -5.7762170000 -21.4911950000
C -2.0022760000 -6.8811120000 -20.6008060000
H -2.6294620000 -4.8480040000 -20.2571290000
C 0.2257330000 -7.1614330000 -21.4896960000
H 1.3374220000 -5.3472110000 -21.8323760000
C -0.9760470000 -7.7181660000 -21.0454370000
H -2.9422210000 -7.3048480000 -20.2575250000
H 1.0313840000 -7.8047870000 -21.8330800000
H -1.1118140000 -8.7962210000 -21.0457160000
C -0.6463890000 -4.9220170000 -29.4647290000
C 0.3735940000 -5.7787950000 -29.9099090000
C -1.8531840000 -5.4872560000 -29.0212750000
C 0.1923720000 -7.1630690000 -29.9097500000
H 1.3144620000 -5.3546690000 -30.2490420000
C -2.0355090000 -6.8714400000 -29.0242890000
H -2.6525970000 -4.8351800000 -28.6809540000
C -1.0130650000 -7.7137010000 -29.4677570000
H 0.9951550000 -7.8105110000 -30.2521830000
H -2.9782300000 -7.2903700000 -28.6827090000
H -1.1545510000 -8.7910200000 -29.4688880000
C -0.6668180000 -4.9175200000 -37.8792010000
C 0.3602330000 -5.7799970000 -38.2957740000
C -1.8852510000 -5.4768590000 -37.4613730000
C 0.1744280000 -7.1637290000 -38.2935950000
H 1.3102170000 -5.3606820000 -38.6153240000
C -2.0720650000 -6.8606340000 -37.4608420000
H -2.6899920000 -4.8204020000 -37.1423790000
C -1.0426670000 -7.7083810000 -37.8766570000
H 0.9826400000 -7.8155460000 -38.6143760000
H -3.0235120000 -7.2748700000 -37.1381810000
H -1.1876130000 -8.7852460000 -37.8757090000

H -0.3500560000 -2.6476710000 -42.4463310000
H 0.3500560000 2.6476710000 -42.4463310000

Table S3.11. Optimized coordinates for **3.9**.

Zn 0.0000000000 0.0000000000 29.4630960000
N -0.2183250000 1.4299370000 28.0195090000
C -0.1768040000 1.2312690000 26.6722670000
C 0.0000000000 0.0000000000 25.9872400000
C 0.1768040000 -1.2312690000 26.6722670000
N 0.2183250000 -1.4299370000 28.0195090000
C 0.4088520000 -2.7868790000 28.2100970000
C 0.5071720000 -3.4291790000 29.4623050000
C 0.4150580000 -2.7853870000 30.7164130000
N 0.1931810000 -1.4346280000 30.9064420000
C 0.1919820000 -1.2288420000 32.2542010000
C 0.0000000000 0.0000000000 32.9379390000
C -0.1919820000 1.2288420000 32.2542010000
N -0.1931810000 1.4346280000 30.9064420000
C -0.4150580000 2.7853870000 30.7164130000
C -0.5071720000 3.4291790000 29.4623050000
C -0.4088520000 2.7868790000 28.2100970000
C -0.4749430000 3.4540030000 26.9361470000
C -0.3399450000 2.4823630000 25.9713910000
C -0.3267610000 2.4840630000 24.5358350000
C -0.1524350000 1.2350980000 23.8352540000
N -0.1666700000 1.4380240000 22.4877270000
Zn 0.0000000000 0.0000000000 21.0440830000
N -0.2040990000 1.4323770000 19.6003410000
C -0.1656410000 1.2333470000 18.2532190000
C 0.0000000000 0.0000000000 17.5677190000
C 0.1656410000 -1.2333470000 18.2532190000
N 0.2040990000 -1.4323770000 19.6003410000
C 0.3703670000 -2.7925910000 19.7909820000
C 0.4419890000 -3.4381950000 21.0436710000
C 0.3485690000 -2.7954010000 22.2975800000
N 0.1666700000 -1.4380240000 22.4877270000
C 0.1524350000 -1.2350980000 23.8352540000
C 0.0000000000 0.0000000000 24.5199850000
C 0.3267610000 -2.4840630000 24.5358350000
C 0.3399450000 -2.4823630000 25.9713910000
C 0.4749430000 -3.4540030000 26.9361470000
H 0.6011030000 -4.5163580000 26.7880680000
C 0.4580190000 -3.4566460000 23.5706890000
H 0.6201370000 -4.5141150000 23.7188430000
C 0.4306360000 -3.4602040000 18.5176480000
C 0.3120500000 -2.4862510000 17.5525370000
C 0.2977060000 -2.4879890000 16.1172170000
C 0.1387310000 -1.2370880000 15.4165210000
N 0.1473430000 -1.4403840000 14.0693080000
Zn 0.0000000000 0.0000000000 12.6250440000
N -0.1814720000 1.4363820000 11.1817080000
C -0.1308970000 1.2380180000 9.8349560000
C 0.0000000000 0.0000000000 9.1495860000
C 0.1308970000 -1.2380180000 9.8349560000
N 0.1814720000 -1.4363820000 11.1817080000
C 0.3097570000 -2.8006690000 11.3723150000
C 0.3790540000 -3.4464530000 12.6254230000
C 0.3074050000 -2.8009350000 13.8791620000

C 0.4121830000 -3.4628690000 15.1520800000
H 0.5594150000 -4.5224590000 15.3004620000
C 0.3315820000 -3.4714800000 10.0997340000
C 0.2277190000 -2.4956720000 9.1344610000
C 0.1900130000 -2.4989370000 7.6995620000
C 0.0793540000 -1.2426320000 6.9992750000
N 0.0591550000 -1.4472250000 5.6527670000
Zn 0.0000000000 0.0000000000 4.2079280000
N -0.0805710000 1.4464070000 2.7635360000
C -0.0328820000 1.2448520000 1.4173850000
C 0.0000000000 0.0000000000 0.7323160000
C 0.0328820000 -1.2448520000 1.4173850000
N 0.0805710000 -1.4464070000 2.7635360000
C 0.1122690000 -2.8160870000 2.9545770000
C 0.1594500000 -3.4639710000 4.2081630000
C 0.1471410000 -2.8143960000 5.4619380000
C 0.2406790000 -3.4792930000 6.7342790000
H 0.3370910000 -4.5447550000 6.8823170000
C 0.0682550000 -3.4869970000 1.6825980000
C 0.0259240000 -2.5062970000 0.7172810000
H 0.0636210000 -4.5568870000 1.5350090000
C -0.0259240000 2.5062970000 0.7172810000
C -0.0682550000 3.4869970000 1.6825980000
C -0.1122690000 2.8160870000 2.9545770000
C -0.1594500000 3.4639710000 4.2081630000
C -0.1471410000 2.8143960000 5.4619380000
N -0.0591550000 1.4472250000 5.6527670000
C -0.0793540000 1.2426320000 6.9992750000
C -0.1900130000 2.4989370000 7.6995620000
C -0.2277190000 2.4956720000 9.1344610000
C -0.3315820000 3.4714800000 10.0997340000
C -0.3097570000 2.8006690000 11.3723150000
C -0.3790540000 3.4464530000 12.6254230000
C -0.3074050000 2.8009350000 13.8791620000
N -0.1473430000 1.4403840000 14.0693080000
C -0.1387310000 1.2370880000 15.4165210000
C -0.2977060000 2.4879890000 16.1172170000
C -0.3120500000 2.4862510000 17.5525370000
C -0.4306360000 3.4602040000 18.5176480000
C -0.3703670000 2.7925910000 19.7909820000
C -0.4419890000 3.4381950000 21.0436710000
C -0.3485690000 2.7954010000 22.2975800000
C -0.4580190000 3.4566460000 23.5706890000
H -0.6201370000 4.5141150000 23.7188430000
H -0.5402720000 4.5244150000 18.3696570000
C -0.4121830000 3.4628690000 15.1520800000
H -0.5594150000 4.5224590000 15.3004620000
C 0.0000000000 0.0000000000 16.1017250000
H -0.4074680000 4.5386650000 9.9520260000
C -0.2406790000 3.4792930000 6.7342790000
H -0.3370910000 4.5447550000 6.8823170000
C 0.0000000000 0.0000000000 7.6844850000
H -0.0636210000 4.5568870000 1.5350090000
H 0.4074680000 -4.5386650000 9.9520260000
H 0.5402720000 -4.5244150000 18.3696570000
H -0.6011030000 4.5163580000 26.7880680000
C -0.5671900000 3.4394610000 31.9893060000
C -0.4206190000 2.4692900000 32.9543310000
C -0.4592000000 2.4629760000 34.3898990000
C -0.2429900000 1.2194080000 35.0911520000
N -0.3147660000 1.4129310000 36.4381900000
Zn 0.0000000000 0.0000000000 37.8783530000
N -0.2928680000 1.4175440000 39.3225800000

C -0.2841940000 1.2090090000 40.6712510000
C -0.6108010000 2.4270800000 41.3714170000
C -0.6567600000 2.4158960000 42.8078780000
C -0.3432070000 1.1915090000 43.5108430000
N -0.4333850000 1.3784620000 44.8583180000
Zn 0.0000000000 0.0000000000 46.3084180000
N 0.4333850000 -1.3784620000 44.8583180000
C 0.3432070000 -1.1915090000 43.5108430000
C 0.0000000000 0.0000000000 42.8285400000
C 0.0000000000 0.0000000000 41.3527880000
C 0.2841940000 -1.2090090000 40.6712510000
N 0.2928680000 -1.4175440000 39.3225800000
C 0.6118630000 -2.7473780000 39.1336320000
C 0.7346960000 -3.3886060000 37.8796640000
C 0.5812120000 -2.7566700000 36.6285380000
N 0.3147660000 -1.4129310000 36.4381900000
C 0.2429900000 -1.2194080000 35.0911520000
C 0.0000000000 0.0000000000 34.4075300000
C 0.4592000000 -2.4629760000 34.3898990000
C 0.4206190000 -2.4692900000 32.9543310000
C 0.5671900000 -3.4394610000 31.9893060000
H 0.7652820000 -4.4908780000 32.1368540000
C 0.6622970000 -3.4227940000 35.3536860000
H 0.8431170000 -4.4772620000 35.2056920000
C 0.8226750000 -3.3852720000 40.4075270000
C 0.6108010000 -2.4270800000 41.3714170000
C 0.6567600000 -2.4158960000 42.8078780000
C 0.9373350000 -3.3549020000 43.7691750000
C 0.8034900000 -2.6965210000 45.0471320000
C 0.9977360000 -3.3178470000 46.2936360000
C 0.8209750000 -2.6900560000 47.5501200000
N 0.4306280000 -1.3893230000 47.7525550000
C 0.3800220000 -1.1939730000 49.1133230000
C 0.0000000000 0.0000000000 49.7622210000
C -0.3800220000 1.1939730000 49.1133230000
N -0.4306280000 1.3893230000 47.7525550000
C -0.8209750000 2.6900560000 47.5501200000
C -0.9977360000 3.3178470000 46.2936360000
C -0.8034900000 2.6965210000 45.0471320000
C -0.9373350000 3.3549020000 43.7691750000
H -1.2020960000 4.3916930000 43.6221160000
C -1.0363870000 3.3348660000 48.8251650000
C -0.7527040000 2.4148640000 49.7903980000
H -0.7928930000 2.5513520000 50.8611040000
H -1.3585050000 4.3562670000 48.9650580000
C 0.7527040000 -2.4148640000 49.7903980000
C 1.0363870000 -3.3348660000 48.8251650000
H 1.3585050000 -4.3562670000 48.9650580000
H 0.7928930000 -2.5513520000 50.8611040000
H 1.2020960000 -4.3916930000 43.6221160000
H 1.0994660000 -4.4187470000 40.5553330000
C -0.8226750000 3.3852720000 40.4075270000
C -0.6118630000 2.7473780000 39.1336320000
C -0.7346960000 3.3886060000 37.8796640000
C -0.5812120000 2.7566700000 36.6285380000
C -0.6622970000 3.4227940000 35.3536860000
H -0.8431170000 4.4772620000 35.2056920000
H -1.0994660000 4.4187470000 40.5553330000
H -0.7652820000 4.4908780000 32.1368540000
C 0.0000000000 0.0000000000 51.2612790000
C -1.2060680000 0.0540290000 51.9785600000
C 1.2060680000 -0.0540290000 51.9785600000
C -1.2062930000 0.0531140000 53.3747990000

H -2.1465530000 0.0899970000 51.4358130000
C 1.2062930000 -0.0531140000 53.3747990000
H 2.1465530000 -0.0899970000 51.4358130000
C 0.0000000000 0.0000000000 54.0773150000
H -2.1498610000 0.0905100000 53.9126020000
H 2.1498610000 -0.0905100000 53.9126020000
H 0.0000000000 0.0000000000 55.1638810000
C 1.4209450000 -4.7553450000 46.2925340000
C 0.5495450000 -5.7617110000 46.7402500000
C 2.6982930000 -5.1253730000 45.8410830000
C 0.9441250000 -7.1008780000 46.7358130000
H -0.4441660000 -5.4902210000 47.0854820000
C 3.0940830000 -6.4643900000 45.8387420000
H 3.3841740000 -4.3560900000 45.4975480000
C 2.2180580000 -7.4563610000 46.2857080000
H 0.2539880000 -7.8662020000 47.0806990000
H 4.0882630000 -6.7308170000 45.4900800000
H 2.5255130000 -8.4985250000 46.2831210000
C 1.0547440000 -4.8513030000 37.8815980000
C 0.1318260000 -5.7868350000 38.3777520000
C 2.2842720000 -5.3175030000 37.3876770000
C 0.4292110000 -7.1507910000 38.3775190000
H -0.8256410000 -5.4403200000 38.7561940000
C 2.5831720000 -6.6811820000 37.3913080000
H 3.0099550000 -4.6038690000 37.0080910000
C 1.6562120000 -7.6022130000 37.8852060000
H -0.3000490000 -7.8602160000 38.7593330000
H 3.5420630000 -7.0224420000 37.0105810000
H 1.8882150000 -8.6637220000 37.8865010000
C 0.7312280000 -4.9098830000 29.4635440000
C 1.9377990000 -5.4535660000 28.9931240000
C -0.2611040000 -5.7842820000 29.9362760000
C 2.1468370000 -6.8338920000 28.9968540000
H 2.7162010000 -4.7876420000 28.6317200000
C -0.0534240000 -7.1647950000 29.9360890000
H -1.2013870000 -5.3768930000 30.2967290000
C 1.1515290000 -7.6938810000 29.4672900000
H 3.0891870000 -7.2359670000 28.6346410000
H -0.8352170000 -7.8261740000 30.2997500000
H 1.3137230000 -8.7682740000 29.4686740000
C 0.6318150000 -4.9238140000 21.0439090000
C 1.8344550000 -5.4930940000 20.5944230000
C -0.3893270000 -5.7767080000 21.4937550000
C 2.0117900000 -6.8778800000 20.5967210000
H 2.6345360000 -4.8438760000 20.2503310000
C -0.2132430000 -7.1616260000 21.4920400000
H -1.3268420000 -5.3491160000 21.8376340000
C 0.9881980000 -7.7164750000 21.0445330000
H 2.9514780000 -7.3001690000 20.2509800000
H -1.0168320000 -7.8062050000 21.8379270000
H 1.1257650000 -8.7942990000 21.0447810000
C 0.5373140000 -4.9355500000 12.6249790000
C 1.7197840000 -5.5304300000 12.1553250000
C -0.4935900000 -5.7665620000 13.0933680000
C 1.8681620000 -6.9185790000 12.1565150000
H 2.5271890000 -4.8984780000 11.7965740000
C -0.3466340000 -7.1548360000 13.0902290000
H -1.4159780000 -5.3191710000 13.4525410000
C 0.8350790000 -7.7351320000 12.6228950000
H 2.7927470000 -7.3607540000 11.7952860000
H -1.1575550000 -7.7821170000 13.4504940000
H 0.9500270000 -8.8156000000 12.6221450000
C 0.2260350000 -4.9597460000 4.2079150000

C 1.3576520000 -5.6266940000 3.7103240000
C -0.8413870000 -5.7255800000 4.7049770000
C 1.4211270000 -7.0212540000 3.7124350000
H 2.1928410000 -5.0458850000 3.3294970000
C -0.7796920000 -7.1202160000 4.7022350000
H -1.7252640000 -5.2220790000 5.0859700000
C 0.3522150000 -7.7723830000 4.2072060000
H 2.3076430000 -7.5196810000 3.3296640000
H -1.6180370000 -7.6962020000 5.0846850000
H 0.4009180000 -8.8578550000 4.2069830000
C -0.2260350000 4.9597460000 4.2079150000
C -1.3576520000 5.6266940000 3.7103240000
C 0.8413870000 5.7255800000 4.7049770000
C -1.4211270000 7.0212540000 3.7124350000
H -2.1928410000 5.0458850000 3.3294970000
C 0.7796920000 7.1202160000 4.7022350000
H 1.7252640000 5.2220790000 5.0859700000
C -0.3522150000 7.7723830000 4.2072060000
H -2.3076430000 7.5196810000 3.3296640000
H 1.6180370000 7.6962020000 5.0846850000
H -0.4009180000 8.8578550000 4.2069830000
C -1.4209450000 4.7553450000 46.2925340000
C -0.5495450000 5.7617110000 46.7402500000
C -2.6982930000 5.1253730000 45.8410830000
C -0.9441250000 7.1008780000 46.7358130000
H 0.4441660000 5.4902210000 47.0854820000
C -3.0940830000 6.4643900000 45.8387420000
H -3.3841740000 4.3560900000 45.4975480000
C -2.2180580000 7.4563610000 46.2857080000
H -0.2539880000 7.8662020000 47.0806990000
H -4.0882630000 6.7308170000 45.4900800000
H -2.5255130000 8.4985250000 46.2831210000
C -1.0547440000 4.8513030000 37.8815980000
C -0.1318260000 5.7868350000 38.3777520000
C -2.2842720000 5.3175030000 37.3876770000
C -0.4292110000 7.1507910000 38.3775190000
H 0.8256410000 5.4403200000 38.7561940000
C -2.5831720000 6.6811820000 37.3913080000
H -3.0099550000 4.6038690000 37.0080910000
C -1.6562120000 7.6022130000 37.8852060000
H 0.3000490000 7.8602160000 38.7593330000
H -3.5420630000 7.0224420000 37.0105810000
H -1.8882150000 8.6637220000 37.8865010000
C -0.7312280000 4.9098830000 29.4635440000
C -1.9377990000 5.4535660000 28.9931240000
C 0.2611040000 5.7842820000 29.9362760000
C -2.1468370000 6.8338920000 28.9968540000
H -2.7162010000 4.7876420000 28.6317200000
C 0.0534240000 7.1647950000 29.9360890000
H 1.2013870000 5.3768930000 30.2967290000
C -1.1515290000 7.6938810000 29.4672900000
H -3.0891870000 7.2359670000 28.6346410000
H 0.8352170000 7.8261740000 30.2997500000
H -1.3137230000 8.7682740000 29.4686740000
C -0.6318150000 4.9238140000 21.0439090000
C -1.8344550000 5.4930940000 20.5944230000
C 0.3893270000 5.7767080000 21.4937550000
C -2.0117900000 6.8778800000 20.5967210000
H -2.6345360000 4.8438760000 20.2503310000
C 0.2132430000 7.1616260000 21.4920400000
H 1.3268420000 5.3491160000 21.8376340000
C -0.9881980000 7.7164750000 21.0445330000
H -2.9514780000 7.3001690000 20.2509800000

H 1.0168320000 7.8062050000 21.8379270000
H -1.1257650000 8.7942990000 21.0447810000
C -0.5373140000 4.9355500000 12.6249790000
C -1.7197840000 5.5304300000 12.1553250000
C 0.4935900000 5.7665620000 13.0933680000
C -1.8681620000 6.9185790000 12.1565150000
H -2.5271890000 4.8984780000 11.7965740000
C 0.3466340000 7.1548360000 13.0902290000
H 1.4159780000 5.3191710000 13.4525410000
C -0.8350790000 7.7351320000 12.6228950000
H -2.7927470000 7.3607540000 11.7952860000
H 1.1575550000 7.7821170000 13.4504940000
H -0.9500270000 8.8156000000 12.6221450000
Zn 0.0000000000 0.0000000000 -21.0440830000
N 0.1666700000 1.4380240000 -22.4877270000
C 0.1524350000 1.2350980000 -23.8352540000
C 0.0000000000 0.0000000000 -24.5199850000
C -0.1524350000 -1.2350980000 -23.8352540000
N -0.1666700000 -1.4380240000 -22.4877270000
C -0.3485690000 -2.7954010000 -22.2975800000
C -0.4419890000 -3.4381950000 -21.0436710000
C -0.3703670000 -2.7925910000 -19.7909820000
N -0.2040990000 -1.4323770000 -19.6003410000
C -0.1656410000 -1.2333470000 -18.2532190000
C 0.0000000000 0.0000000000 -17.5677190000
C 0.1656410000 1.2333470000 -18.2532190000
N 0.2040990000 1.4323770000 -19.6003410000
C 0.3703670000 2.7925910000 -19.7909820000
C 0.4419890000 3.4381950000 -21.0436710000
C 0.3485690000 2.7954010000 -22.2975800000
C 0.4580190000 3.4566460000 -23.5706890000
C 0.3267610000 2.4840630000 -24.5358350000
C 0.3399450000 2.4823630000 -25.9713910000
C 0.1768040000 1.2312690000 -26.6722670000
N 0.2183250000 1.4299370000 -28.0195090000
Zn 0.0000000000 0.0000000000 -29.4630960000
N 0.1931810000 1.4346280000 -30.9064420000
C 0.1919820000 1.2288420000 -32.2542010000
C 0.0000000000 0.0000000000 -32.9379390000
C -0.1919820000 -1.2288420000 -32.2542010000
N -0.1931810000 -1.4346280000 -30.9064420000
C -0.4150580000 -2.7853870000 -30.7164130000
C -0.5071720000 -3.4291790000 -29.4623050000
C -0.4088520000 -2.7868790000 -28.2100970000
N -0.2183250000 -1.4299370000 -28.0195090000
C -0.1768040000 -1.2312690000 -26.6722670000
C 0.0000000000 0.0000000000 -25.9872400000
C -0.3399450000 -2.4823630000 -25.9713910000
C -0.3267610000 -2.4840630000 -24.5358350000
C -0.4580190000 -3.4566460000 -23.5706890000
H -0.6201370000 -4.5141150000 -23.7188430000
C -0.4749430000 -3.4540030000 -26.9361470000
H -0.6011030000 -4.5163580000 -26.7880680000
C -0.5671900000 -3.4394610000 -31.9893060000
C -0.4206190000 -2.4692900000 -32.9543310000
C -0.4592000000 -2.4629760000 -34.3898990000
C -0.2429900000 -1.2194080000 -35.0911520000
N -0.3147660000 -1.4129310000 -36.4381900000
Zn 0.0000000000 0.0000000000 -37.8783530000
N 0.2928680000 1.4175440000 -39.3225800000
C 0.2841940000 1.2090090000 -40.6712510000
C 0.0000000000 0.0000000000 -41.3527880000
C -0.2841940000 -1.2090090000 -40.6712510000

N -0.2928680000 -1.4175440000 -39.3225800000
C -0.6118630000 -2.7473780000 -39.1336320000
C -0.7346960000 -3.3886060000 -37.8796640000
C -0.5812120000 -2.7566700000 -36.6285380000
C -0.6622970000 -3.4227940000 -35.3536860000
H -0.8431170000 -4.4772620000 -35.2056920000
C -0.8226750000 -3.3852720000 -40.4075270000
C -0.6108010000 -2.4270800000 -41.3714170000
C -0.6567600000 -2.4158960000 -42.8078780000
C -0.3432070000 -1.1915090000 -43.5108430000
N -0.4333850000 -1.3784620000 -44.8583180000
Zn 0.0000000000 0.0000000000 -46.3084180000
N 0.4306280000 1.3893230000 -47.7525550000
C 0.3800220000 1.1939730000 -49.1133230000
C 0.0000000000 0.0000000000 -49.7622210000
C -0.3800220000 -1.1939730000 -49.1133230000
N -0.4306280000 -1.3893230000 -47.7525550000
C -0.8209750000 -2.6900560000 -47.5501200000
C -0.9977360000 -3.3178470000 -46.2936360000
C -0.8034900000 -2.6965210000 -45.0471320000
C -0.9373350000 -3.3549020000 -43.7691750000
H -1.2020960000 -4.3916930000 -43.6221160000
C -1.0363870000 -3.3348660000 -48.8251650000
C -0.7527040000 -2.4148640000 -49.7903980000
H -0.7928930000 -2.5513520000 -50.8611040000
H -1.3585050000 -4.3562670000 -48.9650580000
C 0.7527040000 2.4148640000 -49.7903980000
C 1.0363870000 3.3348660000 -48.8251650000
C 0.8209750000 2.6900560000 -47.5501200000
C 0.9977360000 3.3178470000 -46.2936360000
C 0.8034900000 2.6965210000 -45.0471320000
N 0.4333850000 1.3784620000 -44.8583180000
C 0.3432070000 1.1915090000 -43.5108430000
C 0.6567600000 2.4158960000 -42.8078780000
C 0.6108010000 2.4270800000 -41.3714170000
C 0.8226750000 3.3852720000 -40.4075270000
C 0.6118630000 2.7473780000 -39.1336320000
C 0.7346960000 3.3886060000 -37.8796640000
C 0.5812120000 2.7566700000 -36.6285380000
N 0.3147660000 1.4129310000 -36.4381900000
C 0.2429900000 1.2194080000 -35.0911520000
C 0.4592000000 2.4629760000 -34.3898990000
C 0.4206190000 2.4692900000 -32.9543310000
C 0.5671900000 3.4394610000 -31.9893060000
C 0.4150580000 2.7853870000 -30.7164130000
C 0.5071720000 3.4291790000 -29.4623050000
C 0.4088520000 2.7868790000 -28.2100970000
C 0.4749430000 3.4540030000 -26.9361470000
H 0.6011030000 4.5163580000 -26.7880680000
H 0.7652820000 4.4908780000 -32.1368540000
C 0.6622970000 3.4227940000 -35.3536860000
H 0.8431170000 4.4772620000 -35.2056920000
C 0.0000000000 0.0000000000 -34.4075300000
H 1.0994660000 4.4187470000 -40.5553330000
C 0.9373350000 3.3549020000 -43.7691750000
H 1.2020960000 4.3916930000 -43.6221160000
C 0.0000000000 0.0000000000 -42.8285400000
H 1.3585050000 4.3562670000 -48.9650580000
H 0.7928930000 2.5513520000 -50.8611040000
H -1.0994660000 -4.4187470000 -40.5553330000
H -0.7652820000 -4.4908780000 -32.1368540000
H 0.6201370000 4.5141150000 -23.7188430000
C 0.4306360000 3.4602040000 -18.5176480000

C 0.3120500000 2.4862510000 -17.5525370000
C 0.2977060000 2.4879890000 -16.1172170000
C 0.1387310000 1.2370880000 -15.4165210000
N 0.1473430000 1.4403840000 -14.0693080000
Zn 0.0000000000 0.0000000000 -12.6250440000
N 0.1814720000 1.4363820000 -11.1817080000
C 0.1308970000 1.2380180000 -9.8349560000
C 0.2277190000 2.4956720000 -9.1344610000
C 0.1900130000 2.4989370000 -7.6995620000
C 0.0793540000 1.2426320000 -6.9992750000
N 0.0591550000 1.4472250000 -5.6527670000
Zn 0.0000000000 0.0000000000 -4.2079280000
N -0.0591550000 -1.4472250000 -5.6527670000
C -0.0793540000 -1.2426320000 -6.9992750000
C 0.0000000000 0.0000000000 -7.6844850000
C 0.0000000000 0.0000000000 -9.1495860000
C -0.1308970000 -1.2380180000 -9.8349560000
N -0.1814720000 -1.4363820000 -11.1817080000
C -0.3097570000 -2.8006690000 -11.3723150000
C -0.3790540000 -3.4464530000 -12.6254230000
C -0.3074050000 -2.8009350000 -13.8791620000
N -0.1473430000 -1.4403840000 -14.0693080000
C -0.1387310000 -1.2370880000 -15.4165210000
C 0.0000000000 0.0000000000 -16.1017250000
C -0.2977060000 -2.4879890000 -16.1172170000
C -0.3120500000 -2.4862510000 -17.5525370000
C -0.4306360000 -3.4602040000 -18.5176480000
H -0.5402720000 -4.5244150000 -18.3696570000
C -0.4121830000 -3.4628690000 -15.1520800000
H -0.5594150000 -4.5224590000 -15.3004620000
C -0.3315820000 -3.4714800000 -10.0997340000
C -0.2277190000 -2.4956720000 -9.1344610000
C -0.1900130000 -2.4989370000 -7.6995620000
C -0.2406790000 -3.4792930000 -6.7342790000
C -0.1471410000 -2.8143960000 -5.4619380000
C -0.1594500000 -3.4639710000 -4.2081630000
C -0.1122690000 -2.8160870000 -2.9545770000
N -0.0805710000 -1.4464070000 -2.7635360000
C -0.0328820000 -1.2448520000 -1.4173850000
C 0.0000000000 0.0000000000 -0.7323160000
C 0.0328820000 1.2448520000 -1.4173850000
N 0.0805710000 1.4464070000 -2.7635360000
C 0.1122690000 2.8160870000 -2.9545770000
C 0.1594500000 3.4639710000 -4.2081630000
C 0.1471410000 2.8143960000 -5.4619380000
C 0.2406790000 3.4792930000 -6.7342790000
H 0.3370910000 4.5447550000 -6.8823170000
C 0.0682550000 3.4869970000 -1.6825980000
C 0.0259240000 2.5062970000 -0.7172810000
H 0.0636210000 4.5568870000 -1.5350090000
C -0.0259240000 -2.5062970000 -0.7172810000
C -0.0682550000 -3.4869970000 -1.6825980000
H -0.0636210000 -4.5568870000 -1.5350090000
H -0.3370910000 -4.5447550000 -6.8823170000
H -0.4074680000 -4.5386650000 -9.9520260000
C 0.3315820000 3.4714800000 -10.0997340000
C 0.3097570000 2.8006690000 -11.3723150000
C 0.3790540000 3.4464530000 -12.6254230000
C 0.3074050000 2.8009350000 -13.8791620000
C 0.4121830000 3.4628690000 -15.1520800000
H 0.5594150000 4.5224590000 -15.3004620000
H 0.4074680000 4.5386650000 -9.9520260000
H 0.5402720000 4.5244150000 -18.3696570000

C 0.0000000000 0.0000000000 -51.2612790000
C 1.2060680000 0.0540290000 -51.9785600000
C -1.2060680000 -0.0540290000 -51.9785600000
C 1.2062930000 0.0531140000 -53.3747990000
H 2.1465530000 0.0899970000 -51.4358130000
C -1.2062930000 -0.0531140000 -53.3747990000
H -2.1465530000 -0.0899970000 -51.4358130000
C 0.0000000000 0.0000000000 -54.0773150000
H 2.1498610000 0.0905100000 -53.9126020000
H -2.1498610000 -0.0905100000 -53.9126020000
H 0.0000000000 0.0000000000 -55.1638810000
C -0.2260350000 -4.9597460000 -4.2079150000
C -1.3576520000 -5.6266940000 -3.7103240000
C 0.8413870000 -5.7255800000 -4.7049770000
C -1.4211270000 -7.0212540000 -3.7124350000
H -2.1928410000 -5.0458850000 -3.3294970000
C 0.7796920000 -7.1202160000 -4.7022350000
H 1.7252640000 -5.2220790000 -5.0859700000
C -0.3522150000 -7.7723830000 -4.2072060000
H -2.3076430000 -7.5196810000 -3.3296640000
H 1.6180370000 -7.6962020000 -5.0846850000
H -0.4009180000 -8.8578550000 -4.2069830000
C -0.5373140000 -4.9355500000 -12.6249790000
C -1.7197840000 -5.5304300000 -12.1553250000
C 0.4935900000 -5.7665620000 -13.0933680000
C -1.8681620000 -6.9185790000 -12.1565150000
H -2.5271890000 -4.8984780000 -11.7965740000
C 0.3466340000 -7.1548360000 -13.0902290000
H 1.4159780000 -5.3191710000 -13.4525410000
C -0.8350790000 -7.7351320000 -12.6228950000
H -2.7927470000 -7.3607540000 -11.7952860000
H 1.1575550000 -7.7821170000 -13.4504940000
H -0.9500270000 -8.8156000000 -12.6221450000
C -0.6318150000 -4.9238140000 -21.0439090000
C 0.3893270000 -5.7767080000 -21.4937550000
C -1.8344550000 -5.4930940000 -20.5944230000
C 0.2132430000 -7.1616260000 -21.4920400000
H 1.3268420000 -5.3491160000 -21.8376340000
C -2.0117900000 -6.8778800000 -20.5967210000
H -2.6345360000 -4.8438760000 -20.2503310000
C -0.9881980000 -7.7164750000 -21.0445330000
H 1.0168320000 -7.8062050000 -21.8379270000
H -2.9514780000 -7.3001690000 -20.2509800000
H -1.1257650000 -8.7942990000 -21.0447810000
C -0.7312280000 -4.9098830000 -29.4635440000
C 0.2611040000 -5.7842820000 -29.9362760000
C -1.9377990000 -5.4535660000 -28.9931240000
C 0.0534240000 -7.1647950000 -29.9360890000
H 1.2013870000 -5.3768930000 -30.2967290000
C -2.1468370000 -6.8338920000 -28.9968540000
H -2.7162010000 -4.7876420000 -28.6317200000
C -1.1515290000 -7.6938810000 -29.4672900000
H 0.8352170000 -7.8261740000 -30.2997500000
H -3.0891870000 -7.2359670000 -28.6346410000
H -1.3137230000 -8.7682740000 -29.4686740000
C -1.0547440000 -4.8513030000 -37.8815980000
C -0.1318260000 -5.7868350000 -38.3777520000
C -2.2842720000 -5.3175030000 -37.3876770000
C -0.4292110000 -7.1507910000 -38.3775190000
H 0.8256410000 -5.4403200000 -38.7561940000
C -2.5831720000 -6.6811820000 -37.3913080000
H -3.0099550000 -4.6038690000 -37.0080910000
C -1.6562120000 -7.6022130000 -37.8852060000

H 0.3000490000 -7.8602160000 -38.7593330000
H -3.5420630000 -7.0224420000 -37.0105810000
H -1.8882150000 -8.6637220000 -37.8865010000
C -1.4209450000 -4.7553450000 -46.2925340000
C -0.5495450000 -5.7617110000 -46.7402500000
C -2.6982930000 -5.1253730000 -45.8410830000
C -0.9441250000 -7.1008780000 -46.7358130000
H 0.4441660000 -5.4902210000 -47.0854820000
C -3.0940830000 -6.4643900000 -45.8387420000
H -3.3841740000 -4.3560900000 -45.4975480000
C -2.2180580000 -7.4563610000 -46.2857080000
H -0.2539880000 -7.8662020000 -47.0806990000
H -4.0882630000 -6.7308170000 -45.4900800000
H -2.5255130000 -8.4985250000 -46.2831210000
C 1.4209450000 4.7553450000 -46.2925340000
C 0.5495450000 5.7617110000 -46.7402500000
C 2.6982930000 5.1253730000 -45.8410830000
C 0.9441250000 7.1008780000 -46.7358130000
H -0.4441660000 5.4902210000 -47.0854820000
C 3.0940830000 6.4643900000 -45.8387420000
H 3.3841740000 4.3560900000 -45.4975480000
C 2.2180580000 7.4563610000 -46.2857080000
H 0.2539880000 7.8662020000 -47.0806990000
H 4.0882630000 6.7308170000 -45.4900800000
H 2.5255130000 8.4985250000 -46.2831210000
C 0.2260350000 4.9597460000 -4.2079150000
C 1.3576520000 5.6266940000 -3.7103240000
C -0.8413870000 5.7255800000 -4.7049770000
C 1.4211270000 7.0212540000 -3.7124350000
H 2.1928410000 5.0458850000 -3.3294970000
C -0.7796920000 7.1202160000 -4.7022350000
H -1.7252640000 5.2220790000 -5.0859700000
C 0.3522150000 7.7723830000 -4.2072060000
H 2.3076430000 7.5196810000 -3.3296640000
H -1.6180370000 7.6962020000 -5.0846850000
H 0.4009180000 8.8578550000 -4.2069830000
C 0.5373140000 4.9355500000 -12.6249790000
C 1.7197840000 5.5304300000 -12.1553250000
C -0.4935900000 5.7665620000 -13.0933680000
C 1.8681620000 6.9185790000 -12.1565150000
H 2.5271890000 4.8984780000 -11.7965740000
C -0.3466340000 7.1548360000 -13.0902290000
H -1.4159780000 5.3191710000 -13.4525410000
C 0.8350790000 7.7351320000 -12.6228950000
H 2.7927470000 7.3607540000 -11.7952860000
H -1.1575550000 7.7821170000 -13.4504940000
H 0.9500270000 8.8156000000 -12.6221450000
C 0.6318150000 4.9238140000 -21.0439090000
C -0.3893270000 5.7767080000 -21.4937550000
C 1.8344550000 5.4930940000 -20.5944230000
C -0.2132430000 7.1616260000 -21.4920400000
H -1.3268420000 5.3491160000 -21.8376340000
C 2.0117900000 6.8778800000 -20.5967210000
H 2.6345360000 4.8438760000 -20.2503310000
C 0.9881980000 7.7164750000 -21.0445330000
H -1.0168320000 7.8062050000 -21.8379270000
H 2.9514780000 7.3001690000 -20.2509800000
H 1.1257650000 8.7942990000 -21.0447810000
C 0.7312280000 4.9098830000 -29.4635440000
C -0.2611040000 5.7842820000 -29.9362760000
C 1.9377990000 5.4535660000 -28.9931240000
C -0.0534240000 7.1647950000 -29.9360890000
H -1.2013870000 5.3768930000 -30.2967290000

```
C 2.1468370000 6.8338920000 -28.9968540000
H 2.7162010000 4.7876420000 -28.6317200000
C 1.1515290000 7.6938810000 -29.4672900000
H -0.8352170000 7.8261740000 -30.2997500000
H 3.0891870000 7.2359670000 -28.6346410000
H 1.3137230000 8.7682740000 -29.4686740000
C 1.0547440000 4.8513030000 -37.8815980000
C 0.1318260000 5.7868350000 -38.3777520000
C 2.2842720000 5.3175030000 -37.3876770000
C 0.4292110000 7.1507910000 -38.3775190000
H -0.8256410000 5.4403200000 -38.7561940000
C 2.5831720000 6.6811820000 -37.3913080000
H 3.0099550000 4.6038690000 -37.0080910000
C 1.6562120000 7.6022130000 -37.8852060000
H -0.3000490000 7.8602160000 -38.7593330000
H 3.5420630000 7.0224420000 -37.0105810000
H 1.8882150000 8.6637220000 -37.8865010000
```

Table S3.12. TDDFT-predicted band excitation data for **1.1**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	18324	546	0.04	63.5% HOMO => L+1, 35.9% H-1 => LUMO
1	18324	546	0.04	63.5% HOMO => LUMO, 35.9% H-1 => L+1
2	24205	413	1.91	63.7% H-1 => LUMO, 35.9% HOMO => L+1
3	24205	413	1.91	63.7% H-1 => L+1, 35.9% HOMO => LUMO
4	27337	366	0.00	99.6% H-2 => L+1
5	27337	366	0.00	99.6% H-2 => LUMO
6	29230	342	0.00	47.9% H-4 => L+1, 47.9% H-5 => LUMO
7	29586	338	0.00	46.8% H-4 => L+1, 46.8% H-5 => LUMO, 2.02% H-6 => L+1, 2.02% H-7 => LUMO
8	29907	334	0.04	94.9% H-3 => L+1
9	29907	334	0.04	94.9% H-3 => LUMO
10	30595	327	0.00	47.1% H-4 => LUMO, 47.1% H-5 => L+1, 2.02% H-6 => LUMO, 2.02% H-7 => L+1
11	30960	323	0.00	48.9% H-4 => LUMO, 48.9% H-5 => L+1
12	31244	320	0.00	88.8% HOMO => L+2, 3.42% H-6 => L+1, 3.42% H-7 => LUMO
13	31923	313	0.00	47.7% H-6 => LUMO, 47.7% H-7 => L+1
14	31944	313	0.00	40.7% H-6 => L+1, 40.7% H-7 => LUMO, 6.86% HOMO => L+2, 2.82% H-10 => LUMO, 2.82% H-11 => L+1
15	32090	312	0.00	48.6% H-6 => L+1, 48.6% H-7 => LUMO
16	32327	309	0.03	56.1% H-9 => L+1, 39.0% H-8 => LUMO
17	32327	309	0.03	56.1% H-9 => LUMO, 39.0% H-8 => L+1
18	32373	309	0.00	40.6% H-6 => LUMO, 40.6% H-7 => L+1, 14.0% H-1 => L+2, 2.15% H-4 => LUMO, 2.15% H-5 => L+1
19	32844	304	0.01	53.5% H-8 => LUMO, 27.9% H-9 => L+1, 16.0% H-14 => L+1
20	32844	304	0.01	53.5% H-8 => L+1, 27.9% H-9 => LUMO, 16.0% H-14 => LUMO
21	33340	300	0.00	34.1% H-10 => L+1, 34.1% H-11 => LUMO, 22.8% H-1 => L+2, 2.85% H-6 => LUMO, 2.85% H-7 => L+1
22	33375	300	0.07	43.5% H-14 => L+1, 22.2% H-12 => LUMO, 18.1% H-13 => L+1, 9.34% H-9 => L+1, 4.69% H-8 => LUMO
23	33375	300	0.07	43.5% H-14 => LUMO, 22.2% H-12 => L+1, 18.1% H-13 => LUMO, 9.34% H-9 => LUMO, 4.69% H-8 => L+1
24	33460	299	0.00	48.8% H-10 => LUMO, 48.8% H-11 => L+1
25	33678	297	0.00	57.6% H-1 => L+2, 15.1% H-10 => L+1, 15.1% H-11 => LUMO, 4.18% H-6 => LUMO, 4.18% H-7 => L+1
26	33682	297	0.15	35.6% H-14 => L+1, 31.3% H-13 => L+1, 26.3% H-12 => LUMO, 3.14% H-9 => L+1

27	33682	297	0.15	35.6% H-14 => LUMO, 31.3% H-13 => LUMO, 26.3% H-12 => L+1, 3.14% H-9 => LUMO
28	33945	295	0.00	46.7% H-10 => LUMO, 46.7% H-11 => L+1, 2.86% H-6 => L+1, 2.86% H-7 => LUMO
29	33951	295	0.00	48.5% H-10 => L+1, 48.5% H-11 => LUMO
30	34100	293	0.00	49.8% H-12 => LUMO, 48.1% H-13 => L+1
31	34100	293	0.00	49.8% H-12 => L+1, 48.1% H-13 => LUMO
32	34787	287	0.00	98.0% HOMO => L+3
33	34981	286	0.03	97.1% HOMO => L+5
34	34981	286	0.03	97.1% HOMO => L+4
35	35480	282	0.00	97.7% HOMO => L+6
36	35728	280	0.00	98.7% HOMO => L+8
37	35751	280	0.00	98.0% HOMO => L+7
38	36049	277	0.01	97.6% HOMO => L+9
39	36049	277	0.01	97.6% HOMO => L+10
40	36891	271	0.00	98.4% H-1 => L+3
41	37011	270	0.02	98.0% H-1 => L+4
42	37011	270	0.02	98.0% H-1 => L+5
43	37445	267	0.00	97.8% H-1 => L+6
44	37587	266	0.00	48.6% H-15 => LUMO, 48.6% H-16 => L+1
45	37765	265	0.00	99.5% H-1 => L+7
46	37841	264	0.00	94.9% H-1 => L+8, 2.04% H-15 => L+1, 2.04% H-16 => LUMO
47	38095	263	0.00	97.8% H-1 => L+10
48	38095	263	0.00	97.8% H-1 => L+9
49	38503	260	0.00	47.1% H-15 => L+1, 47.1% H-16 => LUMO, 4.18% H-1 => L+8
50	39978	250	0.00	45.9% H-15 => L+1, 45.9% H-16 => LUMO, 3.50% HOMO => L+12, 2.32% H-1 => L+2
51	40168	249	0.00	86.3% H-2 => L+2, 5.92% H-18 => L+1, 5.92% H-19 => LUMO
52	40859	245	0.00	44.4% H-15 => LUMO, 44.4% H-16 => L+1, 3.20% H-1 => L+12
53	42855	233	0.00	96.4% H-3 => L+2
54	42933	233	0.06	96.8% H-4 => L+2
55	42933	233	0.06	96.8% H-5 => L+2
56	43706	229	0.00	96.2% HOMO => L+11
57	44194	226	0.00	9.02% H-8 => L+10, 8.81% H-12 => L+4, 8.30% H-7 => L+7, 8.02% H-6 => L+8, 7.66% H-11 => L+3, 7.60% H-10 => L+6, 7.49% H-13 => L+5, 6.98% H-9 => L+9, 6.20% H-6 => L+2, 4.41% H-11 => L+2, 3.43% H-3 => L+5, 3.18% H-4 => L+8, 3.04% H-5 => L+7
58	44194	226	0.00	9.02% H-8 => L+9, 8.81% H-12 => L+5, 8.30% H-6 => L+7, 8.02% H-7 => L+8, 7.66% H-10 => L+3, 7.60% H-11 => L+6, 7.49% H-13 => L+4, 6.98% H-9 => L+10, 6.20% H-7 => L+2, 4.41% H-10 =>

				L+2, 3.43% H-3 => L+4, 3.18% H-5 => L+8, 3.04% H-4 => L+7
59	44221	226	0.00	11.5% H-8 => L+8, 9.57% H-12 => L+3, 9.00% H-9 => L+7, 8.13% H-13 => L+6, 6.67% H-6 => L+4, 6.67% H-7 => L+5, 5.58% H-12 => L+2, 5.55% H-10 => L+5, 5.55% H-11 => L+4, 4.46% H-6 => L+10, 4.46% H-7 => L+9, 3.72% H-10 => L+9, 3.72% H-11 => L+10, 3.11% H-4 => L+10, 3.11% H-5 => L+9, 3.02% H-3 => L+6
60	44272	226	0.00	11.6% H-8 => L+7, 10.4% H-10 => L+4, 10.4% H-11 => L+5, 9.73% H-12 => L+6, 9.63% H-6 => L+9, 9.63% H-7 => L+10, 8.99% H-9 => L+8, 8.41% H-13 => L+3, 5.62% H-13 => L+2, 3.98% H-3 => L+3
61	44527	225	0.00	48.1% H-18 => L+1, 48.1% H-19 => LUMO
62	44792	223	0.00	48.1% H-18 => LUMO, 48.1% H-19 => L+1, 2.33% H-9 => L+2
63	44875	223	0.00	47.0% H-18 => LUMO, 47.0% H-19 => L+1, 3.15% HOMO => L+11
64	44949	222	0.03	87.5% H-6 => L+2, 2.63% H-11 => L+2
65	44949	222	0.03	87.5% H-7 => L+2, 2.63% H-10 => L+2
66	45158	221	0.00	40.8% H-18 => L+1, 40.8% H-19 => LUMO, 12.1% H-2 => L+2, 4.95% H-8 => L+2
67	45374	220	0.00	90.0% H-9 => L+2, 4.32% H-14 => L+2
68	45524	220	0.00	92.2% H-8 => L+2, 2.12% H-18 => L+1, 2.12% H-19 => LUMO
69	45901	218	0.00	99.7% H-1 => L+11
70	46273	216	0.00	72.7% HOMO => L+12, 12.2% H-12 => L+2, 4.89% H-2 => L+11, 2.58% H-3 => L+6
71	46294	216	0.00	82.0% H-14 => L+2, 4.54% H-9 => L+2, 3.94% H-1 => L+12, 2.27% H-4 => L+5, 2.27% H-5 => L+4
72	46427	215	0.07	90.9% H-17 => LUMO
73	46427	215	0.07	90.9% H-17 => L+1
74	46516	215	0.01	81.0% H-11 => L+2, 5.84% H-3 => L+5, 3.86% H-4 => L+3
75	46516	215	0.01	81.0% H-10 => L+2, 5.84% H-3 => L+4, 3.86% H-5 => L+3
76	46566	215	0.00	50.1% H-13 => L+2, 28.2% H-3 => L+3, 8.79% H-4 => L+5, 8.79% H-5 => L+4
77	46685	214	0.00	97.7% H-2 => L+3
78	46743	214	0.00	75.4% H-12 => L+2, 13.7% HOMO => L+12
79	46805	214	0.06	39.0% H-3 => L+5, 33.1% H-4 => L+3, 8.00% H-11 => L+2, 5.39% H-5 => L+6, 2.90% H-13 => L+5, 2.70% H-11 => L+3
80	46805	214	0.06	39.0% H-3 => L+4, 33.1% H-5 => L+3, 8.00% H-10 => L+2, 5.39% H-4 => L+6, 2.90% H-13 => L+4, 2.70% H-10 => L+3

81	46845	213	0.00	41.7% H-13 => L+2, 24.9% H-3 => L+3, 7.82% H-4 => L+5, 7.82% H-5 => L+4, 5.43% H-13 => L+3, 2.05% H-10 => L+4, 2.05% H-11 => L+5
82	46883	213	0.01	97.0% H-2 => L+4
83	46883	213	0.01	97.0% H-2 => L+5
84	46979	213	0.00	35.6% H-3 => L+6, 24.7% H-4 => L+4, 24.7% H-5 => L+5, 4.31% H-12 => L+2, 2.53% H-13 => L+6
85	47287	211	0.00	31.1% H-4 => L+5, 31.1% H-5 => L+4, 15.7% H-3 => L+8, 5.57% H-14 => L+2, 5.02% H-14 => L+3, 3.16% H-1 => L+12
86	47302	211	0.00	35.7% H-4 => L+4, 35.7% H-5 => L+5, 18.0% H-3 => L+7, 4.07% H-14 => L+6
87	47335	211	0.00	98.0% H-2 => L+6
88	47432	211	0.03	33.9% H-4 => L+3, 31.2% H-5 => L+6, 10.7% H-3 => L+5, 6.13% H-14 => L+5, 4.40% H-3 => L+9, 3.87% H-5 => L+7, 2.71% H-4 => L+8
89	47432	211	0.03	33.9% H-5 => L+3, 31.2% H-4 => L+6, 10.7% H-3 => L+4, 6.13% H-14 => L+4, 4.40% H-3 => L+10, 3.87% H-4 => L+7, 2.71% H-5 => L+8
90	47552	210	0.05	40.1% H-3 => L+9, 22.4% H-4 => L+8, 14.6% H-5 => L+7, 13.2% H-5 => L+6
91	47552	210	0.05	40.1% H-3 => L+10, 22.4% H-5 => L+8, 14.6% H-4 => L+7, 13.2% H-4 => L+6
92	47565	210	0.00	41.2% H-3 => L+8, 18.2% H-4 => L+9, 18.2% H-5 => L+10, 6.65% H-4 => L+5, 6.65% H-5 => L+4, 3.52% H-14 => L+3
93	47642	210	0.00	99.3% H-2 => L+8
94	47652	210	0.00	99.1% H-2 => L+7
95	47663	210	0.00	41.3% H-3 => L+7, 17.8% H-4 => L+10, 17.8% H-5 => L+9, 6.04% H-4 => L+4, 6.04% H-5 => L+5, 2.87% H-14 => L+6
96	47892	209	0.00	98.4% H-2 => L+10
97	47892	209	0.00	98.4% H-2 => L+9
98	48129	208	0.01	42.2% H-5 => L+7, 35.3% H-4 => L+8, 5.46% H-14 => L+9, 4.27% H-7 => L+7, 4.12% H-9 => L+9, 4.07% H-6 => L+8
99	48129	208	0.01	42.2% H-4 => L+7, 35.3% H-5 => L+8, 5.46% H-14 => L+10, 4.27% H-6 => L+7, 4.12% H-9 => L+10, 4.07% H-7 => L+8
100	48169	208	0.00	25.7% H-4 => L+9, 25.7% H-5 => L+10, 10.8% H-4 => L+5, 10.8% H-5 => L+4, 7.17% H-14 => L+8, 7.13% H-3 => L+3, 4.71% H-9 => L+8, 2.95% H-6 => L+9, 2.95% H-7 => L+10
101	48292	207	0.00	29.5% H-4 => L+10, 29.5% H-5 => L+9, 6.89% H-14 => L+7, 5.87% H-4 => L+4, 5.87% H-5 => L+5, 5.33% H-9 => L+7, 5.13% H-3 => L+6, 3.35% H-6 => L+10, 3.35% H-7 => L+9
102	48699	205	0.00	56.5% H-1 => L+12, 8.58% H-6 => L+5, 8.58% H-7 => L+4, 6.38% H-9 => L+3, 3.43% H-8 => L+6, 2.08% H-4 => L+5, 2.08% H-5 => L+4

103	48825	205	0.00	31.2% H-3 => L+3, 19.5% H-4 => L+5, 19.5% H-5 => L+4, 12.7% H-4 => L+9, 12.7% H-5 => L+10
104	48909	204	0.00	34.8% H-5 => L+6, 32.8% H-3 => L+5, 20.5% H-4 => L+3, 2.87% H-4 => L+8, 2.02% H-3 => L+9
105	48909	204	0.00	34.8% H-4 => L+6, 32.8% H-3 => L+4, 20.5% H-5 => L+3, 2.87% H-5 => L+8, 2.02% H-3 => L+10
106	49079	204	0.00	44.9% H-3 => L+6, 16.9% H-4 => L+4, 16.9% H-5 => L+5, 8.76% H-4 => L+10, 8.76% H-5 => L+9
107	49403	202	0.00	25.5% H-3 => L+9, 15.5% H-4 => L+8, 14.9% H-5 => L+7, 11.7% H-6 => L+3, 4.98% H-7 => L+6, 4.14% H-5 => L+6, 4.14% H-9 => L+5, 3.84% H-8 => L+4, 2.16% H-6 => L+8, 2.13% H-7 => L+7, 2.13% H-11 => L+8, 2.08% H-10 => L+7
108	49403	202	0.00	25.5% H-3 => L+10, 15.5% H-5 => L+8, 14.9% H-4 => L+7, 11.7% H-7 => L+3, 4.98% H-6 => L+6, 4.14% H-4 => L+6, 4.14% H-9 => L+4, 3.84% H-8 => L+5, 2.16% H-7 => L+8, 2.13% H-6 => L+7, 2.13% H-10 => L+8, 2.08% H-11 => L+7
109	49468	202	0.00	33.7% H-3 => L+8, 24.8% H-4 => L+9, 24.8% H-5 => L+10, 5.61% H-1 => L+12, 2.39% H-4 => L+5, 2.39% H-5 => L+4
110	49481	202	0.00	32.5% H-3 => L+7, 28.9% H-4 => L+10, 28.9% H-5 => L+9
111	49564	202	0.05	23.4% H-6 => L+3, 19.0% H-3 => L+9, 10.0% H-5 => L+7, 9.49% H-4 => L+8, 5.00% H-9 => L+5, 3.72% H-8 => L+4, 3.28% H-7 => L+6, 2.83% H-13 => L+9, 2.82% H-3 => L+5, 2.71% H-10 => L+7, 2.58% H-12 => L+10, 2.58% H-11 => L+8, 2.27% H-16 => L+2
112	49564	202	0.05	23.4% H-7 => L+3, 19.0% H-3 => L+10, 10.0% H-4 => L+7, 9.49% H-5 => L+8, 5.00% H-9 => L+4, 3.72% H-8 => L+5, 3.28% H-6 => L+6, 2.83% H-13 => L+10, 2.82% H-3 => L+4, 2.71% H-11 => L+7, 2.58% H-12 => L+9, 2.58% H-10 => L+8, 2.27% H-15 => L+2
113	49664	201	0.00	15.4% H-6 => L+4, 15.4% H-7 => L+5, 12.7% H-8 => L+3, 7.38% H-12 => L+8, 7.22% H-13 => L+7, 6.16% H-9 => L+6, 4.72% H-6 => L+10, 4.72% H-7 => L+9, 3.86% H-10 => L+9, 3.86% H-11 => L+10, 3.54% H-3 => L+7, 2.98% H-10 => L+5, 2.98% H-11 => L+4, 2.14% H-4 => L+4, 2.14% H-5 => L+5, 2.11% H-14 => L+6
114	49909	200	0.00	19.9% H-1 => L+12, 16.1% H-6 => L+5, 16.1% H-7 => L+4, 7.28% H-9 => L+3, 6.16% H-12 => L+7, 5.72% H-13 => L+8, 3.77% H-3 => L+8, 3.51% H-10 => L+10, 3.51% H-11 => L+9, 3.44% H-4 => L+9, 3.44% H-5 => L+10
115	50096	200	0.01	80.3% H-20 => L+1, 11.0% HOMO => L+14
116	50096	200	0.01	80.3% H-20 => LUMO, 11.0% HOMO => L+13
117	50246	199	0.08	80.0% HOMO => L+14, 12.3% H-20 => L+1

118	50246	199	0.08	80.0% HOMO => L+13, 12.3% H-20 => LUMO
119	50310	199	0.01	43.1% H-6 => L+5, 43.1% H-7 => L+4, 3.40% H-3 => L+3, 2.35% H-6 => L+9, 2.35% H-7 => L+10
120	50383	198	0.00	38.8% H-6 => L+4, 38.8% H-7 => L+5, 5.50% H-3 => L+6, 3.94% H-6 => L+10, 3.94% H-7 => L+9, 2.23% H-10 => L+5, 2.23% H-11 => L+4
121	50428	198	0.00	40.1% H-6 => L+3, 37.0% H-7 => L+6, 3.87% H-9 => L+5, 2.86% H-10 => L+6, 2.62% H-8 => L+4, 2.26% H-3 => L+5
122	50428	198	0.00	40.1% H-7 => L+3, 37.0% H-6 => L+6, 3.87% H-9 => L+4, 2.86% H-11 => L+6, 2.62% H-8 => L+5, 2.26% H-3 => L+4
123	50784	197	0.00	40.4% H-8 => L+3, 15.8% H-6 => L+4, 15.8% H-7 => L+5, 6.10% H-6 => L+10, 6.10% H-7 => L+9, 4.62% H-14 => L+6
124	50786	197	0.00	61.4% H-9 => L+3, 9.10% H-6 => L+5, 9.10% H-7 => L+4, 8.26% H-8 => L+6, 4.38% H-14 => L+3
125	50808	197	0.01	25.6% H-7 => L+7, 25.3% H-14 => L+5, 24.6% H-6 => L+8, 6.36% H-8 => L+4, 3.46% H-5 => L+6, 2.24% H-7 => L+6, 2.13% H-3 => L+9
126	50808	197	0.01	25.6% H-6 => L+7, 25.3% H-14 => L+4, 24.6% H-7 => L+8, 6.36% H-8 => L+5, 3.46% H-4 => L+6, 2.24% H-6 => L+6, 2.13% H-3 => L+10
127	50873	197	0.00	29.6% H-9 => L+5, 29.6% H-8 => L+4, 15.7% H-7 => L+7, 5.94% H-6 => L+8, 4.09% H-14 => L+5, 2.87% H-7 => L+6, 2.12% H-8 => L+10
128	50873	197	0.00	29.6% H-9 => L+4, 29.6% H-8 => L+5, 15.7% H-6 => L+7, 5.94% H-7 => L+8, 4.09% H-14 => L+4, 2.87% H-6 => L+6, 2.12% H-8 => L+9
129	50927	196	0.00	74.3% H-14 => L+3, 4.43% H-9 => L+3, 2.54% H-4 => L+5, 2.54% H-5 => L+4
130	50960	196	0.00	26.1% H-14 => L+5, 22.0% H-9 => L+5, 12.4% H-6 => L+8, 7.65% H-16 => L+2, 4.53% H-10 => L+7, 4.05% H-7 => L+7, 3.21% H-11 => L+8, 2.84% H-11 => L+3, 2.82% H-7 => L+6
131	50960	196	0.00	26.1% H-14 => L+4, 22.0% H-9 => L+4, 12.4% H-7 => L+8, 7.65% H-15 => L+2, 4.53% H-11 => L+7, 4.05% H-6 => L+7, 3.21% H-10 => L+8, 2.84% H-10 => L+3, 2.82% H-6 => L+6
132	50979	196	0.00	31.1% H-9 => L+6, 23.5% H-8 => L+3, 15.6% H-6 => L+10, 15.6% H-7 => L+9, 4.33% H-6 => L+4, 4.33% H-7 => L+5
133	51107	196	0.00	35.0% H-6 => L+9, 35.0% H-7 => L+10, 8.58% H-8 => L+6, 2.87% H-10 => L+10, 2.87% H-11 => L+9, 2.75% H-3 => L+8, 2.21% H-9 => L+3
134	51190	195	0.00	30.6% H-8 => L+4, 24.8% H-7 => L+6, 15.0% H-14 => L+5, 6.69% H-6 => L+3, 6.00% H-9 => L+5, 3.76% H-11 => L+3, 2.10% H-9 => L+9
135	51190	195	0.00	30.6% H-8 => L+5, 24.8% H-6 => L+6, 15.0% H-14 => L+4, 6.69% H-7 => L+3, 6.00% H-9 => L+4, 3.76% H-10 => L+3, 2.10% H-9 => L+10

136	51227	195	0.00	16.4% H-9 => L+6, 14.8% H-10 => L+5, 14.8% H-11 => L+4, 14.7% H-6 => L+10, 14.7% H-7 => L+9, 12.6% H-14 => L+6
137	51327	195	0.01	28.0% H-8 => L+7, 27.4% H-14 => L+8, 23.1% H-9 => L+8, 5.30% H-4 => L+9, 5.30% H-5 => L+10, 3.11% H-6 => L+9, 3.11% H-7 => L+10
138	51347	195	0.00	29.5% H-8 => L+8, 29.0% H-9 => L+7, 26.0% H-14 => L+7, 4.75% H-4 => L+10, 4.75% H-5 => L+9
139	51409	195	0.01	28.2% H-16 => L+2, 15.7% H-14 => L+9, 15.1% H-6 => L+8, 9.21% H-7 => L+7, 5.49% H-8 => L+10, 4.25% H-11 => L+3, 3.68% H-11 => L+8, 2.22% H-7 => L+6, 2.19% H-5 => L+7, 2.06% H-10 => L+7

Table S3.13. TDDFT-predicted band excitation data for **3.1**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	10034	997	0.67	93.9% HOMO => LUMO, 4.77% H-1 => L+1
1	10710	934	0.00	98.0% H-1 => LUMO
2	15028	665	0.00	94.1% HOMO => L+1, 3.56% H-5 => LUMO
3	16138	620	0.02	65.1% H-2 => LUMO, 32.6% HOMO => L+2
4	16742	597	0.00	82.3% H-3 => LUMO, 13.8% H-1 => L+2, 3.49% H-2 => L+1
5	17434	574	1.64	91.4% H-1 => L+1, 4.38% H-4 => LUMO, 3.89% HOMO => LUMO
6	18523	540	1.05	93.4% H-4 => LUMO, 3.29% H-1 => L+1, 2.83% HOMO => LUMO
7	19325	517	0.61	57.8% HOMO => L+2, 27.3% H-2 => LUMO, 10.6% H-1 => L+3, 4.17% H-3 => L+1
8	19602	510	0.00	56.7% HOMO => L+3, 34.4% H-1 => L+2, 6.40% H-3 => LUMO
9	20645	484	0.00	93.0% H-5 => LUMO, 3.08% HOMO => L+1, 2.56% H-3 => L+2
10	21167	472	0.00	57.1% H-2 => L+1, 30.6% H-1 => L+2, 10.9% HOMO => L+3
11	21753	460	0.04	68.4% H-3 => L+1, 28.8% H-1 => L+3
12	21958	455	0.00	98.3% H-6 => LUMO
13	22992	435	0.00	97.9% H-7 => LUMO
14	23751	421	0.00	94.1% H-4 => L+1, 2.83% H-3 => L+2
15	24104	415	0.10	64.0% H-2 => L+2, 25.6% HOMO => L+4, 4.81% H-3 => L+3, 4.23% H-5 => L+1
16	24448	409	0.00	55.1% H-3 => L+2, 34.1% H-8 => LUMO, 4.00% H-2 => L+3, 3.36% H-1 => L+4
17	24518	408	2.71	59.0% H-1 => L+3, 23.7% H-3 => L+1, 8.38% HOMO => L+2, 6.47% H-2 => LUMO

18	24760	404	0.00	35.8% H-2 => L+1, 30.1% HOMO => L+3, 18.6% H-1 => L+2, 10.0% H-3 => LUMO
19	24904	402	0.01	94.7% H-9 => LUMO, 2.41% H-4 => L+2
20	25081	399	0.00	63.1% H-8 => LUMO, 26.6% H-3 => L+2, 3.23% H-2 => L+3, 2.81% H-4 => L+1, 2.30% H-1 => L+4
21	25362	394	0.30	37.2% HOMO => L+4, 33.1% H-5 => L+1, 25.5% H-2 => L+2, 2.24% H-12 => LUMO
22	25715	389	0.38	58.2% H-5 => L+1, 28.9% HOMO => L+4, 8.52% H-12 => LUMO
23	25947	385	0.01	77.0% H-10 => LUMO, 17.4% H-4 => L+2
24	26144	383	0.00	97.1% H-11 => LUMO
25	26249	381	0.00	94.4% H-13 => LUMO, 2.78% H-15 => LUMO
26	26469	378	0.03	74.2% H-12 => LUMO, 13.5% H-14 => LUMO, 5.21% HOMO => L+4
27	26524	377	0.04	57.0% H-4 => L+2, 20.5% H-6 => L+1, 15.8% H-10 => LUMO, 3.42% H-7 => L+2
28	26613	376	0.00	64.4% H-6 => L+1, 19.0% H-4 => L+2, 10.9% H-7 => L+2, 4.00% H-10 => LUMO
29	26767	374	0.06	83.8% H-14 => LUMO, 11.1% H-12 => LUMO
30	27044	370	0.00	93.4% H-15 => LUMO, 2.64% H-13 => LUMO
31	27187	368	0.00	70.3% H-7 => L+1, 28.2% H-6 => L+2
32	27202	368	0.06	95.6% H-16 => LUMO, 2.02% H-12 => LUMO
33	27440	364	0.00	73.7% H-1 => L+4, 22.5% H-2 => L+3
34	27679	361	0.00	91.5% H-17 => LUMO
35	27914	358	0.00	93.9% H-5 => L+2, 2.29% H-21 => LUMO
36	27925	358	0.00	95.2% H-18 => LUMO, 2.62% H-3 => L+3
37	27999	357	0.00	42.3% H-2 => L+3, 23.3% H-23 => LUMO, 16.6% H-20 => LUMO, 7.55% H-1 => L+4, 5.22% H-3 => L+2
38	28037	357	0.00	92.7% H-21 => LUMO, 2.07% H-17 => LUMO
39	28058	356	0.00	67.7% H-19 => LUMO, 30.3% H-22 => LUMO
40	28139	355	0.00	32.3% H-23 => LUMO, 25.8% H-20 => LUMO, 23.8% H-2 => L+3, 7.94% H-1 => L+4, 4.65% H-3 => L+2
41	28276	354	0.27	85.1% H-3 => L+3, 5.21% H-2 => L+2, 2.25% H-18 => LUMO
42	28294	353	0.00	65.7% H-22 => LUMO, 30.2% H-19 => LUMO
43	28316	353	0.00	55.6% H-20 => LUMO, 42.3% H-23 => LUMO
44	29289	341	0.00	90.4% H-24 => LUMO, 2.08% H-5 => L+3
45	29407	340	0.00	59.5% H-9 => L+1, 28.5% H-4 => L+3, 7.39% H-8 => L+2
46	29565	338	0.03	84.6% H-8 => L+1, 9.33% H-9 => L+2
47	30036	333	0.00	69.2% H-4 => L+3, 25.7% H-9 => L+1, 2.17% H-8 => L+2
48	30752	325	0.14	61.6% H-25 => LUMO, 28.9% H-11 => L+1, 2.84% H-10 => L+2

49	30753	325	0.20	79.8% H-13 => L+1, 7.00% H-14 => L+2, 4.48% H-15 => L+1, 2.43% H-12 => L+2
50	30879	324	0.00	87.3% H-10 => L+1, 6.46% H-11 => L+2
51	30921	323	0.00	51.3% H-12 => L+1, 30.6% H-14 => L+1, 9.17% H-13 => L+2, 2.46% H-16 => L+1
52	31014	322	0.14	56.4% H-11 => L+1, 29.5% H-25 => LUMO, 4.46% H-10 => L+2
53	31362	319	0.00	47.4% H-14 => L+1, 22.3% H-12 => L+1, 11.0% H-26 => LUMO, 5.81% H-16 => L+1, 3.56% H-6 => L+2
54	31376	319	0.07	93.2% H-5 => L+3, 2.21% H-24 => LUMO
55	31412	318	0.00	66.9% H-6 => L+2, 27.2% H-7 => L+1, 2.80% H-12 => L+1
56	31798	314	0.00	63.3% H-15 => L+1, 8.30% H-7 => L+2, 7.63% H-17 => L+1, 5.01% H-2 => L+4, 4.66% H-16 => L+2, 3.28% H-13 => L+1
57	31948	313	0.00	78.1% H-16 => L+1, 6.29% H-15 => L+2, 5.86% H-12 => L+1
58	32045	312	0.00	74.5% H-7 => L+2, 12.5% H-6 => L+1, 7.42% H-15 => L+1, 3.27% H-2 => L+4
59	32063	312	0.00	78.7% H-26 => LUMO, 9.55% H-12 => L+1, 4.40% H-14 => L+1
60	32197	311	0.00	82.3% H-3 => L+4, 12.6% HOMO => L+5
61	32318	309	0.04	82.4% H-2 => L+4, 5.47% H-15 => L+1, 2.33% H-17 => L+1, 2.25% H-21 => L+1
62	32355	309	0.00	82.5% HOMO => L+5, 11.3% H-3 => L+4
63	32419	308	0.05	57.4% H-17 => L+1, 9.09% H-21 => L+1, 8.83% HOMO => L+8, 7.83% H-15 => L+1, 4.94% H-12 => L+2, 2.14% H-14 => L+2
64	32526	307	0.00	91.2% HOMO => L+6, 5.91% HOMO => L+10
65	32632	306	0.00	44.9% HOMO => L+7, 44.2% H-18 => L+1, 2.15% H-17 => L+2
66	32681	306	0.02	61.0% H-21 => L+1, 16.1% H-17 => L+1, 7.84% HOMO => L+8, 5.66% H-18 => L+2, 2.49% H-2 => L+4
67	32694	306	0.00	48.2% HOMO => L+7, 43.1% H-18 => L+1
68	32753	305	0.00	64.8% H-19 => L+1, 23.4% H-22 => L+1, 4.68% H-23 => L+2
69	32774	305	0.01	57.5% H-23 => L+1, 31.0% H-20 => L+1, 5.03% H-19 => L+2
70	32850	304	0.00	77.3% HOMO => L+8, 11.3% H-21 => L+1, 3.00% H-17 => L+1
71	33020	303	0.00	89.1% H-6 => L+3, 6.41% H-7 => L+4
72	33070	302	0.02	84.0% HOMO => L+10, 5.36% HOMO => L+6, 4.96% H-20 => L+1
73	33085	302	0.00	87.3% HOMO => L+9, 4.33% H-19 => L+1, 3.05% H-22 => L+1
74	33266	301	0.00	59.0% H-22 => L+1, 19.1% H-19 => L+1, 6.74% HOMO => L+9, 4.60% H-20 => L+2, 4.04% H-27 => LUMO

75	33293	300	0.01	52.6% H-20 => L+1, 30.8% H-23 => L+1, 5.58% H-22 => L+2, 4.97% HOMO => L+10
76	33301	300	0.00	97.1% HOMO => L+11
77	33398	299	0.00	95.6% HOMO => L+12
78	33440	299	0.00	79.1% H-8 => L+2, 9.26% H-9 => L+1, 6.63% H-27 => LUMO
79	33482	299	0.01	81.4% H-9 => L+2, 9.51% H-8 => L+1, 3.16% HOMO => L+15
80	33491	299	0.00	47.3% H-27 => LUMO, 36.7% HOMO => L+16, 3.86% H-8 => L+2, 2.14% H-24 => L+1
81	33634	297	0.02	92.1% HOMO => L+15, 2.85% H-9 => L+2, 2.05% H-20 => L+1
82	33683	297	0.00	59.1% H-7 => L+3, 21.0% HOMO => L+16, 9.10% H-6 => L+4, 4.37% H-27 => LUMO
83	33689	297	0.00	95.6% HOMO => L+13
84	33734	296	0.00	93.6% HOMO => L+14
85	33741	296	0.00	39.0% HOMO => L+16, 24.4% H-27 => LUMO, 22.2% H-7 => L+3, 3.39% H-6 => L+4
86	34400	291	0.02	54.9% H-10 => L+2, 34.9% H-4 => L+4, 5.57% H-11 => L+1
87	34457	290	0.00	55.3% H-11 => L+2, 31.1% H-24 => L+1, 4.67% H-10 => L+1, 2.76% H-27 => LUMO
88	34484	290	0.00	70.5% H-1 => L+5, 16.1% H-12 => L+2
89	34581	289	0.04	55.5% H-4 => L+4, 32.4% H-10 => L+2, 2.95% H-9 => L+2, 2.88% H-11 => L+1
90	34601	289	0.04	49.3% H-12 => L+2, 22.7% H-1 => L+5, 4.83% H-8 => L+3, 4.57% H-13 => L+1, 4.45% H-14 => L+2, 3.87% H-16 => L+2, 2.98% H-21 => L+1
91	34679	288	0.00	56.0% H-13 => L+2, 24.5% H-1 => L+6, 7.68% H-14 => L+1, 2.65% H-9 => L+3, 2.49% H-12 => L+1
92	34777	288	0.00	64.2% H-1 => L+6, 19.5% H-13 => L+2, 4.16% H-1 => L+10, 4.05% H-9 => L+3, 2.83% H-14 => L+1
93	34842	287	0.04	93.6% H-1 => L+7, 2.23% H-2 => L+8
94	34902	287	0.00	36.1% H-24 => L+1, 34.0% H-1 => L+8, 21.0% H-11 => L+2
95	34957	286	0.00	59.2% H-1 => L+8, 20.4% H-24 => L+1, 11.4% H-11 => L+2, 2.48% H-1 => L+14
96	35237	284	0.04	60.0% H-14 => L+2, 11.4% H-8 => L+3, 5.53% H-16 => L+2, 5.49% H-12 => L+2, 3.48% H-13 => L+1, 3.08% H-17 => L+1, 2.72% H-11 => L+3, 2.40% H-15 => L+1
97	35267	284	0.00	82.7% H-1 => L+10, 6.05% H-9 => L+3, 3.75% H-1 => L+6, 3.24% H-2 => L+9
98	35268	284	0.00	81.4% H-1 => L+9, 5.95% H-8 => L+3, 3.07% H-14 => L+2, 2.80% H-2 => L+10
99	35357	283	0.00	56.5% H-9 => L+3, 10.4% H-25 => L+1, 6.72% H-1 => L+10, 6.53% H-13 => L+2, 5.94% H-15 =>

				L+2, 3.94% H-8 => L+4, 2.59% H-1 => L+6, 2.49% H-5 => L+4
100	35396	283	0.00	57.9% H-8 => L+3, 10.8% H-1 => L+9, 9.07% H-14 => L+2, 7.21% H-16 => L+2, 5.89% H-12 => L+2, 3.71% H-9 => L+4
101	35512	282	0.00	95.9% H-1 => L+11
102	35586	281	0.00	97.0% H-1 => L+12
103	35597	281	0.00	40.6% H-25 => L+1, 17.4% H-17 => L+2, 15.6% H-1 => L+15, 11.8% H-21 => L+2, 5.48% H-9 => L+3, 2.22% H-13 => L+2
104	35639	281	0.00	69.2% H-15 => L+2, 9.91% H-9 => L+3, 9.78% H-17 => L+2, 4.18% H-16 => L+1
105	35713	280	0.00	53.0% H-16 => L+2, 15.3% H-1 => L+16, 7.41% H-14 => L+2, 6.63% H-8 => L+3, 5.16% H-18 => L+2, 4.62% H-15 => L+1, 4.43% H-12 => L+2
106	35822	279	0.00	81.2% H-1 => L+16, 11.7% H-16 => L+2
107	35842	279	0.00	79.8% H-1 => L+15, 8.74% H-25 => L+1, 4.12% H-17 => L+2, 2.18% H-21 => L+2
108	35937	278	0.00	92.5% H-1 => L+13, 3.51% H-2 => L+14
109	35958	278	0.00	91.1% H-1 => L+14, 3.75% H-2 => L+13, 3.05% H-1 => L+8
110	36223	276	0.00	62.0% H-5 => L+4, 21.1% H-17 => L+2, 4.76% H-25 => L+1, 4.31% H-15 => L+2, 2.67% H-9 => L+3
111	36349	275	0.00	34.3% H-17 => L+2, 27.7% H-5 => L+4, 10.9% H-21 => L+2, 7.80% H-15 => L+2, 6.03% H-25 => L+1, 4.25% H-10 => L+3, 3.68% H-18 => L+1
112	36355	275	0.00	67.7% H-19 => L+2, 22.2% H-22 => L+2, 5.35% H-23 => L+1, 2.06% H-20 => L+1
113	36358	275	0.00	84.4% H-18 => L+2, 3.86% H-21 => L+1, 3.84% H-16 => L+2, 3.43% H-17 => L+1, 2.05% H-12 => L+2
114	36381	275	0.00	54.6% H-23 => L+2, 33.7% H-20 => L+2, 5.75% H-19 => L+1, 2.33% H-12 => L+3
115	36405	275	0.00	62.6% H-21 => L+2, 19.9% H-25 => L+1, 8.48% H-10 => L+3, 2.31% H-5 => L+4
116	36784	272	0.00	43.6% H-28 => LUMO, 32.9% HOMO => L+17, 16.5% H-12 => L+3
117	36822	272	0.04	53.1% H-13 => L+3, 13.3% H-22 => L+2, 9.16% H-19 => L+2, 8.29% H-24 => L+2, 3.92% H-26 => L+1, 2.48% H-15 => L+3, 2.47% H-14 => L+4, 2.24% H-20 => L+1
118	36935	271	0.00	68.6% H-12 => L+3, 14.7% HOMO => L+17, 4.66% H-28 => LUMO, 2.81% H-20 => L+2, 2.17% H-13 => L+4
119	36988	270	0.00	52.4% H-20 => L+2, 34.2% H-23 => L+2, 6.02% H-22 => L+1
120	37006	270	0.01	53.6% H-22 => L+2, 20.6% H-13 => L+3, 13.7% H-19 => L+2, 4.57% H-26 => L+1, 2.90% H-20 => L+1

121	37034	270	0.01	71.5% H-29 => LUMO, 11.8% H-11 => L+3, 5.50% H-25 => L+2, 2.69% H-1 => L+17, 2.03% H-12 => L+2
122	37160	269	0.00	80.5% H-10 => L+3, 4.47% H-17 => L+2, 4.07% H-21 => L+2, 3.04% H-5 => L+4, 2.91% H-25 => L+1
123	37167	269	0.05	75.3% H-11 => L+3, 14.8% H-29 => LUMO, 2.40% H-27 => L+1, 2.03% H-10 => L+4
124	37293	268	0.00	72.4% H-14 => L+3, 9.49% H-16 => L+3, 3.92% H-15 => L+4, 2.52% H-18 => L+3, 2.40% HOMO => L+17
125	37410	267	0.03	79.8% H-15 => L+3, 5.36% H-17 => L+3, 3.65% H-12 => L+4, 2.72% H-13 => L+3
126	37589	266	0.02	45.9% H-26 => L+1, 30.2% H-24 => L+2, 13.0% H-13 => L+3, 2.86% H-4 => L+4
127	37887	264	0.00	49.9% H-31 => LUMO, 20.1% H-6 => L+4, 9.27% HOMO => L+17, 9.03% H-7 => L+3, 4.00% H-28 => LUMO, 2.81% H-16 => L+3
128	38019	263	0.02	54.9% H-24 => L+2, 39.2% H-26 => L+1
129	38119	262	0.00	78.5% H-16 => L+3, 12.1% H-14 => L+3
130	38298	261	0.12	56.6% H-27 => L+1, 25.6% H-25 => L+2, 8.24% H-1 => L+17, 3.46% H-11 => L+3
131	38318	261	0.00	33.3% H-28 => LUMO, 30.6% HOMO => L+17, 7.96% H-6 => L+4, 6.58% H-31 => LUMO, 5.66% H-26 => L+2, 3.29% H-18 => L+3
132	38544	259	0.03	79.1% H-17 => L+3, 4.82% H-15 => L+3, 4.75% H-21 => L+3, 3.35% H-30 => LUMO
133	38646	259	0.00	62.6% H-22 => L+3, 14.7% H-19 => L+3, 12.9% HOMO => L+18, 3.69% H-20 => L+4, 2.04% H-23 => L+4
134	38657	259	0.01	59.7% H-20 => L+3, 29.4% H-23 => L+3, 5.15% H-22 => L+4
135	38716	258	0.00	80.5% HOMO => L+18, 10.1% H-22 => L+3, 2.90% H-19 => L+3
136	38915	257	0.00	58.2% H-18 => L+3, 21.4% H-6 => L+4, 10.8% H-31 => LUMO
137	38946	257	0.00	34.4% H-6 => L+4, 28.9% H-18 => L+3, 27.0% H-31 => LUMO, 2.35% H-7 => L+3
138	39014	256	0.00	84.8% H-32 => LUMO, 4.11% H-27 => L+1, 3.56% H-25 => L+2
139	39018	256	0.00	82.8% H-21 => L+3, 4.83% H-17 => L+3

Table S3.14. TDDFT-predicted band excitation data for **3.2**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	7363	1358	1.56	97.2% HOMO => LUMO, 2.30% H-1 => L+2
1	8032	1245	0.00	98.4% H-1 => LUMO

2	11803	847	0.00	86.6% H-3 => LUMO, 9.80% H-1 => L+1
3	12019	832	0.00	90.1% H-2 => LUMO, 3.41% H-6 => LUMO, 2.99% H-1 => L+3
4	12902	775	0.00	91.5% HOMO => L+1, 2.73% H-2 => LUMO, 2.08% H-6 => LUMO
5	13388	747	0.00	96.4% HOMO => L+2
6	14502	690	0.00	88.2% H-1 => L+1, 10.1% H-3 => LUMO
7	15400	649	0.06	75.8% H-4 => LUMO, 20.1% HOMO => L+4, 2.17% H-2 => L+3
8	15475	646	3.12	90.2% H-1 => L+2, 5.79% H-5 => LUMO, 2.96% HOMO => LUMO
9	15708	637	0.00	87.9% HOMO => L+3, 5.65% H-8 => LUMO
10	16417	609	0.00	85.7% H-6 => LUMO, 8.63% H-1 => L+3
11	16436	608	0.01	78.4% H-5 => LUMO, 9.56% H-1 => L+4, 5.45% H-1 => L+2, 3.26% H-3 => L+3
12	17689	565	0.41	66.4% H-7 => LUMO, 21.5% H-2 => L+1, 4.05% H-1 => L+4, 2.13% H-3 => L+3
13	17789	562	0.18	45.5% HOMO => L+4, 34.6% H-3 => L+1, 16.2% H-4 => LUMO
14	18272	547	0.00	65.4% H-2 => L+2, 25.8% H-8 => LUMO, 6.14% HOMO => L+3
15	18486	541	0.14	53.5% H-2 => L+1, 30.3% H-7 => LUMO, 6.96% H-1 => L+4, 3.77% H-5 => LUMO, 2.61% H-3 => L+3
16	18538	539	0.00	80.9% H-1 => L+3, 7.29% H-3 => L+2, 4.93% H-6 => LUMO, 2.44% H-2 => LUMO, 2.20% HOMO => L+1
17	19027	526	0.08	68.8% H-9 => LUMO, 18.0% H-3 => L+1, 6.08% H-2 => L+3, 3.05% HOMO => L+4, 2.00% HOMO => L+2
18	19038	525	0.00	65.0% H-8 => LUMO, 28.7% H-2 => L+2
19	19595	510	0.00	84.6% H-3 => L+2, 3.13% HOMO => L+1, 2.97% H-2 => LUMO, 2.85% H-1 => L+3, 2.61% H-6 => LUMO
20	19602	510	0.49	33.1% H-3 => L+1, 26.6% HOMO => L+4, 24.9% H-9 => LUMO, 6.87% H-2 => L+3, 4.29% H-5 => L+2
21	20092	498	0.06	43.7% H-1 => L+4, 31.1% HOMO => L+5, 11.7% H-2 => L+1, 6.84% H-10 => LUMO, 2.72% H-5 => LUMO
22	20292	493	0.01	87.6% H-10 => LUMO, 3.68% HOMO => L+5, 2.97% H-12 => LUMO, 2.49% H-1 => L+4
23	20891	479	0.04	33.2% HOMO => L+5, 25.2% H-3 => L+3, 19.5% H-1 => L+4, 19.0% H-4 => L+2
24	21275	470	0.61	69.4% H-2 => L+3, 13.3% H-1 => L+5, 7.67% H-3 => L+1, 2.69% H-4 => LUMO
25	21447	466	0.00	92.7% H-11 => LUMO, 3.64% H-10 => L+1, 2.89% H-12 => L+1
26	21679	461	0.00	66.7% H-4 => L+1, 23.9% H-2 => L+4, 2.94% H-6 => L+2, 2.69% H-5 => L+3

27	21864	457	0.00	91.4% H-12 => LUMO, 5.23% H-11 => L+1, 2.39% H-10 => LUMO
28	22066	453	0.00	43.5% H-5 => L+1, 28.7% H-3 => L+4, 10.6% HOMO => L+6, 9.84% H-4 => L+3
29	22133	452	0.42	47.6% H-3 => L+3, 45.1% H-4 => L+2
30	22616	442	0.11	92.4% H-6 => L+1, 2.16% HOMO => L+5
31	22693	441	0.00	60.6% H-6 => L+2, 29.5% H-2 => L+4, 3.46% H-4 => L+1, 2.10% H-1 => L+6
32	22863	437	0.06	70.4% H-5 => L+2, 18.6% H-1 => L+5, 2.86% H-2 => L+3, 2.08% H-14 => LUMO
33	22909	437	0.00	55.8% HOMO => L+6, 36.2% H-5 => L+1, 3.54% H-3 => L+4
34	23089	433	0.00	25.4% H-6 => L+2, 21.7% H-2 => L+4, 20.6% H-4 => L+1, 10.4% H-13 => LUMO, 9.89% H-15 => LUMO, 4.24% H-1 => L+6
35	23555	425	0.00	92.1% H-14 => LUMO, 2.53% H-13 => L+1
36	23580	424	0.00	83.9% H-13 => LUMO, 3.99% H-2 => L+4, 3.08% H-15 => LUMO, 3.05% H-6 => L+2, 2.33% H-14 => L+1
37	23952	417	0.00	53.8% H-3 => L+4, 13.1% HOMO => L+6, 12.3% H-7 => L+1, 6.89% H-5 => L+1, 5.24% H-8 => L+2, 2.82% H-4 => L+3
38	23955	417	0.00	82.0% H-15 => LUMO, 5.54% H-2 => L+4, 3.60% H-1 => L+6, 2.38% H-6 => L+2
39	24226	413	1.82	46.4% H-1 => L+5, 15.6% H-8 => L+1, 10.9% H-5 => L+2, 10.2% H-7 => L+2, 5.20% H-2 => L+3, 2.39% H-4 => LUMO, 2.30% H-3 => L+1, 2.08% HOMO => L+4, 2.03% H-6 => L+3
40	24548	407	0.57	27.6% H-4 => L+2, 22.2% HOMO => L+5, 12.9% H-3 => L+3, 9.48% H-1 => L+4, 7.42% H-2 => L+1, 4.58% H-5 => LUMO, 3.86% H-30 => LUMO, 3.42% H-24 => LUMO
41	24589	407	0.06	71.0% H-16 => LUMO, 12.7% H-7 => L+2, 8.77% H-6 => L+3
42	24604	406	0.00	60.3% H-18 => LUMO, 14.8% H-7 => L+1, 4.99% H-4 => L+3, 4.37% H-8 => L+2, 4.05% H-5 => L+1, 3.64% H-22 => LUMO, 3.17% HOMO => L+6
43	24647	406	0.00	94.8% H-17 => LUMO
44	24692	405	0.00	54.4% H-4 => L+3, 32.7% H-7 => L+1, 4.17% H-3 => L+4, 2.39% HOMO => L+6
45	24810	403	0.21	44.5% H-7 => L+2, 24.3% H-16 => LUMO, 14.6% H-6 => L+3, 5.84% H-5 => L+2, 4.34% H-1 => L+5, 2.16% H-8 => L+1
46	24962	401	0.02	88.5% H-19 => LUMO, 3.63% H-23 => LUMO
47	25082	399	0.60	67.5% H-8 => L+1, 8.67% H-6 => L+3, 8.06% H-1 => L+5, 3.95% H-2 => L+3, 3.05% H-5 => L+4, 2.24% H-5 => L+2

48	25093	399	0.00	48.9% H-20 => LUMO, 19.8% H-18 => LUMO, 11.5% H-7 => L+1, 6.29% H-8 => L+2, 3.59% HOMO => L+6, 2.02% H-5 => L+1
49	25114	398	0.00	47.0% H-5 => L+3, 22.8% H-9 => L+1, 12.0% H-1 => L+6, 6.71% H-2 => L+4, 5.49% H-6 => L+4
50	25223	396	0.00	53.1% H-8 => L+2, 20.2% H-7 => L+1, 16.0% H-4 => L+3, 2.76% H-18 => LUMO, 2.12% H-20 => LUMO
51	25265	396	0.02	54.6% H-21 => LUMO, 21.7% H-9 => L+2, 12.5% H-23 => LUMO, 2.51% H-8 => L+3, 2.35% H-4 => L+4
52	25344	395	0.00	65.4% H-9 => L+1, 20.5% H-1 => L+6, 5.40% H-5 => L+3, 2.66% H-2 => L+4, 2.06% H-3 => L+5
53	25408	394	0.14	63.8% H-9 => L+2, 24.5% H-21 => LUMO, 2.84% H-8 => L+3, 2.41% H-23 => LUMO, 2.25% H-19 => LUMO
54	25410	394	0.00	43.0% H-20 => LUMO, 21.6% H-8 => L+2, 12.1% H-18 => LUMO, 6.09% HOMO => L+6, 4.22% H-7 => L+1, 4.12% H-2 => L+5
55	25665	390	0.46	49.7% H-6 => L+3, 24.0% H-7 => L+2, 8.58% H-8 => L+1, 5.83% H-7 => L+4, 3.31% H-5 => L+4, 2.56% H-1 => L+5
56	25673	390	0.00	92.0% H-22 => LUMO
57	25686	389	0.05	76.5% H-23 => LUMO, 14.3% H-21 => LUMO, 4.53% H-19 => LUMO
58	25887	386	0.01	48.8% H-1 => L+6, 21.2% H-5 => L+3, 8.02% H-9 => L+1, 5.09% H-6 => L+4, 3.43% H-7 => L+3
59	26128	383	0.25	80.1% H-4 => L+4, 4.73% H-9 => L+2, 3.79% H-8 => L+3
60	26195	382	0.00	69.3% H-26 => LUMO, 28.1% H-25 => LUMO
61	26228	381	0.00	42.7% H-27 => LUMO, 32.3% H-10 => L+2, 11.3% H-29 => LUMO, 5.54% H-32 => LUMO, 2.61% H-12 => L+4, 2.59% H-11 => L+3
62	26257	381	0.04	47.2% H-10 => L+2, 24.9% H-27 => LUMO, 9.53% H-29 => LUMO, 5.22% H-32 => LUMO, 3.76% H-12 => L+4, 3.50% H-11 => L+3, 2.03% H-10 => L+4
63	26274	381	0.01	80.4% H-24 => LUMO, 7.83% H-30 => LUMO
64	26316	380	0.00	40.2% H-6 => L+4, 31.9% H-7 => L+3, 12.1% H-5 => L+3, 5.13% H-33 => LUMO, 3.48% H-1 => L+6
65	26406	379	0.00	66.8% H-25 => LUMO, 29.1% H-26 => LUMO
66	26495	377	0.01	83.6% H-30 => LUMO, 11.3% H-24 => LUMO
67	26542	377	0.00	71.6% H-28 => LUMO, 23.4% H-31 => LUMO
68	26551	377	0.01	35.6% H-29 => LUMO, 31.1% H-32 => LUMO, 30.1% H-27 => LUMO
69	26807	373	0.00	51.8% H-32 => LUMO, 40.6% H-29 => LUMO, 2.46% H-5 => L+4
70	26820	373	0.00	70.3% H-31 => LUMO, 24.6% H-28 => LUMO

71	26849	372	0.00	79.4% H-10 => L+1, 7.87% H-2 => L+5, 7.77% H-12 => L+1
72	26912	372	0.00	54.3% H-11 => L+2, 20.4% H-10 => L+3, 15.1% H-12 => L+3, 6.86% H-11 => L+4
73	26944	371	0.00	68.7% H-2 => L+5, 7.90% H-10 => L+1, 6.19% H-34 => LUMO, 4.29% H-4 => L+3
74	27054	370	0.02	51.6% H-5 => L+4, 17.6% H-12 => L+2, 11.0% H-11 => L+3, 4.82% H-10 => L+4, 2.90% H-32 => LUMO, 2.71% H-6 => L+3
75	27232	367	0.01	37.0% H-12 => L+2, 27.9% H-5 => L+4, 18.5% H-11 => L+3, 9.74% H-10 => L+4
76	27362	365	0.01	80.9% H-3 => L+5, 5.09% H-5 => L+3, 3.62% H-33 => LUMO
77	27370	365	0.01	70.7% H-8 => L+3, 16.2% H-9 => L+4, 6.58% H-4 => L+4
78	27437	364	0.00	84.1% H-33 => LUMO, 6.72% H-7 => L+3, 2.94% H-3 => L+5
79	27520	363	0.00	69.5% H-9 => L+3, 24.5% H-8 => L+4
80	28069	356	0.00	52.0% H-7 => L+3, 41.4% H-6 => L+4, 2.93% H-6 => L+2
81	28354	353	0.01	87.4% H-11 => L+1, 4.41% H-12 => LUMO, 2.66% H-2 => L+6, 2.12% H-10 => LUMO
82	28395	352	0.00	70.3% H-35 => LUMO, 12.8% H-3 => L+6, 5.41% H-7 => L+4, 3.30% H-4 => L+5
83	28438	352	0.00	84.7% H-34 => LUMO, 3.26% H-2 => L+5
84	28446	352	0.29	86.0% H-2 => L+6, 2.73% H-11 => L+1, 2.44% H-5 => L+5, 2.26% H-4 => L+4
85	28643	349	0.00	84.5% H-12 => L+1, 6.82% H-10 => L+1, 4.92% H-11 => LUMO, 2.40% H-11 => L+5
86	29019	345	0.10	74.7% H-7 => L+4, 12.3% H-35 => LUMO, 3.96% H-6 => L+3, 3.31% H-3 => L+6
87	29307	341	0.10	67.3% H-3 => L+6, 8.82% H-7 => L+4, 7.90% H-35 => LUMO, 4.53% H-5 => L+4, 2.70% H-4 => L+5
88	29441	340	0.00	64.9% H-13 => L+2, 18.2% H-14 => L+3, 4.60% H-8 => L+4, 2.10% H-9 => L+3
89	29466	339	0.04	68.6% H-14 => L+2, 20.7% H-13 => L+3, 2.67% H-14 => L+4
90	29554	338	0.00	58.4% H-8 => L+4, 21.3% H-9 => L+3, 5.98% H-15 => L+2, 4.80% H-13 => L+2, 2.32% H-14 => L+3
91	29667	337	0.00	69.3% H-15 => L+1, 10.7% H-13 => L+1, 5.22% H-23 => L+2, 2.64% H-21 => L+2, 2.07% H-30 => L+2
92	29752	336	0.01	78.6% H-9 => L+4, 16.2% H-8 => L+3, 2.63% H-9 => L+2
93	29839	335	0.00	65.4% H-15 => L+2, 7.20% H-23 => L+1, 6.42% H-8 => L+4, 3.25% H-15 => L+4, 3.03% H-21 => L+1, 2.88% H-30 => L+1, 2.87% H-19 => L+1, 2.17% H-9 => L+3

94	29889	335	0.00	86.4% H-14 => L+1, 2.98% H-18 => L+2, 2.77% H-13 => LUMO
95	29901	334	0.02	77.2% H-13 => L+1, 8.22% H-15 => L+1, 3.65% H-19 => L+2, 2.60% H-14 => LUMO
96	30122	332	0.00	87.1% H-36 => LUMO, 2.09% H-35 => L+1
97	30273	330	0.02	84.8% H-4 => L+5, 6.59% H-3 => L+6
98	30539	327	0.00	60.2% H-10 => L+3, 31.9% H-11 => L+2, 7.21% H-11 => L+4
99	30586	327	0.14	64.3% H-37 => LUMO, 14.8% H-16 => L+2, 4.32% H-5 => L+5, 3.55% H-17 => L+3, 2.58% H-6 => L+6
100	30730	325	0.05	52.6% H-16 => L+2, 14.2% H-37 => LUMO, 12.1% H-17 => L+3, 5.27% H-5 => L+5, 5.00% H-18 => L+1, 2.09% H-14 => L+2
101	30740	325	0.00	74.1% H-17 => L+2, 16.7% H-16 => L+3
102	30806	325	0.00	53.1% H-18 => L+2, 13.5% H-20 => L+2, 11.5% H-19 => L+3, 6.46% H-14 => L+1, 3.50% H-21 => L+3, 2.39% H-22 => L+2
103	30890	324	0.13	45.7% H-19 => L+2, 14.2% H-21 => L+2, 9.17% H-18 => L+3, 9.11% H-20 => L+3, 5.40% H-13 => L+1, 3.67% H-12 => L+2, 2.89% H-11 => L+3
104	30947	323	0.02	32.9% H-12 => L+2, 32.8% H-11 => L+3, 9.46% H-10 => L+4, 7.74% H-10 => L+2, 7.22% H-12 => L+4, 4.06% H-19 => L+2, 2.26% H-21 => L+2
105	30964	323	0.00	53.3% H-18 => L+1, 9.12% H-26 => L+1, 8.35% H-27 => L+2, 7.57% H-22 => L+1, 5.68% H-16 => L+2, 2.77% H-25 => L+1, 2.23% H-32 => L+2, 2.18% H-29 => L+2
106	31089	322	0.00	82.1% H-16 => L+1, 7.13% H-22 => L+2, 2.84% H-20 => L+2, 2.17% H-17 => LUMO
107	31112	321	0.02	88.5% H-17 => L+1, 3.77% H-23 => L+2
108	31122	321	0.00	81.8% H-6 => L+5, 2.72% H-7 => L+6, 2.63% H-13 => L+2, 2.56% H-5 => L+6, 2.02% H-21 => L+1
109	31128	321	0.00	33.8% H-20 => L+2, 12.3% H-27 => L+1, 11.1% H-26 => L+2, 7.71% H-16 => L+1, 7.19% H-22 => L+2, 4.25% H-29 => L+1, 4.21% H-21 => L+3, 3.93% H-18 => L+2, 3.26% H-32 => L+1, 2.24% H-36 => LUMO
110	31243	320	0.06	71.0% H-5 => L+5, 10.6% H-37 => LUMO, 4.38% HOMO => L+7, 2.08% H-14 => L+2
111	31360	319	0.00	64.3% H-19 => L+1, 7.37% HOMO => L+8, 7.18% HOMO => L+9, 6.86% H-15 => L+2, 4.30% H-38 => LUMO, 3.93% H-23 => L+1
112	31374	319	0.02	70.4% HOMO => L+7, 6.68% H-26 => L+1, 5.22% H-5 => L+5, 4.79% H-27 => L+2, 2.32% H-18 => L+1
113	31436	318	0.00	59.7% H-12 => L+3, 13.0% H-11 => L+4, 11.8% H-10 => L+3, 10.7% H-11 => L+2

114	31452	318	0.00	42.6% HOMO => L+9, 34.1% HOMO => L+8, 15.8% H-19 => L+1, 3.78% H-21 => L+1
115	31469	318	0.00	35.0% H-20 => L+1, 24.4% H-18 => L+1, 11.4% HOMO => L+7, 7.73% H-26 => L+1, 4.30% H-27 => L+2, 2.59% H-22 => L+1, 2.26% H-29 => L+2, 2.07% H-5 => L+5
116	31499	317	0.00	38.5% H-21 => L+2, 13.0% H-23 => L+2, 11.4% H-19 => L+2, 10.8% H-15 => L+1, 7.09% HOMO => L+10, 4.90% HOMO => L+12, 4.07% H-20 => L+3
117	31599	316	0.00	21.4% H-20 => L+2, 20.2% H-26 => L+2, 17.2% H-18 => L+2, 16.9% H-27 => L+1, 5.91% H-21 => L+3, 3.15% H-29 => L+1, 2.50% H-25 => L+2, 2.28% H-32 => L+1
118	31633	316	0.01	45.8% HOMO => L+10, 35.9% HOMO => L+12, 8.78% H-21 => L+2, 3.09% H-19 => L+2
119	31662	316	0.00	45.3% H-21 => L+1, 16.6% H-38 => LUMO, 7.88% H-23 => L+1, 5.97% H-15 => L+2, 3.19% H-30 => L+1, 2.85% HOMO => L+8, 2.80% H-6 => L+5, 2.24% HOMO => L+9, 2.19% H-33 => L+2
120	31699	315	0.01	46.9% H-10 => L+4, 17.4% H-12 => L+4, 8.57% H-10 => L+2, 8.30% H-23 => L+2, 4.99% H-11 => L+3, 3.33% H-12 => L+2, 2.97% HOMO => L+12, 2.37% H-22 => L+3
121	31721	315	0.00	47.6% HOMO => L+8, 38.6% HOMO => L+9, 4.36% H-38 => LUMO, 4.26% HOMO => L+14, 2.31% H-2 => L+7
122	31792	315	0.04	47.9% H-20 => L+1, 8.50% H-18 => L+1, 8.45% H-27 => L+2, 7.95% H-26 => L+1, 7.09% H-22 => L+1, 4.73% HOMO => L+7
123	31800	314	0.00	46.6% H-22 => L+2, 13.9% HOMO => L+11, 8.02% H-23 => L+3, 3.89% H-25 => L+2, 3.77% H-26 => L+2, 3.67% H-4 => L+6, 3.48% H-16 => L+1
124	31861	314	0.01	35.8% H-23 => L+2, 13.1% HOMO => L+12, 9.67% H-22 => L+3, 9.03% H-10 => L+4, 5.56% H-21 => L+2, 3.83% H-17 => L+1, 3.62% HOMO => L+10, 3.24% H-24 => L+2, 2.94% H-12 => L+4, 2.91% H-19 => L+2
125	31869	314	0.00	58.3% H-38 => LUMO, 19.7% H-21 => L+1, 3.96% H-19 => L+1, 2.83% H-15 => L+2, 2.53% HOMO => L+9, 2.40% H-6 => L+5
126	31968	313	0.00	74.7% HOMO => L+11, 7.23% H-22 => L+2, 6.70% H-4 => L+6
127	31999	313	0.02	36.8% HOMO => L+10, 31.1% HOMO => L+12, 13.3% H-23 => L+2
128	32090	312	0.00	66.4% H-23 => L+1, 12.1% H-21 => L+1, 5.22% H-19 => L+1, 3.60% H-15 => L+2, 2.93% H-38 => LUMO

129	32181	311	0.00	51.1% H-4 => L+6, 19.8% HOMO => L+15, 12.8% HOMO => L+17, 3.21% H-8 => L+5, 2.54% H-22 => L+2, 2.05% H-25 => L+2
130	32181	311	0.01	71.0% H-22 => L+1, 8.09% H-26 => L+1, 4.07% H-25 => L+1, 2.94% H-32 => L+2, 2.72% H-29 => L+2
131	32239	310	0.00	48.6% HOMO => L+15, 23.8% H-4 => L+6, 13.3% HOMO => L+17, 4.02% HOMO => L+11, 2.35% HOMO => L+19
132	32279	310	0.00	33.5% H-24 => L+2, 24.1% H-30 => L+2, 7.31% HOMO => L+12, 6.10% H-18 => L+3, 4.28% H-33 => L+1, 3.93% H-20 => L+3, 2.29% HOMO => L+10, 2.12% H-15 => L+1
133	32279	310	0.00	51.4% HOMO => L+13, 29.8% HOMO => L+18, 4.97% HOMO => L+21, 3.74% H-7 => L+5, 3.07% H-6 => L+6
134	32323	309	0.00	83.0% HOMO => L+14, 2.89% H-2 => L+13, 2.35% HOMO => L+9
135	32341	309	0.04	34.8% HOMO => L+13, 34.1% HOMO => L+18, 7.09% H-7 => L+5, 5.41% H-6 => L+6, 5.24% H-13 => L+3, 3.13% H-14 => L+2
136	32426	308	0.03	25.3% HOMO => L+18, 17.5% H-13 => L+3, 17.5% H-7 => L+5, 11.1% H-6 => L+6, 8.38% H-14 => L+2, 3.24% H-14 => L+4, 2.93% H-20 => L+1
137	32465	308	0.00	30.9% H-30 => L+2, 25.2% H-24 => L+2, 20.8% HOMO => L+16, 8.91% H-25 => L+3, 3.10% H-28 => L+1, 3.01% H-26 => L+3
138	32468	308	0.00	49.6% H-25 => L+2, 10.8% H-26 => L+2, 9.44% HOMO => L+17, 8.60% H-24 => L+3, 4.20% H-30 => L+3, 3.25% H-4 => L+6, 2.42% HOMO => L+15
139	32506	308	0.00	28.7% H-14 => L+3, 15.3% H-28 => L+2, 13.5% H-24 => L+1, 9.67% H-13 => L+2, 5.94% H-21 => L+1, 5.41% H-31 => L+2, 5.06% HOMO => L+14, 4.89% H-13 => L+4
140	32521	307	0.00	30.0% H-14 => L+3, 23.1% H-24 => L+1, 13.3% H-28 => L+2, 10.9% H-13 => L+2, 5.34% H-13 => L+4, 4.94% H-31 => L+2
141	32545	307	0.04	16.4% H-27 => L+2, 15.9% H-13 => L+3, 13.7% H-29 => L+2, 11.0% H-32 => L+2, 5.82% H-28 => L+3, 5.55% H-7 => L+5, 4.77% H-25 => L+1, 4.48% H-14 => L+2, 4.23% H-22 => L+1, 3.66% HOMO => L+13, 3.22% H-6 => L+6, 2.73% H-14 => L+4, 2.15% H-31 => L+3, 2.05% H-26 => L+1
142	32586	307	0.00	75.3% HOMO => L+16, 9.43% H-30 => L+2, 6.17% H-24 => L+2
143	32588	307	0.01	21.6% H-13 => L+3, 14.7% H-7 => L+5, 10.6% H-6 => L+6, 8.62% H-25 => L+1, 7.31% H-27 => L+2, 6.74% HOMO => L+21, 5.86% H-14 =>

				L+2, 5.03% H-29 => L+2, 4.52% H-32 => L+2, 3.43% H-14 => L+4, 2.54% H-28 => L+3
144	32589	307	0.00	58.2% HOMO => L+17, 24.9% HOMO => L+15, 7.86% H-25 => L+2
145	32658	306	0.00	26.3% H-30 => L+1, 21.2% H-24 => L+1, 19.8% H-28 => L+2, 7.34% HOMO => L+22, 5.02% H-23 => L+1, 4.84% H-31 => L+2
146	32744	305	0.01	70.9% HOMO => L+21, 13.3% H-25 => L+1, 5.38% HOMO => L+18
147	32847	304	0.00	78.8% HOMO => L+22, 12.2% H-30 => L+1
148	32920	304	0.00	87.9% HOMO => L+19, 2.96% H-2 => L+20, 2.67% HOMO => L+17
149	32923	304	0.00	89.4% HOMO => L+20, 2.90% H-28 => L+1, 2.86% H-2 => L+19
150	32942	304	0.01	53.2% H-25 => L+1, 10.8% H-32 => L+2, 8.74% H-26 => L+1, 7.10% HOMO => L+21, 3.45% H-29 => L+2, 2.69% H-27 => L+2, 2.22% H-31 => L+3
151	32975	303	0.00	41.5% H-30 => L+1, 25.1% H-24 => L+1, 12.2% H-31 => L+2, 5.85% HOMO => L+22, 2.88% H-28 => L+2, 2.69% H-32 => L+3
152	33009	303	0.00	84.1% H-5 => L+6, 3.43% H-24 => L+1, 2.14% H-6 => L+5
153	33021	303	0.00	50.9% H-29 => L+1, 22.9% H-32 => L+1, 8.25% H-25 => L+2, 4.90% H-26 => L+2, 2.65% H-8 => L+5, 2.56% H-27 => L+1
154	33031	303	0.00	60.4% H-28 => L+1, 28.4% H-31 => L+1, 2.82% H-24 => L+2
155	33066	302	0.00	53.8% H-27 => L+1, 27.2% H-26 => L+2, 7.99% H-32 => L+1
156	33092	302	0.00	32.1% H-26 => L+1, 31.5% H-29 => L+2, 22.7% H-27 => L+2, 3.92% H-25 => L+1, 2.15% H-31 => L+3
157	33151	302	0.00	44.9% H-31 => L+2, 25.8% H-28 => L+2, 7.68% H-29 => L+3, 6.45% H-32 => L+3, 3.93% H-30 => L+1, 2.50% H-17 => L+2
158	33153	302	0.00	42.4% H-32 => L+2, 17.0% H-29 => L+2, 12.0% H-26 => L+1, 9.33% H-27 => L+2, 8.12% H-31 => L+3, 3.96% H-28 => L+3
159	33154	302	0.00	80.1% H-8 => L+5, 6.20% H-9 => L+6, 6.02% H-4 => L+6, 2.41% H-29 => L+1
160	33211	301	0.00	63.0% H-31 => L+1, 27.8% H-28 => L+1
161	33217	301	0.00	55.7% H-32 => L+1, 28.6% H-29 => L+1, 4.23% H-27 => L+1, 3.84% H-26 => L+2
162	33272	301	0.00	78.4% H-15 => L+3, 15.0% HOMO => L+23
163	33332	300	0.03	58.2% HOMO => L+23, 15.9% H-15 => L+3, 5.40% H-40 => LUMO, 3.74% H-17 => L+3, 2.58% H-27 => L+2, 2.57% HOMO => L+21

164	33412	299	0.08	61.5% H-9 => L+5, 9.85% H-18 => L+3, 7.05% H-8 => L+6, 6.23% H-33 => L+1, 3.90% H-19 => L+2, 2.48% H-1 => L+7
165	33521	298	0.00	59.9% H-16 => L+3, 16.5% H-17 => L+2, 10.8% H-17 => L+4, 4.60% H-31 => L+2, 3.68% H-33 => L+2
166	33536	298	0.00	58.0% H-17 => L+3, 16.7% H-16 => L+2, 10.3% H-16 => L+4, 3.10% H-32 => L+2, 2.29% H-15 => L+3
167	33543	298	0.00	57.3% H-1 => L+9, 37.7% H-1 => L+8
168	33568	298	0.20	66.2% H-1 => L+7, 17.0% H-39 => LUMO, 3.17% H-18 => L+3, 2.30% H-1 => L+13, 2.10% H-3 => L+8
169	33693	297	0.00	32.4% H-18 => L+3, 21.6% H-9 => L+5, 10.9% H-19 => L+2, 10.1% H-1 => L+7, 5.66% H-39 => LUMO, 4.24% H-19 => L+4, 4.15% H-30 => L+2, 2.00% H-20 => L+3
170	33756	296	0.00	52.1% H-19 => L+3, 10.3% H-18 => L+2, 10.2% H-18 => L+4, 7.85% H-20 => L+2, 3.86% H-1 => L+9, 3.30% H-34 => L+2, 2.51% H-26 => L+2
171	33763	296	0.04	50.8% H-1 => L+12, 41.7% H-1 => L+10
172	33836	296	0.00	49.7% H-6 => L+6, 40.1% H-7 => L+5, 3.00% H-34 => L+1
173	33838	296	0.00	53.8% H-33 => L+1, 8.33% H-39 => LUMO, 7.25% H-18 => L+3, 5.07% H-20 => L+3, 3.49% H-30 => L+2, 3.34% H-1 => L+7, 3.00% H-21 => L+2, 2.71% H-19 => L+2, 2.66% H-9 => L+5
174	33959	294	0.00	71.5% H-11 => L+4, 21.6% H-12 => L+3, 5.68% H-10 => L+3
175	34050	294	0.00	78.2% H-33 => L+2, 3.80% H-30 => L+1, 3.16% H-16 => L+3, 2.11% H-15 => L+4
176	34055	294	0.00	45.4% H-1 => L+8, 30.3% H-1 => L+9, 6.81% H-1 => L+14, 5.33% H-3 => L+7, 2.94% H-19 => L+3, 2.09% H-21 => L+3
177	34079	293	0.00	55.0% H-12 => L+4, 18.7% H-11 => L+3, 11.4% H-10 => L+4, 4.35% H-39 => LUMO, 2.94% H-20 => L+3, 2.31% H-33 => L+1
178	34093	293	0.01	24.2% H-39 => LUMO, 21.3% H-20 => L+3, 17.6% H-33 => L+1, 8.87% H-12 => L+4, 5.14% H-21 => L+2, 3.50% H-30 => L+2, 2.85% H-11 => L+3, 2.59% H-1 => L+7, 2.35% H-21 => L+4
179	34187	293	0.00	34.5% H-21 => L+3, 25.3% H-34 => L+2, 8.80% H-20 => L+2, 6.94% H-20 => L+4, 5.81% H-30 => L+3, 4.41% H-1 => L+8, 3.44% H-23 => L+3

Table S3.15. TDDFT-predicted band excitation data for **3.3**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	5871	1703	2.54	98.4% HOMO => LUMO
1	6707	1491	0.00	97.9% H-1 => LUMO
2	9452	1058	0.00	86.1% H-3 => LUMO, 11.4% H-1 => L+1
3	9738	1027	0.00	91.5% H-2 => LUMO, 5.29% HOMO => L+1
4	10183	982	0.00	90.2% HOMO => L+1, 3.76% H-2 => LUMO, 2.23% H-1 => L+3
5	11885	841	0.00	86.4% H-1 => L+1, 11.8% H-3 => LUMO
6	12386	807	0.00	77.9% H-4 => LUMO, 11.1% H-3 => L+1, 4.04% H-1 => L+4, 2.50% HOMO => L+2
7	12583	795	0.00	94.3% HOMO => L+2, 2.41% H-4 => LUMO
8	12687	788	0.16	82.1% H-5 => LUMO, 6.82% H-7 => LUMO, 3.94% H-2 => L+1
9	14091	710	0.34	37.8% HOMO => L+4, 33.9% H-2 => L+1, 8.55% H-5 => LUMO, 7.41% H-7 => LUMO, 6.40% H-1 => L+2, 2.34% H-3 => L+3
10	14305	699	0.01	92.1% HOMO => L+3, 2.56% H-2 => L+2, 2.37% H-12 => LUMO
11	14395	695	0.00	70.0% H-3 => L+1, 15.5% H-4 => LUMO, 11.0% H-1 => L+4
12	14439	693	2.16	42.5% H-1 => L+2, 38.8% HOMO => L+4, 13.9% H-2 => L+1
13	14872	672	1.29	44.6% H-1 => L+2, 39.3% H-2 => L+1, 11.7% HOMO => L+4
14	15006	666	0.11	81.0% H-6 => LUMO, 13.6% HOMO => L+6, 2.13% H-2 => L+5
15	15730	636	0.00	76.8% H-7 => LUMO, 5.70% H-1 => L+5, 5.38% HOMO => L+4, 3.59% H-3 => L+3, 2.19% H-5 => LUMO
16	15935	628	0.00	68.1% HOMO => L+5, 10.7% H-10 => LUMO, 8.65% H-1 => L+4, 3.08% H-6 => L+1, 2.23% H-2 => L+3
17	16099	621	0.00	88.0% H-8 => LUMO, 4.02% H-1 => L+6, 2.12% H-7 => L+1, 2.00% H-3 => L+5
18	16396	610	0.00	72.7% H-1 => L+4, 13.2% H-3 => L+1, 10.4% HOMO => L+5
19	16530	605	0.00	59.9% H-9 => LUMO, 25.9% H-1 => L+3, 3.54% H-1 => L+6, 3.15% H-3 => L+2, 3.13% H-5 => L+1
20	16737	597	0.00	89.4% H-2 => L+2, 3.79% HOMO => L+3, 3.47% H-12 => LUMO
21	17184	582	0.06	39.1% HOMO => L+6, 37.5% H-4 => L+1, 12.2% H-6 => LUMO, 5.73% H-3 => L+4, 2.02% H-12 => LUMO
22	17207	581	0.00	64.5% H-1 => L+3, 16.7% H-9 => LUMO, 6.59% H-5 => L+1, 3.15% H-3 => L+5, 2.69% H-2 => LUMO
23	17438	573	0.61	93.7% H-11 => LUMO, 2.67% H-9 => L+1

24	17747	563	0.00	66.5% H-10 => LUMO, 13.0% HOMO => L+5, 11.9% H-2 => L+3, 2.06% H-5 => L+2
25	17780	562	0.00	63.8% H-3 => L+2, 18.5% H-5 => L+1, 4.78% H-1 => L+6, 2.80% H-1 => L+3, 2.74% H-4 => L+3, 2.59% H-2 => L+4
26	18051	554	0.00	45.4% H-5 => L+1, 27.7% H-3 => L+2, 16.5% H-9 => LUMO, 2.36% H-2 => L+4, 2.22% H-3 => L+5
27	18198	550	0.00	60.9% H-13 => LUMO, 22.6% H-2 => L+3, 9.32% H-10 => LUMO
28	18330	546	0.17	58.5% H-12 => LUMO, 22.3% H-4 => L+1, 6.64% HOMO => L+6, 3.50% H-2 => L+5, 3.43% H-2 => L+2
29	18623	537	0.37	29.2% H-4 => L+1, 28.3% H-12 => LUMO, 27.1% HOMO => L+6, 8.91% H-3 => L+4
30	18719	534	0.00	45.4% H-2 => L+3, 32.7% H-13 => LUMO, 8.48% H-10 => LUMO, 5.87% H-5 => L+2, 2.78% H-6 => L+1
31	18788	532	0.00	69.0% H-2 => L+4, 15.4% H-5 => L+1, 7.80% H-1 => L+6
32	18898	529	0.02	81.3% H-1 => L+5, 3.97% H-4 => L+2, 3.26% H-7 => LUMO, 2.59% H-8 => L+1
33	19561	511	0.00	92.8% H-14 => LUMO, 2.38% H-15 => L+1
34	19632	509	0.68	83.0% H-3 => L+3, 2.37% H-2 => L+1, 2.16% HOMO => L+8, 2.09% H-1 => L+2
35	19743	507	0.14	66.2% H-3 => L+4, 13.6% H-2 => L+5, 9.24% HOMO => L+6, 3.81% H-5 => L+3, 2.04% H-12 => LUMO
36	20005	500	0.00	74.1% H-6 => L+1, 9.28% H-2 => L+6, 5.75% H-2 => L+3, 2.68% H-5 => L+2, 2.25% HOMO => L+5
37	20206	495	0.00	50.2% H-7 => L+1, 16.6% H-1 => L+6, 12.2% HOMO => L+7, 9.03% H-2 => L+4, 3.89% H-8 => LUMO
38	20286	493	0.00	84.3% H-15 => LUMO, 7.55% H-17 => LUMO, 5.31% H-14 => L+1
39	20310	492	0.00	80.2% H-5 => L+2, 6.30% H-2 => L+3, 3.14% H-6 => L+1, 2.82% H-7 => L+2, 2.11% H-5 => L+5
40	20333	492	0.00	42.9% H-1 => L+6, 31.6% H-7 => L+1, 6.49% H-6 => L+2, 5.04% H-4 => L+3, 4.47% H-2 => L+4, 2.51% H-3 => L+5, 2.07% HOMO => L+7
41	20419	490	0.11	44.8% H-4 => L+2, 38.2% H-8 => L+1, 3.74% H-3 => L+3, 2.99% H-6 => L+3
42	20862	479	0.04	39.1% H-4 => L+2, 31.6% H-8 => L+1, 10.8% H-3 => L+6, 5.90% H-1 => L+5, 4.64% H-4 => L+5
43	20916	478	0.97	66.4% H-2 => L+5, 11.8% H-3 => L+4, 4.12% H-1 => L+7, 3.59% H-4 => L+1, 3.26% H-10 => L+1, 2.16% H-6 => LUMO
44	20925	478	0.00	53.0% HOMO => L+7, 16.4% H-3 => L+5, 10.3% H-7 => L+1, 5.72% H-4 => L+3, 5.46% H-1 => L+6, 3.13% H-6 => L+2
45	21154	473	0.00	87.4% H-16 => LUMO, 5.20% H-15 => L+1, 4.41% H-17 => L+1

46	21343	469	0.00	84.2% H-17 => LUMO, 8.07% H-16 => L+1, 5.88% H-15 => LUMO
47	21538	464	0.00	62.5% H-2 => L+6, 13.2% H-4 => L+4, 10.3% H-6 => L+1, 3.01% H-5 => L+5, 2.53% H-1 => L+8
48	21600	463	0.08	20.1% HOMO => L+8, 18.7% H-3 => L+6, 17.2% H-9 => L+1, 16.6% H-5 => L+4, 9.75% H-8 => L+1, 6.60% H-4 => L+5, 2.83% H-6 => L+3
49	21711	461	0.00	56.2% H-3 => L+5, 17.3% H-6 => L+2, 14.5% H-4 => L+3, 6.36% HOMO => L+7
50	22000	455	0.29	40.0% H-9 => L+1, 38.2% HOMO => L+8, 7.40% H-5 => L+4, 2.15% H-7 => L+4
51	22226	450	0.27	63.1% H-5 => L+3, 15.9% H-10 => L+1, 4.53% H-1 => L+7, 3.86% H-2 => L+5
52	22400	446	0.00	51.1% H-7 => L+2, 32.8% H-4 => L+4, 4.68% H-2 => L+6, 4.09% H-8 => L+3, 2.43% H-18 => LUMO
53	22547	444	0.05	65.3% H-10 => L+1, 10.3% H-5 => L+3, 7.68% H-13 => L+1, 6.85% H-1 => L+7, 2.20% H-7 => L+3, 2.08% H-8 => L+2
54	22651	441	0.00	90.0% H-11 => L+1, 3.48% H-4 => L+3
55	22666	441	0.01	55.6% H-5 => L+4, 29.9% H-9 => L+1, 6.60% HOMO => L+8, 2.05% H-8 => L+1
56	22714	440	0.00	49.0% H-4 => L+3, 41.0% H-6 => L+2, 3.04% H-11 => L+1, 2.21% H-6 => L+5
57	22830	438	0.00	44.2% H-18 => LUMO, 25.2% H-4 => L+4, 15.6% H-20 => LUMO, 5.80% H-7 => L+2
58	22834	438	0.01	70.8% H-19 => LUMO, 10.8% H-8 => L+2, 4.79% H-21 => LUMO, 4.60% H-7 => L+3, 3.46% H-18 => L+1
59	22971	435	0.00	45.9% H-18 => LUMO, 18.9% H-20 => LUMO, 15.5% H-7 => L+2, 7.81% H-4 => L+4, 2.22% H-19 => L+1
60	23102	433	0.01	52.4% H-21 => LUMO, 23.0% H-13 => L+1, 9.04% H-19 => LUMO, 4.60% H-8 => L+2
61	23120	433	0.14	35.8% H-8 => L+2, 25.8% H-13 => L+1, 12.4% H-19 => LUMO, 9.68% H-1 => L+7, 4.62% H-10 => L+1, 3.79% H-7 => L+3
62	23138	432	0.00	77.7% H-12 => L+1, 5.27% H-5 => L+5, 3.17% H-2 => L+6, 2.56% H-4 => L+4
63	23146	432	0.00	57.9% H-3 => L+6, 10.6% HOMO => L+8, 8.52% H-6 => L+3, 4.30% H-4 => L+5, 3.40% H-10 => L+2, 3.14% H-9 => L+1, 3.01% H-4 => L+2, 2.29% H-8 => L+1
64	23247	430	0.00	59.6% H-20 => LUMO, 10.8% H-7 => L+2, 10.3% H-4 => L+4, 6.82% H-12 => L+1, 4.82% H-2 => L+6, 2.70% H-1 => L+8
65	23315	429	0.05	37.5% H-13 => L+1, 35.9% H-21 => LUMO, 13.1% H-8 => L+2, 3.59% H-7 => L+3, 2.89% H-9 => L+2

66	23800	420	0.00	56.9% H-5 => L+5, 9.90% H-1 => L+8, 6.99% H-11 => L+2, 5.33% H-12 => L+1, 4.87% H-2 => L+6, 4.59% H-9 => L+3, 3.42% H-3 => L+7
67	23926	418	0.22	48.0% H-24 => LUMO, 19.0% H-4 => L+5, 4.97% H-6 => L+3, 4.50% H-5 => L+4, 4.37% HOMO => L+8, 2.60% H-26 => LUMO, 2.05% H-7 => L+4, 2.03% H-28 => LUMO
68	23971	417	0.00	85.3% H-22 => LUMO, 3.21% H-23 => L+1, 2.19% H-9 => L+2
69	23989	417	0.00	92.1% H-23 => LUMO, 3.49% H-22 => L+1
70	24106	415	0.47	23.4% H-1 => L+7, 21.1% H-6 => L+4, 18.2% H-9 => L+2, 9.06% H-5 => L+3, 8.81% H-22 => LUMO, 4.77% H-7 => L+3, 3.88% H-10 => L+1, 2.22% H-5 => L+6
71	24113	415	0.00	49.9% H-25 => LUMO, 9.62% H-6 => L+2, 7.58% H-29 => LUMO, 5.82% HOMO => L+7, 3.01% H-4 => L+3, 2.92% H-27 => LUMO, 2.72% H-31 => LUMO, 2.66% H-39 => LUMO, 2.43% H-1 => L+6
72	24223	413	0.19	35.7% H-4 => L+5, 23.3% H-24 => LUMO, 13.5% H-28 => LUMO, 5.70% H-7 => L+4, 4.65% H-10 => L+2, 3.43% HOMO => L+8, 2.46% H-6 => L+6, 2.34% H-30 => LUMO
73	24342	411	0.00	35.9% H-25 => LUMO, 11.7% H-27 => LUMO, 10.4% H-6 => L+2, 9.35% HOMO => L+7, 5.64% H-4 => L+3, 4.36% H-3 => L+5, 3.64% H-39 => LUMO, 2.77% H-2 => L+4, 2.37% H-1 => L+6, 2.18% H-5 => L+1
74	24385	410	1.49	30.4% H-1 => L+7, 14.1% H-6 => L+4, 13.4% H-5 => L+6, 11.4% H-8 => L+2, 9.80% H-7 => L+3, 4.39% H-2 => L+5, 2.74% H-8 => L+5, 2.23% H-5 => L+3
75	24385	410	0.01	46.5% H-26 => LUMO, 18.0% H-28 => LUMO, 15.6% H-24 => LUMO, 4.97% H-30 => LUMO, 4.85% H-6 => L+3
76	24503	408	0.00	32.2% H-27 => LUMO, 21.3% H-4 => L+6, 8.38% H-6 => L+5, 6.47% H-8 => L+4, 3.75% H-29 => LUMO, 3.36% H-3 => L+5, 3.33% H-10 => L+3, 2.72% H-4 => L+3, 2.46% H-12 => L+2, 2.35% H-25 => LUMO
77	24514	408	0.04	33.2% H-6 => L+3, 22.3% H-28 => LUMO, 16.0% H-4 => L+5, 11.0% H-30 => LUMO, 4.99% H-7 => L+4, 2.80% H-10 => L+2
78	24614	406	0.00	28.7% H-8 => L+3, 28.4% H-11 => L+2, 20.4% H-1 => L+8, 7.80% H-7 => L+5, 2.83% H-9 => L+3, 2.32% H-2 => L+6, 2.17% H-3 => L+7
79	24636	406	0.00	39.9% H-26 => LUMO, 16.7% H-6 => L+3, 15.0% H-28 => LUMO, 8.55% H-30 => LUMO, 5.53% H-7 => L+4, 2.79% H-2 => L+7, 2.63% HOMO => L+8, 2.42% H-24 => LUMO

80	24668	405	0.31	36.2% H-9 => L+2, 27.1% H-6 => L+4, 10.4% H-8 => L+2, 8.30% H-7 => L+3, 7.20% H-5 => L+6, 3.87% H-1 => L+7
81	24735	404	0.00	42.0% H-27 => LUMO, 18.9% H-4 => L+6, 7.77% H-8 => L+4, 6.66% H-6 => L+5, 3.89% H-25 => LUMO, 3.16% HOMO => L+7, 3.02% H-2 => L+8, 2.73% H-6 => L+2, 2.56% H-12 => L+2
82	24881	402	0.00	85.3% H-14 => L+1, 4.06% H-15 => LUMO, 2.60% H-15 => L+4, 2.05% H-16 => L+1
83	24950	401	0.07	60.8% H-30 => LUMO, 19.6% H-28 => LUMO, 6.59% H-10 => L+2, 3.80% H-24 => LUMO, 2.32% H-29 => L+1, 2.20% H-26 => LUMO
84	24952	401	0.00	83.2% H-29 => LUMO, 6.05% H-27 => LUMO, 2.99% H-25 => LUMO
85	24996	400	0.02	47.2% H-1 => L+8, 18.3% H-5 => L+5, 15.5% H-11 => L+2, 3.04% H-8 => L+3, 2.48% H-9 => L+3, 2.05% H-4 => L+4
86	25026	400	0.02	35.0% H-10 => L+2, 18.2% H-7 => L+4, 8.44% H-13 => L+2, 6.17% H-28 => LUMO, 5.97% H-2 => L+7, 3.67% H-5 => L+4, 3.44% H-30 => LUMO, 2.99% HOMO => L+8, 2.67% H-26 => LUMO, 2.23% H-14 => L+1
87	25071	399	0.07	40.1% H-7 => L+4, 31.1% H-10 => L+2, 12.9% H-6 => L+3, 3.67% H-12 => L+3, 3.31% H-30 => LUMO, 2.06% H-13 => L+2
88	25144	398	0.87	42.5% H-7 => L+3, 24.2% H-9 => L+2, 11.5% H-6 => L+4, 7.65% H-1 => L+7, 2.63% H-8 => L+5
89	25284	396	0.00	65.3% H-12 => L+2, 16.9% H-4 => L+6, 7.23% H-13 => L+3, 4.23% H-10 => L+3
90	25337	395	0.00	93.8% H-33 => LUMO, 2.39% H-39 => LUMO
91	25354	394	0.25	70.7% H-13 => L+2, 12.1% H-7 => L+4, 8.76% H-12 => L+3
92	25374	394	0.00	45.3% H-5 => L+6, 16.7% H-6 => L+4, 8.42% H-34 => LUMO, 5.03% H-9 => L+5, 4.75% H-7 => L+3, 3.52% H-7 => L+6, 2.76% H-43 => LUMO, 2.54% H-9 => L+2
93	25440	393	0.00	71.9% H-36 => LUMO, 19.0% H-38 => LUMO, 3.50% H-41 => LUMO, 2.09% H-8 => L+3
94	25443	393	0.03	82.9% H-34 => LUMO, 4.04% H-5 => L+6, 3.05% H-37 => LUMO, 2.05% H-40 => LUMO
95	25449	393	0.00	47.5% H-35 => LUMO, 42.7% H-32 => LUMO, 2.62% H-13 => L+2, 2.29% H-2 => L+7
96	25533	392	0.00	74.8% H-15 => L+1, 11.0% H-17 => L+1, 6.34% H-14 => L+4, 2.62% H-14 => LUMO, 2.11% H-16 => LUMO
97	25548	391	0.00	67.2% H-31 => LUMO, 17.2% H-39 => LUMO
98	25556	391	0.00	37.3% H-11 => L+2, 28.3% H-8 => L+3, 11.2% H-7 => L+5, 5.17% H-1 => L+8, 3.04% H-11 => L+5, 2.06% H-41 => LUMO
99	25690	389	0.01	47.2% H-35 => LUMO, 46.9% H-32 => LUMO

100	25724	389	0.00	54.6% H-39 => LUMO, 16.7% H-8 => L+4, 16.6% H-31 => LUMO, 3.93% H-33 => LUMO
101	25773	388	0.00	58.1% H-8 => L+4, 14.9% H-39 => LUMO, 6.26% H-4 => L+6, 5.09% H-31 => LUMO, 4.57% H-12 => L+2
102	25800	388	0.01	57.4% H-37 => LUMO, 24.1% H-40 => LUMO, 5.80% H-34 => LUMO
103	25815	387	0.00	49.2% H-38 => LUMO, 23.1% H-36 => LUMO, 21.6% H-41 => LUMO
104	25941	385	0.00	20.5% H-37 => LUMO, 17.5% H-8 => L+5, 16.1% H-7 => L+6, 10.7% H-11 => L+3, 8.45% H-43 => LUMO, 6.16% H-5 => L+6, 4.56% H-40 => LUMO, 3.71% H-9 => L+5, 2.06% H-7 => L+3
105	26003	385	0.00	22.1% H-9 => L+3, 17.4% H-8 => L+3, 16.7% H-7 => L+5, 11.1% H-41 => LUMO, 8.66% H-38 => LUMO, 7.54% H-8 => L+6, 3.71% H-44 => LUMO, 2.70% H-11 => L+5
106	26072	384	0.28	63.4% H-2 => L+7, 12.3% H-42 => LUMO, 4.18% H-6 => L+3, 3.40% H-32 => LUMO, 3.15% H-4 => L+5
107	26098	383	0.00	56.8% H-41 => LUMO, 18.4% H-38 => LUMO, 7.56% H-9 => L+3, 5.78% H-7 => L+5
108	26106	383	0.00	62.2% H-40 => LUMO, 13.8% H-37 => LUMO, 4.21% H-14 => L+2, 4.09% H-8 => L+5, 3.71% H-7 => L+6, 2.58% H-11 => L+3
109	26149	382	0.07	69.0% H-14 => L+2, 9.15% H-15 => L+3, 3.82% H-17 => L+6, 2.96% H-16 => L+5, 2.80% H-14 => L+5, 2.35% H-40 => LUMO
110	26244	381	0.00	56.6% H-6 => L+5, 21.1% H-4 => L+6, 6.80% H-2 => L+8, 4.93% H-12 => L+2, 2.78% H-10 => L+6
111	26476	378	0.00	81.0% H-16 => L+1, 6.56% H-17 => LUMO, 4.03% H-15 => LUMO, 3.60% H-17 => L+4, 2.48% H-15 => L+4
112	26566	376	0.00	48.1% H-15 => L+2, 20.2% H-14 => L+3, 6.52% H-3 => L+7, 5.93% H-17 => L+5, 3.72% H-17 => L+2, 3.67% H-16 => L+3, 3.32% H-14 => L+6, 3.05% H-16 => L+6
113	26608	376	0.00	67.4% H-17 => L+1, 7.55% H-15 => L+1, 7.04% H-16 => LUMO, 5.91% H-16 => L+4, 4.91% H-2 => L+8, 3.66% H-9 => L+4
114	26617	376	0.01	79.7% H-43 => LUMO, 4.97% H-11 => L+3, 3.88% H-8 => L+5, 3.80% H-7 => L+6, 2.33% H-9 => L+5
115	26617	376	0.01	59.7% H-3 => L+7, 6.37% H-9 => L+3, 5.90% H-8 => L+3, 4.57% H-7 => L+5, 4.44% H-1 => L+8, 2.91% H-15 => L+2, 2.76% H-10 => L+4
116	26657	375	0.00	43.1% H-2 => L+8, 29.2% H-9 => L+4, 8.39% H-17 => L+1, 8.25% H-6 => L+5
117	26799	373	0.00	64.7% H-10 => L+3, 13.0% H-13 => L+3, 5.46% H-13 => L+6, 3.76% H-10 => L+6

118	26870	372	0.01	41.1% H-9 => L+3, 14.1% H-7 => L+5, 13.8% H-44 => LUMO, 13.7% H-3 => L+7, 3.85% H-7 => L+2, 2.31% H-11 => L+2
119	26872	372	0.00	59.1% H-9 => L+4, 24.6% H-2 => L+8, 6.28% H-6 => L+5, 2.34% H-4 => L+6
120	26936	371	0.28	44.8% H-6 => L+6, 22.5% H-12 => L+3, 13.9% H-10 => L+5, 4.83% H-13 => L+5, 4.39% H-13 => L+2
121	27017	370	0.00	41.4% H-44 => LUMO, 36.4% H-10 => L+4, 9.54% H-7 => L+5, 3.94% H-9 => L+3
122	27021	370	0.00	38.8% H-16 => L+2, 19.6% H-15 => L+3, 15.8% H-17 => L+3, 9.23% H-14 => L+5, 8.21% H-16 => L+5, 4.55% H-15 => L+6
123	27128	369	0.11	50.4% H-42 => LUMO, 29.5% H-11 => L+4, 3.32% H-6 => L+6, 3.12% H-2 => L+7, 2.82% H-10 => L+2
124	27167	368	0.00	42.4% H-17 => L+2, 28.6% H-16 => L+3, 15.7% H-15 => L+5, 9.14% H-14 => L+6
125	27234	367	0.07	31.5% H-3 => L+8, 28.3% H-11 => L+3, 14.6% H-8 => L+5, 8.03% H-5 => L+6, 4.09% H-9 => L+5, 2.96% H-4 => L+7
126	27243	367	0.00	42.9% H-10 => L+4, 26.6% H-44 => LUMO, 13.4% H-13 => L+4, 5.41% H-7 => L+5, 2.07% H-3 => L+7
127	27287	366	0.00	53.6% H-13 => L+3, 21.8% H-12 => L+5, 6.49% H-10 => L+6, 5.94% H-12 => L+2, 4.77% H-10 => L+3, 2.01% H-6 => L+5
128	27443	364	0.09	51.2% H-11 => L+4, 13.9% H-6 => L+6, 11.0% H-12 => L+3, 10.2% H-42 => LUMO, 3.39% H-13 => L+5
129	27445	364	0.14	40.1% H-3 => L+8, 21.0% H-11 => L+3, 13.2% H-8 => L+5, 9.20% H-45 => LUMO, 3.54% H-11 => L+6, 2.18% H-4 => L+7
130	27548	363	0.02	26.2% H-6 => L+6, 19.8% H-12 => L+3, 17.9% H-42 => LUMO, 13.4% H-11 => L+4, 5.38% H-13 => L+5, 4.30% H-4 => L+5, 2.19% H-10 => L+5, 2.14% H-12 => L+6, 2.02% H-2 => L+7
131	27745	360	0.02	50.9% H-18 => L+1, 36.4% H-12 => L+4, 2.60% H-19 => LUMO, 2.12% H-45 => LUMO, 2.10% H-19 => L+4
132	27756	360	0.00	71.2% H-19 => L+1, 16.0% H-13 => L+4, 3.70% H-18 => LUMO, 2.85% H-18 => L+4
133	27791	360	0.00	39.6% H-12 => L+4, 27.2% H-18 => L+1, 15.2% H-20 => L+1, 9.85% H-45 => LUMO
134	27859	359	0.00	65.1% H-13 => L+4, 16.0% H-19 => L+1, 9.06% H-10 => L+4
135	27947	358	0.10	70.9% H-20 => L+1, 10.6% H-18 => L+1, 8.83% H-12 => L+4
136	28016	357	0.02	31.4% H-9 => L+5, 21.4% H-8 => L+5, 19.6% H-7 => L+6, 15.5% H-11 => L+3, 2.52% H-11 => L+6, 2.39% H-5 => L+6

137	28024	357	0.00	89.0% H-21 => L+1, 2.21% H-20 => L+4
138	28260	354	0.00	39.3% H-7 => L+6, 28.6% H-9 => L+5, 13.1% H-11 => L+6, 5.18% H-7 => L+3, 4.71% H-3 => L+8, 2.37% H-8 => L+5
139	28363	353	0.00	52.9% H-8 => L+6, 19.2% H-11 => L+5, 15.0% H-7 => L+5, 2.48% H-9 => L+6, 2.40% H-11 => L+2
140	28375	352	0.15	63.1% H-45 => LUMO, 8.11% H-12 => L+4, 6.57% H-3 => L+8, 5.44% H-20 => L+1, 4.17% H-8 => L+5, 2.05% H-44 => L+1, 2.01% H-9 => L+5
141	28585	350	0.00	37.4% H-10 => L+5, 28.3% H-12 => L+3, 18.4% H-12 => L+6, 6.47% H-13 => L+5, 3.39% H-10 => L+2, 2.63% H-13 => L+2
142	28677	349	0.00	33.0% H-9 => L+6, 30.5% H-11 => L+5, 22.1% H-8 => L+6, 2.31% H-4 => L+8
143	28717	348	0.00	39.7% H-12 => L+5, 15.7% H-13 => L+3, 12.9% H-13 => L+6, 10.5% H-10 => L+6, 6.69% H-10 => L+3, 6.59% H-12 => L+2, 3.47% H-46 => LUMO
144	28823	347	0.00	78.3% H-46 => LUMO, 2.78% H-10 => L+3, 2.06% H-2 => L+8
145	28893	346	0.00	85.3% H-22 => L+1, 3.75% H-23 => LUMO, 3.56% H-47 => LUMO, 2.45% H-23 => L+4
146	28913	346	0.01	90.0% H-23 => L+1, 3.77% H-22 => LUMO, 2.56% H-22 => L+4
147	28938	346	0.00	79.6% H-24 => L+1, 6.69% H-28 => L+1, 2.08% H-25 => LUMO
148	28980	345	0.00	63.5% H-25 => L+1, 10.2% H-29 => L+1, 7.98% H-20 => L+2, 2.54% H-27 => L+1, 2.43% H-39 => L+1, 2.35% H-31 => L+1
149	29075	344	0.00	43.8% H-28 => L+1, 23.3% H-30 => L+1, 11.8% H-21 => L+2, 6.42% H-26 => L+1, 2.27% H-24 => L+1
150	29186	343	0.01	39.4% H-27 => L+1, 15.8% H-18 => L+2, 8.97% H-19 => L+3, 8.81% H-25 => L+1, 5.27% H-29 => L+1, 4.80% H-20 => L+2, 2.94% H-39 => L+1, 2.19% H-18 => L+5, 2.15% H-26 => LUMO
151	29236	342	0.00	44.4% H-26 => L+1, 19.5% H-19 => L+2, 11.7% H-18 => L+3, 3.63% H-30 => L+1, 3.58% H-5 => L+7, 2.97% H-19 => L+5
152	29271	342	0.00	82.1% H-47 => LUMO, 5.11% H-22 => L+1, 3.35% H-45 => L+1
153	29332	341	0.06	82.4% H-4 => L+7, 3.91% H-6 => L+8, 3.82% H-3 => L+8
154	29338	341	0.01	54.1% H-13 => L+5, 31.1% H-10 => L+5, 4.55% H-12 => L+6, 2.98% H-13 => L+2, 2.10% H-6 => L+6
155	29409	340	0.00	81.7% H-14 => L+4, 4.34% H-16 => L+4, 4.00% H-15 => L+1, 2.91% H-5 => L+7, 2.11% H-17 => L+1
156	29455	340	0.00	68.9% H-5 => L+7, 12.6% H-26 => L+1, 3.24% H-2 => L+8, 3.18% H-14 => L+4

157	29600	338	0.00	35.8% H-18 => L+2, 19.2% H-19 => L+3, 13.3% H-25 => L+1, 7.65% H-27 => L+1, 4.62% H-18 => L+5, 4.39% H-20 => L+2, 4.20% H-29 => L+1
158	29656	337	0.00	34.2% H-19 => L+2, 20.5% H-26 => L+1, 16.9% H-18 => L+3, 9.46% H-5 => L+7, 3.76% H-19 => L+5, 2.44% H-24 => L+1, 2.01% H-30 => L+1
159	29729	336	0.00	51.1% H-10 => L+6, 25.0% H-13 => L+6, 6.45% H-13 => L+3, 5.33% H-10 => L+3
160	29763	336	0.03	39.1% H-27 => L+1, 29.4% H-29 => L+1, 9.22% H-20 => L+2, 6.10% H-25 => L+1, 2.59% H-18 => L+2, 2.58% H-39 => L+1
161	29801	336	0.00	40.8% H-30 => L+1, 35.4% H-28 => L+1, 4.25% H-24 => L+1, 4.01% H-26 => L+1, 2.71% H-35 => L+1, 2.19% H-29 => LUMO
162	29868	335	0.00	38.5% H-33 => L+1, 26.3% H-29 => L+1, 12.1% H-20 => L+2, 7.70% H-39 => L+1, 2.11% H-28 => L+4, 2.06% H-36 => L+2
163	29914	334	0.00	42.2% H-9 => L+6, 35.7% H-11 => L+5, 8.41% H-4 => L+8, 4.81% H-8 => L+6
164	30016	333	0.00	45.0% H-14 => L+3, 21.1% H-15 => L+2, 20.7% H-34 => L+1, 3.01% H-15 => L+5
165	30039	333	0.00	52.5% H-34 => L+1, 16.3% H-14 => L+3, 7.23% H-15 => L+2, 6.57% H-4 => L+8
166	30072	333	0.00	64.3% H-36 => L+1, 18.1% H-38 => L+1, 5.10% H-33 => L+2, 4.11% H-41 => L+1, 2.57% H-34 => L+4
167	30106	332	0.01	39.0% H-33 => L+1, 14.1% H-5 => L+8, 10.5% H-31 => L+1, 9.45% H-29 => L+1, 8.19% H-20 => L+2, 2.68% H-23 => L+2
168	30125	332	0.00	35.9% H-35 => L+1, 20.4% H-32 => L+1, 13.3% H-30 => L+1, 8.27% HOMO => L+9, 7.95% H-21 => L+2, 2.07% H-22 => L+2, 2.05% H-34 => L+2
169	30134	332	0.00	57.4% H-4 => L+8, 9.11% H-9 => L+6, 8.39% H-6 => L+7, 7.19% H-34 => L+1, 3.22% H-47 => LUMO, 2.48% H-11 => L+5
170	30138	332	0.13	68.2% H-5 => L+8, 6.25% H-33 => L+1, 3.89% H-29 => L+1, 3.51% H-48 => LUMO, 3.44% H-20 => L+2, 2.63% H-8 => L+7, 2.20% H-2 => L+7
171	30187	331	0.01	74.2% H-11 => L+6, 13.8% H-9 => L+5, 3.90% H-11 => L+3, 3.43% H-7 => L+6, 2.14% H-8 => L+5
172	30230	331	0.00	68.4% H-15 => L+4, 22.2% H-17 => L+4, 3.33% H-14 => L+1
173	30311	330	0.00	52.5% H-21 => L+2, 14.3% HOMO => L+9, 7.10% H-30 => L+1, 5.90% H-35 => L+1, 3.26% H-28 => L+1, 2.83% H-49 => LUMO, 2.35% H-20 => L+3
174	30439	329	0.04	32.9% H-31 => L+1, 27.7% H-48 => LUMO, 20.8% H-20 => L+2, 5.24% H-39 => L+1, 2.02% H-29 => L+1
175	30447	328	0.00	52.2% HOMO => L+9, 18.3% H-32 => L+1, 5.42% H-21 => L+2, 2.99% H-22 => L+2

176	30464	328	0.00	38.5% H-15 => L+3, 27.8% H-16 => L+2, 13.6% H-14 => L+2, 5.34% H-14 => L+5, 4.93% H-17 => L+3, 4.76% H-16 => L+5, 3.79% H-17 => L+6
177	30576	327	0.00	48.9% H-32 => L+1, 33.7% H-35 => L+1, 4.09% HOMO => L+9, 3.14% H-22 => L+2
178	30576	327	0.07	42.0% H-31 => L+1, 21.1% H-48 => LUMO, 19.5% H-39 => L+1, 2.49% H-23 => L+2
179	30676	326	0.00	58.4% H-37 => L+1, 22.2% H-40 => L+1, 4.15% H-34 => L+1, 2.30% H-26 => L+2
180	30679	326	0.00	42.1% H-38 => L+1, 22.9% H-41 => L+1, 22.0% H-36 => L+1, 3.21% H-27 => L+2, 2.17% H-37 => LUMO
181	30724	325	0.16	34.4% H-39 => L+1, 34.3% H-48 => LUMO, 10.9% H-20 => L+2, 4.44% H-23 => L+2, 2.13% H-22 => L+3
182	30790	325	0.00	28.8% H-24 => L+2, 16.3% H-25 => L+3, 12.9% H-26 => L+2, 6.46% H-17 => L+2, 4.79% H-27 => L+3, 4.02% H-37 => L+1, 2.47% H-26 => L+5, 2.42% H-30 => L+2, 2.35% H-24 => L+5
183	30799	325	0.15	42.0% H-25 => L+2, 14.5% H-24 => L+3, 9.82% H-26 => L+3, 6.23% H-27 => L+2, 3.98% H-38 => L+1, 3.33% H-25 => L+5, 2.37% H-27 => L+5, 2.27% H-29 => L+2, 2.24% H-41 => L+1, 2.20% H-36 => L+1
184	30814	325	0.00	48.6% H-23 => L+2, 20.6% H-22 => L+3, 13.3% H-39 => L+1, 3.91% H-23 => L+5, 2.37% H-29 => L+1
185	30819	324	0.00	50.9% H-22 => L+2, 21.4% H-23 => L+3, 7.02% H-35 => L+1, 4.00% H-22 => L+5, 2.90% HOMO => L+9, 2.07% H-30 => L+1
186	30840	324	0.00	29.1% H-17 => L+2, 11.2% H-16 => L+3, 7.78% H-15 => L+5, 6.28% H-28 => L+2, 5.93% H-15 => L+2, 5.85% H-24 => L+2, 5.44% H-37 => L+1, 5.05% H-17 => L+5, 4.24% H-14 => L+6, 2.20% H-43 => L+1
187	30935	323	0.00	49.0% H-40 => L+1, 19.1% H-37 => L+1, 3.57% H-17 => L+2, 3.06% H-43 => L+1, 2.48% H-26 => L+2, 2.46% H-28 => L+2, 2.08% H-24 => L+2
188	30936	323	0.03	60.2% H-41 => L+1, 25.2% H-38 => L+1, 3.56% H-25 => L+2, 2.48% H-40 => LUMO
189	30965	323	0.00	19.8% H-28 => L+2, 15.7% H-40 => L+1, 11.5% H-30 => L+2, 9.83% H-43 => L+1, 6.14% H-20 => L+4, 5.54% H-17 => L+2, 5.13% HOMO => L+13, 4.21% HOMO => L+15
190	30971	323	0.00	25.6% H-16 => L+2, 23.8% H-17 => L+3, 15.4% H-15 => L+6, 11.6% H-14 => L+5, 8.16% H-15 => L+3, 4.52% H-16 => L+5, 3.90% H-14 => L+2
191	30990	323	0.00	34.1% H-13 => L+6, 25.4% H-49 => LUMO, 20.5% H-12 => L+5, 8.93% H-10 => L+6
192	31014	322	0.00	68.4% H-12 => L+6, 20.1% H-13 => L+5, 7.74% H-10 => L+5

193	31025	322	0.00	48.8% H-49 => LUMO, 14.7% H-13 => L+6, 9.05% HOMO => L+11, 8.88% H-10 => L+6, 7.11% H-12 => L+5, 2.64% H-7 => L+7
194	31060	322	0.00	55.2% HOMO => L+12, 39.1% HOMO => L+10
195	31068	322	0.00	66.8% HOMO => L+11, 14.6% HOMO => L+16, 9.81% H-49 => LUMO
196	31109	321	0.00	28.5% H-27 => L+2, 12.0% H-29 => L+2, 7.05% HOMO => L+17, 6.39% H-21 => L+4, 5.42% H-26 => L+3, 5.19% H-39 => L+2, 3.73% H-44 => L+1, 3.24% HOMO => L+14, 2.93% H-25 => L+2, 2.12% H-30 => L+3
197	31205	320	0.00	42.4% HOMO => L+13, 40.9% HOMO => L+15, 5.57% H-28 => L+2
198	31298	320	0.00	39.0% H-26 => L+2, 25.2% H-24 => L+2, 10.5% H-27 => L+3, 4.95% H-30 => L+2, 3.39% H-34 => L+1, 2.86% H-37 => L+1
199	31319	319	0.00	50.3% HOMO => L+10, 38.2% HOMO => L+12, 4.13% HOMO => L+18
200	31326	319	0.04	62.2% HOMO => L+17, 22.1% HOMO => L+14, 4.44% H-27 => L+2
201	31382	319	0.00	43.7% H-14 => L+5, 20.4% H-17 => L+3, 16.2% H-16 => L+5, 6.66% H-14 => L+2, 6.06% H-17 => L+6, 2.06% H-15 => L+6
202	31451	318	0.00	80.6% H-16 => L+4, 5.18% H-17 => L+1, 4.40% H-14 => L+4, 3.12% H-15 => L+1, 2.52% H-15 => L+7
203	31525	317	0.00	35.5% HOMO => L+16, 24.9% H-7 => L+7, 10.8% HOMO => L+11, 10.5% HOMO => L+19, 6.31% H-8 => L+8
204	31531	317	0.00	66.2% H-17 => L+4, 19.4% H-15 => L+4, 7.21% H-16 => L+1, 3.11% H-16 => L+7
205	31556	317	0.00	67.9% H-6 => L+7, 13.6% H-4 => L+8, 8.13% H-43 => L+1, 2.91% H-30 => L+2
206	31568	317	0.00	27.6% HOMO => L+15, 26.6% HOMO => L+13, 9.69% H-14 => L+6, 5.24% H-17 => L+5, 3.35% H-15 => L+5, 3.12% H-30 => L+2, 3.08% H-16 => L+3, 2.24% H-2 => L+14, 2.22% HOMO => L+20, 2.19% H-15 => L+2, 2.15% H-29 => L+3
207	31572	317	0.00	30.5% H-42 => L+1, 20.9% H-7 => L+7, 18.1% HOMO => L+16, 6.49% HOMO => L+19, 4.82% H-8 => L+8, 2.19% HOMO => L+11
208	31585	317	0.03	61.6% HOMO => L+14, 21.1% HOMO => L+17, 2.02% H-2 => L+13
209	31602	316	0.00	23.8% H-14 => L+6, 14.8% HOMO => L+13, 14.3% HOMO => L+15, 12.5% H-17 => L+5, 8.16% H-15 => L+5, 7.72% H-16 => L+3, 5.17% H-15 => L+2, 3.40% H-16 => L+6, 2.21% H-17 => L+2
210	31715	315	0.00	63.3% H-43 => L+1, 13.6% H-28 => L+2, 8.67% H-6 => L+7, 2.62% H-20 => L+4

211	31760	315	0.02	19.2% H-29 => L+2, 15.9% H-27 => L+2, 11.3% H-25 => L+2, 8.20% H-24 => L+3, 6.93% H-44 => L+1, 5.65% H-26 => L+3, 5.54% H-30 => L+3, 4.54% H-39 => L+2, 4.31% H-1 => L+9, 3.19% H-28 => L+3, 2.91% H-27 => L+5, 2.16% H-21 => L+4
212	31761	315	0.00	60.0% HOMO => L+20, 22.1% HOMO => L+22, 3.20% H-30 => L+2
213	31802	314	0.01	36.6% H-8 => L+7, 25.2% H-7 => L+8, 9.54% H-18 => L+2, 7.05% H-9 => L+7, 3.80% H-48 => LUMO, 2.94% H-19 => L+3
214	31809	314	0.01	19.8% HOMO => L+23, 16.5% H-29 => L+2, 12.5% H-44 => L+1, 10.2% HOMO => L+21, 5.11% H-39 => L+2, 4.23% H-30 => L+3, 4.11% H-28 => L+3, 3.70% H-31 => L+2, 3.22% H-50 => LUMO, 2.13% H-33 => L+2, 2.05% H-1 => L+9
215	31825	314	0.00	27.6% H-30 => L+2, 15.1% H-28 => L+2, 13.3% H-29 => L+3, 7.13% HOMO => L+20, 4.05% H-6 => L+7, 3.48% H-24 => L+2, 3.46% HOMO => L+13, 2.68% H-27 => L+3, 2.50% HOMO => L+15, 2.22% H-25 => L+3, 2.12% H-14 => L+6
216	31841	314	0.01	42.2% HOMO => L+23, 18.2% HOMO => L+21, 9.26% H-44 => L+1, 6.74% H-29 => L+2, 2.66% HOMO => L+14, 2.15% H-30 => L+3
217	31892	314	0.00	28.1% H-42 => L+1, 14.2% H-7 => L+7, 14.0% HOMO => L+29, 7.61% H-34 => L+2, 6.00% HOMO => L+27, 3.77% HOMO => L+19, 3.68% HOMO => L+16, 2.90% H-19 => L+2, 2.03% H-8 => L+8
218	31931	313	0.01	48.5% HOMO => L+18, 40.7% HOMO => L+26
219	31954	313	0.00	71.7% HOMO => L+19, 17.5% HOMO => L+16, 4.22% H-2 => L+18

Table S3.16. TDDFT-predicted band excitation data for **3.4**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	4899	2041	3.54	98.9% HOMO => LUMO
1	5948	1681	0.00	97.3% H-1 => LUMO
2	8001	1250	0.00	85.1% H-3 => LUMO, 12.5% H-1 => L+1
3	8126	1231	0.00	74.0% H-2 => LUMO, 24.2% HOMO => L+1
4	8558	1169	0.00	72.5% HOMO => L+1, 22.4% H-2 => LUMO
5	10296	971	0.00	84.9% H-1 => L+1, 12.8% H-3 => LUMO
6	10421	960	0.00	78.5% H-4 => LUMO, 13.9% H-3 => L+1, 4.30% H-1 => L+2
7	11029	907	0.18	90.4% H-5 => LUMO, 2.39% H-2 => L+1
8	11810	847	0.03	70.0% HOMO => L+2, 21.1% H-2 => L+1

9	12086	827	0.00	83.3% HOMO => L+3, 8.93% H-3 => L+1, 3.05% H-4 => LUMO
10	12114	826	0.18	68.9% H-2 => L+1, 24.5% HOMO => L+2, 2.11% H-5 => LUMO
11	12290	814	0.00	60.8% H-3 => L+1, 15.2% H-4 => LUMO, 13.5% HOMO => L+3, 7.32% H-1 => L+2
12	12731	786	0.00	75.4% H-6 => LUMO, 12.1% H-4 => L+1, 4.31% H-3 => L+2, 2.42% H-1 => L+6
13	12865	777	0.00	80.9% H-7 => LUMO, 7.04% H-9 => LUMO, 5.16% H-5 => L+1
14	13407	746	0.00	91.1% HOMO => L+4, 3.43% H-2 => L+3
15	14040	712	0.00	83.2% H-1 => L+2, 12.1% H-3 => L+1
16	14141	707	4.38	91.2% H-1 => L+3, 3.83% H-3 => L+4
17	14475	691	0.00	55.1% H-4 => L+1, 19.1% H-6 => LUMO, 14.4% H-3 => L+2, 5.40% H-1 => L+6
18	14724	679	0.00	30.1% HOMO => L+6, 20.7% H-9 => LUMO, 16.7% H-5 => L+1, 13.8% H-7 => LUMO, 13.2% H-2 => L+2, 2.06% H-10 => L+1
19	14758	678	0.15	83.5% H-8 => LUMO, 10.2% HOMO => L+8
20	14944	669	0.00	87.1% HOMO => L+5, 3.66% H-14 => LUMO, 3.29% H-2 => L+4
21	15202	658	0.00	65.6% H-5 => L+1, 24.0% HOMO => L+6, 4.23% H-9 => LUMO
22	15520	644	0.00	54.1% H-9 => LUMO, 21.5% HOMO => L+6, 5.01% H-1 => L+7, 4.41% H-1 => L+4, 4.09% H-2 => L+2, 2.47% H-3 => L+5
23	15631	640	0.00	80.8% H-10 => LUMO, 5.70% H-11 => LUMO, 3.88% H-9 => L+1, 2.59% H-1 => L+5
24	15665	638	0.00	87.5% H-2 => L+3, 4.17% HOMO => L+4
25	15800	633	0.00	71.7% H-2 => L+2, 18.8% HOMO => L+6, 4.48% H-5 => L+1
26	15897	629	0.00	26.5% H-3 => L+2, 21.0% HOMO => L+7, 18.5% H-4 => L+1, 10.8% H-1 => L+6, 10.5% H-13 => LUMO, 2.79% H-2 => L+3, 2.54% H-6 => L+2, 2.46% H-8 => L+1
27	16034	624	0.00	69.1% H-1 => L+4, 11.3% H-3 => L+3, 7.09% H-12 => LUMO, 4.55% H-9 => LUMO, 2.09% H-3 => L+5
28	16153	619	0.00	40.5% HOMO => L+7, 28.1% H-3 => L+2, 9.32% H-4 => L+1, 8.96% H-13 => LUMO, 3.52% H-1 => L+6, 2.48% H-8 => L+1
29	16246	616	0.03	71.7% H-11 => LUMO, 6.45% H-1 => L+8, 6.09% H-10 => LUMO, 5.58% H-7 => L+1, 2.29% H-3 => L+7
30	16771	596	0.00	73.6% H-12 => LUMO, 13.8% H-1 => L+4, 4.39% H-3 => L+3
31	16805	595	0.01	27.7% H-6 => L+1, 25.6% HOMO => L+8, 14.5% H-2 => L+4, 9.03% H-8 => LUMO, 7.52% H-14 => LUMO, 4.94% H-4 => L+2, 2.45% H-2 => L+7

32	16857	593	0.00	58.2% H-2 => L+4, 13.7% H-6 => L+1, 6.77% HOMO => L+8, 4.89% HOMO => L+5, 4.73% H-5 => L+3, 3.02% H-17 => LUMO
33	16903	592	0.00	77.6% H-3 => L+3, 9.06% H-12 => LUMO, 7.37% H-1 => L+4
34	17113	584	0.69	87.9% H-15 => LUMO, 5.08% H-12 => L+1, 2.24% H-5 => L+2
35	17313	578	0.00	69.2% H-13 => LUMO, 21.4% HOMO => L+7
36	17489	572	0.00	71.6% H-1 => L+6, 21.2% H-3 => L+2
37	17516	571	0.00	72.9% H-7 => L+1, 9.35% H-11 => LUMO, 3.07% H-1 => L+8, 2.98% H-5 => L+2, 2.78% H-3 => L+7, 2.75% H-1 => L+5
38	17684	565	0.04	54.0% H-14 => LUMO, 24.0% H-17 => LUMO, 8.27% H-6 => L+1, 3.59% HOMO => L+5, 3.12% H-2 => L+4
39	17901	559	0.00	80.9% H-1 => L+5, 3.75% H-11 => LUMO, 2.70% H-4 => L+3, 2.31% H-9 => L+1
40	17937	558	0.00	76.7% H-16 => LUMO, 10.2% H-2 => L+5, 2.38% H-8 => L+1
41	17939	557	0.37	37.7% H-6 => L+1, 28.4% HOMO => L+8, 16.2% H-17 => LUMO, 6.69% H-4 => L+2, 2.48% H-3 => L+6
42	18091	553	0.02	49.1% H-17 => LUMO, 24.9% H-14 => LUMO, 7.27% H-2 => L+4, 5.15% HOMO => L+8, 5.14% H-4 => L+2, 2.31% H-6 => L+1
43	18177	550	0.60	57.2% H-3 => L+4, 10.8% H-5 => L+2, 5.24% H-1 => L+8, 3.70% H-2 => L+6, 3.39% H-1 => L+3, 2.91% H-9 => L+1, 2.65% H-4 => L+5, 2.60% H-7 => L+1, 2.60% H-15 => LUMO, 2.06% H-4 => L+3
44	18466	542	0.00	42.9% H-2 => L+5, 19.6% H-8 => L+1, 13.7% H-16 => LUMO, 7.45% HOMO => L+7, 5.48% H-5 => L+4, 3.93% H-13 => LUMO
45	18475	541	0.32	25.9% H-3 => L+4, 25.5% H-2 => L+6, 20.5% H-5 => L+2, 7.51% H-7 => L+1, 6.00% H-1 => L+8, 3.70% H-3 => L+7, 3.20% H-11 => LUMO, 2.49% H-9 => L+1
46	18897	529	0.06	68.0% H-5 => L+3, 9.85% H-4 => L+2, 6.79% H-2 => L+4, 3.27% HOMO => L+8, 2.90% H-2 => L+7, 2.11% H-5 => L+5, 2.10% H-17 => LUMO
47	18936	528	0.00	42.8% H-1 => L+7, 31.1% H-10 => L+1, 6.98% H-9 => LUMO, 4.17% H-3 => L+5, 2.69% H-3 => L+8, 2.10% H-7 => L+2
48	18978	527	0.30	54.7% H-4 => L+2, 14.3% H-5 => L+3, 13.9% HOMO => L+8, 5.40% H-2 => L+7, 2.88% H-7 => L+4, 2.70% H-14 => LUMO
49	19070	524	0.04	43.6% H-9 => L+1, 33.4% H-4 => L+3, 9.42% H-5 => L+2, 2.77% H-10 => LUMO, 2.55% H-10 => L+2

50	19080	524	0.00	59.9% H-8 => L+1, 24.3% H-2 => L+5, 7.58% H-2 => L+8
51	19173	522	0.00	77.4% H-18 => LUMO, 7.97% H-4 => L+3, 4.12% H-2 => L+6, 2.69% H-19 => L+1
52	19230	520	0.01	34.6% H-2 => L+6, 24.3% H-5 => L+2, 16.1% H-9 => L+1, 10.3% H-18 => LUMO, 3.40% H-4 => L+3, 2.90% H-1 => L+8
53	19368	516	0.03	41.3% H-4 => L+3, 18.4% H-9 => L+1, 14.3% H-5 => L+2, 11.5% H-2 => L+6, 2.95% H-1 => L+5, 2.76% H-18 => LUMO
54	19510	513	0.00	37.2% H-1 => L+7, 35.6% H-10 => L+1, 7.71% H-3 => L+5, 5.98% H-4 => L+4, 4.33% H-6 => L+3, 2.16% H-9 => L+2
55	19686	508	0.00	84.0% H-19 => LUMO, 6.47% H-18 => L+1, 4.05% H-21 => LUMO
56	19919	502	0.00	69.7% H-3 => L+5, 14.1% H-10 => L+1, 2.20% HOMO => L+10
57	19968	501	0.01	61.5% H-3 => L+6, 18.0% H-2 => L+7, 7.74% H-4 => L+2
58	20052	499	0.00	59.8% H-5 => L+4, 17.4% H-7 => L+3, 11.6% H-2 => L+5, 4.18% H-2 => L+8, 2.47% H-5 => L+7
59	20297	493	0.00	72.7% H-20 => LUMO, 12.5% H-22 => LUMO, 6.37% H-19 => L+1, 2.94% H-1 => L+8
60	20323	492	0.06	58.2% H-1 => L+8, 9.09% H-2 => L+6, 6.42% H-8 => L+3, 5.29% H-6 => L+4, 3.65% H-20 => LUMO, 3.11% H-4 => L+5, 2.88% HOMO => L+9, 2.65% H-5 => L+2, 2.03% H-4 => L+3
61	20458	489	0.00	57.9% H-4 => L+4, 11.1% H-7 => L+2, 4.63% HOMO => L+10, 3.81% H-6 => L+3, 3.72% H-3 => L+5, 3.49% H-10 => L+1, 2.89% H-11 => L+1, 2.72% H-5 => L+6
62	20468	489	0.93	46.3% H-2 => L+7, 22.0% H-3 => L+6, 12.8% H-13 => L+1, 2.70% H-5 => L+8, 2.20% H-4 => L+2
63	20499	488	0.00	37.5% H-11 => L+1, 18.3% H-7 => L+2, 11.2% H-4 => L+4, 10.4% H-3 => L+8, 6.00% H-1 => L+7, 5.97% H-4 => L+7
64	20585	486	0.00	45.5% H-2 => L+8, 29.6% H-6 => L+2, 7.20% H-8 => L+1, 5.58% H-4 => L+6, 3.84% H-5 => L+7
65	20827	480	0.10	48.5% HOMO => L+9, 15.6% H-3 => L+7, 15.2% H-12 => L+1, 3.09% H-4 => L+5, 3.09% H-2 => L+10
66	20920	478	0.22	68.9% H-12 => L+1, 8.64% HOMO => L+9, 5.06% H-3 => L+7, 4.04% H-15 => LUMO, 2.07% H-5 => L+2
67	20959	477	0.00	81.5% H-21 => LUMO, 6.58% H-20 => L+1, 5.60% H-22 => L+1, 2.87% H-19 => LUMO
68	21053	475	0.00	75.8% H-22 => LUMO, 10.4% H-21 => L+1, 9.65% H-20 => LUMO
69	21144	473	0.04	73.0% H-13 => L+1, 13.3% H-2 => L+7, 3.63% H-5 => L+5

70	21151	473	0.00	63.6% H-7 => L+3, 17.7% H-5 => L+4, 5.05% H-9 => L+3, 3.46% H-7 => L+5, 2.44% H-6 => L+2
71	21252	471	0.00	36.7% H-11 => L+1, 19.1% HOMO => L+10, 7.33% H-4 => L+4, 6.92% H-7 => L+2, 6.38% H-3 => L+8, 4.47% H-6 => L+3, 3.85% H-5 => L+6, 3.63% H-4 => L+7
72	21345	469	0.00	47.9% H-6 => L+3, 12.0% HOMO => L+10, 11.2% H-11 => L+1, 8.79% H-7 => L+2, 5.53% H-15 => L+1, 4.06% H-4 => L+4
73	21362	468	0.01	45.6% H-6 => L+2, 20.0% H-2 => L+8, 14.5% H-14 => L+1, 4.94% H-5 => L+4, 3.36% H-17 => L+1
74	21442	466	0.00	22.7% H-7 => L+2, 19.5% H-6 => L+3, 18.7% HOMO => L+10, 14.3% H-3 => L+8, 8.58% H-15 => L+1, 2.78% H-4 => L+4, 2.73% H-4 => L+7
75	21473	466	0.00	73.4% H-15 => L+1, 14.0% H-7 => L+2, 2.89% H-12 => L+2, 2.05% H-12 => LUMO
76	21479	466	0.01	54.0% H-3 => L+7, 13.7% HOMO => L+9, 9.99% H-6 => L+4, 8.74% H-8 => L+3, 5.27% H-4 => L+5
77	21665	462	0.00	58.8% H-14 => L+1, 16.7% H-17 => L+1, 8.33% H-6 => L+2, 6.41% H-2 => L+8
78	21867	457	0.37	46.5% H-16 => L+1, 34.7% H-5 => L+5, 2.09% H-1 => L+9, 2.05% H-7 => L+7
79	21979	455	0.00	69.8% H-17 => L+1, 16.8% H-14 => L+1, 3.32% H-16 => L+2, 2.90% H-16 => LUMO
80	22117	452	0.40	40.7% H-16 => L+1, 33.4% H-5 => L+5, 5.11% H-13 => L+1, 3.80% H-1 => L+9, 2.68% H-7 => L+4, 2.37% H-24 => LUMO
81	22288	449	0.44	65.2% H-4 => L+5, 15.9% H-8 => L+3, 8.41% H-6 => L+4, 2.31% H-6 => L+7
82	22348	447	0.00	61.8% H-5 => L+6, 15.7% HOMO => L+10, 6.85% H-7 => L+2, 4.11% H-3 => L+8, 4.01% H-15 => L+1, 2.61% H-6 => L+3
83	22358	447	0.00	45.9% H-4 => L+6, 16.6% H-9 => L+3, 15.6% H-23 => LUMO, 5.03% H-10 => L+4, 3.44% H-6 => L+2, 2.93% H-2 => L+8, 2.81% H-27 => LUMO
84	22388	447	0.04	34.9% H-8 => L+2, 18.3% H-24 => LUMO, 9.36% H-7 => L+4, 9.35% H-10 => L+3, 7.82% H-9 => L+4, 4.38% H-26 => LUMO, 2.77% H-11 => L+3, 2.34% H-5 => L+8
85	22504	444	0.00	61.4% H-23 => LUMO, 19.6% H-4 => L+6, 10.9% H-25 => LUMO, 3.75% H-24 => L+1
86	22541	444	0.00	65.9% H-24 => LUMO, 14.9% H-8 => L+2, 5.66% H-7 => L+4, 4.03% H-23 => L+1, 3.35% H-5 => L+5
87	22623	442	0.00	71.5% H-25 => LUMO, 11.1% H-27 => LUMO, 7.16% H-23 => LUMO, 3.23% H-9 => L+3
88	22625	442	0.00	50.3% H-3 => L+8, 13.4% H-5 => L+6, 6.51% H-6 => L+5, 5.82% H-6 => L+3, 5.72% H-8 => L+4,

				4.70% H-4 => L+7, 3.26% HOMO => L+10, 2.67% H-13 => L+3
89	22684	441	0.02	46.6% H-26 => LUMO, 23.2% H-8 => L+2, 15.9% H-7 => L+4, 2.52% H-5 => L+5
90	22750	440	0.00	72.3% H-27 => LUMO, 7.48% H-25 => LUMO, 5.45% H-23 => LUMO, 4.46% H-5 => L+7, 2.46% H-26 => L+1
91	22844	438	0.01	39.4% H-26 => LUMO, 35.4% H-7 => L+4, 5.82% H-8 => L+2, 3.36% H-5 => L+8, 2.98% H-5 => L+5, 2.26% H-24 => LUMO, 2.10% H-11 => L+3
92	22857	438	0.00	72.4% H-9 => L+2, 5.47% H-10 => L+1, 5.31% H-4 => L+7, 4.00% HOMO => L+10, 3.20% H-10 => L+6
93	22971	435	0.00	39.4% H-9 => L+3, 20.3% H-5 => L+7, 11.0% H-4 => L+6, 7.19% H-2 => L+8, 6.95% H-10 => L+4, 3.34% H-7 => L+5
94	22996	435	0.00	36.0% H-6 => L+4, 21.6% H-10 => L+2, 19.9% H-8 => L+3, 5.30% H-8 => L+5, 2.38% H-4 => L+8, 2.13% HOMO => L+9
95	23075	433	0.44	52.1% H-10 => L+3, 14.4% H-9 => L+4, 8.47% H-1 => L+9, 6.09% H-7 => L+4, 3.67% H-8 => L+2, 2.30% H-24 => LUMO, 2.07% H-12 => L+4
96	23144	432	0.01	33.1% H-5 => L+7, 10.4% H-1 => L+10, 9.63% H-9 => L+3, 8.14% H-4 => L+6, 6.19% H-7 => L+5, 5.69% H-27 => LUMO, 5.67% H-3 => L+9, 4.59% H-25 => LUMO, 2.82% H-7 => L+3, 2.30% H-23 => LUMO
97	23238	430	0.06	45.5% H-10 => L+2, 18.4% H-8 => L+3, 15.8% H-6 => L+4, 4.51% H-4 => L+8, 2.51% H-9 => L+6, 2.36% H-12 => L+1
98	23452	426	0.09	22.0% H-11 => L+2, 19.8% H-7 => L+6, 18.0% H-4 => L+8, 5.95% H-10 => L+2, 5.70% H-6 => L+7, 3.53% H-35 => LUMO, 2.79% H-8 => L+5, 2.03% H-15 => L+2
99	23545	425	0.00	48.4% H-30 => LUMO, 12.6% H-4 => L+7, 7.56% H-9 => L+2, 7.42% H-32 => LUMO, 3.98% H-34 => LUMO, 3.56% H-18 => L+1, 2.31% H-5 => L+6, 2.13% HOMO => L+10
100	23601	424	0.00	92.6% H-28 => LUMO, 5.06% H-29 => L+1
101	23603	424	0.00	91.9% H-29 => LUMO, 5.00% H-28 => L+1
102	23668	423	0.00	46.1% H-4 => L+7, 9.49% H-18 => L+1, 9.29% H-8 => L+4, 7.23% H-30 => LUMO, 4.77% H-34 => LUMO, 4.43% H-13 => L+3, 2.79% H-9 => L+2, 2.53% H-32 => LUMO, 2.36% H-6 => L+8
103	23672	422	0.00	73.5% H-18 => L+1, 8.42% H-30 => LUMO, 4.59% H-19 => LUMO, 2.78% H-4 => L+7, 2.54% H-19 => L+2
104	23746	421	0.06	64.5% H-31 => LUMO, 5.74% H-35 => LUMO, 3.47% H-8 => L+3, 3.04% H-10 => L+2, 2.51% H-6 => L+4, 2.00% H-48 => LUMO

105	23917	418	0.00	45.0% H-32 => LUMO, 21.9% H-34 => LUMO, 18.4% H-30 => LUMO, 6.80% H-36 => LUMO, 2.32% H-31 => L+1
106	23940	418	0.58	48.3% H-5 => L+8, 10.2% H-1 => L+9, 6.17% H-6 => L+6, 5.55% H-8 => L+2, 4.86% H-7 => L+7, 3.31% H-3 => L+10, 3.13% H-2 => L+7, 2.29% H-7 => L+4, 2.01% H-9 => L+4
107	23987	417	0.00	25.2% H-12 => L+3, 21.3% H-7 => L+5, 12.3% H-10 => L+4, 9.03% H-5 => L+7, 7.67% H-9 => L+5, 4.78% H-11 => L+4, 2.88% H-7 => L+8
108	23994	417	0.00	33.7% H-35 => LUMO, 20.9% H-33 => LUMO, 16.2% H-31 => LUMO, 6.91% H-37 => LUMO, 3.06% H-8 => L+3, 2.58% HOMO => L+9
109	24075	415	0.15	29.8% H-35 => LUMO, 19.4% H-37 => LUMO, 11.8% H-33 => LUMO, 5.11% H-8 => L+3, 4.08% HOMO => L+9, 3.23% H-31 => LUMO, 2.96% H-19 => L+1, 2.44% H-10 => L+2, 2.19% H-4 => L+8, 2.13% H-6 => L+4, 2.08% H-48 => LUMO
110	24114	415	0.00	36.6% H-34 => LUMO, 17.5% H-32 => LUMO, 9.60% H-6 => L+5, 9.40% H-36 => LUMO, 5.24% H-8 => L+4, 3.09% H-2 => L+9, 2.57% H-30 => LUMO, 2.52% H-33 => L+1, 2.18% HOMO => L+10
111	24170	414	0.00	68.6% H-19 => L+1, 8.14% H-33 => LUMO, 5.34% H-18 => L+2, 4.54% H-20 => LUMO, 3.28% H-18 => LUMO, 3.25% H-21 => L+1
112	24222	413	0.80	48.3% H-1 => L+9, 13.9% H-6 => L+6, 6.74% H-11 => L+3, 5.75% H-7 => L+4, 5.71% H-5 => L+8, 5.48% H-8 => L+2, 2.61% H-5 => L+5
113	24272	412	0.13	45.2% H-33 => LUMO, 9.07% H-8 => L+3, 7.17% HOMO => L+9, 3.71% H-6 => L+4, 3.27% H-7 => L+6, 2.39% H-19 => L+1, 2.28% H-4 => L+5, 2.26% H-3 => L+7, 2.18% H-31 => LUMO, 2.18% H-48 => LUMO, 2.15% H-5 => L+2, 2.13% H-32 => L+1
114	24285	412	0.00	26.1% H-6 => L+5, 18.2% H-32 => LUMO, 13.2% H-2 => L+9, 11.7% H-34 => LUMO, 6.75% HOMO => L+10, 5.02% H-8 => L+4, 3.20% H-30 => LUMO, 2.35% H-5 => L+6
115	24385	410	0.01	42.9% H-1 => L+10, 9.36% H-5 => L+7, 8.76% H-10 => L+4, 6.26% H-9 => L+3, 6.11% H-12 => L+3, 4.98% H-7 => L+5, 4.91% H-3 => L+9, 4.22% H-9 => L+5, 2.80% H-13 => L+2
116	24418	410	0.01	41.2% H-4 => L+8, 19.4% H-7 => L+6, 5.88% H-14 => L+3, 5.48% H-10 => L+2, 5.32% H-15 => L+2, 4.74% H-11 => L+2
117	24493	408	0.00	33.8% H-8 => L+4, 31.5% H-6 => L+5, 10.6% H-36 => LUMO, 4.49% H-13 => L+3, 3.18% H-8 => L+7, 2.08% H-4 => L+7

118	24524	408	0.04	62.6% H-37 => LUMO, 21.7% H-35 => LUMO, 3.98% H-33 => LUMO, 3.64% H-36 => L+1, 3.24% H-31 => LUMO
119	24525	408	0.00	63.5% H-36 => LUMO, 12.5% H-34 => LUMO, 9.28% H-8 => L+4, 2.38% H-37 => L+1, 2.19% H-6 => L+5
120	24627	406	0.21	22.8% H-9 => L+4, 20.0% H-10 => L+3, 15.4% H-11 => L+3, 13.0% H-5 => L+8, 8.60% H-10 => L+5, 4.78% H-6 => L+6, 4.58% H-15 => L+3, 3.27% H-1 => L+9
121	24641	406	0.01	40.2% H-7 => L+5, 16.5% H-1 => L+10, 13.8% H-13 => L+2, 7.94% H-12 => L+3, 5.49% H-10 => L+4
122	24671	405	0.47	49.7% H-11 => L+3, 17.6% H-15 => L+3, 3.83% H-7 => L+4, 3.63% H-6 => L+6, 3.20% H-11 => L+5, 3.16% H-9 => L+4, 2.56% H-7 => L+7, 2.32% H-10 => L+5, 2.16% H-42 => LUMO, 2.08% H-14 => L+2
123	24697	405	0.00	67.2% H-20 => L+1, 15.2% H-22 => L+1, 5.82% H-19 => L+2, 4.10% H-19 => LUMO
124	24778	404	0.00	39.8% H-12 => L+2, 16.4% H-40 => LUMO, 8.47% H-13 => L+3, 7.75% H-2 => L+9, 6.56% H-44 => LUMO, 4.36% H-39 => LUMO, 2.97% H-8 => L+4
125	24814	403	0.01	44.3% H-11 => L+2, 11.0% H-2 => L+10, 8.28% H-7 => L+6, 6.36% H-48 => LUMO, 5.12% H-14 => L+3, 4.07% H-6 => L+7, 2.99% H-38 => LUMO, 2.27% H-41 => LUMO
126	24831	403	0.00	73.2% H-40 => LUMO, 10.1% H-12 => L+2, 7.19% H-13 => L+3, 3.29% H-8 => L+4
127	24889	402	0.15	34.6% H-6 => L+6, 31.3% H-42 => LUMO, 10.5% H-45 => LUMO, 4.67% H-15 => L+3, 3.85% H-5 => L+8, 3.64% H-9 => L+4, 2.41% H-1 => L+9
128	24929	401	0.06	50.4% H-42 => LUMO, 27.7% H-6 => L+6, 6.26% H-9 => L+4, 3.20% H-5 => L+8, 2.97% H-45 => LUMO
129	24932	401	0.00	53.9% H-13 => L+3, 14.6% H-12 => L+2, 7.21% H-8 => L+4, 4.34% H-39 => LUMO, 3.73% H-16 => L+3, 3.39% H-40 => LUMO, 2.01% H-14 => L+4
130	24937	401	0.00	59.9% H-13 => L+2, 10.0% H-43 => LUMO, 6.70% H-12 => L+3, 6.03% H-1 => L+10, 2.39% H-7 => L+5, 2.37% H-5 => L+7
131	24948	401	0.00	75.2% H-41 => LUMO, 5.49% H-38 => LUMO, 4.06% H-11 => L+2, 3.98% H-48 => LUMO, 2.76% H-7 => L+6
132	24961	401	0.35	20.9% H-15 => L+3, 16.6% H-9 => L+4, 14.9% H-12 => L+4, 14.8% H-45 => LUMO, 7.26% H-11 => L+3, 5.74% H-7 => L+7, 3.13% H-1 => L+9, 2.92% H-47 => LUMO, 2.18% H-5 => L+8

133	25011	400	0.00	77.0% H-43 => LUMO, 7.48% H-46 => LUMO, 4.44% H-13 => L+2, 2.52% H-49 => LUMO
134	25019	400	0.01	26.5% H-7 => L+6, 11.4% H-14 => L+3, 10.6% H-11 => L+2, 9.07% H-2 => L+10, 6.79% H-8 => L+5, 6.27% H-41 => LUMO, 5.75% H-4 => L+8, 4.26% H-13 => L+4, 4.00% H-6 => L+7, 3.69% H-38 => LUMO, 2.06% H-9 => L+6
135	25024	400	0.13	50.6% H-45 => LUMO, 13.3% H-42 => LUMO, 12.1% H-47 => LUMO, 3.44% H-15 => L+3, 3.22% H-9 => L+4, 2.64% H-50 => LUMO, 2.29% H-12 => L+4
136	25033	399	0.00	39.8% H-39 => LUMO, 29.9% H-44 => LUMO, 16.7% H-12 => L+2, 2.93% H-40 => LUMO
137	25130	398	0.02	50.4% H-38 => LUMO, 17.6% H-48 => LUMO, 4.12% H-14 => L+3, 2.70% H-11 => L+2, 2.63% H-13 => L+4
138	25227	396	0.33	46.2% H-17 => L+3, 19.0% H-14 => L+3, 9.28% H-6 => L+7, 6.21% H-4 => L+8, 3.46% H-16 => L+4, 2.41% H-14 => L+5
139	25243	396	0.00	33.2% H-12 => L+3, 21.3% H-10 => L+4, 12.3% H-9 => L+5, 5.99% H-1 => L+10, 5.30% H-13 => L+2, 4.18% H-15 => L+4
140	25252	396	0.00	50.8% H-44 => LUMO, 26.8% H-39 => LUMO, 5.60% H-16 => L+3, 3.06% H-2 => L+9
141	25291	395	0.01	56.9% H-48 => LUMO, 24.8% H-38 => LUMO, 10.4% H-41 => LUMO
142	25302	395	0.00	47.3% H-16 => L+3, 11.4% H-39 => LUMO, 9.99% H-14 => L+4, 8.52% H-17 => L+4, 4.21% H-44 => LUMO, 2.90% H-12 => L+2, 2.41% H-13 => L+5
143	25359	394	0.01	35.5% H-15 => L+2, 17.3% H-17 => L+3, 15.3% H-6 => L+7, 6.47% H-16 => L+4, 5.18% H-14 => L+3, 4.80% H-4 => L+8, 4.29% H-8 => L+5
144	25377	394	0.00	54.1% H-47 => LUMO, 20.5% H-50 => LUMO, 16.1% H-45 => LUMO, 2.69% H-46 => L+1, 2.43% H-14 => L+2
145	25382	394	0.00	62.8% H-46 => LUMO, 18.6% H-49 => LUMO, 9.10% H-43 => LUMO, 2.28% H-47 => L+1
146	25390	394	0.00	70.0% H-21 => L+1, 8.01% H-22 => LUMO, 5.41% H-20 => LUMO, 4.62% H-22 => L+2, 3.88% H-20 => L+2
147	25446	393	0.04	41.5% H-15 => L+2, 16.3% H-14 => L+3, 11.0% H-17 => L+3, 7.06% H-16 => L+4, 6.10% H-2 => L+10, 4.44% H-6 => L+7, 3.12% H-7 => L+6
148	25465	393	0.00	67.2% H-22 => L+1, 10.9% H-21 => LUMO, 9.46% H-20 => L+1, 8.63% H-21 => L+2
149	25473	393	0.41	66.8% H-14 => L+2, 11.1% H-17 => L+2, 2.93% H-7 => L+7, 2.56% H-9 => L+4, 2.22% H-11 => L+3
150	25498	392	0.00	41.7% H-2 => L+9, 14.2% H-51 => LUMO, 10.8% H-16 => L+3, 5.55% H-39 => LUMO, 3.14% H-6

				=> L+5, 2.78% H-8 => L+4, 2.47% H-17 => L+4, 2.42% H-4 => L+7, 2.09% H-13 => L+3
151	25590	391	0.00	21.5% H-49 => LUMO, 12.8% H-52 => LUMO, 11.6% H-46 => LUMO, 8.96% H-7 => L+8, 5.64% H-15 => L+4, 5.50% H-12 => L+5, 5.34% H-9 => L+8, 5.18% H-10 => L+7, 4.10% H-7 => L+5, 3.53% H-11 => L+7, 3.31% H-16 => L+2
152	25601	391	0.00	52.6% H-50 => LUMO, 21.0% H-47 => LUMO, 4.23% H-9 => L+7, 3.27% H-10 => L+5, 2.96% H-15 => L+3, 2.47% H-49 => L+1, 2.04% H-53 => LUMO, 2.00% H-17 => L+2
153	25633	390	0.00	42.1% H-49 => LUMO, 12.1% H-16 => L+2, 11.5% H-46 => LUMO, 6.55% H-7 => L+8, 2.79% H-11 => L+4, 2.29% H-7 => L+5, 2.08% H-11 => L+7
154	25678	389	0.01	49.3% H-17 => L+2, 9.13% H-50 => LUMO, 6.86% H-9 => L+7, 5.88% H-10 => L+5, 5.44% H-15 => L+3, 5.00% H-14 => L+2, 2.84% H-47 => LUMO, 2.33% H-16 => L+1, 2.26% H-16 => L+6
155	25730	389	0.00	62.2% H-16 => L+2, 8.79% H-52 => LUMO, 4.44% H-10 => L+4, 3.48% H-7 => L+8, 2.10% H-49 => LUMO, 2.02% H-3 => L+9
156	25797	388	0.02	26.2% H-17 => L+2, 16.5% H-15 => L+3, 12.6% H-7 => L+7, 6.58% H-9 => L+7, 6.12% H-53 => LUMO, 4.91% H-10 => L+5, 4.43% H-50 => LUMO, 2.90% H-5 => L+8, 2.89% H-15 => L+5
157	25809	387	0.39	47.5% H-2 => L+10, 21.4% H-6 => L+7, 6.04% H-15 => L+2, 4.04% H-14 => L+3, 3.58% H-55 => LUMO
158	25831	387	0.00	14.6% H-10 => L+4, 12.6% H-9 => L+5, 12.6% H-10 => L+7, 11.9% H-11 => L+4, 8.99% H-8 => L+6, 8.44% H-52 => LUMO, 5.30% H-49 => LUMO, 3.19% H-7 => L+8, 2.36% H-9 => L+3, 2.23% H-9 => L+8
159	25865	387	0.01	42.8% H-7 => L+7, 6.32% H-14 => L+2, 6.04% H-10 => L+5, 5.99% H-3 => L+10, 5.51% H-5 => L+8, 4.57% H-9 => L+4, 3.83% H-50 => LUMO, 3.70% H-9 => L+7, 2.37% H-15 => L+3, 2.26% H-53 => LUMO, 2.05% H-4 => L+9
160	25962	385	0.00	49.4% H-6 => L+8, 18.0% H-8 => L+7, 5.42% H-2 => L+9, 3.98% H-13 => L+5, 3.84% H-16 => L+3, 3.39% H-17 => L+4, 2.55% H-14 => L+4
161	25995	385	0.00	64.0% H-8 => L+5, 12.4% H-6 => L+7, 7.04% H-2 => L+10, 4.34% H-8 => L+8
162	26054	384	0.00	32.3% H-3 => L+9, 21.5% H-11 => L+4, 7.43% H-52 => LUMO, 6.51% H-9 => L+5, 6.22% H-1 => L+10, 5.93% H-10 => L+4, 3.44% H-8 => L+6, 2.54% H-12 => L+3
163	26118	383	0.10	66.8% H-18 => L+3, 13.0% H-19 => L+4, 4.28% H-20 => L+5, 3.04% H-22 => L+8, 2.95% H-18 => L+5, 2.15% H-21 => L+7

164	26157	382	0.00	37.9% H-8 => L+6, 23.3% H-11 => L+4, 15.6% H-52 => LUMO, 3.78% H-12 => L+5, 3.05% H-19 => L+3, 2.27% H-7 => L+8
165	26230	381	0.01	24.6% H-3 => L+9, 24.4% H-52 => LUMO, 6.25% H-16 => L+2, 6.10% H-11 => L+4, 3.90% H-9 => L+5, 3.59% H-54 => LUMO, 3.51% H-19 => L+3, 3.21% H-10 => L+7, 3.04% H-15 => L+4, 2.42% H-8 => L+6, 2.00% H-24 => L+1
166	26415	379	0.00	26.7% H-8 => L+6, 15.1% H-19 => L+3, 10.7% H-52 => LUMO, 7.21% H-9 => L+5, 7.03% H-18 => L+4, 4.72% H-3 => L+9, 3.66% H-15 => L+4, 3.55% H-7 => L+8, 2.68% H-12 => L+5, 2.59% H-20 => L+4, 2.51% H-9 => L+8
167	26424	378	0.01	26.7% H-19 => L+3, 13.0% H-11 => L+4, 12.5% H-18 => L+4, 9.37% H-3 => L+9, 5.13% H-8 => L+6, 4.52% H-9 => L+5, 3.31% H-20 => L+4, 2.42% H-52 => LUMO, 2.30% H-12 => L+5, 2.12% H-22 => L+7
168	26442	378	0.02	70.3% H-53 => LUMO, 5.56% H-23 => L+1, 4.35% H-10 => L+5, 2.65% H-27 => L+1, 2.59% H-3 => L+10, 2.08% H-52 => L+1
169	26462	378	0.28	53.8% H-3 => L+10, 16.0% H-23 => L+1, 4.84% H-7 => L+7, 4.10% H-1 => L+9, 3.81% H-4 => L+9, 2.90% H-12 => L+4
170	26470	378	0.00	63.3% H-13 => L+4, 6.28% H-16 => L+4, 5.86% H-14 => L+3, 4.50% H-14 => L+5, 2.45% H-17 => L+8, 2.38% H-13 => L+7, 2.02% H-17 => L+5
171	26506	377	0.00	69.2% H-51 => LUMO, 5.01% H-2 => L+9, 3.99% H-13 => L+3, 2.43% H-8 => L+4
172	26536	377	0.00	79.0% H-24 => L+1, 5.58% H-23 => LUMO, 4.33% H-23 => L+2, 4.24% H-9 => L+5
173	26557	377	0.03	59.7% H-23 => L+1, 6.01% H-3 => L+10, 5.55% H-12 => L+4, 3.98% H-24 => LUMO, 3.77% H-25 => L+1, 3.59% H-53 => LUMO, 3.12% H-24 => L+2, 3.10% H-7 => L+7
174	26647	375	0.01	69.2% H-25 => L+1, 9.99% H-27 => L+1, 6.83% H-12 => L+4
175	26653	375	0.15	81.5% H-9 => L+6, 5.84% H-7 => L+6, 3.13% H-10 => L+2
176	26712	374	0.08	19.2% H-20 => L+3, 14.0% H-12 => L+4, 11.3% H-10 => L+5, 10.7% H-19 => L+4, 10.2% H-25 => L+1, 4.98% H-18 => L+5, 3.44% H-3 => L+10, 3.34% H-22 => L+5, 2.63% H-22 => L+3, 2.00% H-21 => L+7
177	26791	373	0.00	50.0% H-26 => L+1, 23.7% H-54 => LUMO, 6.56% H-7 => L+8, 6.56% H-9 => L+5, 2.22% H-11 => L+4
178	26799	373	0.08	24.1% H-12 => L+4, 20.1% H-20 => L+3, 8.68% H-19 => L+4, 8.14% H-10 => L+5, 5.72% H-18 => L+5, 3.47% H-22 => L+5, 3.23% H-15 => L+3,

				2.52% H-22 => L+3, 2.46% H-3 => L+10, 2.42% H-15 => L+5
179	26876	372	0.00	75.9% H-27 => L+1, 8.69% H-25 => L+1, 3.70% H-53 => LUMO, 3.24% H-26 => L+2
180	26903	372	0.00	31.6% H-14 => L+4, 31.5% H-17 => L+4, 5.99% H-13 => L+5, 4.91% H-13 => L+8, 4.89% H-8 => L+7, 4.51% H-6 => L+8, 2.45% H-51 => LUMO, 2.13% H-17 => L+7
181	26919	371	0.00	26.2% H-7 => L+8, 26.0% H-26 => L+1, 10.9% H-15 => L+4, 10.1% H-9 => L+5, 7.68% H-54 => LUMO, 3.80% H-12 => L+5, 2.25% H-10 => L+7, 2.07% H-8 => L+6
182	27031	370	0.00	28.5% H-10 => L+6, 15.1% H-6 => L+8, 9.73% H-16 => L+5, 9.36% H-16 => L+3, 9.05% H-14 => L+4, 4.99% H-8 => L+7, 4.59% H-13 => L+5, 4.34% H-17 => L+4, 3.77% H-14 => L+7
183	27082	369	0.00	24.0% H-21 => L+3, 13.9% H-20 => L+4, 13.0% H-54 => LUMO, 12.8% H-22 => L+4, 8.08% H-19 => L+5, 7.26% H-21 => L+5, 4.46% H-18 => L+7, 4.38% H-20 => L+7, 2.72% H-19 => L+8, 2.16% H-26 => L+1
184	27091	369	0.11	31.1% H-16 => L+4, 14.3% H-14 => L+5, 13.7% H-17 => L+5, 9.64% H-17 => L+3, 7.53% H-13 => L+7, 5.66% H-14 => L+3, 5.44% H-8 => L+8, 4.53% H-16 => L+7
185	27102	369	0.00	34.1% H-54 => LUMO, 15.4% H-7 => L+8, 9.82% H-15 => L+4, 9.52% H-26 => L+1, 6.40% H-21 => L+3, 3.54% H-20 => L+4, 3.36% H-22 => L+4, 2.05% H-19 => L+5
186	27103	369	0.00	56.9% H-10 => L+6, 6.82% H-16 => L+5, 6.76% H-17 => L+4, 6.22% H-8 => L+7, 4.02% H-14 => L+4, 2.60% H-16 => L+3, 2.13% H-14 => L+7
187	27169	368	0.00	34.9% H-22 => L+3, 27.7% H-21 => L+4, 16.3% H-20 => L+5, 10.5% H-19 => L+7, 6.68% H-18 => L+8
188	27387	365	0.00	30.4% H-9 => L+7, 25.7% H-10 => L+5, 18.4% H-10 => L+8, 4.62% H-15 => L+3, 4.43% H-9 => L+4, 3.88% H-12 => L+4, 2.95% H-15 => L+5
189	27446	364	0.00	39.7% H-15 => L+4, 17.0% H-10 => L+7, 13.2% H-9 => L+8, 7.80% H-12 => L+3, 6.06% H-9 => L+5, 4.03% H-54 => LUMO, 2.40% H-15 => L+7
190	27468	364	0.00	50.4% H-8 => L+7, 16.3% H-6 => L+8, 13.1% H-17 => L+4, 5.54% H-16 => L+5, 3.92% H-16 => L+3, 3.62% H-14 => L+4, 2.61% H-6 => L+5
191	27474	364	0.00	83.7% H-18 => L+2, 5.53% H-19 => L+1, 4.53% H-19 => L+6
192	27563	363	0.03	60.4% H-11 => L+5, 11.3% H-29 => L+1, 5.74% H-12 => L+7, 2.80% H-15 => L+8, 2.65% H-3 => L+10

193	27627	362	0.01	71.7% H-29 => L+1, 12.0% H-11 => L+5, 4.69% H-28 => LUMO, 3.34% H-28 => L+2, 2.10% H-56 => LUMO
194	27629	362	0.00	85.8% H-28 => L+1, 5.50% H-29 => LUMO, 3.99% H-29 => L+2
195	27662	362	0.03	51.3% H-30 => L+1, 13.0% H-55 => LUMO, 8.70% H-32 => L+1, 7.69% H-34 => L+1, 2.58% H-8 => L+8
196	27720	361	0.10	45.3% H-55 => LUMO, 26.7% H-30 => L+1, 9.00% H-8 => L+8
197	27761	360	0.00	68.2% H-31 => L+1, 14.2% H-35 => L+1, 3.06% H-11 => L+6, 2.89% H-30 => LUMO, 2.28% H-30 => L+2
198	27839	359	0.00	44.0% H-19 => L+2, 29.2% H-11 => L+6, 4.97% H-18 => L+6, 4.24% H-21 => L+2, 2.59% H-20 => L+1
199	27883	359	0.02	34.7% H-8 => L+8, 19.9% H-55 => LUMO, 8.57% H-16 => L+4, 6.39% H-34 => L+1, 5.04% H-32 => L+1, 4.89% H-6 => L+7, 2.52% H-14 => L+5, 2.32% H-14 => L+3
200	27912	358	0.00	19.9% H-19 => L+2, 19.1% H-11 => L+6, 17.8% H-35 => L+1, 12.3% H-31 => L+1, 6.17% H-37 => L+1, 4.42% H-33 => L+1
201	27940	358	0.02	38.5% H-32 => L+1, 19.6% H-34 => L+1, 14.0% H-8 => L+8, 7.29% H-30 => L+1, 4.80% H-36 => L+1
202	27994	357	0.04	66.2% H-56 => LUMO, 11.0% H-4 => L+9, 4.53% H-3 => L+10, 4.30% H-29 => L+1, 3.04% H-54 => L+1
203	28003	357	0.00	24.2% H-35 => L+1, 17.7% H-13 => L+5, 12.9% H-11 => L+6, 8.76% H-14 => L+4, 6.65% H-33 => L+1, 5.48% H-37 => L+1, 4.04% H-14 => L+7, 4.03% H-19 => L+2, 2.35% H-31 => L+1, 2.23% H-16 => L+8, 2.09% H-13 => L+3
204	28048	357	0.00	27.2% H-13 => L+5, 23.9% H-11 => L+6, 13.3% H-14 => L+4, 7.85% H-35 => L+1, 4.77% H-14 => L+7, 3.48% H-19 => L+2, 2.97% H-13 => L+3, 2.72% H-16 => L+8, 2.36% H-33 => L+1
205	28107	356	0.00	41.2% H-12 => L+5, 12.5% H-9 => L+8, 9.99% H-15 => L+7, 7.04% H-11 => L+7, 6.48% H-10 => L+7, 4.81% H-4 => L+10, 3.71% H-12 => L+8, 2.05% H-15 => L+4, 2.00% H-10 => L+4
206	28138	355	0.00	40.0% H-34 => L+1, 33.5% H-32 => L+1, 9.37% H-36 => L+1, 4.39% H-33 => LUMO, 3.64% H-33 => L+2
207	28140	355	0.00	64.0% H-33 => L+1, 14.9% H-37 => L+1, 5.99% H-35 => L+1, 2.40% H-34 => L+2, 2.30% H-32 => LUMO, 2.15% H-34 => LUMO
208	28227	354	0.01	30.2% H-15 => L+5, 20.7% H-13 => L+6, 17.3% H-12 => L+7, 10.3% H-9 => L+7, 6.53% H-11 =>

				L+8, 2.39% H-15 => L+3, 2.34% H-16 => L+6, 2.33% H-56 => LUMO
209	28246	354	0.00	18.6% H-16 => L+7, 18.4% H-14 => L+5, 13.2% H-16 => L+4, 12.8% H-8 => L+8, 4.61% H-13 => L+4, 4.60% H-14 => L+3, 4.60% H-13 => L+7, 4.56% H-17 => L+8, 4.13% H-17 => L+5, 3.55% H-14 => L+8, 2.74% H-17 => L+3
210	28313	353	0.22	78.6% H-5 => L+9, 4.38% H-7 => L+10, 3.62% H-2 => L+10, 3.07% H-55 => LUMO
211	28389	352	0.05	45.4% H-13 => L+6, 26.2% H-4 => L+9, 5.89% H-15 => L+5, 5.72% H-56 => LUMO, 2.07% H-3 => L+10
212	28438	352	0.00	28.4% H-16 => L+5, 15.8% H-17 => L+4, 13.0% H-13 => L+5, 7.87% H-17 => L+7, 7.69% H-16 => L+3, 7.15% H-13 => L+8, 6.62% H-14 => L+7, 5.14% H-5 => L+10
213	28460	351	0.04	73.1% H-12 => L+6, 6.52% H-36 => L+1, 2.76% H-15 => L+2
214	28481	351	0.07	42.6% H-4 => L+9, 19.3% H-13 => L+6, 8.67% H-9 => L+7, 6.71% H-56 => LUMO, 6.30% H-15 => L+5, 2.81% H-16 => L+6, 2.17% H-12 => L+7, 2.12% H-6 => L+10
215	28505	351	0.00	58.4% H-37 => L+1, 19.0% H-35 => L+1, 6.36% H-33 => L+1, 3.85% H-31 => L+1, 3.79% H-36 => LUMO, 3.39% H-36 => L+2
216	28514	351	0.02	63.0% H-36 => L+1, 13.4% H-34 => L+1, 8.32% H-12 => L+6, 2.77% H-37 => LUMO, 2.31% H-37 => L+2
217	28555	350	0.00	70.7% H-5 => L+10, 6.20% H-7 => L+9, 5.00% H-58 => LUMO, 3.97% H-2 => L+9, 2.39% H-17 => L+4
218	28579	350	0.00	33.9% H-4 => L+10, 33.3% H-57 => LUMO, 8.25% H-12 => L+5, 4.93% H-10 => L+7, 4.80% H-6 => L+9, 3.26% H-3 => L+9, 2.54% H-56 => L+1
219	28586	350	0.01	32.7% H-17 => L+5, 19.4% H-14 => L+5, 8.12% H-14 => L+8, 7.26% H-16 => L+4, 5.44% H-17 => L+3, 4.92% H-12 => L+6, 4.33% H-13 => L+4, 4.24% H-17 => L+8, 3.14% H-8 => L+8, 2.74% H-40 => L+1
220	28645	349	0.00	65.2% H-20 => L+2, 20.9% H-22 => L+2, 4.61% H-19 => L+6, 2.67% H-19 => L+1
221	28738	348	0.00	76.6% H-40 => L+1, 8.27% H-44 => L+1, 3.25% H-39 => L+1
222	28745	348	0.00	26.3% H-42 => L+1, 26.1% H-14 => L+6, 17.8% H-17 => L+6, 3.51% H-4 => L+10, 3.43% H-12 => L+8, 3.27% H-9 => L+8, 2.95% H-10 => L+7, 2.70% H-11 => L+7, 2.41% H-45 => L+1
223	28788	347	0.00	34.0% H-42 => L+1, 12.7% H-57 => LUMO, 9.56% H-10 => L+7, 7.25% H-45 => L+1, 6.89%

				H-9 => L+8, 6.60% H-12 => L+8, 4.88% H-12 => L+5, 4.72% H-11 => L+7
224	28800	347	0.00	31.2% H-41 => L+1, 24.5% H-48 => L+1, 17.2% H-15 => L+6, 4.29% H-38 => L+1, 3.11% H-25 => L+3, 2.94% H-58 => LUMO
225	28841	347	0.00	28.0% H-14 => L+6, 15.5% H-42 => L+1, 12.7% H-17 => L+6, 12.2% H-57 => LUMO, 6.86% H-45 => L+1, 5.32% H-9 => L+8, 4.86% H-10 => L+7, 2.63% H-4 => L+10, 2.46% H-12 => L+8
226	28917	346	0.00	27.2% H-4 => L+10, 23.5% H-57 => LUMO, 17.9% H-9 => L+8, 4.97% H-17 => L+6, 4.60% H-10 => L+7, 2.86% H-9 => L+5, 2.56% H-12 => L+8, 2.43% H-7 => L+8
227	28950	345	0.00	52.3% H-15 => L+6, 30.0% H-41 => L+1, 2.99% H-38 => L+1, 2.14% H-5 => L+10
228	28981	345	0.00	83.6% H-43 => L+1, 6.24% H-46 => L+1, 2.17% H-45 => L+2, 2.14% H-49 => L+1
229	28986	345	0.01	41.4% H-39 => L+1, 31.5% H-44 => L+1, 12.2% H-40 => L+1
230	28987	345	0.00	57.4% H-45 => L+1, 17.0% H-42 => L+1, 11.8% H-47 => L+1, 3.21% H-43 => L+2, 2.66% H-50 => L+1
231	29001	345	0.00	42.7% H-38 => L+1, 14.9% H-41 => L+1, 14.7% H-15 => L+6, 10.3% H-48 => L+1, 3.59% H-58 => LUMO
232	29146	343	0.00	54.7% H-11 => L+7, 8.87% H-10 => L+7, 8.27% H-9 => L+8, 6.71% H-12 => L+5, 5.48% H-4 => L+10, 2.87% H-7 => L+8, 2.33% H-12 => L+8
233	29158	343	0.04	36.4% H-12 => L+7, 22.8% H-15 => L+5, 19.7% H-15 => L+8, 6.49% H-11 => L+5, 5.24% H-12 => L+4, 3.79% H-10 => L+5
234	29170	343	0.00	65.9% H-58 => LUMO, 8.42% H-38 => L+1, 3.66% H-60 => LUMO, 2.98% H-41 => L+1, 2.90% H-5 => L+10
235	29228	342	0.00	39.3% H-39 => L+1, 38.8% H-44 => L+1, 4.20% HOMO => L+11, 2.49% H-38 => LUMO, 2.41% H-24 => L+3, 2.17% H-23 => L+4
236	29267	342	0.00	40.2% H-48 => L+1, 25.3% H-38 => L+1, 10.9% H-41 => L+1, 5.58% H-58 => LUMO
237	29292	341	0.00	65.0% H-10 => L+8, 15.7% H-9 => L+7, 5.13% H-15 => L+5, 5.08% H-11 => L+8, 2.02% H-10 => L+5
238	29330	341	0.00	69.8% H-21 => L+2, 7.06% H-19 => L+2, 6.95% H-22 => L+1, 5.18% H-20 => L+1, 3.54% H-22 => L+6, 3.47% H-20 => L+6
239	29376	340	0.00	62.3% H-46 => L+1, 19.3% H-49 => L+1, 8.34% H-43 => L+1, 2.73% H-47 => LUMO, 2.00% H-47 => L+2
240	29377	340	0.00	52.7% H-47 => L+1, 20.0% H-50 => L+1, 16.5% H-45 => L+1, 3.14% H-46 => LUMO, 2.31% H-46 => L+2

241	29380	340	0.00	53.7% H-22 => L+2, 15.3% H-20 => L+2, 8.93% H-21 => L+1, 6.61% H-21 => L+6, 3.92% H-13 => L+7
242	29386	340	0.00	37.0% H-13 => L+7, 11.7% H-17 => L+5, 11.1% HOMO => L+11, 6.41% H-16 => L+7, 6.22% H-22 => L+2, 4.61% H-14 => L+8, 3.86% H-17 => L+8, 2.73% H-44 => L+1, 2.20% H-13 => L+4, 2.13% H-8 => L+8
243	29476	339	0.00	55.2% H-17 => L+6, 35.4% H-14 => L+6, 3.57% H-16 => L+2
244	29479	339	0.07	85.5% H-16 => L+6, 6.23% H-13 => L+6, 2.40% H-17 => L+2
245	29529	339	0.03	34.0% H-24 => L+3, 27.4% H-23 => L+4, 9.47% H-24 => L+5, 4.75% H-13 => L+7, 3.92% HOMO => L+11, 3.76% H-44 => L+1, 3.51% H-39 => L+1, 2.58% H-23 => L+7
246	29542	338	0.00	39.3% H-23 => L+3, 31.2% H-24 => L+4, 10.5% H-23 => L+5, 3.58% H-38 => L+1, 2.78% H-24 => L+7, 2.27% H-48 => L+1
247	29576	338	0.00	47.9% HOMO => L+11, 8.98% H-51 => L+1, 7.30% H-13 => L+7, 5.24% H-24 => L+3, 3.79% H-23 => L+4, 3.76% H-14 => L+5, 2.29% H-44 => L+1, 2.09% H-26 => L+3
248	29587	338	0.00	63.2% H-50 => L+1, 21.8% H-47 => L+1, 3.38% H-49 => LUMO, 2.52% H-49 => L+2
249	29588	338	0.00	68.2% H-49 => L+1, 21.5% H-46 => L+1, 3.55% H-50 => LUMO, 2.62% H-50 => L+2
250	29622	338	0.00	33.1% H-13 => L+8, 22.1% H-17 => L+7, 14.2% H-14 => L+7, 6.61% H-16 => L+8, 5.27% H-16 => L+5, 3.58% H-17 => L+4, 3.32% H-14 => L+4, 2.30% H-8 => L+7, 2.14% H-13 => L+5
251	29629	338	0.00	37.8% H-15 => L+7, 18.9% H-12 => L+8, 12.8% H-11 => L+7, 10.2% H-9 => L+8, 6.04% H-10 => L+7, 4.46% H-15 => L+4, 3.73% H-50 => L+1, 2.44% H-12 => L+5
252	29697	337	0.00	58.7% H-11 => L+8, 7.37% H-15 => L+5, 6.81% H-52 => L+1, 6.76% H-15 => L+8, 4.74% H-11 => L+5, 2.30% H-7 => L+7
253	29747	336	0.00	59.6% H-18 => L+4, 27.4% H-19 => L+3, 5.43% H-19 => L+5, 3.35% H-20 => L+4
254	29937	334	0.00	51.0% H-26 => L+3, 8.95% H-27 => L+4, 7.48% H-51 => L+1, 5.55% H-25 => L+4, 3.07% H-13 => L+7, 2.34% HOMO => L+11
255	29944	334	0.00	21.1% H-16 => L+5, 15.1% H-16 => L+8, 14.8% H-25 => L+3, 11.3% H-17 => L+7, 9.50% H-14 => L+7, 6.77% H-13 => L+5, 3.72% H-27 => L+3, 3.51% H-26 => L+4, 2.70% H-48 => L+1, 2.63% H-17 => L+4
256	30000	333	0.01	29.4% H-16 => L+7, 20.9% H-14 => L+5, 17.1% H-17 => L+8, 12.6% H-17 => L+5, 4.68% H-16 => L+4, 4.01% H-51 => L+1, 3.12% H-14 => L+8

257	30043	333	0.00	21.3% H-25 => L+3, 18.7% H-27 => L+3, 11.9% H-16 => L+5, 10.2% H-26 => L+4, 9.11% H-14 => L+7, 4.80% H-48 => L+1, 4.36% H-16 => L+8, 2.14% H-17 => L+7
258	30105	332	0.01	41.8% H-26 => L+2, 17.4% H-52 => L+1, 6.84% H-11 => L+8, 4.70% H-37 => L+3, 4.19% H-24 => L+2, 2.68% H-35 => L+3, 2.10% H-27 => L+6, 2.07% H-25 => L+6
259	30106	332	0.00	29.4% H-25 => L+2, 26.7% H-27 => L+2, 6.64% H-34 => L+3, 5.01% H-26 => L+6, 4.48% H-23 => L+2, 3.68% H-36 => L+3, 3.60% H-53 => L+1, 3.10% H-26 => L+1, 2.04% H-37 => L+4

Table S3.17. TDDFT-predicted band excitation data for **3.5**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	4205	2378	4.55	99.0% HOMO => LUMO
1	5464	1830	0.00	96.5% H-1 => LUMO, 2.18% H-3 => L+1
2	6961	1436	0.00	62.8% H-2 => LUMO, 35.4% HOMO => L+1
3	7054	1418	0.00	84.3% H-3 => LUMO, 13.0% H-1 => L+1
4	7434	1345	0.00	62.1% HOMO => L+1, 34.3% H-2 => LUMO
5	9016	1109	0.00	76.7% H-5 => LUMO, 15.6% H-3 => L+1, 4.89% H-1 => L+2
6	9237	1083	0.00	83.8% H-1 => L+1, 13.3% H-3 => LUMO
7	9646	1037	0.14	91.2% H-4 => LUMO, 4.01% HOMO => L+2
8	10195	981	0.16	84.1% HOMO => L+2, 7.56% H-2 => L+1
9	10396	962	0.04	86.0% H-2 => L+1, 7.64% HOMO => L+2, 2.09% H-4 => LUMO
10	10793	927	0.00	67.3% H-3 => L+1, 20.0% H-5 => LUMO, 8.22% H-1 => L+2
11	11084	902	0.00	73.2% H-6 => LUMO, 15.1% H-5 => L+1, 5.38% H-3 => L+2, 2.28% H-1 => L+5
12	11739	852	0.00	83.5% H-7 => LUMO, 5.99% H-4 => L+1, 2.34% H-12 => LUMO, 2.29% H-9 => L+1
13	11818	846	0.00	96.2% HOMO => L+3
14	12445	804	0.00	82.8% H-1 => L+2, 11.8% H-3 => L+1
15	12628	792	0.00	44.7% H-5 => L+1, 19.2% H-6 => LUMO, 18.8% HOMO => L+4, 9.11% H-3 => L+2, 2.86% H-1 => L+5
16	12827	780	0.00	46.7% HOMO => L+5, 18.3% H-2 => L+2, 18.2% H-4 => L+1, 6.93% H-7 => LUMO, 2.21% H-12 => LUMO
17	12834	779	0.04	83.9% H-9 => LUMO, 5.29% H-7 => L+1, 3.59% H-11 => LUMO
18	12876	777	0.00	73.6% HOMO => L+4, 12.4% H-5 => L+1, 3.92% H-6 => LUMO, 3.22% H-3 => L+2, 3.12% H-2 => L+3

19	12947	772	0.00	72.4% H-8 => LUMO, 12.5% H-6 => L+1, 4.75% H-5 => L+2, 2.39% H-3 => L+5, 2.10% H-15 => LUMO
20	13115	762	0.00	63.5% H-4 => L+1, 29.3% HOMO => L+5, 3.26% H-7 => LUMO
21	13528	739	0.00	73.3% H-2 => L+2, 18.1% HOMO => L+5, 4.98% H-4 => L+1
22	13815	724	5.21	87.9% H-1 => L+3, 6.16% H-3 => L+4
23	14049	712	0.00	61.1% H-3 => L+2, 23.2% H-5 => L+1, 10.7% H-1 => L+5
24	14081	710	0.00	80.2% HOMO => L+6, 4.31% H-6 => L+1, 4.20% H-2 => L+4, 3.14% H-8 => LUMO
25	14556	687	0.00	40.8% H-6 => L+1, 19.5% H-8 => LUMO, 13.8% H-5 => L+2, 8.88% HOMO => L+6, 6.76% H-3 => L+5, 3.36% H-1 => L+8, 2.79% H-10 => L+1
26	14589	685	0.18	84.7% H-10 => LUMO, 7.85% HOMO => L+10, 2.26% H-8 => L+1
27	14927	670	0.00	88.4% H-2 => L+3, 4.76% HOMO => L+4
28	15016	666	0.00	43.7% H-11 => LUMO, 16.7% HOMO => L+8, 10.9% H-9 => LUMO, 9.93% H-7 => L+1, 6.68% H-2 => L+5, 5.20% H-4 => L+2, 3.93% H-12 => L+1
29	15183	659	0.00	52.8% H-12 => LUMO, 23.2% H-1 => L+4, 10.1% H-3 => L+3, 3.16% H-11 => L+1, 2.66% H-14 => LUMO, 2.50% H-1 => L+7
30	15322	653	0.00	71.5% HOMO => L+7, 6.38% H-1 => L+5, 5.59% H-17 => LUMO, 3.42% H-2 => L+6, 2.73% H-2 => L+3
31	15385	650	0.00	59.0% H-7 => L+1, 18.3% H-11 => LUMO, 4.71% H-13 => LUMO, 3.24% H-4 => L+2, 2.38% H-1 => L+9, 2.25% HOMO => L+8
32	15446	647	0.00	45.0% H-1 => L+4, 26.7% H-12 => LUMO, 14.9% H-3 => L+3, 3.26% H-3 => L+6
33	15515	645	0.00	71.3% H-1 => L+5, 14.6% H-3 => L+2, 7.33% HOMO => L+7, 2.03% H-3 => L+8
34	15658	639	0.01	49.3% HOMO => L+8, 23.1% H-11 => LUMO, 8.68% H-2 => L+5, 4.72% H-7 => L+1, 3.28% H-4 => L+2
35	15743	635	0.00	31.1% H-6 => L+1, 21.4% H-5 => L+2, 11.0% H-15 => LUMO, 9.50% HOMO => L+9, 8.25% H-3 => L+5, 5.88% H-1 => L+8, 3.07% H-8 => L+2, 2.33% H-10 => L+1
36	15873	630	0.00	68.4% H-2 => L+4, 6.07% H-4 => L+3, 5.57% HOMO => L+6, 5.07% H-5 => L+2, 2.23% HOMO => L+9
37	15970	626	0.04	70.4% H-13 => LUMO, 7.29% H-7 => L+1, 6.49% H-1 => L+6, 4.14% H-3 => L+4, 2.74% H-2 => L+5

38	16088	622	0.00	34.7% HOMO => L+9, 18.9% H-15 => LUMO, 17.0% H-5 => L+2, 9.90% H-2 => L+4, 4.27% H-6 => L+1, 4.08% H-10 => L+1
39	16116	621	0.00	73.8% H-14 => LUMO, 5.77% H-9 => L+1, 4.96% H-12 => LUMO, 4.95% H-1 => L+10, 2.10% H-3 => L+9
40	16186	618	0.09	56.9% H-4 => L+2, 19.1% HOMO => L+8, 6.32% H-7 => L+1, 6.04% H-2 => L+5, 3.81% H-18 => LUMO
41	16341	612	0.00	68.6% H-3 => L+3, 25.2% H-1 => L+4, 2.46% H-5 => L+4
42	16561	604	0.00	43.4% H-8 => L+1, 25.8% HOMO => L+10, 9.49% H-10 => LUMO, 6.22% H-17 => LUMO, 6.21% H-6 => L+2, 2.14% H-2 => L+9, 2.07% H-5 => L+5
43	16570	604	0.09	65.7% H-2 => L+5, 12.5% H-4 => L+2, 8.52% HOMO => L+8, 4.83% H-18 => LUMO, 2.62% H-13 => LUMO
44	16663	600	0.00	85.2% H-16 => LUMO, 4.96% H-13 => L+1, 3.12% H-18 => L+1
45	16991	589	0.00	32.3% H-3 => L+5, 29.1% H-5 => L+2, 12.8% HOMO => L+9, 9.90% H-1 => L+8, 8.47% H-15 => LUMO
46	16992	589	0.41	74.1% H-18 => LUMO, 8.50% H-4 => L+2, 7.32% H-1 => L+6, 4.35% H-16 => L+1, 2.37% H-2 => L+5
47	16995	588	0.02	43.4% H-2 => L+6, 20.9% H-17 => LUMO, 12.7% HOMO => L+7, 6.49% H-4 => L+4, 4.86% H-8 => L+1, 3.10% H-20 => LUMO
48	17025	587	0.00	81.9% H-9 => L+1, 9.54% H-14 => LUMO
49	17027	587	0.00	51.7% H-15 => LUMO, 17.0% HOMO => L+9, 13.3% H-3 => L+5, 7.71% H-1 => L+8, 2.68% H-5 => L+2
50	17142	583	0.43	63.0% H-1 => L+6, 12.3% H-3 => L+4, 10.7% H-13 => LUMO, 5.32% H-18 => LUMO
51	17350	576	0.00	56.8% H-19 => LUMO, 16.5% H-4 => L+3, 15.9% H-21 => LUMO
52	17359	576	0.80	64.3% H-3 => L+4, 14.1% H-1 => L+6, 7.64% H-5 => L+3, 5.78% H-1 => L+3
53	17434	574	0.05	41.2% H-17 => LUMO, 21.4% H-20 => LUMO, 20.0% H-2 => L+6, 7.65% H-8 => L+1, 2.32% HOMO => L+7
54	17559	570	0.27	33.5% HOMO => L+10, 32.3% H-8 => L+1, 11.4% H-6 => L+2, 6.57% H-17 => LUMO, 4.93% H-5 => L+5, 3.89% H-20 => LUMO, 2.16% H-3 => L+8
55	17745	564	0.00	64.9% H-21 => LUMO, 15.9% H-19 => LUMO, 3.88% H-10 => L+1, 3.38% H-20 => L+1, 2.87% H-2 => L+7, 2.50% H-2 => L+4
56	17857	560	0.00	63.6% H-20 => LUMO, 16.2% H-2 => L+6, 10.6% H-17 => LUMO, 2.13% H-21 => L+1

57	17869	560	0.00	60.4% H-4 => L+3, 9.91% H-21 => LUMO, 7.44% H-19 => LUMO, 7.14% H-2 => L+4, 4.03% H-2 => L+7, 2.86% H-10 => L+1
58	17981	556	0.00	25.3% H-11 => L+1, 16.6% H-7 => L+2, 9.21% H-4 => L+5, 6.95% H-1 => L+10, 6.69% H-1 => L+7, 6.18% H-3 => L+9, 5.61% H-12 => LUMO, 5.28% H-2 => L+8, 3.55% H-3 => L+6, 3.01% H-5 => L+7, 2.01% H-14 => LUMO
59	18087	553	0.00	48.5% H-10 => L+1, 15.6% H-1 => L+8, 10.4% HOMO => L+9, 5.53% H-2 => L+7, 5.31% H-19 => LUMO, 2.88% H-4 => L+3, 2.68% H-3 => L+5
60	18211	549	0.00	79.8% H-5 => L+3, 6.57% H-3 => L+4, 2.71% H-12 => L+1, 2.44% H-6 => L+4
61	18245	548	0.00	45.7% H-1 => L+8, 24.5% H-3 => L+5, 5.68% HOMO => L+9, 5.27% H-4 => L+3, 4.19% H-19 => LUMO, 2.84% H-2 => L+7, 2.81% H-10 => L+1
62	18253	548	0.00	38.9% H-1 => L+7, 11.2% H-7 => L+2, 10.6% H-11 => L+1, 9.61% H-2 => L+8, 5.80% H-4 => L+5, 5.31% H-1 => L+10, 2.58% H-3 => L+6, 2.22% H-12 => LUMO, 2.19% H-9 => L+1
63	18385	544	0.03	67.0% H-12 => L+1, 8.02% H-11 => LUMO, 5.13% H-11 => L+2, 4.46% H-5 => L+3, 4.01% H-1 => L+9, 2.79% H-3 => L+7
64	18492	541	0.47	61.3% H-6 => L+2, 21.4% HOMO => L+10, 4.53% H-2 => L+9, 3.00% H-4 => L+4, 2.42% H-4 => L+7
65	18660	536	0.00	36.6% H-1 => L+7, 25.8% H-11 => L+1, 8.52% H-3 => L+6, 7.05% H-5 => L+4, 4.49% H-7 => L+2, 3.83% H-6 => L+3, 2.50% H-2 => L+8
66	18710	534	0.00	55.4% H-2 => L+7, 20.7% H-10 => L+1, 6.86% H-2 => L+10, 3.47% H-4 => L+6, 2.05% H-1 => L+8, 2.01% H-19 => LUMO
67	18748	533	0.01	66.7% H-4 => L+4, 9.89% H-7 => L+3, 9.71% H-2 => L+6, 3.89% H-6 => L+2
68	18765	533	0.00	57.6% H-3 => L+6, 14.6% H-11 => L+1, 8.24% H-7 => L+2, 3.73% H-2 => L+8, 2.81% H-22 => LUMO, 2.27% H-1 => L+4
69	18931	528	0.00	42.2% H-7 => L+2, 28.0% H-2 => L+8, 9.38% H-4 => L+5, 7.86% H-3 => L+6, 2.65% H-1 => L+10
70	18940	528	0.00	86.2% H-22 => LUMO, 3.88% H-23 => L+1, 3.42% H-3 => L+6
71	19251	519	0.00	66.4% H-5 => L+4, 4.39% H-3 => L+6, 4.08% H-1 => L+7, 3.23% H-2 => L+8, 3.02% H-3 => L+3, 2.90% H-11 => L+1, 2.83% H-6 => L+3, 2.45% H-4 => L+5
72	19261	519	0.00	37.2% H-1 => L+9, 17.8% H-9 => L+2, 9.52% H-14 => L+1, 8.72% H-12 => L+1, 4.52% H-3 => L+10, 3.31% H-13 => LUMO, 2.55% H-7 => L+5, 2.22% H-3 => L+7

73	19309	518	0.00	81.6% H-23 => LUMO, 7.19% H-22 => L+1, 2.72% H-25 => LUMO, 2.57% H-24 => L+1, 2.06% H-1 => L+9
74	19311	518	0.02	57.4% H-5 => L+5, 14.3% H-2 => L+9, 8.02% H-6 => L+2, 4.64% HOMO => L+10, 4.15% H-3 => L+8
75	19452	514	0.00	53.6% H-4 => L+5, 30.9% H-2 => L+8, 3.42% H-5 => L+4, 2.18% H-7 => L+2
76	19775	506	0.00	46.0% H-24 => LUMO, 31.3% H-13 => L+1, 4.78% H-23 => L+1, 3.89% H-26 => LUMO, 2.36% H-5 => L+4
77	19832	504	0.00	46.6% H-13 => L+1, 33.5% H-24 => LUMO, 3.20% H-23 => L+1, 2.63% H-16 => LUMO, 2.38% H-26 => LUMO
78	19836	504	0.01	33.0% H-1 => L+9, 32.6% H-9 => L+2, 17.4% H-14 => L+1, 2.01% H-8 => L+3
79	19856	504	0.47	46.6% H-15 => L+1, 22.4% H-2 => L+9, 13.3% H-5 => L+5, 3.08% H-10 => L+2
80	19857	504	0.00	39.0% H-2 => L+10, 23.2% H-8 => L+2, 11.8% H-4 => L+6, 7.10% H-4 => L+9, 2.91% H-7 => L+4, 2.91% H-6 => L+5, 2.85% H-10 => L+1, 2.29% H-2 => L+7
81	19889	503	0.00	35.3% H-4 => L+6, 24.2% H-8 => L+2, 14.4% H-2 => L+7, 7.62% H-7 => L+4, 5.08% H-9 => L+3, 2.44% H-6 => L+5, 2.40% H-10 => L+1
82	19946	501	0.06	48.0% H-3 => L+7, 20.1% H-14 => L+1, 8.27% H-5 => L+6, 3.71% H-3 => L+10, 3.63% HOMO => L+12, 2.39% H-12 => L+1, 2.27% H-9 => L+2
83	20082	498	0.00	46.9% H-7 => L+3, 24.3% H-3 => L+8, 10.8% H-4 => L+4, 5.44% H-5 => L+5, 2.11% H-9 => L+4
84	20108	497	0.00	45.9% H-6 => L+3, 26.9% H-1 => L+10, 6.56% H-5 => L+4, 4.65% H-2 => L+8, 3.42% H-6 => L+6, 2.78% H-10 => L+3
85	20219	495	0.44	51.9% H-16 => L+1, 10.5% H-3 => L+7, 5.58% H-14 => L+1, 5.20% H-18 => LUMO, 3.93% H-25 => LUMO, 3.27% H-7 => L+5, 3.07% H-5 => L+6, 2.18% H-13 => L+2
86	20289	493	0.03	64.2% H-25 => LUMO, 17.8% H-27 => LUMO, 6.82% H-24 => L+1, 4.10% H-16 => L+1
87	20343	492	0.01	32.2% H-3 => L+8, 23.9% H-7 => L+3, 20.8% H-15 => L+1, 6.81% H-5 => L+5, 6.61% H-2 => L+9
88	20368	491	0.00	21.8% H-14 => L+1, 19.4% H-3 => L+7, 18.6% H-16 => L+1, 16.6% H-9 => L+2, 5.09% H-5 => L+6, 4.16% H-6 => L+4, 3.92% H-1 => L+9
89	20403	490	0.57	33.3% H-2 => L+9, 24.4% H-3 => L+8, 19.3% H-15 => L+1, 3.70% H-7 => L+3, 2.02% H-4 => L+10
90	20421	490	0.00	35.4% H-1 => L+10, 34.2% H-6 => L+3, 7.63% H-8 => L+4, 3.21% H-10 => L+3, 3.10% H-2 => L+8, 2.23% H-13 => L+1

91	20529	487	0.00	36.7% H-17 => L+1, 22.3% H-8 => L+2, 18.5% H-2 => L+10, 3.37% H-4 => L+6, 3.28% H-20 => L+1, 2.24% H-9 => L+3
92	20554	487	0.27	47.2% H-5 => L+6, 13.7% H-14 => L+1, 13.6% H-9 => L+2, 7.55% HOMO => L+12, 2.86% H-6 => L+4
93	20701	483	0.00	81.6% H-18 => L+1, 4.19% HOMO => L+11, 3.50% H-16 => L+2, 3.15% H-16 => LUMO
94	20745	482	0.00	41.8% H-17 => L+1, 16.8% H-8 => L+2, 12.2% H-2 => L+10, 8.12% H-4 => L+6, 5.61% H-20 => L+1, 4.52% H-6 => L+5
95	20785	481	0.00	45.1% HOMO => L+11, 20.9% H-3 => L+9, 6.88% H-18 => L+1, 3.97% H-5 => L+7, 3.59% H-2 => L+12, 3.18% H-4 => L+5, 2.63% H-5 => L+10, 2.18% H-1 => L+7
96	20828	480	0.00	75.4% H-26 => LUMO, 7.59% H-25 => L+1, 6.60% H-27 => L+1, 4.36% H-24 => LUMO
97	20859	479	0.00	70.3% H-19 => L+1, 21.0% H-21 => L+1
98	20871	479	0.00	66.4% H-27 => LUMO, 13.8% H-25 => LUMO, 12.3% H-26 => L+1, 2.60% H-25 => L+2
99	20905	478	0.00	35.0% H-9 => L+3, 25.3% H-7 => L+4, 19.0% H-4 => L+6, 4.70% H-17 => L+1, 2.97% H-20 => L+1, 2.67% H-7 => L+7
100	20910	478	0.12	22.5% HOMO => L+12, 16.4% H-3 => L+10, 8.04% H-5 => L+9, 7.51% H-5 => L+6, 7.00% H-4 => L+8, 5.16% H-7 => L+5, 4.21% H-14 => L+1, 4.14% H-9 => L+2, 3.89% H-11 => L+2, 2.87% H-8 => L+6, 2.77% H-2 => L+11, 2.54% H-6 => L+7, 2.10% H-1 => L+9
101	21062	475	0.06	47.0% H-6 => L+4, 12.0% H-5 => L+6, 10.4% H-8 => L+3, 6.52% H-3 => L+10, 3.33% HOMO => L+12, 3.26% H-6 => L+7, 2.64% H-7 => L+5, 2.12% H-5 => L+9, 2.09% H-14 => L+1
102	21187	472	0.07	64.4% H-21 => L+1, 16.7% H-19 => L+1, 4.45% H-20 => L+2, 4.31% H-20 => LUMO, 2.89% H-4 => L+7
103	21220	471	0.00	72.7% H-20 => L+1, 5.00% H-17 => L+1, 4.98% H-4 => L+6, 3.57% H-21 => L+2, 2.76% H-21 => LUMO, 2.50% H-6 => L+5
104	21269	470	0.00	77.2% H-10 => L+2, 4.13% H-2 => L+9, 2.43% H-8 => L+5
105	21333	469	0.00	48.6% H-3 => L+9, 20.2% HOMO => L+11, 5.53% H-8 => L+4, 5.11% H-6 => L+6, 4.70% H-10 => L+3, 3.04% H-1 => L+10, 2.24% H-5 => L+7
106	21433	467	0.00	55.3% H-6 => L+5, 12.3% H-9 => L+3, 8.15% H-2 => L+10, 4.52% H-11 => L+3, 3.26% H-9 => L+6, 3.08% H-20 => L+1, 2.70% H-7 => L+4
107	21580	463	0.05	35.9% H-7 => L+5, 32.9% HOMO => L+12, 7.70% H-4 => L+8, 6.52% H-6 => L+4, 5.38% H-11 => L+2, 2.64% H-9 => L+2

108	21700	461	0.86	67.2% H-4 => L+7, 3.31% H-10 => L+2, 2.78% H-1 => L+11, 2.48% H-3 => L+8, 2.35% H-21 => L+1, 2.08% H-7 => L+6
109	21711	461	0.03	68.6% H-11 => L+2, 5.43% H-7 => L+5, 5.24% H-12 => L+5, 5.04% H-12 => L+1, 4.79% H-4 => L+8, 2.65% H-16 => L+1
110	21755	460	0.00	75.8% H-12 => L+2, 5.53% H-11 => L+1, 5.28% H-11 => L+5, 3.16% HOMO => L+11, 2.61% H-13 => L+1
111	21771	459	0.00	42.9% H-7 => L+4, 24.0% H-9 => L+3, 13.5% H-6 => L+5, 4.11% H-9 => L+6, 2.92% H-2 => L+10, 2.34% H-4 => L+3
112	21820	458	0.00	39.7% H-8 => L+3, 21.1% H-6 => L+4, 18.0% H-3 => L+10, 7.33% H-7 => L+5, 5.81% H-10 => L+4
113	22036	454	0.00	67.3% H-5 => L+7, 9.26% H-10 => L+3, 7.15% H-8 => L+4, 2.25% H-6 => L+9, 2.25% HOMO => L+11
114	22046	454	0.04	57.0% H-4 => L+8, 19.5% H-7 => L+5, 5.35% H-8 => L+3, 3.39% HOMO => L+12, 2.90% H-9 => L+8, 2.37% H-13 => L+2
115	22178	451	0.00	36.1% H-28 => LUMO, 24.7% H-5 => L+8, 9.27% H-4 => L+9, 7.16% H-32 => LUMO, 4.49% H-6 => L+5, 3.08% H-29 => L+1, 2.93% H-2 => L+10, 2.20% H-7 => L+7
116	22242	450	0.00	46.4% H-5 => L+8, 20.5% H-28 => LUMO, 16.0% H-30 => LUMO, 4.28% H-4 => L+9, 2.08% H-11 => L+3
117	22242	450	0.01	74.3% H-29 => LUMO, 9.08% H-31 => LUMO, 5.91% H-28 => L+1, 2.07% H-4 => L+7
118	22336	448	0.00	39.4% H-3 => L+10, 22.3% H-8 => L+3, 7.88% H-4 => L+8, 6.87% H-5 => L+9, 5.49% H-8 => L+6, 5.44% H-6 => L+7
119	22347	447	0.00	66.3% H-30 => LUMO, 14.0% H-28 => LUMO, 6.33% H-5 => L+8, 2.20% H-2 => L+10
120	22367	447	0.01	56.0% H-31 => LUMO, 23.3% H-33 => LUMO, 9.29% H-29 => LUMO, 3.41% H-7 => L+6
121	22389	447	0.00	27.7% H-9 => L+5, 25.7% H-14 => L+2, 10.8% H-5 => L+10, 5.61% H-7 => L+8, 3.99% H-8 => L+7, 3.65% H-6 => L+9, 2.90% H-10 => L+6, 2.72% H-3 => L+9, 2.49% H-1 => L+10, 2.48% H-5 => L+7
122	22393	447	0.00	32.9% H-4 => L+9, 19.1% H-32 => LUMO, 18.0% H-28 => LUMO, 5.48% H-30 => LUMO, 2.85% H-11 => L+3, 2.20% H-7 => L+10
123	22449	445	0.22	31.6% H-33 => LUMO, 15.2% H-31 => LUMO, 15.2% H-7 => L+6, 14.1% H-9 => L+4, 4.08% H-12 => L+3, 2.85% H-32 => L+1, 2.44% H-11 => L+4
124	22591	443	0.00	61.6% H-32 => LUMO, 13.6% H-4 => L+9, 5.16% H-30 => LUMO, 3.62% H-11 => L+3, 2.17% H-12 => L+4, 2.11% H-33 => L+1

125	22623	442	0.03	34.1% H-33 => LUMO, 21.4% H-9 => L+4, 11.1% H-7 => L+6, 6.76% H-31 => LUMO, 4.71% H-4 => L+7, 4.61% H-12 => L+3, 3.07% H-4 => L+10, 2.14% H-14 => L+3
126	22719	440	0.00	68.2% H-6 => L+6, 11.4% H-10 => L+3, 6.29% H-8 => L+4, 2.26% H-14 => L+2, 2.10% H-5 => L+4
127	22788	439	0.30	26.2% H-7 => L+6, 23.6% H-12 => L+3, 11.8% H-11 => L+4, 6.92% H-8 => L+5, 4.08% H-31 => LUMO, 3.20% H-29 => LUMO, 2.88% H-10 => L+2, 2.64% H-1 => L+11, 2.48% H-4 => L+7, 2.34% H-9 => L+7, 2.23% H-6 => L+8
128	22846	438	0.00	84.6% H-22 => L+1, 6.14% H-23 => LUMO, 3.52% H-23 => L+2, 2.03% H-24 => L+1
129	22915	436	0.19	31.7% H-4 => L+10, 31.0% H-8 => L+5, 7.23% H-7 => L+6, 4.05% H-10 => L+2, 3.93% H-6 => L+8, 3.34% H-7 => L+9, 3.31% H-9 => L+4, 2.21% H-2 => L+9
130	22947	436	0.16	66.0% H-13 => L+2, 6.27% H-5 => L+9, 3.79% H-7 => L+5, 2.85% H-16 => L+1, 2.09% H-8 => L+3
131	23021	434	0.01	39.0% H-11 => L+3, 22.5% H-12 => L+4, 6.34% H-15 => L+2, 4.32% H-5 => L+8, 2.68% H-13 => L+3, 2.56% H-1 => L+12, 2.45% H-32 => LUMO, 2.27% H-9 => L+3
132	23127	432	0.00	50.7% H-5 => L+9, 7.06% H-36 => LUMO, 6.68% H-13 => L+2, 4.92% HOMO => L+12, 4.58% H-8 => L+3, 3.73% H-11 => L+2, 2.87% H-10 => L+4, 2.49% H-6 => L+10
133	23183	431	0.34	34.4% H-9 => L+4, 17.7% H-12 => L+3, 11.6% H-7 => L+6, 8.07% H-11 => L+4, 4.71% H-4 => L+10, 3.94% H-9 => L+7, 2.76% H-13 => L+4
134	23222	431	0.00	69.1% H-23 => L+1, 6.00% H-24 => LUMO, 5.94% H-22 => L+2, 4.41% H-22 => LUMO, 3.06% H-25 => L+1, 2.09% H-14 => L+2
135	23293	429	0.11	47.8% H-36 => LUMO, 21.4% H-38 => LUMO, 5.07% H-5 => L+9, 3.57% H-13 => L+2, 3.54% H-40 => LUMO, 2.65% H-10 => L+4, 2.39% H-8 => L+6, 2.08% H-6 => L+7
136	23316	429	0.00	41.4% H-9 => L+5, 27.1% H-14 => L+2, 9.08% H-10 => L+3, 4.95% H-8 => L+4, 2.56% H-23 => L+1
137	23341	428	0.00	71.0% H-35 => LUMO, 13.6% H-15 => L+2, 4.99% H-34 => L+1
138	23342	428	0.00	43.3% H-8 => L+4, 21.1% H-10 => L+3, 14.1% H-5 => L+10, 6.75% H-9 => L+5, 2.87% H-6 => L+3, 2.17% H-10 => L+6
139	23344	428	0.00	87.6% H-34 => LUMO, 6.14% H-35 => L+1
140	23367	428	0.00	56.9% H-15 => L+2, 19.3% H-35 => LUMO, 4.12% H-1 => L+12, 3.38% H-11 => L+3, 2.24% H-3 => L+11

141	23426	427	0.00	62.4% H-37 => LUMO, 7.65% H-41 => LUMO, 3.86% H-39 => LUMO, 3.47% H-14 => L+2, 2.92% H-10 => L+3, 2.77% H-36 => L+1
142	23463	426	0.06	42.4% H-8 => L+5, 27.3% H-4 => L+10, 6.41% H-1 => L+11, 3.63% H-34 => LUMO, 3.21% H-3 => L+12, 2.41% H-17 => L+2, 2.30% H-12 => L+3
143	23519	425	0.00	34.1% H-16 => L+2, 21.9% H-5 => L+10, 9.17% H-14 => L+2, 5.13% H-8 => L+4, 3.67% H-9 => L+5, 2.90% H-37 => LUMO, 2.54% H-6 => L+9, 2.16% H-2 => L+12, 2.12% H-18 => L+1
144	23547	425	0.01	41.1% H-38 => LUMO, 15.5% H-36 => LUMO, 13.1% H-40 => LUMO, 12.5% H-42 => LUMO, 3.10% H-18 => L+2, 2.43% H-37 => L+1
145	23608	424	0.00	25.6% H-7 => L+7, 17.8% H-9 => L+6, 11.3% H-4 => L+9, 6.29% H-15 => L+2, 6.16% H-13 => L+3, 4.35% H-1 => L+12, 2.70% H-9 => L+3, 2.26% H-10 => L+5, 2.20% H-19 => L+2, 2.07% H-14 => L+4
146	23672	422	0.00	53.8% H-41 => LUMO, 14.1% H-39 => LUMO, 8.29% H-43 => LUMO, 5.32% H-37 => LUMO, 3.14% H-5 => L+10, 2.84% H-16 => L+2, 2.39% H-14 => L+2
147	23687	422	0.00	67.2% H-24 => L+1, 6.14% H-23 => L+2, 5.24% H-23 => LUMO, 4.87% H-26 => L+1, 4.83% H-25 => LUMO
148	23722	422	0.11	63.2% H-42 => LUMO, 15.5% H-44 => LUMO, 7.96% H-38 => LUMO, 4.09% H-6 => L+7
149	23750	421	0.14	23.7% H-6 => L+7, 12.7% H-2 => L+11, 12.2% H-36 => LUMO, 11.3% H-40 => LUMO, 7.38% HOMO => L+12, 4.45% H-8 => L+6, 4.10% H-38 => LUMO
150	23776	421	0.00	39.4% H-16 => L+2, 12.5% H-37 => LUMO, 10.7% H-39 => LUMO, 7.72% H-14 => L+2, 6.27% H-2 => L+12, 4.68% H-5 => L+10, 3.04% HOMO => L+11
151	23855	419	0.00	69.0% H-17 => L+2, 6.08% H-1 => L+11, 4.31% H-4 => L+10, 3.83% H-20 => L+2, 2.04% H-15 => L+5
152	23858	419	0.00	23.3% H-39 => LUMO, 16.3% H-41 => LUMO, 10.6% H-10 => L+3, 8.26% H-43 => LUMO, 7.67% H-14 => L+2, 5.66% H-5 => L+10, 4.10% H-57 => LUMO, 3.03% H-16 => L+2, 2.87% H-40 => L+1
153	23859	419	0.00	28.9% H-7 => L+7, 14.9% H-13 => L+3, 8.46% H-11 => L+3, 6.73% H-10 => L+5, 5.34% H-9 => L+6, 5.12% H-9 => L+9, 3.62% H-11 => L+6, 3.07% H-4 => L+9, 2.91% H-15 => L+2, 2.69% H-18 => L+3, 2.64% H-12 => L+4, 2.54% H-7 => L+4, 2.27% H-19 => L+2

154	23926	418	0.01	47.9% H-18 => L+2, 25.7% H-40 => LUMO, 2.73% H-2 => L+11, 2.64% H-16 => L+5, 2.32% H-6 => L+7
155	23942	418	0.04	27.6% H-18 => L+2, 26.1% H-40 => LUMO, 11.0% H-6 => L+7, 10.4% H-38 => LUMO, 7.00% H-44 => LUMO, 4.04% H-42 => LUMO, 2.42% H-39 => L+1
156	24008	417	0.00	36.0% H-39 => LUMO, 11.6% H-10 => L+3, 7.94% HOMO => L+11, 6.18% H-2 => L+12, 3.25% H-57 => LUMO, 2.67% H-41 => LUMO, 2.59% H-6 => L+6, 2.55% H-8 => L+4, 2.29% H-5 => L+7, 2.03% H-14 => L+2
157	24064	416	0.08	24.3% H-6 => L+7, 23.2% H-10 => L+4, 13.1% H-2 => L+11, 12.7% H-8 => L+6, 3.76% HOMO => L+12, 3.30% H-15 => L+3, 3.25% H-38 => LUMO, 2.86% H-40 => LUMO
158	24104	415	0.00	64.3% H-19 => L+2, 15.4% H-21 => L+2, 6.88% H-1 => L+12, 2.02% H-4 => L+9
159	24110	415	0.00	61.2% H-25 => L+1, 20.2% H-27 => L+1, 6.44% H-24 => L+2, 4.90% H-24 => LUMO
160	24173	414	0.68	38.4% H-1 => L+11, 18.4% H-6 => L+8, 5.70% H-14 => L+3, 4.74% H-12 => L+3, 4.36% H-9 => L+4, 3.94% H-3 => L+12, 3.08% H-17 => L+2, 3.02% H-8 => L+5, 2.27% H-12 => L+6, 2.09% H-4 => L+7
161	24212	413	0.00	20.5% H-5 => L+10, 9.65% H-7 => L+8, 9.17% H-6 => L+9, 7.72% H-8 => L+7, 7.37% H-43 => LUMO, 6.07% H-10 => L+6, 5.61% H-2 => L+12, 4.16% H-17 => L+3, 3.61% H-15 => L+4, 3.08% H-9 => L+5, 2.67% H-8 => L+4
162	24249	412	0.05	65.1% H-44 => LUMO, 14.5% H-42 => LUMO, 8.26% H-40 => LUMO, 4.46% H-43 => L+1, 2.22% H-36 => LUMO
163	24254	412	0.00	65.2% H-43 => LUMO, 10.6% H-41 => LUMO, 3.49% H-44 => L+1, 2.63% H-2 => L+12, 2.44% H-7 => L+8, 2.39% H-37 => LUMO, 2.21% H-5 => L+10
164	24276	412	0.14	50.8% H-6 => L+8, 20.2% H-20 => L+2, 5.29% H-4 => L+10, 4.57% H-12 => L+3, 4.37% H-1 => L+11
165	24299	412	0.01	34.0% H-21 => L+2, 20.1% H-1 => L+12, 14.9% H-10 => L+5, 8.27% H-9 => L+6, 3.09% H-3 => L+11, 2.23% H-20 => L+5, 2.11% H-20 => L+1, 2.10% H-11 => L+3
166	24364	410	0.00	43.3% H-20 => L+2, 9.13% H-16 => L+3, 8.97% H-12 => L+6, 6.82% H-12 => L+3, 5.76% H-6 => L+8, 5.61% H-11 => L+4, 2.67% H-4 => L+10, 2.62% H-21 => L+1, 2.27% H-11 => L+7, 2.27% H-13 => L+4, 2.15% H-21 => L+5
167	24385	410	0.00	30.7% H-10 => L+5, 30.4% H-21 => L+2, 9.04% H-19 => L+2, 4.13% H-13 => L+3, 2.53% H-20 =>

				L+5, 2.42% H-15 => L+2, 2.39% H-1 => L+12, 2.37% H-20 => L+1
168	24416	410	0.52	16.6% H-16 => L+3, 11.8% H-20 => L+2, 7.35% H-17 => L+2, 7.26% H-13 => L+4, 6.85% H-7 => L+6, 5.75% H-1 => L+11, 5.71% H-6 => L+8, 5.31% H-9 => L+7, 4.37% H-14 => L+3, 3.72% H-7 => L+9, 3.60% H-12 => L+6, 2.73% H-4 => L+10, 2.33% H-18 => L+4
169	24447	409	0.01	18.2% H-10 => L+5, 18.0% H-1 => L+12, 9.43% H-7 => L+7, 8.19% H-9 => L+6, 6.74% H-18 => L+3, 6.06% H-11 => L+3, 5.64% H-19 => L+2, 5.16% H-11 => L+6, 2.83% H-4 => L+9, 2.77% H-12 => L+7, 2.11% H-16 => L+4
170	24458	409	0.00	36.7% H-8 => L+6, 27.2% H-10 => L+4, 6.96% H-10 => L+7, 4.40% H-6 => L+7, 4.03% H-48 => LUMO, 2.79% H-15 => L+3, 2.37% H-6 => L+4
171	24463	409	0.00	45.5% H-7 => L+8, 14.9% H-47 => LUMO, 8.83% H-11 => L+5, 4.86% H-6 => L+9, 4.15% H-9 => L+5, 3.61% H-50 => LUMO
172	24485	408	0.00	72.9% H-47 => LUMO, 9.91% H-7 => L+8, 3.36% H-45 => LUMO, 2.21% H-50 => LUMO
173	24553	407	0.01	25.1% H-9 => L+6, 19.8% H-13 => L+3, 9.43% H-1 => L+12, 7.25% H-21 => L+2, 6.41% H-16 => L+4, 3.94% H-10 => L+5, 3.53% H-11 => L+3, 3.19% H-12 => L+4, 2.54% H-9 => L+9, 2.43% H-19 => L+2, 2.31% H-7 => L+10
174	24568	407	0.00	63.8% H-48 => LUMO, 11.3% H-54 => LUMO, 5.64% H-8 => L+6, 4.27% H-46 => LUMO, 3.89% H-2 => L+11
175	24590	407	0.00	88.5% H-49 => LUMO, 3.31% H-52 => LUMO, 2.11% H-14 => L+3
176	24610	406	0.00	76.3% H-51 => LUMO, 19.5% H-53 => LUMO
177	24670	405	0.00	63.9% H-50 => LUMO, 12.3% H-57 => LUMO, 5.45% H-11 => L+5, 4.00% H-47 => LUMO
178	24670	405	0.00	42.4% H-26 => L+1, 7.78% H-46 => LUMO, 6.54% H-27 => LUMO, 5.07% H-48 => LUMO, 4.79% H-25 => LUMO, 3.94% H-54 => LUMO, 3.69% H-2 => L+11, 3.67% H-27 => L+2, 3.53% H-12 => L+5, 3.16% H-25 => L+2
179	24682	405	0.00	22.8% H-26 => L+1, 19.6% H-48 => LUMO, 15.7% H-46 => LUMO, 5.70% H-2 => L+11, 5.46% H-54 => LUMO, 3.38% H-27 => LUMO, 2.40% H-25 => LUMO, 2.38% H-12 => L+5
180	24714	405	0.00	56.4% H-27 => L+1, 13.6% H-26 => LUMO, 10.9% H-25 => L+1, 9.61% H-26 => L+2
181	24728	404	0.11	55.9% H-52 => LUMO, 13.3% H-14 => L+3, 5.69% H-7 => L+9, 5.58% H-55 => LUMO, 2.49% H-13 => L+4, 2.18% H-58 => LUMO
182	24737	404	0.00	32.9% H-45 => LUMO, 15.3% H-2 => L+12, 10.5% H-57 => LUMO, 10.0% H-11 => L+5,

				6.87% H-50 => LUMO, 3.51% H-47 => LUMO, 3.37% H-6 => L+9, 3.07% H-7 => L+8
183	24740	404	0.02	22.4% H-52 => LUMO, 20.3% H-7 => L+9, 10.9% H-14 => L+3, 6.17% H-49 => LUMO, 3.52% H-11 => L+4, 3.31% H-12 => L+6, 3.00% H-12 => L+3, 2.80% H-20 => L+2, 2.74% H-9 => L+7, 2.28% H-9 => L+10, 2.22% H-9 => L+4
184	24742	404	0.00	63.8% H-53 => LUMO, 17.3% H-51 => LUMO, 9.40% H-56 => LUMO, 3.26% H-52 => L+1, 2.44% H-59 => LUMO
185	24767	404	0.02	30.6% H-12 => L+5, 14.7% H-46 => LUMO, 14.7% H-15 => L+3, 7.49% H-10 => L+4, 4.77% H-54 => LUMO, 2.82% H-13 => L+2, 2.80% H-11 => L+8, 2.30% H-9 => L+8, 2.27% H-21 => L+3
186	24853	402	0.00	16.4% H-6 => L+10, 10.2% H-54 => LUMO, 9.25% H-19 => L+3, 7.96% H-46 => LUMO, 7.23% H-9 => L+8, 6.41% H-8 => L+6, 5.52% H-8 => L+9, 4.47% H-14 => L+5, 4.01% H-60 => LUMO, 4.00% H-15 => L+6, 3.43% H-17 => L+4, 2.58% H-10 => L+7, 2.43% H-18 => L+2
187	24862	402	1.42	31.9% H-14 => L+3, 14.0% H-1 => L+11, 10.7% H-13 => L+4, 10.1% H-11 => L+4, 6.35% H-7 => L+9, 4.99% H-16 => L+3, 3.70% H-9 => L+7, 2.93% H-52 => LUMO, 2.28% H-17 => L+2
188	24864	402	0.03	46.5% H-15 => L+3, 21.2% H-12 => L+5, 6.22% H-10 => L+4, 5.03% H-17 => L+4, 2.57% H-13 => L+2, 2.40% H-8 => L+6, 2.15% H-9 => L+8
189	24885	402	0.00	27.0% H-13 => L+3, 12.8% H-18 => L+3, 10.0% H-11 => L+6, 9.28% H-12 => L+4, 7.52% H-1 => L+12, 4.21% H-7 => L+7, 3.13% H-10 => L+5, 2.89% H-12 => L+7, 2.85% H-9 => L+6, 2.65% H-13 => L+6, 2.42% H-11 => L+3
190	24915	401	0.00	26.3% H-45 => LUMO, 18.4% H-11 => L+5, 12.3% H-2 => L+12, 7.74% H-7 => L+8, 5.02% H-57 => LUMO, 3.92% H-17 => L+3, 2.58% H-15 => L+4, 2.38% H-10 => L+3
191	24957	401	0.00	27.7% H-6 => L+9, 24.1% H-17 => L+3, 18.3% H-11 => L+5, 6.67% H-15 => L+4, 3.45% H-57 => LUMO, 2.56% H-19 => L+4, 2.26% H-10 => L+6
192	24980	400	0.02	54.6% H-54 => LUMO, 29.7% H-46 => LUMO, 2.38% H-48 => LUMO, 2.21% H-45 => L+1, 2.15% H-2 => L+11
193	25007	400	0.00	50.1% H-57 => LUMO, 20.1% H-45 => LUMO, 13.5% H-50 => LUMO, 2.60% H-54 => L+1, 2.55% H-11 => L+5
194	25010	400	0.02	20.8% H-11 => L+4, 18.6% H-7 => L+9, 10.8% H-14 => L+3, 8.97% H-12 => L+3, 8.41% H-9 => L+10, 5.20% H-61 => LUMO, 3.47% H-9 => L+7, 2.99% H-13 => L+4, 2.64% H-13 => L+7, 2.36% H-6 => L+8

195	25101	398	0.02	62.7% H-55 => LUMO, 17.5% H-58 => LUMO, 9.64% H-52 => LUMO, 3.40% H-56 => L+1
196	25102	398	0.00	59.8% H-56 => LUMO, 16.3% H-59 => LUMO, 10.8% H-53 => LUMO, 3.49% H-55 => L+1
197	25123	398	0.03	21.1% H-2 => L+11, 17.8% H-19 => L+3, 11.6% H-60 => LUMO, 9.44% H-21 => L+3, 7.96% H-46 => LUMO, 4.31% H-9 => L+8, 2.87% H-17 => L+4, 2.40% H-10 => L+4, 2.26% H-15 => L+3
198	25161	397	0.00	27.0% H-18 => L+3, 16.6% H-16 => L+4, 15.6% H-12 => L+4, 8.62% H-7 => L+7, 7.32% H-9 => L+6, 5.13% H-11 => L+3, 2.52% H-56 => LUMO, 2.13% H-14 => L+4
199	25215	397	0.39	23.6% H-19 => L+3, 22.1% H-6 => L+10, 9.50% H-2 => L+11, 8.65% H-21 => L+3, 4.36% H-12 => L+5, 4.12% H-60 => LUMO, 4.10% H-8 => L+9, 3.04% H-10 => L+4, 2.08% H-9 => L+8, 2.02% H-46 => LUMO
200	25256	396	0.00	25.9% H-20 => L+3, 16.2% H-17 => L+3, 14.1% H-6 => L+9, 8.92% H-21 => L+4, 8.74% H-2 => L+12, 3.12% H-7 => L+8, 2.84% H-64 => LUMO, 2.20% H-15 => L+4
201	25311	395	0.03	31.8% H-58 => LUMO, 14.4% H-55 => LUMO, 10.2% H-9 => L+7, 7.61% H-61 => LUMO, 7.43% H-16 => L+3, 4.74% H-18 => L+4, 4.45% H-11 => L+4, 2.36% H-9 => L+10
202	25325	395	0.00	67.8% H-59 => LUMO, 20.0% H-56 => LUMO, 3.71% H-58 => L+1
203	25329	395	0.06	33.5% H-58 => LUMO, 16.8% H-16 => L+3, 13.5% H-9 => L+7, 6.89% H-55 => LUMO, 5.57% H-18 => L+4, 3.54% H-61 => LUMO, 2.48% H-9 => L+10, 2.46% H-7 => L+9
204	25356	394	0.33	44.0% H-21 => L+3, 26.4% H-20 => L+4, 8.07% H-19 => L+3, 5.86% H-6 => L+10, 3.82% H-17 => L+4, 2.32% H-12 => L+5, 2.22% H-19 => L+6
205	25385	394	0.00	38.7% H-7 => L+10, 7.76% H-12 => L+4, 7.36% H-9 => L+9, 5.74% H-10 => L+5, 4.82% H-62 => LUMO, 4.48% H-13 => L+3, 2.77% H-9 => L+6, 2.51% H-4 => L+9, 2.43% H-8 => L+8, 2.36% H-18 => L+3, 2.15% H-11 => L+3, 2.11% H-33 => L+1
206	25395	394	0.00	28.9% H-20 => L+3, 12.8% H-2 => L+12, 12.3% H-21 => L+4, 11.1% H-11 => L+5, 7.94% H-17 => L+3, 7.25% H-19 => L+4, 2.73% H-64 => LUMO, 2.56% H-15 => L+4
207	25460	393	0.00	32.3% H-10 => L+6, 25.4% H-8 => L+7, 7.17% H-2 => L+12, 6.38% H-6 => L+9, 4.56% H-17 => L+3, 3.59% H-19 => L+4, 2.62% H-20 => L+3, 2.30% H-64 => LUMO, 2.28% H-11 => L+5
208	25546	391	0.00	15.9% H-28 => L+1, 12.0% H-11 => L+7, 9.42% H-61 => LUMO, 8.31% H-12 => L+6, 7.42% H-16 => L+3, 7.34% H-12 => L+9, 6.83% H-58 =>

				LUMO, 4.04% H-11 => L+4, 2.78% H-3 => L+12, 2.59% H-16 => L+6, 2.33% H-13 => L+7, 2.24% H-29 => LUMO
209	25576	391	0.00	18.6% H-29 => L+1, 10.4% H-12 => L+7, 8.40% H-18 => L+3, 7.96% H-3 => L+11, 7.72% H-11 => L+6, 7.37% H-12 => L+4, 5.35% H-62 => LUMO, 4.90% H-11 => L+9, 4.22% H-59 => LUMO, 3.01% H-1 => L+12, 2.43% H-28 => LUMO, 2.29% H-11 => L+3
210	25705	389	0.00	52.0% H-29 => L+1, 19.1% H-3 => L+11, 4.82% H-28 => LUMO, 4.74% H-1 => L+12, 3.59% H-28 => L+2, 2.17% H-11 => L+6, 2.07% H-5 => L+12
211	25710	389	0.02	49.5% H-9 => L+8, 12.6% H-12 => L+5, 9.78% H-6 => L+10, 8.37% H-19 => L+3, 3.34% H-14 => L+5, 2.29% H-17 => L+4
212	25718	389	0.01	60.9% H-28 => L+1, 9.75% H-61 => LUMO, 5.42% H-29 => LUMO, 4.08% H-29 => L+2, 4.02% H-3 => L+12, 2.34% H-32 => L+1, 2.04% H-12 => L+6
213	25769	388	0.00	40.4% H-8 => L+7, 38.4% H-10 => L+6, 7.55% H-10 => L+9, 3.25% H-6 => L+9, 2.59% H-6 => L+6, 2.37% H-8 => L+4
214	25823	387	0.00	21.9% H-14 => L+4, 14.1% H-3 => L+11, 13.2% H-62 => LUMO, 7.68% H-8 => L+8, 6.31% H-29 => L+1, 4.77% H-31 => L+1, 4.12% H-13 => L+6, 3.60% H-1 => L+12, 2.62% H-11 => L+9, 2.39% H-12 => L+7
215	25823	387	0.19	62.7% H-30 => L+1, 11.0% H-61 => LUMO, 7.44% H-3 => L+12
216	25847	387	0.02	30.9% H-61 => LUMO, 25.7% H-30 => L+1, 13.7% H-3 => L+12, 7.25% H-32 => L+1, 2.72% H-7 => L+9, 2.49% H-63 => LUMO
217	25893	386	0.00	64.4% H-31 => L+1, 20.1% H-33 => L+1, 3.97% H-62 => LUMO
218	25931	386	0.01	22.6% H-3 => L+11, 19.5% H-14 => L+4, 17.2% H-11 => L+6, 7.40% H-33 => L+1, 4.17% H-62 => LUMO, 3.80% H-18 => L+3, 3.37% H-12 => L+7, 2.91% H-29 => L+1
219	25970	385	0.26	35.0% H-3 => L+12, 10.8% H-9 => L+7, 10.7% H-61 => LUMO, 4.56% H-1 => L+11, 4.23% H-12 => L+6, 3.44% H-28 => L+1, 3.38% H-63 => LUMO, 2.57% H-16 => L+6, 2.56% H-11 => L+7, 2.42% H-5 => L+11, 2.36% H-16 => L+3, 2.31% H-12 => L+9, 2.22% H-13 => L+7
220	26021	384	0.13	66.1% H-60 => LUMO, 4.89% H-2 => L+11, 4.32% H-15 => L+3, 2.79% H-14 => L+5, 2.15% H-10 => L+4
221	26049	384	0.00	29.3% H-8 => L+8, 19.6% H-62 => LUMO, 15.3% H-14 => L+4, 4.10% H-11 => L+6, 3.44% H-12 => L+7, 3.05% H-13 => L+6, 2.68% H-31 => L+1,

				2.44% H-12 => L+4, 2.32% H-23 => L+3, 2.00% H-65 => LUMO
222	26063	384	0.01	57.0% H-32 => L+1, 7.89% H-12 => L+6, 5.14% H-7 => L+9, 4.30% H-63 => LUMO, 3.66% H-30 => L+1, 3.39% H-11 => L+4, 2.31% H-33 => L+2
223	26086	383	0.14	54.3% H-22 => L+3, 13.4% H-23 => L+4, 5.07% H-13 => L+4, 4.89% H-24 => L+6, 2.89% H-22 => L+6, 2.24% H-25 => L+7, 2.19% H-9 => L+7, 2.15% H-27 => L+10
224	26094	383	0.00	85.9% H-13 => L+5, 2.27% H-16 => L+2, 2.25% H-18 => L+5
225	26120	383	0.00	56.9% H-33 => L+1, 14.1% H-31 => L+1, 9.29% H-62 => LUMO, 3.72% H-32 => L+2, 2.99% H-14 => L+4, 2.59% H-32 => LUMO, 2.39% H-3 => L+11
226	26125	383	0.00	82.5% H-22 => L+2, 5.75% H-23 => L+1, 3.91% H-23 => L+5, 2.50% H-22 => LUMO
227	26169	382	0.03	33.5% H-13 => L+4, 15.1% H-9 => L+7, 6.93% H-18 => L+4, 4.36% H-7 => L+9, 4.36% H-22 => L+3, 3.48% H-14 => L+3, 2.86% H-16 => L+3, 2.80% H-32 => L+1, 2.48% H-15 => L+5, 2.46% H-23 => L+4, 2.25% H-13 => L+7, 2.24% H-12 => L+3
228	26203	382	0.00	44.8% H-8 => L+8, 21.4% H-7 => L+10, 14.4% H-62 => LUMO, 4.89% H-14 => L+4, 2.14% H-11 => L+6
229	26221	381	0.19	34.6% H-8 => L+9, 22.6% H-6 => L+10, 15.3% H-10 => L+7, 5.76% H-10 => L+10, 2.70% H-15 => L+6, 2.52% H-19 => L+3, 2.12% H-6 => L+7, 2.01% H-5 => L+9
230	26252	381	0.00	55.1% H-15 => L+4, 8.73% H-19 => L+4, 8.60% H-17 => L+3, 3.27% H-17 => L+6, 3.15% H-15 => L+7, 2.71% H-19 => L+7
231	26269	381	0.03	16.1% H-12 => L+6, 15.5% H-63 => LUMO, 12.3% H-32 => L+1, 9.69% H-13 => L+4, 7.94% H-16 => L+6, 7.24% H-15 => L+5, 3.96% H-7 => L+9, 3.74% H-11 => L+4, 2.30% H-12 => L+9, 2.15% H-16 => L+3, 2.07% H-12 => L+3
232	26289	380	0.00	28.8% H-23 => L+3, 14.5% H-22 => L+4, 5.06% H-24 => L+4, 5.02% H-62 => LUMO, 5.01% H-13 => L+6, 4.05% H-11 => L+6, 2.85% H-16 => L+4, 2.62% H-14 => L+4, 2.29% H-11 => L+9, 2.02% H-22 => L+7, 2.00% H-25 => L+6
233	26316	380	0.00	12.4% H-11 => L+6, 11.6% H-23 => L+3, 8.18% H-14 => L+4, 7.08% H-62 => LUMO, 5.86% H-22 => L+4, 5.52% H-18 => L+3, 5.01% H-16 => L+4, 4.35% H-7 => L+10, 4.21% H-18 => L+6, 3.99% H-13 => L+6, 3.74% H-11 => L+9, 3.28% H-9 => L+9, 3.27% H-24 => L+4, 3.18% H-8 => L+8, 2.55% H-12 => L+4

234	26389	379	0.04	35.7% H-63 => LUMO, 14.7% H-15 => L+5, 7.04% H-9 => L+7, 6.74% H-16 => L+6, 5.23% H-18 => L+4, 4.49% H-61 => LUMO, 2.99% H-9 => L+10, 2.64% H-12 => L+9, 2.06% H-7 => L+9
235	26397	379	0.00	64.0% H-14 => L+5, 9.50% H-23 => L+2, 8.75% H-9 => L+8, 2.56% H-60 => LUMO
236	26490	378	0.00	62.9% H-23 => L+2, 10.7% H-14 => L+5, 5.46% H-22 => L+5, 5.03% H-24 => L+1, 3.44% H-22 => L+1, 2.56% H-24 => L+5
237	26495	377	0.01	55.1% H-15 => L+5, 17.2% H-63 => LUMO, 3.56% H-12 => L+6, 2.60% H-13 => L+4, 2.53% H-32 => L+1, 2.17% H-10 => L+8, 2.01% H-7 => L+9
238	26534	377	0.00	19.5% H-8 => L+10, 14.7% H-17 => L+6, 14.3% H-19 => L+4, 9.13% H-21 => L+4, 7.86% H-10 => L+9, 5.93% H-15 => L+7, 4.04% H-15 => L+4, 3.59% H-17 => L+3, 2.22% H-6 => L+9
239	26558	377	0.00	37.9% H-24 => L+3, 17.4% H-23 => L+4, 12.2% H-22 => L+6, 5.22% H-25 => L+4, 4.27% H-27 => L+7, 3.05% H-26 => L+3, 2.98% H-22 => L+9, 2.21% H-23 => L+10, 2.09% H-26 => L+9, 2.03% H-27 => L+4
240	26675	375	0.01	34.2% H-17 => L+4, 14.2% H-15 => L+6, 9.90% H-20 => L+4, 9.47% H-8 => L+9, 5.03% H-21 => L+6, 4.31% H-19 => L+3, 2.88% H-10 => L+10, 2.56% H-15 => L+3, 2.31% H-15 => L+9
241	26757	374	0.00	68.2% H-34 => L+1, 9.45% H-65 => LUMO, 6.35% H-35 => LUMO, 4.30% H-35 => L+2
242	26766	374	0.00	41.4% H-36 => L+1, 13.4% H-38 => L+1, 12.5% H-18 => L+5, 8.09% H-64 => LUMO, 2.61% H-40 => L+1, 2.03% H-4 => L+11
243	26774	373	0.00	83.2% H-35 => L+1, 7.19% H-34 => LUMO, 5.20% H-34 => L+2
244	26774	373	0.01	68.1% H-16 => L+5, 11.3% H-37 => L+1, 2.64% H-18 => L+2, 2.28% H-13 => L+8, 2.25% H-9 => L+8, 2.15% H-18 => L+8
245	26836	373	0.00	37.2% H-9 => L+9, 20.8% H-17 => L+5, 4.91% H-7 => L+10, 3.61% H-20 => L+5, 3.55% H-65 => LUMO, 3.15% H-7 => L+7, 2.76% H-25 => L+3, 2.32% H-14 => L+10, 2.21% H-11 => L+6, 2.19% H-34 => L+1, 2.00% H-14 => L+4
246	26882	372	0.00	29.1% H-25 => L+3, 15.6% H-24 => L+4, 9.62% H-23 => L+6, 6.78% H-27 => L+6, 5.79% H-22 => L+7, 4.46% H-27 => L+3, 3.60% H-26 => L+7, 3.54% H-17 => L+5, 3.06% H-22 => L+10, 2.98% H-65 => LUMO, 2.49% H-25 => L+9, 2.16% H-26 => L+4
247	26887	372	0.00	47.6% H-65 => LUMO, 17.1% H-17 => L+5, 13.7% H-34 => L+1, 2.86% H-16 => L+4, 2.59% H-63 => L+1

248	26900	372	0.00	23.6% H-36 => L+1, 20.9% H-24 => L+2, 20.2% H-64 => LUMO, 4.01% H-18 => L+5, 3.49% H-19 => L+4, 2.44% H-23 => L+5, 2.24% H-26 => L+2, 2.17% H-21 => L+4
249	26925	371	0.00	45.0% H-24 => L+2, 9.07% H-64 => LUMO, 6.71% H-36 => L+1, 5.20% H-23 => L+5, 4.71% H-26 => L+2, 2.90% H-25 => L+1, 2.62% H-23 => L+1, 2.35% H-19 => L+4, 2.14% H-21 => L+4
250	26928	371	0.05	35.5% H-10 => L+7, 20.5% H-37 => L+1, 13.7% H-8 => L+9, 4.92% H-10 => L+10, 3.18% H-41 => L+1, 3.16% H-16 => L+5, 3.00% H-8 => L+6
251	26941	371	0.00	34.8% H-16 => L+4, 15.5% H-17 => L+5, 10.4% H-9 => L+9, 7.54% H-13 => L+3, 7.22% H-18 => L+3, 4.17% H-11 => L+9, 4.08% H-12 => L+7, 3.85% H-18 => L+6
252	26949	371	0.01	44.2% H-37 => L+1, 18.1% H-10 => L+7, 10.1% H-16 => L+5, 3.78% H-8 => L+9, 3.50% H-41 => L+1, 2.25% H-36 => LUMO, 2.00% H-36 => L+2
253	26959	371	0.02	17.5% H-11 => L+7, 13.8% H-12 => L+6, 10.6% H-9 => L+10, 9.56% H-12 => L+9, 9.11% H-10 => L+8, 4.42% H-15 => L+5, 4.23% H-63 => LUMO, 3.03% H-16 => L+3, 3.00% H-7 => L+9, 2.42% H-11 => L+4
254	26979	371	0.00	18.4% H-18 => L+5, 15.2% H-38 => L+1, 13.2% H-21 => L+4, 7.02% H-64 => LUMO, 6.99% H-20 => L+6, 4.81% H-19 => L+4, 4.68% H-20 => L+3, 4.13% H-40 => L+1, 3.55% H-42 => L+1, 3.31% H-8 => L+10, 3.17% H-10 => L+9, 3.02% H-19 => L+7
255	27042	370	0.00	32.1% H-38 => L+1, 13.5% H-42 => L+1, 8.04% H-36 => L+1, 7.64% H-21 => L+4, 7.10% H-40 => L+1, 6.23% H-20 => L+6, 4.52% H-20 => L+3, 2.42% H-10 => L+9, 2.21% H-8 => L+10, 2.09% H-19 => L+7
256	27081	369	0.00	27.0% H-14 => L+6, 20.7% H-19 => L+5, 14.0% H-21 => L+5, 5.24% H-18 => L+4, 4.95% H-10 => L+8, 4.14% H-9 => L+10, 3.39% H-13 => L+7
257	27091	369	0.00	17.2% H-17 => L+5, 16.0% H-65 => LUMO, 12.3% H-9 => L+9, 5.78% H-20 => L+5, 5.63% H-12 => L+7, 5.43% H-11 => L+9, 4.09% H-11 => L+6, 2.86% H-26 => L+4, 2.83% H-16 => L+4, 2.57% H-18 => L+3, 2.47% H-27 => L+3, 2.05% H-5 => L+12
258	27109	369	0.02	28.6% H-41 => L+1, 14.3% H-39 => L+1, 6.28% H-21 => L+6, 5.97% H-20 => L+4, 5.96% H-21 => L+3, 5.33% H-37 => L+1, 4.01% H-19 => L+6, 3.03% H-43 => L+1, 2.88% H-20 => L+7, 2.73% H-19 => L+3, 2.39% H-10 => L+7, 2.27% H-17 => L+7, 2.08% H-17 => L+4
259	27115	369	0.00	20.9% H-26 => L+3, 13.8% H-27 => L+4, 12.8% H-25 => L+4, 10.1% H-10 => L+8, 8.50% H-26 =>

				L+6, 8.36% H-24 => L+6, 5.32% H-23 => L+7, 5.30% H-25 => L+7, 3.49% H-24 => L+9, 3.22% H-22 => L+9, 2.25% H-23 => L+10
260	27135	369	0.00	39.1% H-18 => L+5, 19.5% H-64 => LUMO, 3.86% H-4 => L+11, 3.74% H-20 => L+6, 3.72% H-36 => L+1, 3.64% H-38 => L+1, 3.21% H-20 => L+3, 2.22% H-16 => L+8, 2.03% H-19 => L+4
261	27152	368	0.01	30.8% H-10 => L+8, 24.8% H-19 => L+5, 13.0% H-18 => L+4, 4.32% H-16 => L+3, 3.81% H-21 => L+5, 2.96% H-11 => L+7
262	27157	368	0.02	20.9% H-41 => L+1, 11.9% H-39 => L+1, 10.8% H-20 => L+4, 9.39% H-21 => L+6, 8.54% H-21 => L+3, 5.11% H-19 => L+6, 4.84% H-10 => L+7, 4.76% H-19 => L+3, 3.53% H-20 => L+7, 2.97% H-17 => L+7, 2.40% H-37 => L+1, 2.03% H-17 => L+4
263	27175	368	0.00	52.0% H-42 => L+1, 15.1% H-38 => L+1, 8.65% H-44 => L+1, 5.41% H-18 => L+5, 3.90% H-40 => L+1
264	27180	368	0.00	27.2% H-27 => L+3, 23.1% H-26 => L+4, 14.7% H-25 => L+6, 9.76% H-24 => L+7, 6.84% H-23 => L+9, 4.80% H-22 => L+10, 3.21% H-9 => L+9
265	27218	367	0.00	22.5% H-8 => L+10, 16.2% H-19 => L+4, 7.77% H-4 => L+11, 7.20% H-20 => L+6, 5.92% H-64 => LUMO, 5.59% H-17 => L+3, 5.36% H-20 => L+3, 5.22% H-42 => L+1, 4.95% H-10 => L+9, 3.13% H-21 => L+7
266	27280	367	0.06	21.8% H-14 => L+6, 21.5% H-18 => L+4, 13.2% H-9 => L+10, 8.49% H-19 => L+5, 6.62% H-13 => L+7, 4.81% H-16 => L+3, 3.53% H-10 => L+8, 2.96% H-11 => L+10, 2.40% H-12 => L+9
267	27320	366	0.00	52.7% H-39 => L+1, 21.4% H-41 => L+1, 9.03% H-43 => L+1, 5.03% H-40 => LUMO, 4.10% H-40 => L+2
268	27321	366	0.03	29.4% H-10 => L+8, 15.3% H-9 => L+10, 14.1% H-19 => L+5, 12.5% H-14 => L+6, 6.86% H-18 => L+4, 4.86% H-21 => L+5
269	27327	366	0.00	60.2% H-40 => L+1, 10.7% H-44 => L+1, 7.28% H-38 => L+1, 4.73% H-39 => LUMO, 4.00% H-42 => L+1, 3.48% H-39 => L+2
270	27374	365	0.00	52.6% H-13 => L+6, 4.23% H-11 => L+9, 3.71% H-18 => L+6, 3.64% H-16 => L+4, 3.43% H-14 => L+4, 3.25% H-20 => L+5, 2.57% H-12 => L+10, 2.55% H-17 => L+5, 2.32% H-14 => L+7, 2.31% H-18 => L+9, 2.18% H-9 => L+9, 2.18% H-13 => L+3, 2.13% H-12 => L+4, 2.08% H-5 => L+12
271	27445	364	0.00	59.6% H-25 => L+2, 23.4% H-27 => L+2, 4.34% H-24 => L+5, 3.90% H-24 => L+1
272	27448	364	0.01	55.5% H-21 => L+5, 19.4% H-19 => L+5, 6.48% H-5 => L+11, 4.90% H-20 => L+2, 4.87% H-20 => L+8

273	27454	364	0.00	63.6% H-4 => L+11, 9.67% H-64 => LUMO, 4.53% H-7 => L+12
274	27468	364	0.00	67.6% H-20 => L+5, 6.58% H-17 => L+5, 5.78% H-5 => L+12, 3.92% H-21 => L+8, 3.48% H-21 => L+2
275	27487	364	0.20	70.3% H-4 => L+12, 6.18% H-7 => L+11, 5.79% H-67 => LUMO, 4.48% H-2 => L+11
276	27556	363	0.02	50.8% H-5 => L+11, 17.3% H-66 => LUMO, 7.63% H-3 => L+12, 5.00% H-6 => L+12, 4.82% H-14 => L+6, 4.57% H-21 => L+5
277	27578	363	0.00	48.8% H-15 => L+6, 23.9% H-17 => L+4, 8.10% H-15 => L+3, 7.47% H-17 => L+7
278	27645	362	0.02	71.6% H-43 => L+1, 9.61% H-41 => L+1, 4.76% H-44 => LUMO, 3.80% H-44 => L+2, 2.30% H-39 => L+1, 2.22% H-37 => L+1
279	27648	362	0.00	65.3% H-44 => L+1, 12.4% H-42 => L+1, 6.70% H-40 => L+1, 5.35% H-43 => LUMO, 4.31% H-43 => L+2
280	27754	360	0.00	57.5% H-5 => L+12, 6.13% H-6 => L+11, 5.82% H-68 => LUMO, 5.79% H-3 => L+11, 4.65% H-13 => L+6, 3.27% H-20 => L+5
281	27795	360	0.00	25.9% H-16 => L+6, 19.8% H-11 => L+7, 12.4% H-9 => L+10, 8.15% H-18 => L+4, 7.52% H-18 => L+7, 7.34% H-14 => L+6, 4.58% H-13 => L+7, 3.78% H-16 => L+3, 2.26% H-12 => L+6, 2.14% H-13 => L+4
282	27822	359	0.00	28.4% H-17 => L+6, 10.4% H-19 => L+4, 9.70% H-17 => L+3, 8.78% H-19 => L+7, 8.15% H-8 => L+10, 7.15% H-15 => L+4, 6.18% H-20 => L+9, 5.27% H-15 => L+7, 3.39% H-21 => L+10, 2.68% H-21 => L+4, 2.15% HOMO => L+13
283	27852	359	0.00	30.7% H-12 => L+7, 23.4% H-18 => L+6, 12.0% H-16 => L+7, 6.61% H-12 => L+10, 5.75% H-18 => L+3, 5.26% H-11 => L+6, 4.70% H-16 => L+4
284	27863	359	0.02	71.3% H-11 => L+8, 6.90% H-47 => L+1, 3.80% H-12 => L+5, 3.16% H-9 => L+8, 2.61% H-4 => L+12, 2.51% H-50 => L+1, 2.22% H-67 => LUMO
285	27870	359	0.01	69.8% H-47 => L+1, 9.86% H-11 => L+8, 8.37% H-50 => L+1, 2.30% H-45 => L+1
286	27953	358	0.00	69.1% H-12 => L+8, 8.65% H-48 => L+1, 3.81% H-11 => L+5, 2.94% H-54 => L+1, 2.15% H-18 => L+5
287	27975	357	0.00	56.5% H-26 => L+2, 7.68% H-27 => L+1, 6.27% H-24 => L+2, 6.12% H-25 => L+1, 4.78% H-48 => L+1, 4.63% H-25 => L+5, 4.59% H-27 => L+5, 3.78% H-12 => L+8
288	27977	357	0.00	91.1% H-49 => L+1, 3.24% H-52 => L+1
289	27991	357	0.07	16.9% H-20 => L+4, 12.5% H-19 => L+6, 6.91% H-19 => L+3, 6.50% H-10 => L+10, 5.92% H-17 => L+7, 5.89% H-20 => L+7, 4.84% H-15 => L+9, 4.57% H-27 => L+2, 4.06% H-57 => L+1, 3.68%

				H-21 => L+3, 3.32% H-67 => LUMO, 3.23% H-50 => L+1, 3.12% H-21 => L+9, 2.13% H-15 => L+6
290	27996	357	0.00	57.5% H-48 => L+1, 10.6% H-54 => L+1, 10.1% H-12 => L+8, 5.70% H-26 => L+2, 3.60% H-46 => L+1
291	27999	357	0.05	60.3% H-51 => L+1, 13.8% H-53 => L+1, 13.0% H-66 => LUMO, 3.22% H-5 => L+11
292	28006	357	0.00	44.4% H-27 => L+2, 13.9% H-25 => L+2, 10.9% H-26 => L+1, 8.08% H-26 => L+5, 2.91% H-20 => L+4, 2.27% H-19 => L+6
293	28017	357	0.17	46.3% H-66 => LUMO, 15.8% H-51 => L+1, 11.7% H-5 => L+11, 4.13% H-53 => L+1, 2.99% H-65 => L+1, 2.66% H-11 => L+7, 2.03% H-19 => L+5
294	28033	357	0.00	27.7% H-57 => L+1, 22.4% H-50 => L+1, 9.51% H-45 => L+1, 7.89% H-47 => L+1, 3.16% H-67 => LUMO, 2.72% H-27 => L+2, 2.58% H-20 => L+4
295	28043	357	0.00	29.5% H-10 => L+9, 16.9% H-21 => L+4, 8.74% H-17 => L+6, 8.25% H-20 => L+3, 6.41% H-8 => L+10, 6.31% H-20 => L+6, 5.56% H-15 => L+10, 4.08% H-17 => L+9, 3.28% H-21 => L+7, 2.39% H-8 => L+7
296	28160	355	0.00	35.3% H-45 => L+1, 33.9% H-50 => L+1, 7.30% H-47 => L+1, 6.81% H-67 => LUMO, 2.74% H-46 => LUMO, 2.21% H-46 => L+2
297	28169	355	0.00	42.1% H-46 => L+1, 18.1% H-54 => L+1, 12.1% H-48 => L+1, 2.80% H-10 => L+9, 2.58% H-20 => L+6, 2.28% H-45 => LUMO, 2.01% H-45 => L+2
298	28183	355	0.00	26.4% H-10 => L+9, 12.0% H-8 => L+10, 10.6% H-20 => L+6, 7.93% H-21 => L+7, 7.09% H-46 => L+1, 4.75% H-21 => L+4, 4.39% H-20 => L+3, 4.37% H-48 => L+1, 3.27% H-17 => L+9, 2.80% H-19 => L+4, 2.62% H-19 => L+10, 2.14% H-8 => L+7
299	28189	355	0.00	78.1% H-52 => L+1, 6.55% H-55 => L+1, 3.12% H-53 => L+2, 3.05% H-49 => L+1, 2.49% H-53 => LUMO

Table S3.18. TDDFT-predicted band excitation data for **3.7**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	3274	3055	6.56	98.8% HOMO => LUMO
1	4898	2042	0.00	94.8% H-2 => LUMO, 3.00% H-3 => L+1
2	5416	1846	0.00	54.1% H-1 => LUMO, 43.7% HOMO => L+1
3	5924	1688	0.00	54.3% HOMO => L+1, 43.7% H-1 => LUMO
4	5930	1686	0.00	82.9% H-3 => LUMO, 13.3% H-2 => L+1

5	7269	1376	0.00	74.9% H-5 => LUMO, 16.5% H-3 => L+1, 5.41% H-2 => L+2
6	7634	1310	0.06	75.0% H-4 => LUMO, 22.5% HOMO => L+2
7	7929	1261	0.00	82.2% H-2 => L+1, 13.5% H-3 => LUMO, 2.26% H-3 => L+2
8	8059	1241	0.31	65.2% HOMO => L+2, 18.7% H-4 => LUMO, 12.0% H-1 => L+1
9	8225	1216	0.11	83.1% H-1 => L+1, 9.01% HOMO => L+2, 2.40% H-4 => LUMO
10	8789	1138	0.00	69.0% H-6 => LUMO, 18.0% H-5 => L+1, 7.01% H-3 => L+2, 2.83% H-2 => L+3
11	8973	1114	0.00	65.0% H-3 => L+1, 21.1% H-5 => LUMO, 8.23% H-2 => L+2, 2.31% H-2 => LUMO
12	9597	1042	0.00	88.0% H-7 => LUMO, 3.63% H-4 => L+1, 3.56% HOMO => L+3
13	10190	981	0.00	80.9% HOMO => L+3, 9.84% H-1 => L+2
14	10309	970	0.00	54.1% H-5 => L+1, 27.0% H-6 => LUMO, 10.6% H-3 => L+2, 3.00% H-2 => L+3
15	10329	968	0.00	84.3% H-4 => L+1, 4.87% H-7 => LUMO, 3.55% H-1 => L+2, 2.30% H-1 => LUMO
16	10371	964	0.00	63.7% H-8 => LUMO, 17.1% H-6 => L+1, 7.93% H-5 => L+2, 2.87% H-2 => L+2, 2.29% H-3 => L+3
17	10445	957	0.00	77.9% H-2 => L+2, 11.3% H-3 => L+1, 3.38% H-3 => L+3, 2.54% H-8 => LUMO, 2.27% H-2 => LUMO
18	10559	947	0.00	80.7% H-1 => L+2, 9.41% HOMO => L+3, 5.35% H-4 => L+1, 2.01% HOMO => L+1
19	11209	892	0.09	81.7% H-9 => LUMO, 7.81% H-7 => L+1
20	11453	873	0.00	95.5% HOMO => L+4
21	11520	868	0.00	62.7% H-3 => L+2, 21.7% H-5 => L+1, 9.23% H-2 => L+3
22	11777	849	0.00	46.1% H-6 => L+1, 29.6% H-8 => LUMO, 12.3% H-5 => L+2, 4.62% H-3 => L+3
23	11896	841	0.00	65.9% H-10 => LUMO, 15.3% H-8 => L+1, 6.38% H-6 => L+2, 3.28% H-5 => L+3
24	12114	826	0.00	90.0% HOMO => L+5, 5.24% H-1 => L+4
25	12166	822	0.02	44.0% HOMO => L+6, 15.1% H-1 => L+3, 11.8% H-7 => L+1, 11.6% H-4 => L+2, 5.67% H-9 => LUMO, 2.50% H-12 => LUMO
26	12316	812	0.00	76.5% H-11 => LUMO, 7.67% H-9 => L+1, 4.11% H-12 => L+1, 2.90% H-15 => LUMO, 2.18% H-7 => L+2
27	12345	810	0.00	61.4% H-7 => L+1, 23.8% HOMO => L+6, 6.31% H-9 => LUMO, 2.59% H-1 => L+3
28	12668	789	0.23	66.3% H-12 => LUMO, 7.78% H-4 => L+2, 7.16% HOMO => L+6, 4.63% H-11 => L+1, 4.59% H-7 => L+1, 2.08% H-9 => L+2
29	12719	786	0.45	48.5% H-4 => L+2, 17.0% H-12 => LUMO, 10.6% HOMO => L+6, 7.09% H-1 => L+3, 5.65% H-7 => L+1, 2.82% H-2 => L+4

30	12836	779	0.00	50.8% H-5 => L+2, 29.1% H-6 => L+1, 10.0% H-3 => L+3, 3.43% H-2 => L+6
31	12840	779	0.00	78.8% H-2 => L+3, 13.5% H-3 => L+2, 2.39% H-2 => L+1, 2.28% H-3 => L+6
32	12935	773	0.52	66.1% H-1 => L+3, 14.9% H-4 => L+2, 9.26% HOMO => L+6, 3.71% H-2 => L+4
33	13028	768	0.00	86.2% HOMO => L+7, 5.47% H-1 => L+5
34	13196	758	0.00	66.9% H-13 => LUMO, 12.7% H-10 => L+1, 5.16% H-8 => L+2, 2.71% H-6 => L+3, 2.66% H-19 => LUMO
35	13239	755	0.00	40.7% H-8 => L+1, 28.1% H-10 => LUMO, 12.9% H-6 => L+2, 5.81% H-5 => L+3, 2.87% H-3 => L+6
36	13593	736	5.51	74.4% H-2 => L+4, 8.83% H-3 => L+5, 7.81% H-4 => L+2
37	13886	720	0.00	59.3% H-3 => L+3, 22.5% H-5 => L+2, 10.4% H-2 => L+6
38	13937	718	0.00	26.3% H-9 => L+1, 16.8% HOMO => L+9, 16.1% H-11 => LUMO, 9.70% H-7 => L+2, 7.30% H-4 => L+3, 7.11% H-1 => L+6, 6.28% H-15 => LUMO, 2.01% H-16 => L+1
39	13961	716	0.00	74.4% H-1 => L+4, 11.4% HOMO => L+8, 5.71% HOMO => L+5, 3.74% H-1 => L+7
40	14084	710	0.00	70.8% HOMO => L+8, 14.7% H-1 => L+4, 3.18% H-1 => L+7, 2.93% H-4 => L+5
41	14182	705	0.00	46.4% H-9 => L+1, 29.3% HOMO => L+9, 8.26% H-1 => L+6, 2.66% H-4 => L+3, 2.53% H-15 => LUMO, 2.41% H-2 => L+5
42	14275	701	0.02	32.9% H-8 => L+1, 28.9% H-6 => L+2, 14.0% H-14 => LUMO, 10.0% H-5 => L+3, 4.06% H-3 => L+6, 2.03% H-2 => L+9
43	14384	695	0.22	71.9% H-14 => LUMO, 7.20% H-6 => L+2, 4.92% H-8 => L+1, 4.81% HOMO => L+14, 3.01% H-13 => L+1
44	14438	693	0.00	39.3% H-2 => L+5, 27.6% H-3 => L+4, 11.0% HOMO => L+9, 9.29% H-7 => L+2, 2.19% H-5 => L+5
45	14492	690	0.00	30.3% H-10 => L+1, 24.4% H-13 => LUMO, 11.3% H-8 => L+2, 6.15% H-6 => L+3, 5.59% HOMO => L+10, 5.25% H-14 => L+1, 4.06% H-5 => L+6, 3.12% H-19 => LUMO, 2.30% H-3 => L+9
46	14609	685	0.00	76.0% H-1 => L+5, 7.42% H-4 => L+4, 6.72% HOMO => L+7, 2.10% HOMO => L+4
47	14813	675	0.00	41.3% H-7 => L+2, 16.7% HOMO => L+9, 10.8% H-9 => L+1, 10.7% H-2 => L+5, 7.59% H-4 => L+3, 5.93% H-3 => L+4, 2.51% H-1 => L+6
48	14960	668	0.04	64.1% H-16 => LUMO, 7.30% H-15 => L+1, 5.71% H-17 => LUMO, 5.22% H-11 => L+1, 3.11% H-12 => LUMO
49	15027	665	0.00	40.5% H-15 => LUMO, 18.0% HOMO => L+9, 17.9% H-7 => L+2, 7.56% H-1 => L+6, 5.25% H-4 => L+3, 2.64% H-16 => L+1

50	15043	665	0.00	65.8% HOMO => L+10, 6.22% H-2 => L+6, 3.98% H-1 => L+8, 3.87% H-24 => LUMO, 2.85% H-1 => L+5
51	15088	663	0.00	30.2% H-15 => LUMO, 22.3% H-4 => L+3, 19.7% H-1 => L+6, 10.8% H-7 => L+2, 3.11% H-18 => LUMO
52	15139	661	0.00	68.3% H-2 => L+6, 14.4% H-3 => L+3, 6.39% HOMO => L+10, 2.40% H-2 => L+2
53	15231	657	0.00	39.1% H-5 => L+3, 36.1% H-6 => L+2, 12.2% H-3 => L+6, 4.98% H-2 => L+9
54	15291	654	0.00	44.9% H-4 => L+3, 43.2% H-1 => L+6
55	15370	651	0.07	55.9% H-11 => L+1, 13.1% H-16 => LUMO, 7.70% H-17 => LUMO, 4.58% H-9 => L+2, 4.37% H-12 => LUMO
56	15475	646	0.00	59.9% H-1 => L+7, 8.08% HOMO => L+8, 8.05% HOMO => L+11, 6.99% H-4 => L+5, 4.06% H-1 => L+10, 2.07% H-7 => L+4, 2.04% H-22 => LUMO
57	15550	643	0.07	56.1% H-17 => LUMO, 8.56% HOMO => L+12, 5.72% H-2 => L+7, 4.85% H-3 => L+5, 3.73% H-11 => L+1, 3.57% H-21 => LUMO, 2.26% H-12 => LUMO
58	15567	642	0.00	41.3% H-10 => L+1, 17.2% H-19 => LUMO, 6.47% HOMO => L+13, 5.75% H-8 => L+2, 4.39% H-6 => L+3, 4.15% H-13 => L+2, 3.17% H-14 => L+1, 2.93% H-5 => L+6, 2.62% H-3 => L+9
59	15589	641	0.00	76.1% H-18 => LUMO, 2.97% H-1 => L+6, 2.39% H-15 => LUMO, 2.37% H-3 => L+7, 2.08% H-2 => L+8
60	15683	638	0.00	47.8% HOMO => L+11, 14.4% H-1 => L+7, 10.4% H-22 => LUMO, 7.88% H-13 => L+1, 2.81% H-1 => L+10, 2.40% H-4 => L+8, 2.00% H-14 => L+2
61	15718	636	0.63	30.4% H-2 => L+7, 27.1% H-3 => L+5, 8.34% H-17 => LUMO, 7.39% H-5 => L+4, 5.93% H-21 => LUMO, 2.71% H-11 => L+1, 2.48% H-16 => LUMO, 2.21% HOMO => L+12
62	15775	634	0.00	54.3% H-3 => L+4, 37.2% H-2 => L+5, 3.44% H-5 => L+5, 2.45% H-3 => L+7
63	15923	628	0.00	24.7% H-19 => LUMO, 22.7% H-8 => L+2, 18.0% HOMO => L+13, 8.13% H-10 => L+1, 5.99% H-6 => L+3, 4.35% H-14 => L+1, 2.59% H-1 => L+11, 2.47% H-5 => L+6
64	15953	627	0.01	47.5% HOMO => L+12, 11.8% H-11 => L+1, 10.1% H-1 => L+9, 8.56% H-17 => LUMO, 5.02% H-4 => L+6, 2.93% H-7 => L+3, 2.80% H-16 => LUMO
65	16000	625	0.00	44.1% H-12 => L+1, 36.1% H-20 => LUMO, 3.13% H-2 => L+14, 2.72% H-11 => L+2, 2.31% H-15 => LUMO
66	16135	620	0.00	43.2% H-12 => L+1, 41.3% H-20 => LUMO, 4.69% H-17 => L+1, 2.91% H-18 => LUMO
67	16143	619	0.01	25.6% H-3 => L+6, 21.1% H-13 => L+1, 19.7% H-5 => L+3, 7.48% H-2 => L+9, 5.27% HOMO =>

				L+14, 5.09% H-22 => LUMO, 3.69% H-14 => LUMO, 2.63% H-10 => L+2
68	16149	619	0.08	58.7% H-21 => LUMO, 10.8% H-9 => L+2, 4.93% HOMO => L+12, 4.24% H-2 => L+7, 4.20% H-18 => L+1, 2.65% H-3 => L+5, 2.64% H-25 => LUMO
69	16237	616	0.01	24.0% H-3 => L+6, 23.5% H-13 => L+1, 10.9% H-5 => L+3, 10.7% HOMO => L+14, 8.25% H-22 => LUMO, 4.39% H-14 => LUMO, 3.96% H-2 => L+9, 2.91% HOMO => L+11, 2.66% H-10 => L+2
70	16259	615	0.00	78.3% H-4 => L+4, 7.84% H-1 => L+5, 3.74% H-27 => LUMO, 2.20% H-7 => L+5
71	16368	611	0.90	41.3% H-2 => L+7, 23.7% H-3 => L+5, 11.1% H-2 => L+4, 6.61% H-25 => LUMO, 6.03% H-5 => L+4, 2.63% H-3 => L+8, 2.46% H-7 => L+3
72	16446	608	0.00	49.6% H-1 => L+8, 10.2% HOMO => L+10, 6.56% H-4 => L+7, 5.60% H-24 => LUMO, 4.50% H-8 => L+2, 3.78% H-19 => LUMO, 3.22% H-27 => LUMO, 3.00% H-7 => L+5
73	16527	605	0.00	33.3% H-9 => L+2, 13.6% HOMO => L+12, 11.6% H-25 => LUMO, 10.9% H-21 => LUMO, 10.7% H-7 => L+3, 5.65% H-3 => L+5, 5.21% H-11 => L+1
74	16571	603	0.00	81.6% H-23 => LUMO, 6.24% H-21 => L+1, 5.14% H-25 => L+1
75	16628	601	0.00	39.4% H-19 => LUMO, 14.7% HOMO => L+13, 13.4% H-14 => L+1, 6.92% H-8 => L+2, 5.54% H-6 => L+3, 3.13% H-5 => L+6, 2.52% H-2 => L+12, 2.33% H-3 => L+9, 2.16% H-10 => L+3
76	16650	601	0.00	35.2% H-8 => L+2, 16.8% H-6 => L+3, 10.1% HOMO => L+13, 7.68% H-1 => L+8, 7.27% H-5 => L+6, 5.26% H-14 => L+1, 4.64% H-3 => L+9, 3.05% H-2 => L+12, 2.38% H-19 => LUMO
77	16694	599	0.46	56.0% H-25 => LUMO, 10.8% H-9 => L+2, 7.85% H-23 => L+1, 7.08% H-21 => LUMO, 6.09% H-2 => L+7, 5.11% H-5 => L+4
78	16813	595	0.07	44.6% H-22 => LUMO, 29.5% HOMO => L+11, 12.1% H-13 => L+1, 2.71% H-4 => L+5
79	16853	593	0.01	52.2% H-4 => L+5, 16.0% H-26 => LUMO, 11.7% H-1 => L+7, 8.04% H-7 => L+4
80	16972	589	0.01	18.7% H-1 => L+9, 17.1% H-9 => L+2, 16.6% H-4 => L+6, 12.7% HOMO => L+12, 10.9% H-7 => L+3, 9.92% H-5 => L+4, 5.41% H-25 => LUMO
81	17015	588	0.00	61.9% H-24 => LUMO, 14.8% H-27 => LUMO, 6.77% H-1 => L+8, 3.31% H-14 => L+1, 2.97% HOMO => L+10
82	17017	588	0.00	58.4% H-5 => L+4, 13.8% H-3 => L+5, 6.26% H-9 => L+2, 4.96% H-4 => L+6, 3.29% H-2 => L+4, 2.89% H-1 => L+9, 2.80% H-6 => L+5
83	17057	586	0.07	26.7% HOMO => L+14, 14.0% H-13 => L+1, 12.6% H-10 => L+2, 11.8% H-22 => LUMO, 10.2% H-26 => LUMO, 5.47% H-4 => L+5, 5.13% H-8 => L+3, 2.84% H-6 => L+6

84	17072	586	0.00	40.9% H-3 => L+7, 34.7% H-2 => L+8, 6.10% H-18 => LUMO, 5.22% H-5 => L+5
85	17113	584	0.03	44.9% H-26 => LUMO, 11.3% H-29 => LUMO, 7.17% H-1 => L+10, 6.86% H-4 => L+5, 6.29% HOMO => L+14, 6.06% H-13 => L+1, 3.44% H-10 => L+2
86	17184	582	0.00	51.3% H-27 => LUMO, 23.9% H-28 => LUMO, 6.31% H-24 => LUMO, 3.77% H-4 => L+7, 2.65% H-4 => L+4
87	17281	579	0.00	62.7% H-2 => L+9, 19.3% H-3 => L+6, 5.06% H-29 => LUMO, 3.89% H-3 => L+12, 2.76% H-2 => L+3
88	17318	577	0.00	30.8% H-1 => L+9, 28.1% H-7 => L+3, 18.0% H-15 => L+1, 3.64% H-16 => LUMO, 2.78% H-9 => L+2, 2.57% H-16 => L+2, 2.53% H-25 => LUMO, 2.06% HOMO => L+12
89	17348	576	0.00	42.2% H-2 => L+8, 19.3% H-3 => L+7, 18.0% H-5 => L+5, 5.15% H-6 => L+4, 3.93% H-2 => L+5, 3.13% H-3 => L+10, 2.30% H-16 => L+1
90	17378	575	0.00	29.9% H-14 => L+1, 14.0% H-6 => L+3, 12.0% HOMO => L+13, 11.9% H-28 => LUMO, 8.38% H-5 => L+6, 7.87% H-2 => L+12, 6.31% H-3 => L+9
91	17414	574	0.00	46.3% H-15 => L+1, 17.3% H-7 => L+3, 9.33% H-1 => L+9, 7.42% H-16 => LUMO, 6.02% H-16 => L+2
92	17439	573	0.00	32.5% H-6 => L+3, 15.0% H-28 => LUMO, 10.5% H-5 => L+6, 9.08% HOMO => L+13, 7.95% H-14 => L+1, 6.49% H-3 => L+9, 4.89% H-27 => LUMO, 3.64% H-2 => L+12
93	17439	573	0.00	64.0% H-29 => LUMO, 9.53% H-1 => L+10, 5.32% H-28 => L+1, 3.44% H-2 => L+9, 3.13% H-4 => L+8, 3.11% H-26 => LUMO
94	17466	573	0.00	60.5% H-16 => L+1, 9.71% H-15 => LUMO, 7.85% H-15 => L+2, 3.90% H-2 => L+8
95	17481	572	0.00	28.0% H-28 => LUMO, 15.2% HOMO => L+13, 14.4% H-27 => LUMO, 12.0% H-14 => L+1, 8.17% H-1 => L+8, 5.54% H-24 => LUMO, 2.87% H-4 => L+7, 2.86% H-29 => L+1, 2.71% H-6 => L+3
96	17569	569	0.00	60.4% H-4 => L+6, 17.3% H-1 => L+9, 14.1% H-7 => L+3
97	17679	566	0.01	43.6% H-1 => L+10, 13.6% H-26 => LUMO, 6.44% H-22 => LUMO, 6.09% H-29 => LUMO, 4.33% H-10 => L+2, 3.97% H-4 => L+5, 3.96% HOMO => L+11, 3.77% H-4 => L+8, 2.60% HOMO => L+14
98	17695	565	0.00	48.8% H-5 => L+5, 24.0% H-3 => L+7, 5.97% H-6 => L+4, 4.82% H-2 => L+8, 3.76% H-3 => L+4, 2.08% H-2 => L+5, 2.02% H-11 => L+2
99	17734	564	0.00	42.4% H-11 => L+2, 8.30% H-20 => LUMO, 7.51% H-9 => L+3, 5.68% H-2 => L+14, 4.01% H-16 => L+1, 3.96% H-7 => L+6, 3.81% H-17 => L+1, 3.16% H-1 => L+12, 3.00% H-4 => L+9, 2.87% H-3 => L+13, 2.77% H-5 => L+5

100	17868	560	0.50	60.2% H-10 => L+2, 22.2% HOMO => L+14, 5.86% H-1 => L+10
101	17879	559	0.00	56.5% H-4 => L+7, 9.19% H-1 => L+8, 8.86% H-28 => LUMO, 8.35% H-7 => L+5, 3.60% H-24 => LUMO, 3.00% H-9 => L+4
102	18111	552	0.01	33.0% H-2 => L+10, 23.3% H-3 => L+8, 16.0% H-12 => L+2, 4.73% H-17 => LUMO, 4.56% H-15 => L+1, 2.64% H-20 => L+1, 2.43% H-2 => L+13
103	18203	549	0.00	39.3% H-5 => L+6, 13.4% H-3 => L+9, 11.8% H-1 => L+11, 11.4% H-2 => L+12, 4.31% HOMO => L+13, 3.05% H-6 => L+9, 2.51% H-13 => L+2
104	18280	547	0.02	53.4% H-12 => L+2, 12.4% H-2 => L+10, 6.77% H-18 => L+1, 6.25% H-3 => L+8, 3.04% H-11 => L+3
105	18304	546	0.00	33.5% H-11 => L+2, 21.4% H-1 => L+12, 9.90% H-4 => L+9, 6.69% H-7 => L+6, 5.54% H-2 => L+14, 3.65% H-9 => L+3, 3.47% H-6 => L+4
106	18354	545	0.26	27.0% H-5 => L+7, 21.4% H-2 => L+10, 17.5% H-3 => L+8, 11.4% H-18 => L+1, 6.26% H-6 => L+5
107	18401	543	0.00	78.9% H-7 => L+4, 9.14% H-4 => L+5, 3.51% H-9 => L+5, 2.07% H-26 => LUMO
108	18403	543	0.00	30.8% H-1 => L+11, 14.0% H-13 => L+2, 12.6% H-3 => L+9, 9.70% H-5 => L+6, 5.77% H-14 => L+1, 5.45% H-2 => L+12, 3.85% H-4 => L+10, 2.81% H-1 => L+14
109	18491	541	0.00	72.5% H-6 => L+4, 10.1% H-5 => L+5, 3.14% H-8 => L+5, 2.25% H-3 => L+4, 2.09% H-1 => L+12
110	18518	540	0.26	53.9% H-8 => L+3, 12.4% HOMO => L+14, 8.32% H-1 => L+13, 6.11% H-6 => L+6, 4.25% H-10 => L+2, 2.88% H-4 => L+11
111	18606	537	0.00	70.3% H-17 => L+1, 6.33% H-30 => LUMO, 3.12% H-20 => LUMO, 2.24% H-11 => L+2
112	18629	537	0.06	34.3% H-3 => L+8, 28.1% H-18 => L+1, 9.95% H-2 => L+10, 6.93% H-5 => L+7, 2.72% H-2 => L+7, 2.60% H-20 => L+1, 2.35% H-21 => LUMO, 2.06% H-5 => L+10
113	18669	536	0.00	81.7% H-30 => LUMO, 5.68% H-17 => L+1, 5.22% H-31 => L+1
114	18712	534	0.52	38.6% H-5 => L+7, 29.3% H-18 => L+1, 4.12% H-2 => L+10, 3.06% H-21 => LUMO, 2.72% H-3 => L+8, 2.24% H-3 => L+5
115	18740	534	0.01	36.1% H-19 => L+1, 22.5% H-4 => L+8, 11.6% H-1 => L+10, 5.23% H-7 => L+7, 5.22% H-14 => L+2, 2.94% H-22 => LUMO, 2.47% H-9 => L+5
116	18839	531	0.09	33.4% H-19 => L+1, 24.4% H-4 => L+8, 8.97% H-8 => L+3, 7.72% H-1 => L+13, 5.20% H-1 => L+10, 4.08% H-7 => L+7, 2.06% H-4 => L+11
117	18861	530	0.00	18.9% H-2 => L+11, 17.4% H-1 => L+12, 16.9% H-9 => L+3, 14.2% H-21 => L+1, 5.99% H-3 => L+10, 4.17% H-16 => L+1, 2.82% H-23 => LUMO, 2.20% H-11 => L+2

118	18882	530	0.00	44.5% H-13 => L+2, 19.6% H-1 => L+14, 14.9% H-1 => L+11, 2.26% H-10 => L+3
119	18884	530	0.00	80.0% H-31 => LUMO, 8.51% H-30 => L+1, 3.62% H-32 => L+1
120	18952	528	0.00	48.0% H-7 => L+5, 13.7% H-4 => L+7, 10.4% H-9 => L+4, 7.45% H-2 => L+12, 5.86% H-3 => L+9, 2.03% H-4 => L+4
121	19043	525	0.00	27.9% H-2 => L+11, 18.7% H-9 => L+3, 13.6% H-3 => L+10, 11.3% H-1 => L+12, 3.82% H-21 => L+1, 3.11% H-4 => L+9
122	19112	523	0.00	32.4% H-2 => L+12, 28.0% H-3 => L+9, 11.4% H-7 => L+5, 6.25% H-22 => L+1, 6.13% H-13 => L+2, 3.65% H-5 => L+12, 2.67% H-2 => L+6
123	19119	523	0.04	33.0% H-6 => L+5, 18.1% H-20 => L+1, 6.92% H-12 => L+2, 6.28% H-5 => L+7, 5.98% H-2 => L+13, 3.83% H-8 => L+4, 3.19% H-3 => L+14, 2.84% H-15 => L+1, 2.31% H-5 => L+4, 2.09% H-2 => L+10
124	19143	522	0.00	37.0% H-20 => L+1, 27.0% H-6 => L+5, 7.87% H-18 => L+1, 6.82% H-12 => L+2, 4.76% H-5 => L+7, 3.49% H-8 => L+4
125	19185	521	0.00	57.2% H-21 => L+1, 13.3% H-9 => L+3, 6.43% H-1 => L+12, 2.67% H-23 => LUMO, 2.27% H-18 => L+2, 2.12% H-7 => L+6, 2.04% H-11 => L+2
126	19190	521	0.00	33.5% H-6 => L+6, 18.7% H-8 => L+3, 9.74% H-1 => L+13, 8.99% H-19 => L+1, 8.63% H-5 => L+9, 5.38% H-4 => L+8, 2.74% H-14 => L+2
127	19214	520	0.00	76.6% H-32 => LUMO, 8.97% H-31 => L+1, 3.24% H-34 => LUMO, 2.86% H-33 => L+1, 2.42% H-30 => L+2
128	19365	516	0.00	45.5% H-22 => L+1, 19.0% H-1 => L+14, 6.28% H-26 => L+1, 5.29% H-2 => L+12, 4.05% H-4 => L+13, 2.34% H-19 => L+2, 2.13% H-3 => L+9, 2.07% H-7 => L+5, 2.05% H-4 => L+10
129	19392	516	0.00	23.5% H-9 => L+3, 22.6% H-7 => L+6, 15.5% H-1 => L+12, 7.70% H-4 => L+9, 7.57% H-2 => L+11, 4.66% H-5 => L+8, 2.88% H-6 => L+7, 2.33% H-25 => L+1
130	19448	514	0.00	35.7% H-3 => L+10, 13.5% H-5 => L+8, 12.9% H-2 => L+11, 8.61% H-7 => L+6, 3.50% H-4 => L+9, 3.50% H-1 => L+12, 2.47% H-2 => L+8, 2.38% H-17 => L+1
131	19462	514	0.18	63.5% H-23 => L+1, 8.13% H-25 => LUMO, 4.07% H-21 => L+2, 3.56% H-25 => L+2, 2.89% H-20 => L+1, 2.86% H-21 => LUMO, 2.31% H-2 => L+13
132	19473	514	0.00	25.0% H-22 => L+1, 20.1% H-1 => L+14, 18.2% H-1 => L+11, 8.34% H-13 => L+2, 6.12% H-4 => L+10, 3.61% H-4 => L+13, 2.64% H-7 => L+8
133	19532	512	0.35	39.7% H-14 => L+2, 19.9% H-6 => L+6, 11.9% H-1 => L+13, 8.94% H-19 => L+1, 2.59% H-13 => L+1, 2.43% H-4 => L+14, 2.23% H-13 => L+3

134	19571	511	0.00	74.3% H-33 => LUMO, 9.83% H-32 => L+1, 5.26% H-35 => LUMO, 2.69% H-31 => L+2, 2.12% H-34 => L+1
135	19620	510	0.00	37.8% H-25 => L+1, 33.2% H-4 => L+9, 7.70% H-7 => L+6, 5.98% H-1 => L+12, 3.85% H-23 => LUMO, 2.75% H-23 => L+2
136	19630	509	0.13	18.1% H-2 => L+13, 14.4% H-20 => L+1, 9.81% H-23 => L+1, 8.94% H-3 => L+11, 8.21% H-6 => L+5, 4.22% H-16 => L+2, 3.90% H-15 => L+1, 3.45% H-12 => L+2, 3.15% H-4 => L+12, 3.05% HOMO => L+16, 2.03% H-7 => L+9, 2.03% H-5 => L+10, 2.00% H-11 => L+3
137	19642	509	0.01	63.4% H-24 => L+1, 17.9% H-27 => L+1, 3.14% H-22 => L+2, 2.89% H-14 => L+2, 2.18% H-22 => LUMO
138	19703	508	0.00	40.3% H-5 => L+8, 19.8% H-3 => L+10, 8.58% H-7 => L+6, 7.48% H-6 => L+7, 5.05% H-2 => L+11, 2.29% H-2 => L+8
139	19719	507	0.00	29.4% H-10 => L+3, 21.4% H-4 => L+10, 9.33% H-13 => L+2, 6.09% H-8 => L+6, 5.84% H-1 => L+11, 5.27% H-2 => L+12, 4.64% H-7 => L+8, 2.39% H-9 => L+7
140	19753	506	0.12	20.8% H-4 => L+8, 15.9% H-7 => L+7, 15.0% H-6 => L+6, 9.91% H-14 => L+2, 9.65% H-1 => L+13, 6.74% H-5 => L+9, 5.58% H-9 => L+5, 3.08% H-11 => L+4
141	19794	505	0.00	41.2% H-25 => L+1, 21.1% H-4 => L+9, 20.4% H-7 => L+6, 2.53% H-23 => L+2, 2.45% H-23 => LUMO
142	19840	504	0.00	68.3% H-26 => L+1, 12.2% H-29 => L+1, 2.98% H-24 => L+2, 2.73% H-7 => L+5, 2.66% H-22 => L+1, 2.31% H-24 => LUMO
143	19861	504	0.02	64.4% H-27 => L+1, 11.7% H-28 => L+1, 9.34% H-24 => L+1, 3.10% H-26 => L+2, 2.71% H-6 => L+6
144	19924	502	0.00	60.9% H-34 => LUMO, 9.08% H-36 => LUMO, 8.41% H-33 => L+1, 8.12% H-15 => L+2, 2.39% H-32 => L+2
145	19924	502	0.00	25.5% H-16 => L+2, 24.0% H-2 => L+13, 10.2% H-8 => L+4, 5.44% H-15 => L+1, 3.47% H-5 => L+10, 3.27% H-15 => L+3, 2.95% H-11 => L+3, 2.92% H-8 => L+7, 2.63% H-6 => L+8, 2.63% H-6 => L+5, 2.49% H-2 => L+10
146	19935	502	0.45	28.6% H-1 => L+13, 20.2% H-14 => L+2, 10.3% H-5 => L+9, 9.82% H-3 => L+12, 7.13% H-7 => L+7, 3.09% H-11 => L+4, 2.81% H-9 => L+5, 2.29% H-24 => L+1
147	19957	501	0.00	54.9% H-15 => L+2, 9.09% H-16 => L+1, 8.72% H-34 => LUMO, 6.01% H-16 => L+3, 4.19% H-5 => L+8
148	19990	500	0.06	37.6% H-5 => L+9, 22.7% H-7 => L+7, 7.17% H-6 => L+6, 5.17% H-4 => L+8, 4.09% H-3 => L+12,

				3.23% H-14 => L+2, 2.92% H-24 => L+1, 2.78% H-9 => L+5
149	20014	500	0.00	48.7% H-8 => L+4, 18.2% H-16 => L+2, 4.43% H-6 => L+5, 4.12% H-10 => L+5, 3.58% H-11 => L+3, 2.69% H-15 => L+3, 2.64% H-3 => L+11, 2.14% H-15 => L+1
150	20033	499	0.00	34.1% H-6 => L+7, 16.1% H-5 => L+8, 14.6% H-2 => L+14, 7.25% H-8 => L+5, 3.49% H-15 => L+2, 3.37% H-6 => L+10, 2.91% H-2 => L+11
151	20162	496	0.01	37.2% H-11 => L+3, 9.00% H-3 => L+11, 6.94% H-2 => L+13, 6.75% H-16 => L+2, 6.63% H-8 => L+4, 4.60% H-9 => L+6, 2.50% H-17 => L+2, 2.22% H-20 => L+1, 2.08% H-7 => L+9
152	20164	496	0.00	46.9% H-9 => L+4, 16.4% H-29 => L+1, 8.07% H-7 => L+5, 6.36% H-26 => L+1, 4.49% H-11 => L+5, 2.66% H-10 => L+3, 2.45% H-28 => LUMO
153	20211	495	0.00	36.5% H-2 => L+14, 17.1% H-6 => L+7, 8.75% H-12 => L+3, 4.16% H-8 => L+8, 3.48% H-1 => L+12, 2.50% H-18 => L+2, 2.09% H-14 => L+4
154	20217	495	0.07	64.9% H-28 => L+1, 7.12% H-29 => LUMO, 6.30% H-27 => L+1, 6.20% H-29 => L+2, 4.44% H-24 => L+1, 2.23% H-1 => L+13
155	20242	494	0.00	50.3% H-29 => L+1, 19.4% H-9 => L+4, 5.14% H-7 => L+5, 4.75% H-28 => LUMO, 4.51% H-28 => L+2, 4.18% H-26 => L+1, 2.39% H-4 => L+10
156	20247	494	0.00	54.3% H-35 => LUMO, 30.1% H-37 => LUMO, 7.43% H-34 => L+1, 2.12% H-33 => L+2
157	20331	492	0.01	44.5% H-10 => L+3, 24.9% H-4 => L+10, 12.2% H-1 => L+14, 3.65% H-9 => L+4
158	20350	491	0.01	32.2% H-3 => L+11, 12.3% H-16 => L+2, 11.4% H-8 => L+4, 10.0% H-5 => L+10, 8.05% H-2 => L+13, 5.95% H-3 => L+14, 3.79% HOMO => L+16, 2.47% H-20 => L+1
159	20504	488	0.02	58.7% H-3 => L+12, 19.9% H-5 => L+9, 6.05% H-7 => L+7, 4.98% H-2 => L+9, 2.74% H-6 => L+12
160	20532	487	0.00	24.6% H-8 => L+5, 18.4% H-12 => L+3, 18.1% H-6 => L+7, 6.97% H-10 => L+4, 5.20% H-18 => L+2, 4.65% HOMO => L+15, 2.44% H-3 => L+13
161	20552	487	0.06	20.4% H-3 => L+11, 19.6% H-5 => L+10, 13.0% H-6 => L+8, 8.21% H-17 => L+2, 6.57% H-5 => L+13, 6.23% HOMO => L+16, 5.19% H-8 => L+7, 2.88% H-2 => L+10, 2.75% H-2 => L+13
162	20657	484	0.00	65.7% H-36 => LUMO, 9.26% H-35 => L+1, 8.04% H-37 => L+1, 7.16% H-34 => LUMO, 2.78% H-36 => L+2, 2.19% H-34 => L+2
163	20665	484	0.00	24.4% H-4 => L+10, 14.9% H-12 => L+4, 14.5% H-7 => L+8, 9.30% H-11 => L+5, 8.71% H-9 => L+7, 8.47% H-8 => L+6, 3.15% H-6 => L+9, 2.76% H-10 => L+3, 2.64% H-7 => L+11, 2.16% H-2 => L+12

164	20668	484	0.00	49.6% H-37 => LUMO, 19.9% H-35 => LUMO, 14.5% H-36 => L+1, 3.49% H-35 => L+2, 2.38% H-33 => LUMO, 2.17% H-34 => L+1
165	20678	484	0.01	24.8% H-11 => L+3, 12.0% H-4 => L+12, 11.6% HOMO => L+16, 7.74% H-3 => L+14, 6.36% H-2 => L+13, 5.58% H-7 => L+9, 5.42% H-5 => L+13, 3.56% H-16 => L+2, 3.15% H-9 => L+6, 3.02% H-5 => L+10
166	20748	482	0.00	21.9% H-3 => L+13, 19.4% H-8 => L+5, 15.8% HOMO => L+15, 5.21% H-5 => L+14, 5.16% H-2 => L+11, 3.93% H-5 => L+11, 2.11% H-10 => L+7, 2.03% H-6 => L+13
167	20760	482	0.00	35.8% H-9 => L+5, 23.2% H-7 => L+7, 19.6% H-11 => L+4, 5.67% H-3 => L+12, 3.17% H-12 => L+5, 2.14% H-7 => L+4
168	20825	480	0.00	31.6% HOMO => L+15, 28.5% H-12 => L+3, 7.69% H-8 => L+5, 5.48% H-2 => L+14, 3.48% H-1 => L+16, 3.34% H-15 => L+2, 3.21% H-18 => L+2, 2.30% H-10 => L+7
169	20903	478	0.01	52.9% H-8 => L+6, 10.3% H-1 => L+14, 8.48% H-12 => L+4, 5.57% H-4 => L+13, 2.24% H-10 => L+3, 2.24% H-6 => L+9
170	20922	478	0.51	46.8% H-4 => L+11, 19.1% H-13 => L+3, 4.69% H-7 => L+13, 3.54% H-14 => L+2, 2.82% H-10 => L+6, 2.19% H-1 => L+13
171	20948	477	0.19	40.9% H-5 => L+10, 11.3% H-6 => L+8, 8.11% H-8 => L+7, 6.55% H-17 => L+2, 5.38% H-6 => L+11, 4.17% H-3 => L+14, 3.94% H-10 => L+5, 3.79% H-3 => L+11, 2.90% H-3 => L+8, 2.09% H-9 => L+6, 2.02% H-13 => L+4
172	21066	475	0.09	36.3% HOMO => L+16, 15.0% H-17 => L+2, 10.3% H-9 => L+6, 6.45% H-4 => L+12, 4.26% H-21 => L+2, 3.58% H-5 => L+10, 3.09% H-1 => L+15, 2.25% H-2 => L+13, 2.19% H-7 => L+9
173	21074	475	0.00	61.2% H-18 => L+2, 17.5% H-12 => L+3, 3.04% H-21 => L+1, 2.80% H-3 => L+13
174	21161	473	0.00	30.8% H-3 => L+13, 15.4% H-8 => L+5, 12.8% HOMO => L+15, 6.51% H-2 => L+14, 5.68% H-10 => L+4, 4.75% H-18 => L+2, 3.37% H-13 => L+5, 3.17% H-12 => L+3, 2.12% H-2 => L+11
175	21217	471	0.26	39.5% H-17 => L+2, 16.6% H-6 => L+8, 13.3% H-9 => L+6, 6.42% H-11 => L+3, 4.73% HOMO => L+16, 2.92% H-3 => L+14
176	21244	471	0.00	28.4% H-19 => L+2, 21.6% H-7 => L+8, 10.2% H-4 => L+13, 6.56% H-8 => L+6, 5.21% H-14 => L+3, 3.58% H-6 => L+9, 3.17% H-22 => L+1, 2.64% H-9 => L+10, 2.55% H-12 => L+4
177	21249	471	0.42	48.2% H-13 => L+3, 24.0% H-4 => L+11, 3.91% H-4 => L+14, 3.31% H-22 => L+2, 2.70% H-14 => L+2, 2.68% H-10 => L+6, 2.30% H-3 => L+12

178	21316	469	0.00	28.0% H-12 => L+4, 20.6% H-7 => L+8, 13.4% H-4 => L+13, 8.93% H-19 => L+2, 5.29% H-11 => L+5, 3.34% H-14 => L+3
179	21322	469	0.09	34.9% H-4 => L+12, 8.97% H-9 => L+6, 7.35% H-7 => L+9, 7.00% H-17 => L+2, 6.78% H-21 => L+2, 5.12% H-8 => L+7, 4.39% HOMO => L+16, 4.08% H-3 => L+14, 2.61% H-10 => L+5, 2.08% H-6 => L+8
180	21445	466	0.05	36.9% H-6 => L+8, 15.9% H-9 => L+6, 11.7% H-3 => L+14, 4.97% H-4 => L+12, 4.67% H-8 => L+7, 4.50% H-10 => L+5, 3.53% H-13 => L+4, 2.14% H-21 => L+2, 2.01% H-7 => L+9
181	21449	466	0.00	38.7% H-6 => L+9, 17.1% H-19 => L+2, 11.3% H-8 => L+6, 7.94% H-5 => L+12, 6.71% H-4 => L+13, 3.75% H-7 => L+8, 3.39% H-1 => L+14
182	21478	466	0.00	40.8% H-10 => L+4, 27.2% H-20 => L+2, 4.39% H-12 => L+3, 3.57% H-18 => L+2, 3.41% H-8 => L+5, 2.99% H-17 => L+3, 2.29% H-11 => L+6, 2.25% H-13 => L+5
183	21491	465	0.00	39.4% H-11 => L+4, 31.1% H-9 => L+5, 9.69% H-12 => L+5, 3.95% H-7 => L+4, 3.08% H-12 => L+8, 2.92% H-11 => L+7
184	21611	463	0.00	26.6% H-20 => L+2, 19.7% H-10 => L+4, 14.5% H-3 => L+13, 5.83% H-2 => L+14, 4.46% H-6 => L+13, 4.43% H-5 => L+11, 3.37% H-8 => L+5, 2.93% H-12 => L+3, 2.83% H-17 => L+3, 2.39% H-5 => L+14
185	21616	463	0.08	34.4% H-21 => L+2, 22.5% H-7 => L+9, 14.5% H-4 => L+12, 5.61% H-17 => L+2, 4.57% H-25 => L+2, 2.31% H-18 => L+3
186	21622	462	0.01	28.3% H-19 => L+2, 18.2% H-4 => L+13, 12.0% H-7 => L+8, 11.6% H-6 => L+9, 6.75% H-5 => L+12
187	21698	461	0.00	61.3% H-5 => L+11, 5.61% H-10 => L+4, 4.95% HOMO => L+15, 3.61% H-14 => L+4, 3.44% H-10 => L+7, 3.00% H-5 => L+14, 2.23% H-3 => L+10, 2.22% H-13 => L+5, 2.18% H-2 => L+14
188	21737	460	0.03	25.5% H-8 => L+7, 18.7% H-3 => L+14, 14.8% H-21 => L+2, 6.31% H-7 => L+9, 5.85% H-4 => L+12, 5.54% H-9 => L+6, 2.12% H-8 => L+10
189	21771	459	0.02	27.9% H-7 => L+9, 15.5% H-9 => L+6, 13.1% H-3 => L+14, 12.3% H-21 => L+2, 9.05% H-8 => L+7
190	21783	459	0.03	31.7% H-4 => L+14, 15.9% H-22 => L+2, 13.9% H-13 => L+3, 6.90% H-41 => LUMO, 4.63% H-10 => L+6, 2.57% H-1 => L+13, 2.47% H-8 => L+9, 2.17% H-26 => L+2, 2.10% H-7 => L+13
191	21829	458	0.04	41.8% H-22 => L+2, 12.2% H-7 => L+10, 8.36% H-4 => L+11, 4.46% H-41 => LUMO, 3.63% H-9 => L+8, 3.59% H-39 => LUMO, 3.14% H-38 => LUMO, 2.15% H-4 => L+14
192	21831	458	0.00	81.1% H-30 => L+1, 6.98% H-31 => LUMO, 4.40% H-31 => L+2, 2.78% H-32 => L+1

193	21890	457	0.00	52.5% H-5 => L+12, 16.9% H-6 => L+9, 5.69% H-14 => L+3, 3.59% H-42 => LUMO, 2.50% H-3 => L+9, 2.32% H-40 => LUMO, 2.10% H-8 => L+12
194	21926	456	0.00	46.3% H-40 => LUMO, 12.9% H-9 => L+7, 8.77% H-38 => LUMO, 7.67% H-39 => LUMO, 3.67% H-14 => L+3, 2.40% H-24 => L+2
195	21960	455	0.00	27.5% H-38 => LUMO, 24.1% H-39 => LUMO, 13.0% H-40 => LUMO, 8.06% H-5 => L+12, 4.11% H-14 => L+3, 3.72% H-4 => L+13, 3.33% H-6 => L+9, 2.89% H-39 => L+1, 2.53% H-38 => L+1
196	21967	455	0.00	37.4% H-39 => LUMO, 32.7% H-38 => LUMO, 6.24% H-41 => LUMO, 4.37% H-4 => L+14, 3.86% H-38 => L+1, 3.37% H-39 => L+1, 2.56% H-22 => L+2, 2.17% H-43 => LUMO
197	21996	455	0.00	30.5% H-14 => L+3, 23.6% H-42 => LUMO, 20.3% H-40 => LUMO, 3.67% H-9 => L+7, 3.35% H-4 => L+13, 2.45% H-44 => LUMO, 2.35% H-24 => L+2
198	22013	454	0.01	25.5% H-10 => L+5, 24.9% H-8 => L+7, 9.36% H-5 => L+13, 8.65% H-13 => L+4, 6.66% H-3 => L+14, 2.99% H-10 => L+8, 2.53% H-6 => L+11, 2.45% H-8 => L+4
199	22014	454	0.00	23.5% H-9 => L+7, 22.6% H-14 => L+3, 6.27% H-44 => LUMO, 6.22% H-38 => LUMO, 5.44% H-39 => LUMO, 4.47% H-5 => L+12, 4.17% H-42 => LUMO, 4.16% H-12 => L+4, 2.41% H-24 => L+2, 2.27% H-19 => L+2
200	22036	454	0.00	66.1% H-23 => L+2, 6.20% H-25 => L+1, 3.54% H-25 => L+3, 3.34% H-20 => L+2, 3.23% H-21 => L+1, 3.04% H-21 => L+3
201	22057	453	0.00	38.9% H-41 => LUMO, 32.3% H-43 => LUMO, 5.37% H-10 => L+6, 3.38% H-45 => LUMO, 2.91% H-22 => L+2, 2.90% H-4 => L+14
202	22079	453	0.00	67.5% H-31 => L+1, 7.60% H-32 => LUMO, 7.28% H-30 => L+2, 5.70% H-30 => LUMO, 3.48% H-33 => L+1, 2.48% H-32 => L+2
203	22083	453	0.12	28.6% H-43 => LUMO, 26.5% H-41 => LUMO, 20.6% H-45 => LUMO, 8.18% H-7 => L+10, 2.66% H-42 => L+1
204	22126	452	0.00	45.1% H-42 => LUMO, 11.3% H-40 => LUMO, 9.16% H-9 => L+7, 4.85% H-44 => LUMO, 4.39% H-12 => L+4, 3.97% H-24 => L+2, 2.83% H-4 => L+13, 2.30% H-41 => L+1, 2.11% H-6 => L+9
205	22193	451	0.00	66.1% H-24 => L+2, 7.08% H-9 => L+7, 3.39% H-28 => L+2, 2.72% H-22 => L+3, 2.21% H-22 => L+1
206	22204	450	0.00	20.4% H-6 => L+10, 12.6% H-20 => L+2, 12.0% H-11 => L+6, 7.55% H-23 => L+2, 5.15% H-16 => L+3, 4.52% HOMO => L+15, 4.24% H-9 => L+9, 3.37% H-5 => L+11, 3.17% H-8 => L+11, 2.56% H-15 => L+2, 2.53% H-14 => L+4, 2.45% H-7 => L+12, 2.22% H-5 => L+14

207	22211	450	0.43	29.9% H-7 => L+10, 14.4% H-43 => LUMO, 10.5% H-26 => L+2, 8.18% H-10 => L+6, 5.44% H-22 => L+2, 4.43% H-45 => LUMO, 2.36% H-4 => L+14, 2.21% H-9 => L+8
208	22217	450	0.00	67.8% H-25 => L+2, 6.31% H-15 => L+3, 5.20% H-23 => L+3, 4.68% H-23 => L+1, 4.31% H-7 => L+9
209	22267	449	0.33	54.0% H-45 => LUMO, 10.1% H-43 => LUMO, 6.27% H-7 => L+10, 6.03% H-44 => L+1, 5.78% H-26 => L+2, 2.95% H-22 => L+2, 2.01% H-41 => LUMO
210	22268	449	0.00	67.5% H-44 => LUMO, 8.34% H-42 => LUMO, 6.08% H-45 => L+1, 2.82% H-9 => L+7
211	22285	449	0.00	48.1% H-6 => L+10, 10.1% H-20 => L+2, 6.67% H-5 => L+14, 4.88% H-11 => L+6, 4.12% H-6 => L+13, 2.96% H-14 => L+4, 2.96% H-9 => L+9, 2.73% H-13 => L+5, 2.51% H-7 => L+12, 2.03% H-5 => L+8
212	22310	448	0.12	23.6% H-10 => L+6, 23.4% H-26 => L+2, 14.2% H-4 => L+14, 7.03% H-7 => L+10, 5.21% H-29 => L+2, 3.74% H-41 => LUMO, 2.67% H-22 => L+2
213	22347	447	0.00	38.7% H-15 => L+3, 12.7% H-10 => L+5, 9.13% H-16 => L+2, 8.42% H-25 => L+2, 4.45% H-16 => L+6, 3.89% H-5 => L+13, 3.80% HOMO => L+16, 3.69% H-32 => L+1
214	22381	447	0.04	33.1% H-26 => L+2, 16.1% H-10 => L+6, 9.55% H-4 => L+14, 6.46% H-29 => L+2, 4.56% H-15 => L+4, 4.02% H-12 => L+5, 4.01% H-16 => L+5, 2.01% H-11 => L+7
215	22396	447	0.00	72.9% H-27 => L+2, 7.08% H-28 => L+2, 3.04% H-44 => LUMO, 2.76% H-11 => L+5
216	22402	446	0.00	61.3% H-32 => L+1, 7.39% H-33 => LUMO, 7.05% H-31 => L+2, 6.81% H-31 => LUMO, 4.17% H-34 => L+1, 3.12% H-15 => L+3
217	22442	446	0.00	53.3% H-16 => L+3, 11.2% H-11 => L+6, 7.55% H-15 => L+2, 7.45% H-15 => L+6, 4.12% H-18 => L+2, 2.83% H-23 => L+2
218	22464	445	0.00	37.4% H-5 => L+13, 14.4% H-15 => L+3, 14.2% H-10 => L+5, 3.39% H-14 => L+5, 3.22% H-6 => L+14, 3.13% H-12 => L+6, 2.90% H-10 => L+8
219	22508	444	0.00	39.9% H-11 => L+5, 10.0% H-12 => L+7, 7.63% H-9 => L+4, 6.47% H-9 => L+7, 6.39% H-27 => L+2, 5.72% H-12 => L+4, 4.72% H-42 => LUMO, 4.58% H-14 => L+3, 3.48% H-17 => L+4
220	22640	442	0.00	56.9% H-28 => L+2, 7.30% H-29 => L+1, 6.24% H-29 => L+3, 5.33% H-27 => L+2, 4.79% H-7 => L+11, 2.71% H-4 => L+13
221	22659	441	0.03	61.9% H-29 => L+2, 9.52% H-26 => L+2, 7.36% H-28 => L+1, 6.80% H-28 => L+3, 2.51% H-7 => L+10
222	22721	440	0.04	36.4% H-13 => L+4, 11.9% H-5 => L+13, 11.5% H-10 => L+5, 5.60% H-12 => L+6, 5.13% H-6 =>

				L+11, 3.78% H-13 => L+7, 3.17% H-8 => L+10, 2.39% H-50 => LUMO, 2.30% H-48 => LUMO
223	22738	440	0.00	32.3% H-33 => L+1, 17.8% H-8 => L+8, 12.2% H-5 => L+14, 4.14% H-32 => LUMO, 3.92% H-32 => L+2, 3.61% H-34 => LUMO, 2.87% H-11 => L+6, 2.85% H-35 => L+1, 2.64% H-6 => L+10, 2.39% H-14 => L+4
224	22746	440	0.00	30.3% H-33 => L+1, 25.0% H-8 => L+8, 9.06% H-5 => L+14, 3.79% H-32 => L+2, 3.54% H-32 => LUMO, 3.30% H-34 => LUMO, 2.86% H-6 => L+10, 2.86% H-14 => L+4, 2.81% H-35 => L+1, 2.35% H-11 => L+6
225	22770	439	0.15	20.9% H-12 => L+5, 14.0% H-11 => L+7, 13.4% H-10 => L+6, 6.24% H-7 => L+10, 5.54% H-11 => L+4, 5.21% H-9 => L+8, 4.85% H-15 => L+4, 4.34% H-16 => L+5, 3.01% H-29 => L+2, 2.96% H-45 => LUMO, 2.39% H-4 => L+14, 2.15% H-6 => L+12
226	22840	438	0.42	20.1% H-9 => L+8, 15.5% H-8 => L+9, 8.44% H-15 => L+4, 7.76% H-10 => L+6, 7.14% H-11 => L+7, 7.13% H-16 => L+5, 6.88% H-7 => L+10, 6.75% H-6 => L+12
227	22840	438	0.00	41.6% H-7 => L+11, 10.0% H-28 => L+2, 9.90% H-4 => L+13, 7.30% H-9 => L+10, 4.66% H-24 => L+2, 3.59% H-11 => L+8, 2.04% H-15 => L+5
228	22844	438	0.00	29.4% H-8 => L+8, 24.7% H-5 => L+14, 18.9% H-11 => L+6, 3.09% H-16 => L+3, 2.89% H-13 => L+5, 2.12% H-10 => L+4
229	22871	437	0.00	30.8% H-50 => LUMO, 21.7% H-12 => L+6, 12.4% H-48 => LUMO, 3.78% H-5 => L+13, 2.92% H-11 => L+9, 2.49% H-52 => LUMO, 2.37% H-10 => L+5, 2.35% H-20 => L+3, 2.05% H-3 => L+14
230	22909	437	0.00	27.1% H-48 => LUMO, 17.7% H-13 => L+4, 17.2% H-12 => L+6, 11.3% H-50 => LUMO, 2.32% H-18 => L+3, 2.25% H-54 => LUMO, 2.03% HOMO => L+16
231	22984	435	0.01	26.5% H-15 => L+5, 25.9% H-16 => L+4, 7.91% H-16 => L+7, 7.81% H-11 => L+5, 3.60% H-13 => L+6, 3.54% H-14 => L+3, 2.68% H-3 => L+15, 2.40% H-2 => L+16
232	23029	434	0.01	52.2% H-46 => LUMO, 34.9% H-47 => LUMO, 4.91% H-47 => L+1, 3.37% H-46 => L+1
233	23030	434	0.00	52.2% H-47 => LUMO, 34.9% H-46 => LUMO, 4.88% H-46 => L+1, 3.34% H-47 => L+1
234	23049	434	0.00	49.6% H-49 => LUMO, 20.5% H-51 => LUMO, 8.44% H-53 => LUMO, 3.34% H-48 => L+1, 2.05% H-10 => L+7, 2.03% H-13 => L+5, 2.02% H-16 => L+3
235	23073	433	0.00	60.1% H-34 => L+1, 7.79% H-33 => L+2, 7.55% H-36 => L+1, 7.50% H-33 => LUMO, 4.60% H-35 => LUMO, 2.27% H-37 => L+2

236	23122	432	0.03	33.4% H-6 => L+11, 9.30% H-12 => L+6, 9.00% H-50 => LUMO, 5.78% H-15 => L+3, 5.41% H-1 => L+15, 4.53% H-13 => L+4, 4.01% HOMO => L+16, 3.18% H-18 => L+3, 3.10% H-48 => LUMO
237	23128	432	0.29	36.0% H-8 => L+9, 10.6% H-16 => L+5, 8.87% H-9 => L+8, 8.48% H-15 => L+4, 5.10% H-6 => L+12, 3.69% H-4 => L+14, 3.14% H-15 => L+7, 2.26% H-18 => L+4
238	23148	432	0.00	29.0% H-7 => L+12, 10.0% H-5 => L+14, 9.14% H-9 => L+9, 8.95% H-11 => L+6, 8.59% H-10 => L+7, 4.93% H-49 => LUMO, 4.79% H-1 => L+16, 2.51% HOMO => L+15, 2.19% H-13 => L+8
239	23180	431	0.11	31.1% H-12 => L+5, 15.3% H-9 => L+8, 9.73% H-11 => L+4, 6.50% H-16 => L+5, 5.53% H-12 => L+8, 5.07% H-18 => L+4, 3.25% H-8 => L+9, 3.03% H-15 => L+4, 2.55% H-15 => L+7, 2.42% H-11 => L+10, 2.07% H-7 => L+10
240	23181	431	0.00	18.0% H-55 => LUMO, 15.4% H-17 => L+3, 15.1% H-53 => LUMO, 8.37% H-51 => LUMO, 6.96% H-49 => LUMO, 5.19% H-11 => L+6, 4.11% H-10 => L+7, 4.01% H-6 => L+13, 2.25% H-7 => L+12
241	23186	431	0.02	28.3% H-48 => LUMO, 20.9% H-50 => LUMO, 12.2% H-54 => LUMO, 9.54% H-6 => L+11, 3.77% H-49 => L+1, 3.74% H-12 => L+6, 3.74% H-52 => LUMO, 3.70% H-1 => L+15, 2.87% H-13 => L+4, 2.12% HOMO => L+16
242	23260	430	0.00	49.5% H-10 => L+7, 7.17% H-11 => L+6, 5.25% H-17 => L+3, 4.95% H-9 => L+9, 4.68% H-5 => L+14, 3.49% H-14 => L+4, 3.08% H-6 => L+13, 2.53% H-8 => L+5, 2.10% H-13 => L+5
243	23278	430	0.00	19.5% H-17 => L+3, 19.3% H-51 => LUMO, 12.4% H-49 => LUMO, 11.1% H-53 => LUMO, 7.23% H-7 => L+12, 4.07% H-10 => L+7, 2.74% H-13 => L+5, 2.58% H-11 => L+6, 2.20% H-55 => LUMO, 2.20% H-50 => L+1
244	23303	429	0.01	32.3% H-56 => LUMO, 32.2% H-54 => LUMO, 7.50% H-48 => LUMO, 5.50% H-52 => LUMO, 4.80% H-1 => L+15, 3.46% H-12 => L+6, 3.32% H-50 => LUMO
245	23313	429	0.06	31.5% H-11 => L+7, 18.7% H-9 => L+8, 7.96% H-8 => L+9, 5.47% H-15 => L+4, 5.38% H-12 => L+8, 4.08% H-9 => L+5, 2.99% H-18 => L+4, 2.99% H-11 => L+4, 2.38% H-12 => L+11, 2.26% H-11 => L+10
246	23329	429	0.00	38.6% H-35 => L+1, 22.1% H-37 => L+1, 8.70% H-55 => LUMO, 5.72% H-34 => L+2, 4.65% H-34 => LUMO, 3.32% H-51 => LUMO, 2.34% H-49 => LUMO
247	23341	428	0.05	31.3% H-56 => LUMO, 11.7% H-6 => L+11, 9.04% H-18 => L+3, 7.09% H-1 => L+15, 2.93% H-58 => LUMO, 2.76% H-52 => LUMO, 2.65% H-13 =>

				L+7, 2.32% H-48 => LUMO, 2.26% H-10 => L+8, 2.21% H-50 => LUMO
248	23366	428	0.00	14.4% H-1 => L+16, 12.6% H-55 => LUMO, 9.36% H-35 => L+1, 6.81% H-49 => LUMO, 5.87% H-37 => L+1, 5.80% HOMO => L+15, 5.30% H-13 => L+5, 5.22% H-14 => L+4, 4.03% H-51 => LUMO, 3.93% H-17 => L+3, 3.91% H-7 => L+12, 2.01% H-4 => L+15
249	23369	428	0.01	35.0% H-6 => L+12, 21.1% H-7 => L+13, 6.22% H-8 => L+9, 5.53% H-19 => L+3, 3.33% H-14 => L+6, 2.85% H-9 => L+14, 2.81% H-10 => L+12, 2.52% H-4 => L+11, 2.02% H-9 => L+11
250	23392	428	0.04	19.7% H-54 => LUMO, 15.9% H-1 => L+15, 8.66% H-6 => L+11, 7.58% H-56 => LUMO, 6.59% H-58 => LUMO, 5.97% H-50 => LUMO, 4.66% H-8 => L+10, 3.82% HOMO => L+16, 3.55% H-10 => L+8, 2.74% H-13 => L+7, 2.48% H-52 => LUMO, 2.04% H-4 => L+16, 2.00% H-18 => L+3
251	23414	427	0.00	38.4% H-55 => LUMO, 12.7% H-1 => L+16, 7.34% H-57 => LUMO, 6.28% H-7 => L+12, 5.13% H-51 => LUMO, 3.64% H-6 => L+13, 3.48% HOMO => L+15
252	23418	427	0.00	47.7% H-13 => L+6, 5.81% H-7 => L+14, 5.80% H-14 => L+3, 4.80% H-10 => L+9, 3.87% H-16 => L+4, 3.42% H-2 => L+16, 2.66% H-9 => L+13, 2.47% H-3 => L+15, 2.31% H-11 => L+8
253	23468	426	0.31	46.9% H-18 => L+3, 15.0% H-56 => LUMO, 4.31% H-21 => L+2, 3.81% H-11 => L+9, 3.64% H-52 => LUMO, 2.51% H-20 => L+3
254	23497	426	0.18	34.6% H-6 => L+12, 23.1% H-7 => L+13, 9.05% H-8 => L+9, 5.49% H-19 => L+3, 4.34% H-4 => L+14, 3.96% H-9 => L+11, 2.87% H-14 => L+6
255	23584	424	0.00	43.5% H-52 => LUMO, 13.1% H-54 => LUMO, 6.58% H-58 => LUMO, 4.60% H-20 => L+3, 4.24% H-1 => L+15, 3.81% H-50 => LUMO, 3.28% H-6 => L+14, 3.04% H-53 => L+1, 2.76% H-12 => L+6, 2.48% H-51 => L+1
256	23586	424	0.00	31.2% H-53 => LUMO, 19.7% H-51 => LUMO, 14.6% H-9 => L+9, 8.36% H-7 => L+12, 4.72% H-57 => LUMO, 4.08% H-52 => L+1, 2.69% H-17 => L+3, 2.02% H-1 => L+16
257	23593	424	0.00	17.5% H-52 => LUMO, 16.1% H-20 => L+3, 14.3% H-6 => L+14, 13.2% H-12 => L+6, 5.88% H-18 => L+3, 4.71% H-8 => L+13, 2.53% H-5 => L+13, 2.23% H-17 => L+6
258	23594	424	0.00	38.2% H-9 => L+9, 13.0% H-53 => LUMO, 10.9% H-7 => L+12, 7.49% H-51 => LUMO, 3.94% H-17 => L+3, 3.56% H-1 => L+16, 3.23% H-21 => L+3, 2.49% H-11 => L+12, 2.33% H-57 => LUMO

259	23665	423	0.00	21.2% H-7 => L+11, 18.8% H-9 => L+10, 14.4% H-12 => L+7, 9.36% H-11 => L+8, 8.58% H-13 => L+6, 6.23% H-12 => L+4, 3.05% H-11 => L+5
260	23674	422	0.00	30.3% H-13 => L+5, 19.7% H-6 => L+13, 12.5% H-17 => L+3, 9.68% H-14 => L+4, 4.07% H-10 => L+4, 3.71% H-5 => L+14, 3.66% H-14 => L+7, 2.55% H-8 => L+11
261	23776	421	0.00	53.7% H-36 => L+1, 12.5% H-37 => LUMO, 10.6% H-35 => LUMO, 6.72% H-37 => L+2, 5.77% H-35 => L+2, 3.77% H-34 => L+1, 2.07% H-36 => L+3
262	23784	420	0.00	42.6% H-37 => L+1, 19.9% H-36 => LUMO, 15.0% H-35 => L+1, 11.7% H-36 => L+2, 2.71% H-34 => LUMO, 2.33% H-35 => L+3
263	23805	420	0.28	56.7% H-8 => L+10, 9.72% H-14 => L+5, 7.25% H-13 => L+7, 3.50% H-1 => L+15, 3.17% H-19 => L+4, 2.87% H-6 => L+8, 2.62% H-10 => L+11, 2.40% H-18 => L+3, 2.18% H-13 => L+4
264	23831	420	0.26	59.3% H-19 => L+3, 8.58% H-7 => L+13, 5.49% H-2 => L+15, 3.47% H-3 => L+16, 3.15% H-22 => L+2, 3.11% H-11 => L+7, 2.40% H-14 => L+6
265	23834	420	0.00	33.2% H-14 => L+4, 13.0% H-17 => L+3, 8.51% H-75 => LUMO, 5.48% H-68 => LUMO, 4.17% H-13 => L+5, 3.64% H-6 => L+13, 2.52% H-14 => L+7, 2.36% H-7 => L+12
266	23883	419	0.01	15.7% H-12 => L+7, 12.4% H-7 => L+14, 7.16% H-12 => L+10, 5.61% H-13 => L+6, 4.99% H-11 => L+5, 4.45% H-18 => L+5, 4.23% H-21 => L+4, 3.39% H-22 => L+3, 3.19% H-12 => L+4, 3.00% H-9 => L+10, 2.30% H-17 => L+4, 2.29% H-17 => L+7, 2.21% H-2 => L+16, 2.10% H-11 => L+11
267	23898	418	0.04	68.6% H-58 => LUMO, 7.59% H-54 => LUMO, 6.22% H-57 => L+1, 5.27% H-56 => LUMO, 3.57% H-52 => LUMO, 2.59% H-48 => LUMO
268	23900	418	0.00	67.6% H-57 => LUMO, 8.22% H-55 => LUMO, 6.98% H-53 => LUMO, 5.90% H-58 => L+1, 2.94% H-49 => LUMO
269	23955	417	0.00	30.8% H-7 => L+14, 14.2% H-9 => L+10, 7.77% H-12 => L+7, 6.74% H-17 => L+4, 6.07% H-11 => L+5, 5.98% H-13 => L+6, 3.78% H-9 => L+13, 2.56% H-12 => L+4
270	23972	417	0.00	21.1% H-6 => L+13, 14.6% H-21 => L+3, 11.2% H-13 => L+5, 9.01% H-1 => L+16, 6.53% H-75 => LUMO, 2.77% H-60 => LUMO, 2.52% H-19 => L+5, 2.21% H-13 => L+8
271	24071	415	0.00	16.3% H-9 => L+10, 14.1% H-11 => L+8, 11.0% H-21 => L+4, 4.31% H-18 => L+5, 4.15% H-13 => L+6, 3.98% H-16 => L+4, 3.89% H-16 => L+7, 3.82% H-11 => L+11, 3.80% H-12 => L+7, 3.80% H-15 => L+8, 3.57% H-9 => L+7, 2.34% H-12 => L+13, 2.28% H-17 => L+7, 2.27% H-25 => L+4
272	24078	415	0.00	87.2% H-59 => LUMO, 5.45% H-63 => LUMO

273	24085	415	0.16	15.1% H-14 => L+6, 14.3% H-18 => L+4, 11.5% H-11 => L+7, 11.3% H-12 => L+5, 8.92% H-19 => L+3, 8.06% H-15 => L+4, 3.93% H-15 => L+7, 3.28% H-21 => L+5, 2.27% H-2 => L+15
274	24096	415	0.00	50.7% H-21 => L+3, 9.14% H-6 => L+13, 4.26% H-25 => L+3, 4.12% H-9 => L+9, 2.58% H-18 => L+6, 2.39% H-7 => L+12, 2.09% H-8 => L+11
275	24131	414	0.00	54.2% H-62 => LUMO, 21.1% H-64 => LUMO, 7.09% H-20 => L+3, 6.50% H-6 => L+14
276	24174	414	0.60	36.1% H-2 => L+15, 9.64% H-15 => L+4, 8.61% H-3 => L+16, 5.55% H-67 => LUMO, 5.39% H-7 => L+13, 5.22% H-19 => L+3, 4.29% H-18 => L+4, 2.68% H-15 => L+7, 2.60% H-12 => L+5, 2.46% H-14 => L+6
277	24188	413	0.00	29.1% H-62 => LUMO, 16.9% H-6 => L+14, 16.1% H-20 => L+3, 4.61% H-10 => L+8, 4.34% H-72 => LUMO, 3.97% H-64 => LUMO, 3.58% H-61 => LUMO, 2.10% H-13 => L+7, 2.06% H-18 => L+3
278	24198	413	0.01	31.7% H-2 => L+16, 16.9% H-22 => L+3, 7.94% H-3 => L+15, 6.75% H-13 => L+6, 5.78% H-10 => L+9, 4.76% H-7 => L+14, 2.70% H-9 => L+10, 2.69% H-66 => LUMO, 2.16% H-8 => L+12, 2.03% H-11 => L+8
279	24201	413	0.01	85.0% H-65 => LUMO, 5.66% H-67 => LUMO
280	24202	413	0.00	66.3% H-63 => LUMO, 14.1% H-68 => LUMO, 5.52% H-59 => LUMO, 3.02% H-60 => LUMO, 2.35% H-62 => L+1
281	24204	413	0.00	17.2% H-64 => LUMO, 16.3% H-6 => L+14, 12.8% H-72 => LUMO, 11.4% H-61 => LUMO, 7.74% H-23 => L+3, 6.40% H-1 => L+15, 3.92% H-10 => L+8
282	24214	413	0.00	59.6% H-66 => LUMO, 34.9% H-69 => LUMO
283	24231	413	0.00	50.6% H-10 => L+8, 14.3% H-14 => L+5, 4.75% H-64 => LUMO, 4.03% H-13 => L+10, 3.99% H-8 => L+10, 3.48% H-62 => LUMO, 2.88% H-8 => L+7, 2.87% H-19 => L+4, 2.11% H-13 => L+4
284	24264	412	0.02	74.7% H-67 => LUMO, 9.51% H-70 => LUMO, 7.43% H-65 => LUMO
285	24264	412	0.00	49.1% H-69 => LUMO, 28.2% H-66 => LUMO, 11.7% H-71 => LUMO, 3.06% H-22 => L+3, 2.95% H-67 => L+1
286	24332	411	0.00	49.6% H-22 => L+3, 8.63% H-2 => L+16, 6.05% H-71 => LUMO, 3.35% H-12 => L+7, 2.91% H-26 => L+3, 2.59% H-9 => L+10, 2.33% H-19 => L+6, 2.26% H-17 => L+4
287	24347	411	0.00	39.5% H-64 => LUMO, 17.0% H-61 => LUMO, 7.33% H-62 => LUMO, 6.67% H-13 => L+7, 5.10% H-20 => L+3, 2.06% H-60 => L+1

288	24358	411	0.00	40.8% H-68 => LUMO, 19.5% H-63 => LUMO, 18.4% H-60 => LUMO, 2.69% H-64 => L+1, 2.15% H-75 => LUMO
289	24372	410	0.00	15.8% H-75 => LUMO, 14.5% H-8 => L+11, 9.59% H-60 => LUMO, 8.54% H-15 => L+6, 6.89% H-68 => LUMO, 5.16% H-30 => L+2, 4.92% H-10 => L+10, 3.73% H-1 => L+16, 2.81% H-16 => L+3, 2.81% H-6 => L+13, 2.38% H-13 => L+8
290	24383	410	0.25	42.8% H-14 => L+6, 6.49% H-7 => L+13, 6.40% H-24 => L+3, 5.27% H-2 => L+15, 4.38% H-18 => L+4, 3.72% H-21 => L+5, 2.32% H-15 => L+4, 2.24% H-23 => L+4, 2.12% H-15 => L+7
291	24406	410	0.00	51.6% H-71 => LUMO, 8.58% H-10 => L+9, 7.94% H-69 => LUMO, 4.94% H-74 => LUMO, 4.53% H-70 => L+1, 2.73% H-17 => L+4, 2.44% H-7 => L+14, 2.33% H-66 => LUMO
292	24413	410	0.01	70.2% H-70 => LUMO, 7.80% H-67 => LUMO, 6.65% H-73 => LUMO, 5.34% H-71 => L+1
293	24414	410	0.00	72.8% H-30 => L+2, 5.89% H-31 => L+1, 4.09% H-31 => L+3, 3.58% H-30 => LUMO
294	24453	409	0.00	20.1% H-10 => L+9, 12.8% H-71 => LUMO, 11.7% H-16 => L+4, 7.49% H-7 => L+14, 4.66% H-16 => L+7, 3.66% H-2 => L+16, 3.25% H-15 => L+8, 2.93% H-11 => L+8, 2.74% H-17 => L+4, 2.61% H-8 => L+12, 2.32% H-69 => LUMO
295	24482	408	0.00	27.7% H-23 => L+3, 12.9% H-61 => LUMO, 12.8% H-13 => L+7, 5.99% H-11 => L+9, 4.77% H-20 => L+3, 4.20% H-14 => L+5, 4.06% H-72 => LUMO, 2.99% H-21 => L+6, 2.69% H-18 => L+3, 2.47% H-25 => L+2
296	24510	408	0.00	23.6% H-13 => L+7, 22.1% H-20 => L+3, 10.4% H-14 => L+5, 7.83% H-11 => L+9, 5.40% H-14 => L+8, 4.55% H-10 => L+8, 2.45% H-9 => L+12, 2.21% H-10 => L+5
297	24517	408	0.03	30.5% H-24 => L+3, 14.3% H-9 => L+11, 5.69% H-7 => L+13, 4.87% H-14 => L+6, 4.64% H-12 => L+8, 2.50% H-11 => L+10, 2.46% H-7 => L+10, 2.22% H-38 => L+1, 2.14% H-17 => L+5, 2.03% H-11 => L+7
298	24539	408	0.01	12.7% H-9 => L+11, 9.83% H-11 => L+10, 9.24% H-18 => L+4, 8.53% H-23 => L+4, 6.34% H-20 => L+4, 5.92% H-11 => L+7, 4.90% H-2 => L+15, 4.37% H-14 => L+6, 3.89% H-24 => L+3, 3.83% H-17 => L+5, 2.75% H-25 => L+5, 2.67% H-12 => L+8, 2.01% H-17 => L+8
299	24558	407	0.00	25.0% H-60 => LUMO, 10.9% H-75 => LUMO, 10.4% H-8 => L+11, 5.76% H-25 => L+3, 5.34% H-1 => L+16, 4.20% H-15 => L+6, 3.69% H-13 => L+5, 2.82% H-22 => L+4
300	24559	407	0.00	37.3% H-17 => L+4, 13.3% H-26 => L+3, 11.5% H-10 => L+9, 6.03% H-12 => L+7, 5.04% H-20 =>

				L+5, 3.64% H-18 => L+5, 2.86% H-7 => L+14, 2.42% H-29 => L+3
301	24570	407	0.00	37.5% H-25 => L+3, 5.96% H-12 => L+9, 5.54% H-21 => L+3, 4.60% H-8 => L+11, 4.14% H-23 => L+2, 4.01% H-23 => L+6, 3.83% H-7 => L+12, 3.53% H-22 => L+4, 3.23% H-26 => L+4, 2.36% H-1 => L+16, 2.26% H-14 => L+7, 2.01% H-19 => L+5
302	24582	407	0.00	17.9% H-39 => L+1, 15.7% H-38 => L+1, 9.61% H-10 => L+9, 6.23% H-11 => L+8, 5.26% H-17 => L+4, 4.90% H-2 => L+16, 3.11% H-38 => LUMO, 2.70% H-39 => LUMO, 2.60% H-26 => L+3, 2.41% H-12 => L+7, 2.04% H-8 => L+12
303	24585	407	0.00	19.8% H-38 => L+1, 17.4% H-39 => L+1, 15.8% H-24 => L+3, 4.47% H-23 => L+4, 4.30% H-18 => L+4, 3.79% H-27 => L+3, 3.31% H-39 => LUMO, 2.89% H-38 => LUMO, 2.70% H-18 => L+7, 2.15% H-39 => L+2, 2.07% H-16 => L+8
304	24603	406	0.07	20.0% H-23 => L+3, 19.9% H-11 => L+9, 14.4% H-16 => L+6, 5.62% H-72 => LUMO, 4.88% H-9 => L+12, 4.04% H-15 => L+9, 2.93% H-18 => L+3, 2.53% H-12 => L+6, 2.19% H-78 => LUMO
305	24608	406	0.09	31.6% H-72 => LUMO, 11.3% H-78 => LUMO, 10.8% H-1 => L+15, 7.61% H-31 => L+2, 5.32% H-23 => L+3, 4.29% H-13 => L+7, 3.80% H-14 => L+5
306	24644	406	0.00	39.9% H-75 => LUMO, 24.2% H-60 => LUMO, 20.9% H-68 => LUMO, 4.12% H-72 => L+1, 2.17% H-61 => L+1
307	24650	406	0.01	28.8% H-31 => L+2, 19.8% H-72 => LUMO, 19.1% H-61 => LUMO, 3.19% H-32 => L+1, 2.86% H-30 => L+3, 2.77% H-14 => L+5, 2.54% H-64 => LUMO, 2.48% H-11 => L+9, 2.14% H-30 => L+1
308	24657	406	0.04	30.8% H-31 => L+2, 19.8% H-61 => LUMO, 6.11% H-1 => L+15, 3.97% H-14 => L+5, 3.45% H-78 => LUMO, 3.30% H-72 => LUMO, 3.19% H-30 => L+3, 3.10% H-32 => L+1, 2.08% H-13 => L+7, 2.03% H-11 => L+9
309	24680	405	0.00	19.0% H-39 => L+1, 16.6% H-38 => L+1, 11.1% H-11 => L+8, 6.59% H-16 => L+4, 5.70% H-10 => L+9, 5.28% H-21 => L+4, 4.33% H-16 => L+7, 2.87% H-23 => L+5, 2.50% H-74 => LUMO, 2.34% H-38 => LUMO, 2.04% H-39 => LUMO
310	24686	405	0.00	15.3% H-16 => L+6, 15.3% H-14 => L+5, 10.8% H-6 => L+14, 6.39% H-8 => L+13, 5.85% H-13 => L+7, 3.81% H-19 => L+4, 3.67% H-10 => L+11, 3.66% H-19 => L+7, 3.38% H-23 => L+3, 3.05% H-24 => L+4, 2.81% H-13 => L+10, 2.70% H-15 => L+3, 2.11% H-15 => L+9, 2.02% H-13 => L+4
311	24687	405	0.03	16.1% H-38 => L+1, 14.1% H-39 => L+1, 12.8% H-27 => L+3, 5.24% H-23 => L+4, 5.03% H-24 =>

				L+3, 3.83% H-12 => L+8, 3.51% H-21 => L+5, 2.85% H-9 => L+11, 2.47% H-18 => L+7, 2.30% H-40 => L+1, 2.10% H-15 => L+4
312	24710	405	0.00	27.3% H-15 => L+6, 17.5% H-8 => L+11, 9.21% H-25 => L+3, 5.25% H-16 => L+3, 4.85% H-14 => L+7, 4.74% H-22 => L+4, 2.95% H-16 => L+9, 2.90% H-75 => LUMO, 2.86% H-12 => L+9, 2.34% H-19 => L+5, 2.06% H-13 => L+8, 2.06% H-1 => L+16
313	24750	404	0.00	54.6% H-73 => LUMO, 11.2% H-76 => LUMO, 8.25% H-27 => L+3, 7.52% H-70 => LUMO, 4.30% H-74 => L+1, 2.89% H-74 => LUMO
314	24753	404	0.00	55.5% H-74 => LUMO, 11.1% H-77 => LUMO, 7.61% H-71 => LUMO, 4.36% H-73 => L+1, 4.19% H-26 => L+3, 2.94% H-73 => LUMO
315	24760	404	0.02	42.1% H-27 => L+3, 18.9% H-40 => L+1, 6.00% H-42 => L+1, 4.24% H-28 => L+3, 3.41% H-20 => L+4
316	24779	404	0.00	52.7% H-19 => L+4, 9.52% H-22 => L+5, 5.19% H-14 => L+5, 4.50% H-16 => L+6, 3.27% H-78 => LUMO, 3.19% H-24 => L+7, 2.48% H-8 => L+13, 2.38% H-13 => L+4, 2.06% H-13 => L+7
317	24780	404	0.27	48.2% H-40 => L+1, 6.25% H-44 => L+1, 4.97% H-9 => L+11, 4.08% H-18 => L+4, 3.32% H-11 => L+13, 2.59% H-12 => L+8, 2.05% H-79 => LUMO
318	24798	403	0.01	49.9% H-26 => L+3, 9.61% H-17 => L+4, 5.60% H-29 => L+3, 5.15% H-2 => L+16, 2.74% H-7 => L+14, 2.21% H-74 => LUMO
319	24806	403	0.00	17.1% H-40 => L+1, 15.6% H-12 => L+8, 13.5% H-42 => L+1, 10.8% H-27 => L+3, 4.93% H-44 => L+1, 3.72% H-73 => LUMO, 2.37% H-28 => L+3, 2.05% H-11 => L+13

Table S3.19. TDDFT-predicted band excitation data for **3.8**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	2668	3748	8.55	98.5% HOMO => LUMO, 2.16% H-1 => L+1
1	4430	2258	0.00	50.5% H-1 => LUMO, 46.7% HOMO => L+1
2	4584	2181	0.00	93.3% H-2 => LUMO, 3.72% H-3 => L+1
3	4933	2027	0.00	51.4% HOMO => L+1, 47.2% H-1 => LUMO
4	5307	1884	0.00	81.8% H-3 => LUMO, 13.2% H-2 => L+1, 2.33% H-5 => L+1
5	6274	1594	0.00	74.0% H-5 => LUMO, 16.4% H-3 => L+1, 5.56% H-2 => L+2
6	6293	1589	0.03	62.8% H-4 => LUMO, 34.4% HOMO => L+2

7	6658	1502	0.27	42.4% HOMO => L+2, 30.9% H-1 => L+1, 22.6% H-4 => LUMO
8	6897	1450	0.38	64.4% H-1 => L+1, 20.2% HOMO => L+2, 11.1% H-4 => LUMO
9	7148	1399	0.00	80.8% H-2 => L+1, 13.3% H-3 => LUMO, 2.66% H-3 => L+2
10	7408	1350	0.00	67.5% H-7 => LUMO, 18.1% H-5 => L+1, 7.69% H-3 => L+2, 2.99% H-2 => L+3
11	7899	1266	0.00	63.2% H-3 => L+1, 20.9% H-5 => LUMO, 8.54% H-2 => L+2, 2.85% H-2 => LUMO
12	8019	1247	0.00	78.3% H-6 => LUMO, 15.1% HOMO => L+3, 2.11% H-4 => L+1
13	8461	1182	0.00	67.8% HOMO => L+3, 16.4% H-6 => LUMO, 11.1% H-4 => L+1
14	8626	1159	0.00	80.7% H-4 => L+1, 12.8% HOMO => L+3, 2.26% H-1 => LUMO
15	8646	1157	0.00	62.7% H-8 => LUMO, 19.2% H-7 => L+1, 8.77% H-5 => L+2, 3.87% H-3 => L+3
16	8720	1147	0.00	93.2% H-1 => L+2, 2.52% HOMO => L+1
17	8886	1125	0.00	53.0% H-5 => L+1, 27.5% H-7 => LUMO, 9.96% H-3 => L+2, 2.94% H-2 => L+3, 2.60% H-3 => LUMO
18	9238	1082	0.00	78.8% H-2 => L+2, 11.7% H-3 => L+1, 3.20% H-2 => LUMO, 2.99% H-3 => L+3
19	9561	1046	0.07	84.7% H-9 => LUMO, 6.23% H-6 => L+1, 3.10% HOMO => L+4
20	9925	1008	0.00	57.5% H-10 => LUMO, 18.3% H-8 => L+1, 9.77% H-7 => L+2, 3.35% H-5 => L+3, 2.54% H-3 => L+2
21	10011	999	0.00	59.6% H-3 => L+2, 20.0% H-5 => L+1, 8.29% H-2 => L+3, 2.89% H-10 => LUMO, 2.69% H-5 => L+3
22	10021	998	0.00	44.5% H-7 => L+1, 32.5% H-8 => LUMO, 11.3% H-5 => L+2, 4.15% H-3 => L+3, 2.15% H-5 => LUMO
23	10175	983	0.07	77.4% HOMO => L+4, 10.8% H-1 => L+3, 2.88% H-9 => LUMO
24	10287	972	0.02	73.2% H-6 => L+1, 12.1% H-4 => L+2, 6.68% H-9 => LUMO, 2.48% H-4 => LUMO
25	10529	950	0.05	43.5% H-4 => L+2, 29.2% H-1 => L+3, 11.8% HOMO => L+4, 10.0% H-6 => L+1
26	10695	935	0.14	52.5% H-1 => L+3, 35.9% H-4 => L+2, 3.03% HOMO => L+4, 2.72% H-6 => L+1
27	10872	920	0.00	79.7% H-11 => LUMO, 9.11% H-9 => L+1, 2.10% H-13 => L+1, 2.01% H-6 => L+2
28	10980	911	0.00	50.3% H-5 => L+2, 28.4% H-7 => L+1, 9.01% H-3 => L+3, 2.97% H-2 => L+4, 2.28% H-3 => L+1
29	11189	894	0.00	58.9% H-12 => LUMO, 16.9% H-10 => L+1, 7.69% H-8 => L+2, 4.53% H-7 => L+3, 2.58% HOMO => L+5, 2.32% H-5 => L+4
30	11210	892	0.00	71.0% H-2 => L+3, 11.3% H-3 => L+2, 3.58% H-10 => LUMO, 2.98% H-2 => L+1, 2.79% H-8 => L+1, 2.31% H-5 => L+3

31	11229	891	0.00	35.2% H-8 => L+1, 31.4% H-10 => LUMO, 10.8% H-7 => L+2, 6.57% H-2 => L+3, 3.90% H-3 => L+4, 3.74% H-5 => L+3
32	11251	889	0.00	90.9% HOMO => L+5, 2.16% H-1 => L+6
33	11704	854	0.00	88.8% HOMO => L+6, 6.13% H-1 => L+5
34	11772	849	0.00	43.8% HOMO => L+7, 13.4% H-1 => L+4, 9.61% H-4 => L+3, 8.70% H-9 => L+1, 7.91% H-6 => L+2, 4.59% H-11 => LUMO, 2.16% H-15 => LUMO
35	11869	843	0.05	73.1% H-13 => LUMO, 9.16% H-11 => L+1, 2.86% H-9 => L+2, 2.69% H-16 => LUMO, 2.33% H-15 => L+1
36	11873	842	0.00	57.2% H-9 => L+1, 19.8% HOMO => L+7, 9.04% H-11 => LUMO, 5.16% H-6 => L+2, 3.82% H-1 => L+4, 2.21% H-6 => LUMO
37	11962	836	0.00	60.6% H-3 => L+3, 20.4% H-5 => L+2, 9.40% H-2 => L+4, 2.10% H-2 => L+2
38	12120	825	0.00	40.0% H-7 => L+2, 35.2% H-8 => L+1, 10.9% H-5 => L+3, 4.04% H-3 => L+4
39	12241	817	0.00	38.6% H-6 => L+2, 18.9% HOMO => L+7, 15.6% H-9 => L+1, 15.4% H-4 => L+3, 3.70% H-1 => L+4
40	12357	809	0.00	62.8% H-14 => LUMO, 15.2% H-12 => L+1, 6.63% H-10 => L+2, 3.88% H-8 => L+3, 2.11% H-7 => L+4
41	12362	809	0.00	79.8% HOMO => L+8, 6.01% H-1 => L+6, 3.63% H-12 => LUMO
42	12435	804	0.00	59.6% H-15 => LUMO, 14.2% H-6 => L+2, 5.93% H-13 => L+1, 4.59% H-16 => L+1, 2.51% H-1 => L+4, 2.16% HOMO => L+7, 2.00% H-9 => L+3
43	12442	804	0.00	33.2% H-10 => L+1, 30.7% H-12 => LUMO, 11.0% H-8 => L+2, 7.30% HOMO => L+8, 5.45% H-7 => L+3, 3.01% H-5 => L+4
44	12464	802	0.00	29.2% H-1 => L+4, 21.5% H-6 => L+2, 18.2% H-4 => L+3, 12.1% H-15 => LUMO, 8.59% HOMO => L+7
45	12523	799	0.01	82.9% H-16 => LUMO, 7.88% H-15 => L+1
46	12619	792	0.00	48.7% H-4 => L+3, 40.5% H-1 => L+4, 3.20% H-6 => L+2
47	12972	771	0.00	46.7% H-5 => L+3, 31.0% H-7 => L+2, 10.8% H-3 => L+4, 3.65% H-2 => L+7
48	13116	762	0.00	74.2% H-2 => L+4, 13.4% H-3 => L+3, 3.26% H-2 => L+2, 2.24% H-3 => L+7
49	13165	760	0.00	81.9% HOMO => L+9, 8.16% H-1 => L+8
50	13216	757	0.12	32.5% H-11 => L+1, 16.9% H-13 => LUMO, 11.5% HOMO => L+10, 10.5% H-9 => L+2, 5.38% H-6 => L+3, 4.73% H-4 => L+4, 4.31% H-1 => L+7, 2.01% H-19 => LUMO
51	13319	751	0.00	25.1% H-10 => L+1, 20.5% H-17 => LUMO, 19.9% H-8 => L+2, 7.46% H-7 => L+3, 5.90% H-12 => L+2, 4.97% H-14 => L+1, 3.20% H-5 => L+4, 2.20% H-3 => L+7

52	13323	751	0.00	43.9% H-17 => LUMO, 13.9% H-10 => L+1, 10.8% H-8 => L+2, 8.28% H-14 => L+1, 4.00% H-7 => L+3, 3.28% H-10 => L+3
53	13325	750	7.28	63.8% H-2 => L+5, 12.1% H-3 => L+6, 4.49% H-6 => L+3, 3.26% H-5 => L+8, 2.99% H-2 => L+8, 2.88% HOMO => L+10
54	13390	747	0.54	36.3% HOMO => L+10, 33.7% H-11 => L+1, 11.5% H-1 => L+7, 5.04% H-2 => L+5, 4.69% H-4 => L+4
55	13394	747	0.00	85.4% H-1 => L+5, 5.29% HOMO => L+6, 4.00% H-4 => L+6, 2.36% HOMO => L+9
56	13574	737	0.00	32.9% H-12 => L+1, 30.7% H-14 => LUMO, 12.0% H-10 => L+2, 6.41% H-8 => L+3, 4.04% H-7 => L+4, 2.11% H-5 => L+7
57	13832	723	0.00	70.1% H-1 => L+6, 7.75% H-4 => L+5, 7.25% HOMO => L+8, 5.05% HOMO => L+11, 3.72% H-1 => L+9, 2.71% HOMO => L+5
58	13840	723	0.02	45.2% H-9 => L+2, 19.1% HOMO => L+10, 14.5% H-11 => L+1, 11.9% H-6 => L+3, 2.58% H-4 => L+4
59	13874	721	0.00	55.9% H-3 => L+4, 24.4% H-5 => L+3, 9.92% H-2 => L+7, 2.04% H-2 => L+3
60	14028	713	0.00	74.1% HOMO => L+11, 6.56% H-1 => L+6, 5.38% H-1 => L+9, 2.93% H-4 => L+8
61	14046	712	0.00	44.0% H-2 => L+6, 38.4% H-3 => L+5, 4.93% H-5 => L+6, 2.39% H-3 => L+8, 2.13% H-2 => L+9
62	14089	710	0.00	39.8% H-8 => L+2, 33.7% H-7 => L+3, 9.83% H-5 => L+4, 4.40% H-3 => L+7, 2.22% HOMO => L+11, 2.04% H-2 => L+10
63	14151	707	0.03	26.0% H-9 => L+2, 21.7% H-4 => L+4, 20.7% HOMO => L+10, 17.3% H-1 => L+7, 7.76% H-6 => L+3
64	14225	703	0.27	83.8% H-18 => LUMO, 4.66% H-17 => L+1, 3.62% HOMO => L+18, 2.08% H-12 => L+1
65	14359	696	0.00	41.3% H-13 => L+1, 17.0% H-15 => LUMO, 8.73% H-20 => LUMO, 7.03% H-11 => L+2, 3.39% HOMO => L+13, 3.33% H-9 => L+3, 2.70% H-19 => L+1, 2.58% H-11 => LUMO, 2.02% H-6 => L+4
66	14389	695	0.01	42.3% H-1 => L+7, 39.5% H-6 => L+3, 6.09% H-9 => L+2, 3.36% HOMO => L+10, 2.55% H-2 => L+5
67	14455	692	0.01	40.8% H-1 => L+8, 14.2% H-12 => L+1, 8.99% H-10 => L+2, 7.27% HOMO => L+9, 4.73% H-4 => L+6, 4.29% H-8 => L+3, 2.68% HOMO => L+12, 2.38% H-1 => L+11, 2.26% H-7 => L+4
68	14481	691	0.00	26.9% H-17 => LUMO, 22.9% H-14 => L+1, 9.91% H-12 => L+2, 8.32% H-18 => L+1, 5.91% H-10 => L+3, 5.24% H-24 => LUMO, 4.86% H-8 => L+4, 2.89% H-7 => L+7, 2.11% H-5 => L+10
69	14526	688	0.04	55.5% H-4 => L+4, 21.4% H-6 => L+3, 14.8% H-1 => L+7
70	14529	688	0.01	29.1% H-1 => L+8, 26.0% H-12 => L+1, 14.4% H-10 => L+2, 6.71% H-8 => L+3, 3.83% H-7 => L+4,

				3.07% H-4 => L+6, 2.51% H-5 => L+7, 2.18% HOMO => L+9
71	14668	682	0.00	30.4% H-13 => L+1, 22.0% HOMO => L+13, 21.0% H-20 => LUMO, 7.94% H-1 => L+10, 4.22% H-4 => L+7, 3.60% H-16 => L+1, 2.37% H-19 => L+1
72	14799	676	0.24	58.3% H-19 => LUMO, 6.58% H-20 => L+1, 4.77% H-2 => L+8, 4.22% H-3 => L+6, 2.95% H-15 => L+1, 2.75% H-22 => LUMO, 2.58% H-5 => L+5, 2.09% H-4 => L+4
73	14825	675	0.00	70.5% HOMO => L+12, 5.72% H-1 => L+11, 3.55% H-1 => L+8, 3.54% H-2 => L+7, 3.28% H-31 => LUMO, 2.70% H-4 => L+9, 2.07% H-12 => L+1
74	14848	673	0.00	41.0% H-5 => L+4, 33.7% H-7 => L+3, 11.1% H-3 => L+7, 4.30% H-2 => L+10
75	14963	668	0.82	28.8% H-2 => L+8, 26.7% H-3 => L+6, 14.1% H-5 => L+5, 6.93% H-15 => L+1, 4.46% H-22 => LUMO, 4.28% H-19 => LUMO
76	14970	668	0.00	69.4% H-2 => L+7, 14.6% H-3 => L+4, 4.14% HOMO => L+12, 3.33% H-2 => L+3, 3.05% H-3 => L+10
77	15018	666	0.00	43.7% H-20 => LUMO, 12.3% HOMO => L+13, 10.7% H-21 => LUMO, 4.47% H-16 => L+1, 4.19% H-19 => L+1, 3.35% H-11 => L+2, 2.40% H-1 => L+10, 2.09% H-9 => L+3
78	15170	659	0.02	61.0% H-15 => L+1, 12.6% H-19 => LUMO, 6.72% H-16 => LUMO, 4.56% H-13 => L+2, 2.10% H-2 => L+8
79	15220	657	0.00	41.6% H-1 => L+9, 9.48% HOMO => L+11, 9.23% HOMO => L+14, 7.48% H-4 => L+8, 5.46% H-14 => L+1, 4.70% H-1 => L+12, 3.94% H-4 => L+5, 2.46% H-24 => LUMO
80	15229	657	0.00	51.7% H-21 => LUMO, 13.6% H-11 => L+2, 7.71% H-13 => L+1, 4.22% H-9 => L+3, 3.34% H-20 => LUMO, 2.20% H-16 => L+1, 2.17% HOMO => L+13
81	15262	655	0.00	49.8% H-10 => L+2, 20.2% H-8 => L+3, 10.1% H-7 => L+4, 5.14% H-5 => L+7, 3.18% H-3 => L+10
82	15269	655	0.00	30.0% H-11 => L+2, 24.1% HOMO => L+13, 19.8% H-21 => LUMO, 4.05% H-9 => L+3, 3.99% H-13 => L+1, 3.79% H-20 => LUMO, 2.74% H-1 => L+10, 2.41% H-25 => LUMO
83	15323	653	0.00	43.0% H-4 => L+5, 10.7% H-14 => L+1, 9.16% HOMO => L+14, 6.17% H-24 => LUMO, 5.94% H-1 => L+6, 4.36% H-1 => L+9, 2.43% H-17 => L+2
84	15337	652	0.03	72.0% H-22 => LUMO, 4.88% H-23 => LUMO, 2.86% H-19 => LUMO, 2.44% H-25 => L+1
85	15385	650	0.00	32.8% H-4 => L+5, 18.7% H-1 => L+9, 13.2% H-14 => L+1, 7.51% H-24 => LUMO, 4.02% H-6 => L+6, 2.63% H-1 => L+6, 2.22% HOMO => L+14, 2.13% H-17 => L+2

86	15451	647	0.00	71.8% H-16 => L+1, 8.55% H-11 => L+2, 6.66% HOMO => L+13, 2.54% H-15 => LUMO, 2.51% H-15 => L+2
87	15500	645	0.00	44.1% H-3 => L+5, 43.3% H-2 => L+6, 4.58% H-5 => L+6, 3.62% H-3 => L+8
88	15530	644	0.00	40.9% HOMO => L+14, 12.6% H-14 => L+1, 10.3% H-29 => LUMO, 6.04% H-24 => LUMO, 4.45% HOMO => L+17, 3.99% H-1 => L+9, 3.15% H-1 => L+12, 2.96% H-5 => L+4
89	15636	640	0.02	28.4% HOMO => L+15, 24.3% H-17 => L+1, 13.8% H-27 => LUMO, 5.21% H-1 => L+14, 3.86% H-18 => L+2, 3.20% H-8 => L+3, 2.40% H-18 => LUMO, 2.13% H-14 => L+2
90	15680	638	0.03	67.4% H-23 => LUMO, 5.74% H-21 => L+1, 5.45% H-22 => LUMO, 3.96% H-26 => L+1, 3.51% HOMO => L+16
91	15688	637	0.00	39.4% H-25 => LUMO, 11.2% H-3 => L+8, 7.37% H-9 => L+3, 7.34% H-2 => L+9, 4.78% H-5 => L+6, 3.24% H-22 => L+1, 2.87% H-26 => LUMO, 2.60% H-6 => L+4, 2.18% H-21 => LUMO, 2.01% H-30 => LUMO
92	15721	636	0.00	21.6% H-11 => L+2, 14.0% HOMO => L+13, 12.3% H-9 => L+3, 12.3% H-4 => L+7, 11.8% H-6 => L+4, 6.23% H-25 => LUMO, 6.03% H-1 => L+10, 2.20% H-16 => L+1, 2.03% H-2 => L+9
93	15725	636	0.00	48.4% H-3 => L+7, 25.7% H-5 => L+4, 9.61% H-2 => L+10, 2.86% HOMO => L+14
94	15760	635	0.00	67.1% H-4 => L+6, 11.0% H-1 => L+8, 8.32% H-6 => L+5, 3.68% H-1 => L+5, 2.34% H-4 => L+9
95	15812	632	0.00	24.0% H-12 => L+2, 23.9% H-24 => LUMO, 13.0% H-14 => L+1, 8.56% HOMO => L+17, 7.38% H-10 => L+3, 3.68% H-8 => L+4, 3.22% H-18 => L+1
96	15912	628	0.02	25.6% H-17 => L+1, 20.0% H-8 => L+3, 17.2% H-27 => LUMO, 5.54% HOMO => L+18, 4.67% H-18 => LUMO, 3.99% H-7 => L+4, 3.19% H-5 => L+7, 3.11% H-14 => L+2, 2.33% H-24 => L+1, 2.10% H-3 => L+10
97	15930	628	0.52	47.9% H-2 => L+8, 18.8% H-3 => L+6, 14.6% H-2 => L+5, 9.19% H-5 => L+5, 3.91% H-3 => L+9
98	15960	627	0.00	23.6% H-1 => L+10, 20.9% H-9 => L+3, 17.9% H-26 => LUMO, 8.15% H-25 => LUMO, 6.34% HOMO => L+13, 6.12% H-4 => L+7, 2.42% H-11 => L+2
99	15995	625	0.00	32.8% H-26 => LUMO, 18.5% H-9 => L+3, 9.54% H-25 => LUMO, 7.84% H-1 => L+10, 4.60% H-3 => L+8, 3.93% H-2 => L+9, 2.94% H-23 => L+1, 2.10% H-5 => L+6, 2.02% H-4 => L+7
100	16022	624	0.01	25.5% H-8 => L+3, 17.8% H-7 => L+4, 8.15% H-17 => L+1, 7.34% H-27 => LUMO, 7.31% H-5 => L+7, 6.85% H-1 => L+11, 3.61% HOMO => L+18, 2.97%

				H-3 => L+10, 2.57% HOMO => L+12, 2.20% HOMO => L+15
101	16032	624	0.00	46.6% HOMO => L+16, 9.09% H-1 => L+13, 6.43% H-15 => L+1, 5.75% H-13 => L+2, 4.97% H-4 => L+10, 3.78% H-6 => L+7, 3.78% H-11 => L+3, 3.34% H-9 => L+4
102	16112	621	0.00	50.2% H-1 => L+11, 8.51% HOMO => L+12, 7.00% H-4 => L+9, 4.88% H-27 => LUMO, 3.56% H-7 => L+4, 3.18% H-6 => L+8, 2.30% HOMO => L+15, 2.29% H-8 => L+3
103	16142	620	0.00	21.0% H-26 => LUMO, 20.7% H-3 => L+8, 12.3% H-25 => LUMO, 11.8% H-2 => L+9, 8.36% H-5 => L+6, 3.67% H-1 => L+10, 3.37% H-30 => LUMO, 2.29% H-7 => L+5, 2.23% H-23 => L+1
104	16156	619	0.01	71.5% H-28 => LUMO, 6.89% H-32 => LUMO, 5.35% H-25 => L+1, 2.70% HOMO => L+16
105	16202	617	0.00	42.5% H-6 => L+4, 26.3% H-1 => L+10, 15.1% H-9 => L+3, 4.55% H-4 => L+7
106	16274	614	0.00	35.7% H-18 => L+1, 34.6% H-24 => LUMO, 11.7% HOMO => L+17, 3.78% H-17 => LUMO, 3.52% H-17 => L+2
107	16351	612	0.00	52.6% H-4 => L+7, 20.0% H-6 => L+4, 10.1% H-1 => L+10, 3.93% H-30 => LUMO, 2.01% H-25 => LUMO
108	16367	611	0.17	56.1% H-5 => L+5, 18.8% H-3 => L+6, 7.17% H-2 => L+5, 4.35% H-7 => L+6, 2.29% H-28 => LUMO
109	16374	611	0.00	55.8% H-4 => L+8, 13.6% H-1 => L+9, 7.10% H-6 => L+6, 3.04% H-33 => LUMO, 3.02% H-1 => L+6, 2.78% H-35 => LUMO, 2.70% H-9 => L+5
110	16417	609	0.00	49.0% H-12 => L+2, 10.5% H-10 => L+3, 8.07% H-8 => L+4, 5.77% H-7 => L+7, 4.09% H-5 => L+10, 3.36% HOMO => L+14, 3.12% H-3 => L+13, 2.75% H-2 => L+16, 2.28% H-29 => LUMO
111	16453	608	0.04	45.0% H-13 => L+2, 18.9% HOMO => L+16, 6.64% H-11 => L+3, 5.31% H-32 => LUMO, 3.74% H-23 => LUMO, 3.65% H-15 => L+1, 2.45% H-9 => L+4, 2.12% H-5 => L+5, 2.01% H-16 => L+2
112	16526	605	0.00	63.8% H-30 => LUMO, 5.92% H-6 => L+4, 5.70% H-32 => L+1, 5.65% H-28 => L+1, 4.54% H-4 => L+7
113	16545	604	0.61	66.9% H-32 => LUMO, 10.3% H-30 => L+1, 5.86% H-13 => L+2, 3.75% H-28 => LUMO, 2.65% H-3 => L+6, 2.60% H-28 => L+2
114	16617	602	0.00	44.9% H-29 => LUMO, 17.8% HOMO => L+14, 6.89% H-1 => L+12, 5.39% H-18 => L+1, 2.90% H-31 => L+1, 2.45% H-33 => LUMO, 2.30% H-10 => L+3
115	16634	601	0.00	53.8% H-2 => L+9, 16.1% H-5 => L+6, 7.11% H-7 => L+5, 4.94% H-30 => LUMO, 3.41% H-2 => L+6, 3.32% H-3 => L+11, 2.81% H-3 => L+5, 2.70% H-3 => L+8

116	16641	601	0.08	33.3% HOMO => L+15, 22.5% H-27 => LUMO, 17.0% H-17 => L+1, 8.39% H-31 => LUMO, 2.82% HOMO => L+18, 2.01% H-29 => L+1
117	16687	599	0.00	43.5% H-7 => L+4, 29.0% H-5 => L+7, 10.5% H-3 => L+10, 5.00% H-2 => L+13
118	16707	599	0.00	68.3% H-2 => L+10, 17.8% H-3 => L+7, 3.78% H-2 => L+4, 3.51% H-3 => L+13
119	16736	598	0.00	22.6% H-31 => LUMO, 15.9% H-27 => LUMO, 13.8% HOMO => L+18, 11.9% HOMO => L+15, 8.67% H-14 => L+2, 4.86% H-34 => LUMO, 2.83% H-12 => L+3
120	16783	596	0.01	25.1% H-34 => LUMO, 14.3% H-31 => LUMO, 11.5% HOMO => L+18, 9.79% H-14 => L+2, 6.84% H-17 => L+1, 5.14% H-6 => L+5, 3.21% H-12 => L+3, 2.24% H-4 => L+9
121	16806	595	0.00	50.9% H-33 => LUMO, 17.7% H-1 => L+12, 12.9% H-29 => LUMO, 2.17% H-4 => L+8, 2.07% HOMO => L+11
122	16862	593	0.00	33.3% H-3 => L+8, 20.1% H-5 => L+6, 16.3% H-19 => L+1, 4.35% H-2 => L+9, 4.32% H-7 => L+5, 4.14% H-2 => L+6, 3.51% H-20 => LUMO, 3.10% H-5 => L+9, 2.83% H-20 => L+2, 2.76% H-3 => L+5
123	16884	592	0.01	59.0% H-20 => L+1, 12.2% H-19 => LUMO, 10.1% H-19 => L+2
124	16886	592	0.00	45.8% H-19 => L+1, 11.0% H-5 => L+6, 8.93% H-20 => LUMO, 8.24% H-3 => L+8, 7.58% H-20 => L+2
125	16928	591	0.00	28.2% H-31 => LUMO, 22.3% H-34 => LUMO, 11.1% H-6 => L+5, 7.18% H-37 => LUMO, 4.16% H-36 => LUMO, 3.03% H-1 => L+11, 2.52% H-33 => L+1, 2.15% H-1 => L+14
126	16954	590	0.00	82.8% H-35 => LUMO, 3.03% H-6 => L+6, 2.80% H-1 => L+9, 2.23% H-34 => L+1
127	17024	587	0.27	38.5% H-3 => L+9, 20.7% H-2 => L+11, 17.6% H-5 => L+8, 4.42% H-23 => LUMO, 3.07% H-22 => LUMO, 2.59% H-7 => L+6
128	17043	587	0.00	21.8% HOMO => L+17, 20.4% H-18 => L+1, 14.4% H-10 => L+3, 5.60% H-1 => L+12, 5.28% H-33 => LUMO, 4.27% H-2 => L+16, 3.20% H-3 => L+13, 3.00% H-5 => L+10, 2.39% H-12 => L+4, 2.39% H-7 => L+7
129	17051	586	0.00	19.4% H-13 => L+2, 15.5% HOMO => L+16, 13.4% H-11 => L+3, 9.81% H-9 => L+4, 8.57% H-6 => L+7, 7.96% H-4 => L+10, 6.93% H-1 => L+13, 3.77% H-20 => L+1
130	17126	584	0.00	20.3% H-1 => L+12, 19.3% H-10 => L+3, 12.0% H-36 => LUMO, 7.97% H-33 => LUMO, 6.97% H-37 => LUMO, 4.41% H-29 => LUMO, 4.08% H-4 => L+11, 3.09% H-8 => L+4, 2.61% H-7 => L+7

131	17134	584	0.00	23.7% H-4 => L+9, 17.0% H-37 => LUMO, 11.4% H-1 => L+11, 10.1% H-6 => L+5, 9.87% H-36 => LUMO, 4.41% H-4 => L+6, 3.33% H-9 => L+6, 3.03% H-1 => L+8, 2.85% H-34 => LUMO, 2.69% H-36 => L+1, 2.64% H-6 => L+8
132	17157	583	0.00	27.1% H-10 => L+3, 25.8% HOMO => L+17, 12.1% H-18 => L+1, 5.36% H-29 => LUMO, 4.89% H-36 => LUMO, 3.33% H-8 => L+4, 2.84% H-37 => LUMO, 2.67% H-1 => L+12, 2.13% H-7 => L+7
133	17232	580	0.00	67.5% H-15 => L+2, 4.57% H-13 => L+3, 3.69% H-26 => LUMO, 3.20% H-16 => L+3, 2.18% H-22 => L+1, 2.12% H-13 => L+1
134	17249	580	0.00	50.0% H-6 => L+5, 30.1% H-34 => LUMO, 4.05% H-1 => L+11, 3.59% H-4 => L+6
135	17319	577	0.00	32.3% H-36 => LUMO, 18.7% H-37 => LUMO, 12.4% H-33 => LUMO, 10.1% H-1 => L+12, 7.30% H-4 => L+8, 4.00% H-37 => L+1, 2.84% H-29 => LUMO, 2.32% H-36 => L+1
136	17330	577	0.07	61.6% H-16 => L+2, 4.75% H-1 => L+13, 4.09% H-15 => L+3, 3.30% H-5 => L+8
137	17372	576	0.36	32.8% H-2 => L+11, 25.0% H-5 => L+8, 11.1% H-7 => L+6, 7.55% H-16 => L+2, 4.62% H-8 => L+5, 3.76% H-3 => L+6
138	17381	575	0.16	28.3% H-14 => L+2, 12.2% H-37 => LUMO, 11.2% H-4 => L+9, 9.25% HOMO => L+18, 7.06% H-36 => LUMO, 6.54% H-1 => L+14, 2.36% H-4 => L+12, 2.16% HOMO => L+15
139	17395	575	0.19	25.9% H-14 => L+2, 15.5% HOMO => L+18, 12.8% H-37 => LUMO, 10.4% H-4 => L+9, 7.45% H-36 => LUMO, 4.15% H-5 => L+7, 2.79% H-3 => L+10, 2.77% H-31 => LUMO
140	17426	574	0.06	46.0% H-11 => L+3, 21.0% H-1 => L+13, 5.84% H-4 => L+10, 4.34% HOMO => L+16, 3.90% H-5 => L+8, 3.68% H-16 => L+2
141	17450	573	0.00	31.7% H-3 => L+10, 30.2% H-5 => L+7, 10.1% H-2 => L+13, 4.06% H-4 => L+9, 3.75% H-37 => LUMO, 2.17% H-36 => LUMO, 2.09% H-3 => L+4, 2.09% H-6 => L+5
142	17480	572	0.00	69.6% H-7 => L+5, 15.3% H-5 => L+6, 4.71% H-3 => L+5, 4.32% H-8 => L+6
143	17609	568	0.00	61.0% H-6 => L+6, 10.1% H-4 => L+8, 8.28% H-9 => L+5, 4.03% H-33 => LUMO, 3.65% H-35 => LUMO, 3.13% H-4 => L+5, 2.03% H-1 => L+12
144	17611	568	0.17	38.6% H-3 => L+9, 24.3% H-2 => L+11, 9.09% H-5 => L+8, 7.21% H-2 => L+8, 4.01% H-9 => L+4, 2.43% H-1 => L+13, 2.24% H-3 => L+12, 2.04% H-21 => L+1
145	17722	564	0.07	40.9% H-1 => L+14, 8.14% H-4 => L+9, 6.10% HOMO => L+15, 5.87% H-4 => L+12, 4.50% H-14 => L+2, 4.06% H-31 => LUMO, 3.86% H-6 => L+11, 3.43% H-18 => L+2, 3.27% H-24 => L+1,

				2.91% H-27 => LUMO, 2.74% H-3 => L+10, 2.10% H-1 => L+17
146	17722	564	0.00	60.5% H-8 => L+4, 6.43% H-5 => L+10, 6.04% H-3 => L+13, 5.66% H-2 => L+16, 5.20% H-7 => L+7, 3.52% HOMO => L+17, 2.91% H-10 => L+7, 2.42% H-7 => L+3
147	17754	563	0.00	29.8% H-1 => L+13, 22.0% H-9 => L+4, 11.6% H-11 => L+3, 9.79% H-6 => L+7, 9.39% H-21 => L+1, 2.69% H-3 => L+9, 2.21% H-7 => L+6
148	17777	563	0.01	61.5% H-21 => L+1, 6.80% H-23 => LUMO, 3.88% H-6 => L+7, 3.02% H-5 => L+8, 2.85% H-2 => L+11, 2.75% H-11 => L+3, 2.71% H-9 => L+4, 2.59% H-23 => L+2
149	17796	562	0.00	18.5% H-23 => L+1, 13.8% H-3 => L+11, 11.9% H-22 => L+1, 7.91% H-2 => L+12, 7.09% H-5 => L+9, 6.36% H-26 => LUMO, 4.47% H-21 => LUMO, 4.06% H-13 => L+3, 2.16% H-15 => L+2
150	17860	560	0.00	25.5% H-22 => L+1, 10.1% H-15 => L+2, 9.09% H-1 => L+16, 4.96% H-2 => L+18, 4.24% H-4 => L+13, 3.85% H-11 => L+4, 3.77% H-9 => L+7, 3.76% H-6 => L+10, 3.39% H-3 => L+17, 3.36% H-26 => LUMO, 3.05% H-3 => L+11, 2.90% H-5 => L+9, 2.87% H-13 => L+3, 2.23% H-19 => L+1, 2.20% H-25 => LUMO
151	17914	558	0.03	42.9% H-7 => L+6, 10.7% H-5 => L+8, 7.29% H-8 => L+5, 6.03% H-9 => L+4, 5.29% H-6 => L+7, 4.63% H-5 => L+5, 4.23% H-4 => L+10, 3.58% H-1 => L+13, 2.53% H-2 => L+11, 2.08% H-3 => L+6
152	17919	558	0.00	45.2% H-17 => L+2, 13.1% H-1 => L+15, 8.82% HOMO => L+17, 5.54% H-18 => L+1, 4.02% H-14 => L+3, 2.95% H-4 => L+14, 2.93% H-7 => L+7
153	17943	557	0.00	34.5% H-22 => L+1, 18.7% H-2 => L+12, 16.7% H-3 => L+11, 3.92% H-13 => L+3, 2.57% H-25 => LUMO, 2.44% H-5 => L+9
154	18010	555	0.00	33.7% H-4 => L+10, 29.4% H-9 => L+4, 8.86% H-7 => L+6, 7.60% H-5 => L+8, 7.37% H-1 => L+13, 2.49% H-6 => L+7
155	18043	554	0.44	53.2% H-12 => L+3, 15.2% H-24 => L+1, 12.8% HOMO => L+18, 3.50% H-10 => L+4, 2.75% H-14 => L+2, 2.10% H-10 => L+2
156	18054	554	0.00	44.0% H-4 => L+11, 17.3% H-1 => L+12, 8.86% H-6 => L+9, 4.50% H-17 => L+2, 4.03% H-9 => L+8, 2.83% H-4 => L+14, 2.49% H-1 => L+15
157	18124	552	0.03	54.6% H-24 => L+1, 8.36% H-12 => L+3, 6.68% H-1 => L+17, 6.58% H-1 => L+14, 4.10% HOMO => L+18, 3.84% H-18 => L+2, 2.12% H-29 => L+1
158	18151	551	0.00	52.6% H-6 => L+7, 28.9% H-4 => L+10, 8.00% H-9 => L+4
159	18169	550	0.00	21.9% H-2 => L+12, 17.3% H-5 => L+9, 15.1% H-7 => L+8, 9.52% H-23 => L+1, 8.62% H-22 => L+1, 5.73% H-8 => L+6, 2.30% H-10 => L+5

160	18207	549	0.00	43.4% H-6 => L+8, 13.9% H-4 => L+9, 12.5% H-2 => L+13, 7.66% H-9 => L+6, 4.56% H-3 => L+10, 3.49% H-11 => L+5, 2.14% H-4 => L+6
161	18301	546	0.01	43.6% H-2 => L+13, 21.2% H-3 => L+10, 14.5% H-6 => L+8, 4.42% H-3 => L+16, 3.59% H-2 => L+7, 2.59% H-4 => L+9
162	18306	546	0.00	30.1% H-23 => L+1, 16.1% H-5 => L+9, 14.4% H-1 => L+16, 7.63% H-3 => L+11, 3.79% H-4 => L+13, 2.70% H-2 => L+12, 2.23% H-2 => L+15, 2.14% H-7 => L+8, 2.06% H-2 => L+18
163	18320	546	0.00	39.1% H-7 => L+7, 10.4% H-17 => L+2, 7.55% H-27 => L+1, 7.35% H-1 => L+15, 6.01% H-2 => L+16, 5.44% H-3 => L+13, 4.18% H-4 => L+11, 2.53% H-8 => L+10, 2.51% H-5 => L+10
164	18338	545	0.02	67.8% H-25 => L+1, 6.83% H-28 => LUMO, 4.26% H-26 => L+1, 2.94% H-22 => L+2, 2.34% H-22 => LUMO, 2.08% H-28 => L+2
165	18425	543	0.00	20.5% H-7 => L+7, 19.7% H-27 => L+1, 16.7% H-1 => L+15, 8.80% H-1 => L+18, 6.76% H-17 => L+2, 5.57% H-5 => L+10, 3.35% H-3 => L+13, 3.14% H-2 => L+16, 2.32% H-24 => L+2
166	18477	541	0.00	35.9% H-3 => L+11, 23.9% H-2 => L+12, 14.5% H-5 => L+9, 6.65% H-2 => L+9, 2.90% H-13 => L+3, 2.49% H-5 => L+12, 2.15% H-23 => L+1, 2.14% H-3 => L+14, 2.02% H-7 => L+8
167	18504	540	0.00	50.0% H-26 => L+1, 5.76% H-16 => L+2, 4.97% H-21 => L+1, 4.49% H-15 => L+3, 3.79% H-25 => L+1, 3.14% H-23 => LUMO, 2.45% H-13 => L+4, 2.41% H-23 => L+2, 2.21% H-3 => L+18, 2.04% H-20 => L+1, 2.02% H-19 => L+2
168	18522	540	0.00	83.8% H-38 => LUMO, 6.53% H-39 => L+1
169	18529	540	0.01	21.2% H-10 => L+4, 16.1% H-12 => L+3, 15.0% H-18 => L+2, 13.7% H-1 => L+17, 7.52% H-8 => L+7, 4.71% H-24 => L+1, 3.07% H-7 => L+10, 2.34% HOMO => L+18, 2.31% H-4 => L+15
170	18565	539	0.00	34.6% H-13 => L+3, 23.0% H-1 => L+16, 6.57% H-23 => L+1, 3.98% H-5 => L+9, 3.63% H-11 => L+4, 2.73% H-28 => L+1, 2.54% H-4 => L+13, 2.51% H-2 => L+12, 2.38% H-3 => L+11, 2.16% H-15 => L+2
171	18594	538	0.03	44.0% H-18 => L+2, 12.0% H-1 => L+14, 6.62% H-24 => L+1, 5.97% H-10 => L+4, 5.40% H-4 => L+12, 3.41% HOMO => L+18, 2.28% H-17 => L+3, 2.17% H-12 => L+3, 2.07% H-6 => L+11
172	18610	537	0.01	26.4% H-2 => L+14, 19.9% H-3 => L+12, 9.22% H-8 => L+5, 8.23% H-20 => L+1, 5.73% H-19 => L+2, 5.03% H-5 => L+11, 2.54% H-7 => L+6
173	18626	537	0.00	46.4% H-27 => L+1, 11.8% H-1 => L+18, 10.2% H-1 => L+15, 7.26% H-4 => L+11, 5.59% H-31 => L+1, 3.83% H-17 => L+2, 2.43% H-24 => L+2

174	18641	536	0.00	24.0% H-28 => L+1, 19.4% H-7 => L+8, 14.4% H-13 => L+3, 9.30% H-5 => L+9, 2.72% H-30 => LUMO, 2.11% H-23 => L+1
175	18661	536	0.00	75.7% H-39 => LUMO, 9.03% H-38 => L+1, 4.25% H-40 => L+1
176	18666	536	0.00	35.5% H-28 => L+1, 22.6% H-7 => L+8, 11.7% H-5 => L+9, 4.39% H-8 => L+6, 3.76% H-30 => LUMO, 2.27% H-25 => L+2
177	18714	534	0.00	59.2% H-8 => L+5, 9.54% H-7 => L+6, 5.55% H-3 => L+12, 4.51% H-10 => L+6, 2.89% H-5 => L+11, 2.47% H-5 => L+5
178	18758	533	0.00	56.6% H-9 => L+5, 10.1% H-6 => L+6, 5.86% H-5 => L+10, 4.22% H-11 => L+6, 3.92% H-1 => L+18
179	18802	532	0.00	24.6% H-1 => L+18, 13.4% H-9 => L+5, 13.3% H-14 => L+3, 10.1% H-5 => L+10, 6.19% H-17 => L+2, 3.85% H-12 => L+4, 3.41% H-4 => L+17, 2.61% HOMO => L+17, 2.05% H-4 => L+11
180	18826	531	0.00	24.8% H-20 => L+2, 10.9% H-19 => L+1, 6.75% H-28 => L+1, 5.48% H-19 => L+3, 4.88% H-40 => LUMO, 4.83% H-7 => L+8, 4.19% H-13 => L+3, 3.89% H-2 => L+15, 3.44% H-3 => L+14, 2.08% H-5 => L+12, 2.08% H-16 => L+3
181	18833	531	0.07	31.6% H-29 => L+1, 17.0% H-4 => L+12, 11.5% H-1 => L+14, 11.0% H-10 => L+4, 3.89% H-6 => L+11, 2.75% H-18 => L+2, 2.49% H-27 => LUMO
182	18890	529	0.11	18.6% H-19 => L+2, 16.0% H-2 => L+14, 9.54% H-26 => L+1, 5.98% H-20 => L+1, 5.63% H-7 => L+9, 5.10% H-30 => L+1, 4.09% H-2 => L+17, 3.58% H-8 => L+8, 3.00% H-10 => L+6, 2.96% H-25 => L+1, 2.93% H-20 => L+3, 2.59% H-3 => L+12
183	18891	529	0.14	37.3% H-29 => L+1, 16.9% H-10 => L+4, 11.4% H-33 => L+1, 9.19% H-4 => L+12, 4.62% H-1 => L+17, 2.41% H-27 => L+2, 2.14% H-18 => L+2
184	18895	529	0.00	71.0% H-40 => LUMO, 8.85% H-39 => L+1, 3.72% H-41 => L+1, 2.77% H-38 => L+2, 2.19% H-42 => LUMO
185	18948	528	0.00	24.5% H-6 => L+9, 23.1% H-31 => L+1, 14.3% H-4 => L+11, 7.00% H-34 => L+1, 5.40% H-9 => L+8, 4.89% H-5 => L+10, 3.22% H-11 => L+6
186	18981	527	0.25	56.3% H-30 => L+1, 9.51% H-32 => LUMO, 7.63% H-19 => L+2, 4.62% H-32 => L+2, 4.05% H-28 => LUMO, 3.75% H-28 => L+2, 2.06% H-15 => L+3, 2.01% H-2 => L+14
187	19025	526	0.00	34.3% H-15 => L+3, 17.0% H-19 => L+2, 5.99% H-26 => L+1, 5.38% H-30 => L+1, 4.20% H-5 => L+11, 2.93% H-13 => L+4, 2.47% H-16 => L+4, 2.17% H-20 => L+3, 2.17% H-7 => L+9, 2.07% H-16 => L+2
188	19027	526	0.00	37.9% H-32 => L+1, 8.16% H-8 => L+6, 7.88% H-1 => L+16, 5.55% H-9 => L+7, 5.47% H-20 => L+2, 5.39% H-11 => L+4, 4.55% H-30 => LUMO, 3.02%

				H-13 => L+3, 2.85% H-30 => L+2, 2.84% H-28 => L+1
189	19034	525	0.00	27.3% H-5 => L+10, 17.5% H-14 => L+3, 14.0% H-2 => L+16, 9.13% H-3 => L+13, 6.86% H-6 => L+9, 4.10% H-17 => L+2, 2.19% H-31 => L+1, 2.07% H-4 => L+11, 2.05% H-12 => L+4
190	19081	524	0.00	25.2% H-16 => L+3, 23.2% H-20 => L+2, 11.9% H-2 => L+15, 4.37% H-3 => L+14, 3.41% H-4 => L+13, 2.60% H-15 => L+4, 2.54% H-19 => L+3, 2.16% H-19 => L+1
191	19118	523	0.00	35.7% H-33 => L+1, 20.2% H-9 => L+6, 10.3% H-6 => L+8, 6.86% H-35 => L+1, 5.43% H-11 => L+5, 2.56% H-31 => LUMO, 2.24% H-31 => L+2, 2.06% H-29 => L+1
192	19119	523	0.00	38.5% H-31 => L+1, 13.3% H-6 => L+9, 11.4% H-34 => L+1, 6.37% H-5 => L+10, 3.46% H-3 => L+13, 2.99% H-27 => L+1, 2.81% H-29 => L+2, 2.69% H-4 => L+11
193	19119	523	0.00	37.3% H-32 => L+1, 11.7% H-1 => L+16, 9.39% H-11 => L+4, 7.22% H-8 => L+6, 5.04% H-13 => L+3, 4.94% H-30 => LUMO, 4.70% H-30 => L+2, 2.40% H-6 => L+10
194	19136	523	0.10	27.1% H-5 => L+11, 8.32% H-7 => L+9, 7.71% H-41 => LUMO, 7.45% H-15 => L+3, 7.36% H-26 => L+1, 6.22% H-2 => L+14, 6.16% H-3 => L+12, 5.36% H-19 => L+2, 2.73% H-8 => L+5, 2.20% H-3 => L+15
195	19144	522	0.00	47.1% H-35 => L+1, 8.38% H-8 => L+7, 7.55% H-9 => L+6, 6.82% H-10 => L+4, 6.04% H-4 => L+12, 2.49% H-1 => L+17, 2.17% H-34 => L+2
196	19154	522	0.01	65.5% H-41 => LUMO, 9.40% H-40 => L+1, 3.38% H-5 => L+11, 3.20% H-43 => LUMO, 2.88% H-39 => L+2, 2.69% H-42 => L+1
197	19164	522	0.00	37.3% H-8 => L+6, 10.2% H-7 => L+8, 8.03% H-1 => L+16, 7.45% H-16 => L+3, 5.46% H-10 => L+5, 4.62% H-13 => L+3, 3.16% H-7 => L+5, 2.46% H-20 => L+2
198	19172	522	0.00	21.6% H-1 => L+15, 20.8% H-14 => L+3, 12.2% H-1 => L+18, 12.1% H-34 => L+1, 6.28% H-4 => L+14, 4.12% H-4 => L+17, 2.65% H-5 => L+10, 2.40% H-6 => L+12
199	19175	522	0.01	17.7% H-10 => L+4, 12.5% H-35 => L+1, 10.1% H-9 => L+6, 9.63% H-8 => L+7, 8.87% H-33 => L+1, 7.85% H-4 => L+12, 5.69% H-7 => L+10, 5.50% H-1 => L+17, 3.46% H-18 => L+2, 2.93% H-6 => L+8, 2.17% H-5 => L+13, 2.07% H-11 => L+5
200	19299	518	0.00	48.3% H-34 => L+1, 8.74% H-31 => L+1, 5.89% H-37 => L+1, 4.07% H-1 => L+18, 3.92% H-1 => L+15, 3.55% H-33 => L+2, 3.41% H-36 => L+1, 3.38% H-14 => L+3, 2.09% H-9 => L+5, 2.03% H-33 => LUMO, 2.00% H-35 => L+2

201	19304	518	0.03	41.3% H-3 => L+12, 19.8% H-2 => L+14, 9.77% H-5 => L+11, 6.79% H-7 => L+9, 6.57% H-2 => L+11, 3.33% H-5 => L+14
202	19343	517	0.10	20.0% H-33 => L+1, 18.9% H-35 => L+1, 16.9% H-9 => L+6, 6.31% H-1 => L+17, 5.75% H-4 => L+12, 4.39% H-29 => L+1, 2.93% H-34 => L+2, 2.81% H-11 => L+5, 2.80% H-6 => L+8, 2.68% H-18 => L+2
203	19412	515	0.00	46.7% H-11 => L+4, 19.7% H-4 => L+13, 7.45% H-1 => L+16, 6.68% H-6 => L+10, 5.65% H-16 => L+3
204	19440	514	0.00	70.5% H-42 => LUMO, 10.9% H-41 => L+1, 4.93% H-44 => LUMO, 3.48% H-40 => L+2, 2.35% H-43 => L+1
205	19446	514	0.72	33.2% H-8 => L+7, 25.6% H-1 => L+17, 5.25% H-36 => L+1, 3.08% H-4 => L+12, 3.04% H-37 => L+1, 2.84% H-18 => L+2, 2.25% H-4 => L+18
206	19461	514	0.37	33.1% H-7 => L+9, 29.0% H-5 => L+11, 8.71% H-8 => L+8, 3.62% H-3 => L+12, 3.46% H-3 => L+9, 3.09% H-7 => L+12, 2.53% H-5 => L+8, 2.20% H-2 => L+14
207	19507	513	0.00	25.3% H-3 => L+13, 11.2% H-14 => L+3, 10.2% H-2 => L+16, 5.63% H-5 => L+16, 5.57% H-37 => L+1, 4.81% H-4 => L+14, 4.69% H-6 => L+9, 4.13% H-2 => L+10, 3.23% H-36 => L+1, 2.50% H-12 => L+4, 2.05% H-9 => L+11
208	19521	512	0.00	33.0% H-16 => L+3, 22.7% H-2 => L+15, 9.46% H-3 => L+14, 3.69% H-10 => L+8, 3.37% H-11 => L+4, 3.16% H-8 => L+6, 2.08% H-8 => L+9
209	19600	510	0.08	33.3% H-36 => L+1, 19.2% H-37 => L+1, 5.85% H-37 => LUMO, 5.42% H-33 => L+1, 5.24% H-1 => L+17, 4.28% H-37 => L+2, 3.40% H-36 => LUMO, 2.92% H-35 => L+1, 2.49% H-36 => L+2, 2.42% H-8 => L+7, 2.17% H-4 => L+12
210	19606	510	0.04	18.8% H-15 => L+3, 15.1% H-2 => L+17, 7.25% H-22 => L+2, 6.76% H-4 => L+16, 5.28% H-3 => L+15, 5.02% H-19 => L+2, 4.14% H-3 => L+18, 3.74% H-6 => L+13, 2.91% H-9 => L+10, 2.69% H-26 => L+1, 2.61% H-7 => L+9, 2.05% H-16 => L+4
211	19615	510	0.00	33.2% H-37 => L+1, 19.2% H-36 => L+1, 5.45% H-36 => LUMO, 5.19% H-3 => L+13, 4.70% H-2 => L+16, 4.36% H-34 => L+1, 4.14% H-36 => L+2, 3.16% H-37 => LUMO, 2.86% H-31 => L+1, 2.55% H-4 => L+14, 2.41% H-37 => L+2
212	19677	508	0.00	37.4% H-4 => L+13, 29.8% H-9 => L+7, 5.71% H-21 => L+2, 5.71% H-11 => L+4, 4.88% H-6 => L+10, 3.22% H-3 => L+14
213	19729	507	0.01	66.8% H-43 => LUMO, 10.8% H-42 => L+1, 7.06% H-45 => LUMO, 3.43% H-41 => L+2
214	19732	507	0.00	40.8% H-21 => L+2, 9.42% H-5 => L+12, 6.16% H-7 => L+11, 4.04% H-16 => L+3, 3.92% H-10 => L+5, 3.67% H-23 => L+1, 3.55% H-8 => L+6,

				2.70% H-8 => L+9, 2.45% H-20 => L+2, 2.40% H-2 => L+15
215	19740	507	0.06	20.9% H-7 => L+10, 18.9% H-8 => L+7, 10.3% H-5 => L+13, 9.01% H-4 => L+12, 5.61% H-3 => L+16, 5.46% H-6 => L+11, 3.04% H-9 => L+9, 2.45% H-2 => L+13, 2.35% H-10 => L+10
216	19744	506	0.00	20.5% H-2 => L+16, 19.7% H-12 => L+4, 14.4% H-14 => L+3, 13.0% H-4 => L+14, 9.04% H-3 => L+13, 4.66% H-10 => L+7, 2.49% H-1 => L+15
217	19787	505	0.12	31.8% H-8 => L+8, 23.3% H-7 => L+9, 12.5% H-22 => L+2, 8.14% H-10 => L+6, 3.16% H-8 => L+11, 3.05% H-12 => L+5, 2.44% H-5 => L+8, 2.15% H-7 => L+6
218	19798	505	0.00	19.2% H-9 => L+7, 17.5% H-3 => L+14, 15.4% H-21 => L+2, 9.60% H-5 => L+12, 6.53% H-2 => L+15, 3.73% H-2 => L+12, 3.48% H-6 => L+10, 3.07% H-10 => L+5, 2.08% H-7 => L+11
219	19801	505	0.08	20.1% H-7 => L+10, 19.7% H-6 => L+11, 13.4% H-4 => L+12, 6.85% H-17 => L+3, 5.88% H-9 => L+9, 3.94% H-8 => L+7, 3.40% H-5 => L+13, 3.10% H-11 => L+8, 2.78% H-36 => L+1
220	19843	504	0.00	40.5% H-9 => L+8, 22.4% H-6 => L+9, 9.65% H-11 => L+6, 5.40% H-13 => L+5, 2.69% H-3 => L+13, 2.64% H-6 => L+6, 2.39% H-2 => L+16
221	19887	503	0.00	54.2% H-6 => L+10, 14.9% H-9 => L+7, 8.16% H-4 => L+13, 5.47% H-21 => L+2, 4.17% H-3 => L+14
222	19950	501	0.00	48.8% H-10 => L+5, 7.96% H-5 => L+12, 7.10% H-8 => L+6, 6.95% H-2 => L+18, 5.21% H-7 => L+11, 4.69% H-12 => L+6
223	19985	500	0.01	49.4% H-22 => L+2, 18.5% H-8 => L+8, 4.29% H-15 => L+3, 2.47% H-25 => L+1, 2.25% H-2 => L+14, 2.09% H-4 => L+16
224	19986	500	0.00	62.9% H-44 => LUMO, 13.6% H-46 => LUMO, 10.1% H-43 => L+1, 3.21% H-42 => L+2, 3.11% H-47 => L+1
225	19990	500	0.01	54.2% H-17 => L+3, 7.01% H-6 => L+11, 5.60% H-4 => L+15, 4.61% H-1 => L+17, 2.97% H-14 => L+4, 2.91% H-18 => L+2, 2.38% H-18 => L+4, 2.22% H-6 => L+17, 2.00% H-14 => L+2
226	20053	499	0.01	33.7% H-12 => L+4, 31.3% H-4 => L+14, 9.47% H-24 => L+2, 7.38% H-1 => L+18
227	20096	498	0.01	22.7% H-2 => L+17, 15.2% H-13 => L+4, 11.0% H-23 => L+2, 4.97% H-8 => L+8, 4.64% H-3 => L+15, 4.14% H-15 => L+3, 3.94% H-11 => L+7, 2.47% H-9 => L+10
228	20121	497	0.00	21.2% H-3 => L+14, 19.3% H-2 => L+15, 16.6% H-10 => L+5, 5.90% H-21 => L+2, 5.45% H-2 => L+18, 5.23% H-5 => L+12, 4.24% H-7 => L+11, 2.98% H-3 => L+17, 2.49% H-2 => L+12

229	20161	496	0.00	24.2% H-2 => L+18, 18.5% H-5 => L+12, 12.1% H-3 => L+14, 3.06% H-2 => L+15, 2.89% H-25 => L+2, 2.71% H-7 => L+14, 2.55% H-3 => L+17
230	20181	496	0.00	44.0% H-24 => L+2, 10.7% H-18 => L+3, 9.91% H-12 => L+4, 6.33% H-4 => L+17, 3.03% H-27 => L+1, 2.95% H-1 => L+18, 2.93% H-9 => L+8
231	20183	495	0.01	36.6% H-11 => L+5, 17.9% H-5 => L+13, 12.7% H-7 => L+10, 9.53% H-9 => L+6, 3.86% H-13 => L+6, 3.77% H-3 => L+16, 2.08% H-3 => L+10, 2.03% H-6 => L+5
232	20208	495	0.00	46.2% H-45 => LUMO, 36.4% H-47 => LUMO, 7.04% H-44 => L+1, 2.22% H-43 => L+2
233	20249	494	0.00	25.2% H-11 => L+5, 17.1% H-7 => L+10, 15.9% H-5 => L+13, 12.1% H-3 => L+16, 6.13% H-6 => L+11, 6.02% H-9 => L+6, 2.16% H-2 => L+13
234	20264	493	0.01	15.4% H-23 => L+2, 11.9% H-5 => L+14, 8.12% H-3 => L+15, 7.41% H-3 => L+18, 7.14% HOMO => L+20, 7.01% H-7 => L+12, 5.76% H-2 => L+17, 3.72% H-8 => L+8, 3.34% H-10 => L+6, 3.27% H-8 => L+11, 2.67% H-10 => L+9, 2.35% H-26 => L+1, 2.20% H-19 => L+2, 2.11% H-21 => L+3, 2.08% H-2 => L+14
235	20305	492	0.00	23.5% H-5 => L+12, 22.0% H-7 => L+11, 9.95% H-25 => L+2, 8.75% H-8 => L+9, 3.29% HOMO => L+19, 3.17% H-10 => L+8, 2.72% H-15 => L+4, 2.50% H-16 => L+3, 2.26% H-22 => L+3
236	20336	492	0.01	28.6% H-23 => L+2, 22.6% H-3 => L+15, 9.94% H-4 => L+16, 4.71% H-2 => L+14, 3.95% H-5 => L+14, 3.45% H-3 => L+18, 2.36% H-6 => L+13
237	20415	490	0.00	59.0% H-25 => L+2, 5.77% H-28 => L+1, 5.42% H-7 => L+11, 3.43% H-22 => L+3, 3.29% H-2 => L+18, 2.92% H-26 => L+2
238	20416	490	0.00	47.4% H-10 => L+6, 9.60% H-8 => L+8, 6.92% H-12 => L+5, 5.69% HOMO => L+20, 4.30% H-2 => L+17, 3.96% H-8 => L+5, 3.69% H-12 => L+8
239	20441	489	0.00	21.4% H-24 => L+2, 13.4% H-4 => L+14, 8.97% H-18 => L+3, 7.83% H-6 => L+12, 4.94% H-10 => L+7, 4.37% H-4 => L+17, 3.92% H-9 => L+11, 3.81% H-11 => L+9, 3.49% H-6 => L+15, 3.24% H-16 => L+5, 3.11% H-12 => L+4, 2.12% H-2 => L+16
240	20444	489	0.56	31.2% H-27 => L+2, 30.2% H-4 => L+15, 6.13% H-17 => L+3, 4.30% H-6 => L+11, 2.52% H-24 => L+3, 2.43% H-29 => L+1, 2.11% H-24 => L+1
241	20471	488	0.00	26.6% H-10 => L+7, 17.2% H-18 => L+3, 10.2% H-12 => L+4, 8.54% H-4 => L+17, 6.10% H-8 => L+10, 5.75% H-24 => L+2, 3.04% H-1 => L+18, 2.56% H-4 => L+14, 2.43% H-7 => L+13, 2.02% H-2 => L+16
242	20498	488	0.00	23.6% H-26 => L+2, 15.5% H-7 => L+11, 6.46% H-3 => L+17, 4.63% HOMO => L+19, 3.62% H-2 =>

				L+15, 3.30% H-2 => L+18, 3.23% H-15 => L+4, 2.70% H-5 => L+18, 2.48% H-23 => L+1, 2.07% H-10 => L+8
243	20541	487	0.00	45.7% H-13 => L+4, 15.4% H-4 => L+16, 10.6% H-23 => L+2, 3.80% H-2 => L+17, 3.67% HOMO => L+20, 2.63% H-6 => L+13
244	20549	487	0.00	27.0% H-6 => L+11, 13.7% H-5 => L+13, 13.1% H-9 => L+9, 7.28% H-11 => L+8, 7.26% H-13 => L+6, 7.12% H-15 => L+5, 4.69% H-3 => L+16, 2.22% H-27 => L+2, 2.01% H-16 => L+6
245	20556	486	0.00	56.9% H-46 => LUMO, 9.87% H-45 => L+1, 8.92% H-47 => L+1, 8.58% H-44 => LUMO, 3.96% H-46 => L+2, 2.58% H-44 => L+2
246	20559	486	0.00	39.4% H-47 => LUMO, 22.7% H-45 => LUMO, 15.9% H-46 => L+1, 4.07% H-45 => L+2, 3.83% H-43 => LUMO, 3.32% H-44 => L+1
247	20611	485	0.00	22.3% H-11 => L+6, 14.3% H-9 => L+8, 13.0% H-18 => L+3, 12.3% H-13 => L+5, 10.7% H-10 => L+7, 2.56% H-11 => L+9, 2.27% H-16 => L+8
248	20636	485	0.00	19.3% H-18 => L+3, 12.7% H-11 => L+6, 12.3% H-9 => L+8, 6.00% H-6 => L+12, 5.50% H-10 => L+7, 4.69% H-1 => L+18, 4.43% H-13 => L+5, 4.15% H-15 => L+6, 3.79% H-4 => L+17, 3.68% H-16 => L+5, 3.35% H-13 => L+8, 2.62% H-4 => L+14, 2.18% H-9 => L+11, 2.07% H-6 => L+15
249	20636	485	0.00	20.4% H-7 => L+11, 20.3% H-8 => L+9, 12.7% H-26 => L+2, 7.71% HOMO => L+19, 6.35% H-10 => L+8, 3.31% H-2 => L+18, 3.10% H-3 => L+17, 2.84% H-2 => L+15, 2.80% H-10 => L+11
250	20646	484	0.01	31.5% H-3 => L+16, 18.5% H-5 => L+13, 7.33% H-4 => L+18, 6.72% H-9 => L+9, 4.54% H-6 => L+11, 4.12% H-2 => L+13, 3.78% H-7 => L+16, 2.85% H-11 => L+8, 2.61% H-1 => L+17, 2.61% H-27 => L+2
251	20653	484	0.28	48.4% H-28 => L+2, 5.25% H-30 => L+1, 4.74% H-11 => L+7, 3.95% H-25 => L+3, 3.84% H-32 => L+2, 2.96% H-4 => L+16, 2.74% H-3 => L+15, 2.20% H-25 => L+1
252	20711	483	0.00	25.9% HOMO => L+19, 11.5% H-8 => L+9, 7.71% H-26 => L+2, 7.06% H-19 => L+3, 4.16% H-3 => L+17, 4.14% H-5 => L+15, 3.53% H-1 => L+20, 3.06% H-15 => L+4, 2.79% H-20 => L+2
253	20712	483	0.13	30.3% H-27 => L+2, 21.2% H-4 => L+15, 8.61% H-3 => L+16, 8.00% H-17 => L+3, 6.66% H-14 => L+4, 2.17% H-12 => L+7, 2.02% H-6 => L+17
254	20743	482	0.05	25.2% H-3 => L+15, 10.6% H-2 => L+17, 7.72% H-23 => L+2, 7.60% H-28 => L+2, 7.46% H-5 => L+14, 5.37% H-5 => L+17, 4.75% H-7 => L+12, 4.04% HOMO => L+20, 3.53% H-2 => L+14, 2.72% H-8 => L+11, 2.02% H-4 => L+16

255	20856	479	0.08	24.9% H-4 => L+16, 14.2% H-20 => L+3, 6.96% HOMO => L+20, 5.75% H-3 => L+18, 4.93% H-5 => L+17, 3.95% H-7 => L+15, 3.49% H-19 => L+2, 3.40% H-10 => L+6, 2.62% H-19 => L+4, 2.30% H-7 => L+12, 2.28% H-22 => L+2, 2.27% H-23 => L+2
256	20896	479	0.23	30.8% H-14 => L+4, 17.5% H-4 => L+15, 9.82% H-4 => L+18, 8.27% H-27 => L+2, 7.85% H-3 => L+16, 4.38% H-12 => L+7, 3.11% H-17 => L+3
257	20899	478	0.00	38.6% H-29 => L+2, 15.4% H-4 => L+17, 10.3% H-10 => L+7, 5.57% H-18 => L+3, 2.55% H-31 => L+1, 2.49% H-8 => L+10, 2.26% H-27 => L+3, 2.21% H-27 => L+1, 2.02% H-1 => L+18
258	20933	478	0.00	42.5% H-19 => L+3, 10.2% H-26 => L+2, 9.38% H-20 => L+2, 7.46% H-15 => L+4, 6.66% H-20 => L+4, 3.92% HOMO => L+19, 2.86% H-3 => L+17, 2.21% H-21 => L+2
259	20937	478	0.00	27.5% HOMO => L+20, 25.7% H-5 => L+14, 14.8% H-20 => L+3, 3.81% H-19 => L+2, 2.96% H-10 => L+6, 2.62% H-1 => L+19, 2.09% H-19 => L+4, 2.08% H-4 => L+16
260	20956	477	0.00	29.6% H-29 => L+2, 19.7% H-10 => L+7, 17.6% H-8 => L+10, 6.44% H-7 => L+13, 4.01% H-4 => L+17, 3.57% H-33 => L+2, 2.47% H-5 => L+16
261	20969	477	0.00	31.7% H-8 => L+9, 17.5% H-10 => L+8, 10.8% H-3 => L+17, 6.86% H-12 => L+6, 5.19% H-15 => L+4, 3.77% H-14 => L+5, 2.97% H-2 => L+15, 2.54% H-2 => L+18, 2.39% H-7 => L+8
262	21001	476	0.02	23.2% H-20 => L+3, 22.0% H-5 => L+14, 6.56% H-3 => L+18, 5.46% H-19 => L+2, 4.05% H-2 => L+17, 3.91% H-7 => L+15, 3.71% H-11 => L+7, 3.29% H-19 => L+4, 3.14% HOMO => L+20, 3.12% H-8 => L+11, 2.34% H-3 => L+15, 2.32% H-10 => L+9, 2.22% H-23 => L+2
263	21029	476	0.01	15.6% H-9 => L+10, 15.3% H-11 => L+7, 11.0% H-32 => L+2, 9.13% H-4 => L+16, 8.67% H-13 => L+4, 5.31% H-28 => L+2, 5.31% HOMO => L+20, 5.27% H-20 => L+3, 5.15% H-6 => L+13, 3.59% H-16 => L+4
264	21044	475	0.00	18.2% H-15 => L+4, 15.0% HOMO => L+19, 13.4% H-26 => L+2, 13.1% H-19 => L+3, 9.39% H-30 => L+2, 3.65% H-20 => L+2, 2.96% H-13 => L+7, 2.77% H-3 => L+17, 2.76% H-25 => L+2
265	21068	475	0.00	38.6% H-6 => L+12, 25.5% H-16 => L+5, 7.95% H-15 => L+6, 4.44% H-13 => L+8, 2.71% H-33 => L+2, 2.42% H-9 => L+14, 2.12% H-16 => L+8
266	21093	474	0.00	54.6% H-31 => L+2, 5.82% H-14 => L+4, 5.49% H-4 => L+18, 4.54% H-9 => L+9, 3.49% H-29 => L+1, 2.97% H-34 => L+2, 2.95% H-29 => L+3, 2.17% H-15 => L+5

267	21107	474	0.01	20.3% H-8 => L+10, 14.4% H-4 => L+17, 9.42% H-6 => L+12, 7.39% H-16 => L+5, 5.77% H-33 => L+2, 5.36% H-7 => L+13, 5.14% H-29 => L+2, 4.80% H-5 => L+16, 2.90% H-15 => L+6, 2.84% H-18 => L+3, 2.15% H-6 => L+18
268	21112	474	0.00	60.1% H-30 => L+2, 7.51% H-15 => L+4, 7.21% H-32 => L+1, 4.52% H-32 => L+3, 3.98% H-28 => L+1, 3.71% H-28 => L+3, 2.66% H-26 => L+2
269	21144	473	0.01	37.8% H-32 => L+2, 12.9% H-12 => L+5, 10.4% H-11 => L+7, 6.48% H-30 => L+3, 5.80% H-28 => L+2, 5.11% H-30 => L+1, 2.43% H-20 => L+3, 2.34% H-10 => L+6
270	21155	473	0.03	41.6% H-9 => L+9, 15.1% H-15 => L+5, 8.59% H-31 => L+2, 7.29% H-13 => L+6, 5.50% H-11 => L+8, 4.89% H-16 => L+6, 2.20% H-11 => L+11, 2.10% H-6 => L+8
271	21159	473	0.00	26.0% H-16 => L+4, 25.8% H-12 => L+5, 13.5% H-32 => L+2, 6.33% H-10 => L+6, 2.33% H-30 => L+1, 2.06% H-14 => L+6, 2.05% H-22 => L+2
272	21200	472	0.00	27.0% H-10 => L+8, 24.0% H-3 => L+17, 13.7% H-2 => L+18, 7.24% H-15 => L+4, 2.77% HOMO => L+19, 2.23% H-2 => L+15
273	21204	472	0.02	25.1% H-38 => L+1, 20.7% H-12 => L+5, 16.5% H-16 => L+4, 5.46% H-11 => L+7, 3.64% H-2 => L+17, 2.50% H-39 => LUMO, 2.10% H-3 => L+15
274	21221	471	0.02	51.9% H-38 => L+1, 8.69% H-16 => L+4, 6.97% H-12 => L+5, 4.71% H-39 => LUMO, 3.92% H-11 => L+7, 3.39% H-39 => L+2, 2.63% H-40 => L+1
275	21276	470	0.00	62.3% H-33 => L+2, 4.42% H-6 => L+12, 3.42% H-31 => L+1, 3.18% H-4 => L+17, 3.06% H-31 => L+3, 2.99% H-36 => L+2
276	21287	470	0.02	43.0% H-7 => L+12, 8.50% H-6 => L+13, 7.65% H-3 => L+18, 5.42% H-32 => L+2, 5.30% H-11 => L+7, 4.26% H-4 => L+16, 3.14% HOMO => L+20, 2.55% H-5 => L+11, 2.04% H-2 => L+17
277	21291	470	0.06	30.6% H-34 => L+2, 24.2% H-4 => L+18, 17.0% H-14 => L+4, 5.05% H-31 => L+2, 3.08% H-3 => L+16
278	21317	469	0.00	72.7% H-35 => L+2, 4.12% H-13 => L+5, 3.63% H-34 => L+1, 3.18% H-34 => L+3
279	21318	469	0.01	43.4% H-34 => L+2, 11.6% H-14 => L+4, 11.3% H-4 => L+18, 7.17% H-31 => L+2, 3.46% H-33 => L+1, 3.28% H-37 => L+2, 2.54% H-33 => L+3, 2.00% H-35 => L+1
280	21326	469	0.01	27.4% H-6 => L+13, 15.7% H-11 => L+7, 11.0% H-7 => L+12, 10.8% H-16 => L+4, 6.43% H-9 => L+10, 3.81% H-4 => L+16, 3.76% H-3 => L+18
281	21358	468	0.00	32.2% H-13 => L+5, 25.3% H-11 => L+6, 8.41% H-35 => L+2, 5.78% H-15 => L+6, 4.38% H-9 => L+5, 3.09% H-13 => L+8, 3.01% H-16 => L+8, 2.29% H-5 => L+16

282	21396	467	0.00	64.6% H-39 => L+1, 8.48% H-38 => L+2, 7.88% H-40 => LUMO, 6.72% H-38 => LUMO, 4.46% H-41 => L+1, 2.60% H-40 => L+2
283	21409	467	0.00	30.7% H-8 => L+10, 27.9% H-7 => L+13, 22.5% H-5 => L+16, 2.66% H-10 => L+13, 2.19% H-2 => L+16
284	21454	466	0.00	44.4% H-5 => L+15, 10.7% H-10 => L+8, 5.73% H-3 => L+17, 5.51% H-12 => L+6, 4.90% H-3 => L+14, 2.98% H-14 => L+8, 2.56% H-17 => L+6, 2.52% H-7 => L+17, 2.17% HOMO => L+19, 2.06% H-7 => L+14
285	21510	465	0.06	24.3% H-9 => L+10, 15.5% H-3 => L+18, 12.3% H-6 => L+13, 9.97% H-8 => L+11, 4.27% H-32 => L+2, 4.00% H-21 => L+3, 3.52% H-7 => L+12, 2.29% H-8 => L+14
286	21549	464	0.02	28.7% H-9 => L+10, 14.7% H-6 => L+13, 14.1% H-3 => L+18, 7.16% H-8 => L+11, 4.93% H-11 => L+7, 4.16% H-10 => L+9, 3.10% H-16 => L+4, 2.89% H-7 => L+12
287	21575	464	0.38	22.6% H-6 => L+14, 16.5% H-37 => L+2, 9.60% H-36 => L+2, 4.94% H-11 => L+8, 3.59% H-12 => L+7, 3.41% H-14 => L+4, 3.24% H-36 => L+1, 2.89% H-4 => L+18, 2.57% H-36 => L+3, 2.47% H-34 => L+2, 2.20% H-9 => L+12
288	21585	463	0.00	36.4% H-12 => L+6, 12.5% H-5 => L+15, 12.3% H-10 => L+8, 8.53% H-14 => L+5, 4.33% H-22 => L+3, 3.99% H-5 => L+18, 3.95% H-2 => L+18, 2.97% H-12 => L+9, 2.57% H-10 => L+5
289	21603	463	0.00	36.3% H-36 => L+2, 21.0% H-37 => L+2, 6.92% H-37 => L+1, 5.69% H-9 => L+11, 5.14% H-37 => L+3, 4.55% H-33 => L+2, 4.01% H-36 => L+1, 2.98% H-36 => L+3, 2.11% H-6 => L+12
290	21633	462	0.00	59.4% H-40 => L+1, 8.87% H-41 => LUMO, 8.49% H-39 => LUMO, 8.26% H-39 => L+2, 5.12% H-42 => L+1, 2.26% H-41 => L+2, 2.13% H-38 => L+3
291	21633	462	0.00	18.6% H-11 => L+8, 15.4% H-37 => L+2, 8.89% H-36 => L+2, 8.46% H-15 => L+5, 8.03% H-12 => L+7, 4.46% H-16 => L+6, 2.71% H-36 => L+1, 2.64% H-14 => L+4, 2.22% H-10 => L+10, 2.01% H-36 => L+3
292	21661	462	0.38	30.7% H-6 => L+14, 9.70% H-11 => L+8, 8.58% H-37 => L+2, 4.97% H-36 => L+2, 3.82% H-15 => L+5, 2.65% H-55 => LUMO, 2.46% H-48 => LUMO, 2.44% H-49 => LUMO
293	21687	461	0.00	26.0% H-5 => L+16, 15.7% H-7 => L+13, 15.0% H-9 => L+11, 2.99% H-49 => LUMO, 2.98% H-48 => LUMO, 2.87% H-8 => L+16, 2.69% H-36 => L+2, 2.56% H-16 => L+5, 2.46% H-6 => L+12
294	21704	461	0.00	20.9% H-15 => L+4, 9.70% H-6 => L+16, 7.67% H-13 => L+7, 7.28% H-5 => L+18, 7.12% H-9 => L+13, 6.99% H-11 => L+10, 5.33% H-22 => L+3,

				4.38% H-26 => L+2, 3.88% H-7 => L+17, 2.55% H-2 => L+18, 2.44% HOMO => L+19
295	21721	460	0.00	20.1% H-7 => L+13, 15.6% H-5 => L+16, 15.4% H-9 => L+11, 8.95% H-49 => LUMO, 8.94% H-48 => LUMO, 6.24% H-50 => LUMO
296	21725	460	0.27	47.1% H-8 => L+11, 8.21% H-21 => L+3, 4.36% H-12 => L+8, 4.29% H-5 => L+17, 3.29% H-14 => L+6, 3.16% H-10 => L+12, 2.88% H-17 => L+5, 2.62% H-7 => L+9, 2.03% H-3 => L+18
297	21754	460	0.00	28.4% H-50 => LUMO, 13.0% H-9 => L+11, 9.03% H-52 => LUMO, 6.17% H-48 => LUMO, 6.15% H-49 => LUMO, 5.44% H-16 => L+5, 4.91% H-6 => L+15, 4.46% H-17 => L+4, 3.51% H-4 => L+17
298	21758	460	0.00	52.2% H-50 => LUMO, 10.3% H-48 => LUMO, 10.3% H-49 => LUMO, 5.24% H-17 => L+4, 3.01% H-9 => L+11
299	21769	459	0.00	27.8% H-12 => L+7, 25.4% H-51 => LUMO, 7.62% H-11 => L+8, 6.79% H-49 => LUMO, 6.79% H-48 => LUMO, 3.66% H-10 => L+10, 3.27% H-4 => L+18, 2.24% H-14 => L+4
300	21782	459	0.06	24.6% H-48 => LUMO, 24.6% H-49 => LUMO, 20.4% H-51 => LUMO, 8.08% H-53 => LUMO, 5.56% H-6 => L+14, 3.04% H-49 => L+1, 3.01% H-48 => L+1
301	21826	458	0.08	23.0% H-51 => LUMO, 21.6% H-53 => LUMO, 9.26% H-12 => L+7, 6.53% H-11 => L+8, 6.30% H-6 => L+14, 4.62% H-48 => LUMO, 4.57% H-49 => LUMO, 3.12% H-4 => L+18, 2.78% H-13 => L+6, 2.06% H-55 => LUMO
302	21836	458	0.00	56.4% H-22 => L+3, 7.58% H-13 => L+7, 7.32% H-25 => L+2, 3.19% H-12 => L+6, 2.33% H-7 => L+14
303	21837	458	0.00	37.3% H-17 => L+4, 11.8% H-49 => LUMO, 11.7% H-48 => LUMO, 4.61% H-52 => LUMO, 4.36% H-18 => L+3, 3.49% H-14 => L+7, 2.96% H-9 => L+11, 2.44% H-5 => L+16, 2.19% H-6 => L+15
304	21867	457	0.00	44.3% H-52 => LUMO, 27.3% H-54 => LUMO, 7.84% H-17 => L+4, 2.92% H-50 => LUMO, 2.13% H-51 => L+1
305	21875	457	0.00	61.6% H-21 => L+3, 7.05% H-5 => L+17, 3.05% H-3 => L+18, 2.71% H-10 => L+9
306	21891	457	0.00	56.2% H-41 => L+1, 9.33% H-40 => LUMO, 8.43% H-40 => L+2, 8.39% H-42 => LUMO, 5.50% H-43 => L+1, 2.18% H-39 => L+3
307	21904	457	0.01	55.8% H-55 => LUMO, 11.7% H-53 => LUMO, 6.54% H-11 => L+8, 6.15% H-51 => LUMO, 2.94% H-57 => LUMO, 2.47% H-12 => L+7
308	21940	456	0.00	43.7% H-54 => LUMO, 24.2% H-52 => LUMO, 11.9% H-56 => LUMO, 4.99% H-53 => L+1
309	21943	456	0.02	36.2% H-53 => LUMO, 16.9% H-55 => LUMO, 14.6% H-57 => LUMO, 10.9% H-51 => LUMO,

				3.50% H-54 => L+1, 3.21% H-52 => L+1, 2.41% H-12 => L+7
310	21966	455	0.00	58.8% H-7 => L+14, 8.70% H-5 => L+15, 3.79% H-5 => L+12, 3.30% H-8 => L+12, 3.19% H-22 => L+3, 2.74% H-18 => L+5, 2.64% H-8 => L+15, 2.48% H-17 => L+6
311	21987	455	0.01	33.5% H-10 => L+9, 21.4% H-5 => L+17, 4.18% H-7 => L+18, 4.17% H-25 => L+3, 2.75% H-10 => L+12, 2.54% H-8 => L+11, 2.43% HOMO => L+20, 2.41% H-3 => L+15, 2.12% H-18 => L+6, 2.04% H-16 => L+4
312	22061	453	0.00	41.6% H-56 => LUMO, 14.7% H-6 => L+15, 6.00% H-57 => L+1, 5.28% H-17 => L+4, 4.58% H-9 => L+11, 2.45% H-4 => L+17, 2.19% H-9 => L+14
313	22075	453	0.10	37.5% H-24 => L+3, 18.0% H-18 => L+4, 7.67% H-57 => LUMO, 4.58% H-6 => L+17, 2.97% H-12 => L+7, 2.80% H-17 => L+7, 2.41% H-27 => L+2
314	22115	452	0.07	52.2% H-57 => LUMO, 10.2% H-55 => LUMO, 7.92% H-56 => L+1, 6.72% H-53 => LUMO, 3.38% H-24 => L+3
315	22129	452	0.00	35.5% H-23 => L+3, 15.9% H-6 => L+16, 6.19% H-14 => L+5, 3.47% H-13 => L+7, 2.84% H-15 => L+10, 2.82% H-21 => L+4, 2.69% H-26 => L+4, 2.29% H-5 => L+15, 2.09% H-9 => L+13, 2.04% H-3 => L+17, 2.02% H-12 => L+6
316	22165	451	0.00	29.0% H-14 => L+5, 18.9% H-5 => L+18, 18.5% H-12 => L+6, 7.13% H-13 => L+7, 4.20% H-3 => L+17, 2.90% H-10 => L+5, 2.41% H-17 => L+6, 2.16% H-18 => L+8
317	22167	451	0.00	56.1% H-42 => L+1, 9.50% H-41 => LUMO, 8.69% H-41 => L+2, 7.66% H-43 => LUMO, 6.83% H-44 => L+1, 2.32% H-40 => L+3
318	22173	451	0.00	27.8% H-6 => L+15, 23.1% H-56 => LUMO, 9.94% H-54 => LUMO, 3.27% H-17 => L+4, 3.26% H-9 => L+14, 3.17% H-57 => L+1, 2.58% H-4 => L+17
319	22183	451	0.00	31.1% H-13 => L+6, 8.23% H-24 => L+3, 7.92% H-11 => L+5, 7.29% H-12 => L+7, 5.37% H-15 => L+8, 4.74% H-15 => L+5, 4.72% H-16 => L+9, 4.34% H-10 => L+10, 3.66% H-16 => L+6, 2.78% H-57 => LUMO, 2.76% H-8 => L+13, 2.43% H-21 => L+5
320	22192	451	0.06	27.8% H-10 => L+9, 16.4% H-25 => L+3, 11.7% H-12 => L+8, 6.27% H-14 => L+6, 4.25% H-12 => L+11, 2.84% H-3 => L+18, 2.79% H-7 => L+15, 2.24% H-17 => L+5, 2.18% H-62 => LUMO
321	22256	449	0.03	26.2% H-25 => L+3, 22.6% H-5 => L+17, 7.61% H-12 => L+8, 4.57% H-21 => L+3, 3.20% H-3 => L+18, 2.46% H-22 => L+4
322	22266	449	0.00	27.3% H-10 => L+10, 12.9% H-8 => L+13, 11.1% H-12 => L+7, 7.33% H-7 => L+16, 6.72% H-13 =>

				L+6, 4.18% H-18 => L+4, 3.65% H-4 => L+18, 2.59% H-15 => L+5, 2.13% H-11 => L+5
323	22303	448	0.00	46.1% H-11 => L+9, 9.35% H-13 => L+8, 9.12% H-9 => L+11, 7.34% H-16 => L+5, 4.77% H-56 => LUMO, 2.93% H-16 => L+8, 2.51% H-9 => L+8
324	22367	447	0.00	32.5% H-8 => L+12, 12.0% H-23 => L+3, 7.61% H-13 => L+7, 7.49% H-14 => L+5, 5.98% H-7 => L+14, 3.71% H-5 => L+18, 3.45% H-10 => L+11, 3.31% H-17 => L+6, 2.86% H-7 => L+11
325	22404	446	0.67	33.3% H-9 => L+12, 9.55% H-11 => L+11, 8.90% H-6 => L+14, 5.09% H-15 => L+8, 4.73% H-13 => L+9, 4.64% H-10 => L+10, 3.30% H-18 => L+4, 3.13% H-24 => L+3, 2.21% H-6 => L+17
326	22415	446	0.16	24.0% H-26 => L+3, 16.6% H-25 => L+3, 5.39% H-5 => L+17, 4.65% H-23 => L+4, 4.31% H-28 => L+2, 3.77% H-15 => L+7, 3.63% H-13 => L+10, 3.37% H-3 => L+18, 2.92% H-8 => L+17, 2.35% H-12 => L+8
327	22435	446	0.24	30.9% H-18 => L+4, 29.6% H-24 => L+3, 5.58% H-9 => L+12, 4.36% H-6 => L+17, 3.46% H-13 => L+6, 2.24% H-17 => L+3, 2.12% H-17 => L+7
328	22441	446	0.00	54.6% H-43 => L+1, 9.38% H-42 => LUMO, 8.84% H-42 => L+2, 8.43% H-45 => L+1, 6.55% H-44 => LUMO, 2.33% H-41 => L+3
329	22485	445	0.00	27.2% H-8 => L+12, 26.3% H-13 => L+7, 15.2% H-23 => L+3, 6.93% H-6 => L+16, 3.14% H-7 => L+14, 3.03% H-14 => L+5
330	22509	444	0.00	31.0% H-12 => L+8, 15.9% H-7 => L+15, 6.25% H-26 => L+3, 6.07% HOMO => L+20, 4.34% H-1 => L+19, 4.16% H-20 => L+3, 3.21% H-19 => L+4, 2.79% H-60 => LUMO, 2.31% H-8 => L+14
331	22523	444	0.00	34.6% H-5 => L+18, 16.4% H-6 => L+16, 14.8% H-14 => L+5, 4.89% H-8 => L+12, 4.56% H-9 => L+13, 4.23% H-13 => L+7, 2.38% H-3 => L+17
332	22576	443	0.00	26.8% H-27 => L+3, 15.5% H-14 => L+7, 10.4% H-17 => L+4, 7.31% H-6 => L+18, 5.48% H-12 => L+10, 2.69% H-10 => L+13, 2.56% H-18 => L+7, 2.14% H-4 => L+17, 2.06% H-24 => L+4
333	22583	443	0.01	26.8% H-7 => L+16, 21.6% H-10 => L+10, 11.1% H-6 => L+17, 8.40% H-8 => L+13, 6.74% H-18 => L+4, 2.44% H-19 => L+6
334	22617	442	0.00	24.6% H-27 => L+3, 7.13% H-20 => L+6, 6.59% H-11 => L+9, 6.19% H-13 => L+8, 6.03% H-16 => L+8, 5.12% H-19 => L+5, 4.83% H-13 => L+5, 4.81% H-15 => L+6, 4.25% H-17 => L+4, 3.69% H-14 => L+7, 3.51% H-19 => L+8, 2.32% H-16 => L+5
335	22639	442	0.02	40.6% H-62 => LUMO, 19.9% H-60 => LUMO, 15.1% H-7 => L+15, 3.06% H-12 => L+8, 2.36% H-15 => L+7

336	22644	442	0.00	11.1% H-1 => L+20, 10.7% H-6 => L+16, 7.95% HOMO => L+19, 7.38% H-20 => L+4, 5.69% H-19 => L+3, 4.36% H-61 => LUMO, 4.13% H-28 => L+3, 3.97% H-7 => L+17, 3.73% H-22 => L+3, 3.11% H-23 => L+3, 3.00% H-14 => L+5, 2.85% H-4 => L+19, 2.37% H-13 => L+7, 2.01% H-19 => L+7
337	22676	441	0.24	28.1% H-6 => L+17, 14.1% H-10 => L+10, 9.30% H-8 => L+13, 5.70% H-7 => L+16, 5.61% H-18 => L+4, 4.38% H-4 => L+18, 4.17% H-29 => L+3, 3.54% H-9 => L+12, 2.92% H-9 => L+15, 2.59% H-19 => L+6, 2.37% H-13 => L+6
338	22677	441	0.00	53.5% H-44 => L+1, 9.39% H-43 => LUMO, 9.36% H-46 => L+1, 9.07% H-43 => L+2, 3.86% H-45 => LUMO, 3.41% H-47 => L+2, 2.40% H-47 => LUMO, 2.39% H-42 => L+3
339	22681	441	0.00	19.8% H-27 => L+3, 13.6% H-11 => L+9, 13.6% H-13 => L+8, 9.67% H-14 => L+7, 7.88% H-6 => L+18, 3.86% H-15 => L+6, 2.42% H-16 => L+8, 2.40% H-11 => L+6, 2.29% H-6 => L+15

Table S3.20. TDDFT-predicted band excitation data for **3.9**.

Index	*Energy (cm^{-1})*	*λ (nm)*	*Osc.Strength*	*Contributions*
0	2228	4489	10.55	98.2% HOMO => LUMO, 2.46% H-1 => L+1
1	3722	2687	0.00	48.4% HOMO => L+1, 48.4% H-1 => LUMO
2	4216	2372	0.00	49.6% HOMO => L+1, 49.3% H-1 => LUMO
3	4385	2280	0.00	91.9% H-2 => LUMO, 4.26% H-4 => L+1
4	4923	2031	0.00	80.8% H-4 => LUMO, 13.0% H-2 => L+1, 2.86% H-5 => L+1
5	5332	1875	0.02	55.6% H-3 => LUMO, 41.2% HOMO => L+2
6	5656	1768	0.00	73.4% H-5 => LUMO, 16.0% H-4 => L+1, 5.55% H-2 => L+2, 2.02% H-7 => L+1
7	5662	1766	0.29	37.1% H-1 => L+1, 33.3% HOMO => L+2, 24.9% H-3 => LUMO
8	5948	1681	0.60	58.0% H-1 => L+1, 22.5% HOMO => L+2, 16.0% H-3 => LUMO
9	6528	1532	0.00	66.5% H-7 => LUMO, 18.7% H-5 => L+1, 6.41% H-4 => L+2, 3.39% H-2 => L+3
10	6620	1511	0.00	78.9% H-2 => L+1, 13.2% H-4 => LUMO, 4.52% H-4 => L+2
11	6848	1460	0.00	67.6% H-6 => LUMO, 25.8% HOMO => L+3
12	7198	1389	0.00	61.8% H-4 => L+1, 20.4% H-5 => LUMO, 8.98% H-2 => L+2, 3.17% H-2 => LUMO

13	7215	1386	0.00	52.5% HOMO => L+3, 23.5% H-6 => LUMO, 17.3% H-3 => L+1
14	7384	1354	0.00	52.1% H-3 => L+1, 31.5% H-1 => L+2, 10.1% HOMO => L+3
15	7505	1332	0.00	61.7% H-8 => LUMO, 18.9% H-7 => L+1, 9.18% H-5 => L+2, 4.17% H-4 => L+3
16	7512	1331	0.00	59.2% H-1 => L+2, 22.7% H-3 => L+1, 7.78% HOMO => L+3, 4.42% H-6 => LUMO
17	7957	1257	0.00	52.2% H-5 => L+1, 26.9% H-7 => LUMO, 9.80% H-4 => L+2, 3.16% H-4 => LUMO, 3.00% H-2 => L+3
18	8251	1212	0.05	78.6% H-9 => LUMO, 10.9% HOMO => L+4, 4.77% H-6 => L+1
19	8425	1187	0.00	76.9% H-2 => L+2, 11.7% H-4 => L+1, 4.05% H-2 => LUMO, 3.28% H-4 => L+3
20	8547	1170	0.00	57.6% H-10 => LUMO, 19.5% H-8 => L+1, 10.1% H-7 => L+2, 4.81% H-5 => L+3, 2.55% H-4 => L+4
21	8711	1148	0.07	66.0% HOMO => L+4, 15.0% H-9 => LUMO, 10.4% H-6 => L+1, 2.32% H-1 => L+3
22	8850	1130	0.00	44.0% H-7 => L+1, 32.5% H-8 => LUMO, 10.6% H-5 => L+2, 4.00% H-4 => L+3, 2.74% H-5 => LUMO
23	8883	1126	0.10	71.5% H-6 => L+1, 16.2% HOMO => L+4, 4.07% H-3 => L+2, 2.39% H-3 => LUMO
24	9008	1110	0.00	47.2% H-3 => L+2, 44.2% H-1 => L+3
25	9009	1110	0.00	61.0% H-4 => L+2, 20.3% H-5 => L+1, 8.59% H-2 => L+3, 2.45% H-2 => L+1, 2.08% H-5 => L+3
26	9124	1096	0.12	45.3% H-1 => L+3, 41.5% H-3 => L+2, 5.74% H-6 => L+1
27	9521	1050	0.00	81.8% H-11 => LUMO, 7.96% H-9 => L+1, 2.81% HOMO => L+5, 2.12% H-13 => L+1
28	9619	1040	0.00	54.3% H-12 => LUMO, 19.0% H-10 => L+1, 10.8% H-8 => L+2, 4.67% H-7 => L+3, 2.75% H-5 => L+4
29	9766	1024	0.00	50.2% H-5 => L+2, 27.1% H-7 => L+1, 8.56% H-4 => L+3, 2.76% H-2 => L+4, 2.72% H-4 => L+1, 2.16% H-7 => L+3
30	9829	1017	0.00	37.1% H-8 => L+1, 36.8% H-10 => LUMO, 11.3% H-7 => L+2, 4.91% H-5 => L+3, 2.21% H-7 => LUMO, 2.01% H-12 => L+1, 2.01% H-4 => L+4
31	10109	989	0.00	75.9% H-2 => L+3, 12.3% H-4 => L+2, 3.98% H-2 => L+1, 3.33% H-4 => L+4
32	10145	986	0.00	69.6% HOMO => L+5, 10.9% H-1 => L+4, 6.10% H-9 => L+1, 5.11% H-11 => LUMO
33	10244	976	0.00	61.0% H-9 => L+1, 13.6% H-6 => L+2, 6.86% H-11 => LUMO, 4.92% HOMO => L+5, 4.09% H-3 => L+3, 2.46% H-6 => LUMO
34	10486	954	0.00	32.9% H-6 => L+2, 23.7% H-3 => L+3, 13.6% H-1 => L+4, 12.5% H-9 => L+1, 11.2% HOMO => L+5
35	10628	941	0.06	77.7% H-13 => LUMO, 10.0% H-11 => L+1, 2.64% H-9 => L+2, 2.22% H-15 => L+1

36	10639	940	0.00	40.9% H-6 => L+2, 32.1% H-1 => L+4, 10.3% H-3 => L+3, 5.76% HOMO => L+5, 4.55% H-9 => L+1
37	10647	939	0.00	34.5% H-7 => L+2, 29.4% H-8 => L+1, 8.67% H-5 => L+3, 7.56% H-14 => LUMO, 5.51% H-10 => L+2, 3.40% H-4 => L+4, 3.16% H-12 => L+1
38	10679	936	0.00	59.9% H-4 => L+3, 19.1% H-5 => L+2, 9.06% H-2 => L+4, 2.44% H-2 => L+2, 2.14% H-4 => L+1
39	10698	935	0.00	48.0% H-14 => LUMO, 15.1% H-12 => L+1, 6.85% H-7 => L+2, 6.33% H-8 => L+3, 5.53% H-10 => L+2, 5.20% H-8 => L+1, 3.07% H-7 => L+4
40	10763	929	0.00	53.0% H-3 => L+3, 35.3% H-1 => L+4, 4.21% H-6 => L+2
41	10850	922	0.00	38.7% H-12 => LUMO, 32.0% H-10 => L+1, 11.6% H-8 => L+2, 5.24% H-7 => L+3, 3.11% H-5 => L+4, 2.08% H-14 => L+1
42	11103	901	0.00	93.0% HOMO => L+6, 2.81% H-1 => L+7
43	11438	874	0.00	80.3% HOMO => L+7, 6.20% H-1 => L+6, 5.16% H-5 => L+3
44	11461	873	0.00	43.4% H-5 => L+3, 27.2% H-7 => L+2, 9.08% H-4 => L+4, 7.94% HOMO => L+7, 2.95% H-2 => L+5, 2.02% H-4 => L+2
45	11496	870	0.03	46.5% HOMO => L+8, 12.6% H-1 => L+5, 8.37% H-3 => L+4, 6.19% H-6 => L+3, 5.63% H-11 => L+1, 5.22% H-9 => L+2, 3.27% H-13 => LUMO, 2.16% H-17 => LUMO
46	11522	868	0.00	71.9% H-15 => LUMO, 10.2% H-13 => L+1, 3.40% H-11 => L+2, 2.45% H-19 => LUMO, 2.39% H-17 => L+1
47	11538	867	0.00	54.7% H-11 => L+1, 14.7% HOMO => L+8, 11.8% H-13 => LUMO, 8.14% H-9 => L+2, 3.76% H-1 => L+5, 2.52% H-9 => LUMO
48	11621	861	0.00	37.9% H-10 => L+1, 30.1% H-8 => L+2, 9.88% H-7 => L+3, 5.07% H-5 => L+4, 2.86% H-12 => L+2, 2.73% H-2 => L+4
49	11714	854	0.00	55.2% H-16 => LUMO, 16.0% H-14 => L+1, 7.27% H-12 => L+2, 5.06% H-10 => L+3, 2.82% H-8 => L+4
50	11748	851	0.00	70.3% H-2 => L+4, 12.4% H-4 => L+3, 4.26% H-4 => L+5, 3.66% H-2 => L+2
51	11872	842	0.00	38.8% H-14 => LUMO, 29.0% H-12 => L+1, 11.8% H-10 => L+2, 6.04% H-8 => L+3, 3.65% H-7 => L+4, 2.17% H-16 => L+1
52	11897	841	0.03	32.2% H-9 => L+2, 19.2% H-11 => L+1, 16.6% HOMO => L+8, 16.5% H-6 => L+3, 6.41% H-3 => L+4
53	11941	837	0.00	83.7% HOMO => L+9, 6.74% H-1 => L+7
54	12092	827	0.09	34.8% H-9 => L+2, 13.4% H-17 => LUMO, 12.7% H-1 => L+5, 12.0% H-3 => L+4, 11.2% HOMO => L+8, 3.62% H-6 => L+3, 2.11% H-11 => L+3

55	12130	824	0.00	51.5% H-17 => LUMO, 7.06% H-15 => L+1, 7.02% H-20 => LUMO, 6.21% H-3 => L+4, 5.99% H-1 => L+5, 3.80% H-6 => L+3, 2.57% H-13 => L+2, 2.22% H-9 => L+2, 2.12% HOMO => L+8
56	12259	816	0.57	46.7% H-6 => L+3, 34.5% H-1 => L+5, 6.26% H-9 => L+2, 3.24% HOMO => L+8
57	12317	812	0.00	56.9% H-4 => L+4, 22.1% H-5 => L+3, 9.34% H-2 => L+5, 2.41% H-2 => L+3, 2.17% H-4 => L+2
58	12344	810	0.00	38.7% H-7 => L+3, 36.9% H-8 => L+2, 9.68% H-5 => L+4, 4.03% H-4 => L+5, 2.09% H-5 => L+2
59	12380	808	0.20	58.6% H-3 => L+4, 22.1% H-1 => L+5, 11.0% H-6 => L+3
60	12389	807	0.00	71.5% H-19 => LUMO, 7.72% H-20 => L+1, 6.99% H-17 => L+1, 2.40% H-15 => LUMO
61	12427	805	0.01	75.7% H-20 => LUMO, 10.7% H-19 => L+1, 3.77% H-17 => LUMO, 2.49% H-17 => L+2
62	12535	798	0.00	68.7% HOMO => L+10, 8.38% H-12 => L+1, 7.10% H-1 => L+9, 3.99% H-10 => L+2
63	12636	791	0.00	47.2% H-18 => LUMO, 12.4% H-16 => L+1, 8.93% H-14 => L+2, 7.96% H-12 => L+1, 4.30% H-10 => L+2, 2.36% H-12 => L+3, 2.06% H-8 => L+3
64	12681	789	0.00	28.0% H-12 => L+1, 17.6% H-10 => L+2, 14.1% HOMO => L+10, 12.5% H-18 => LUMO, 7.56% H-8 => L+3, 3.68% H-7 => L+4, 2.39% H-16 => L+1, 2.27% H-5 => L+5
65	12713	787	0.00	43.7% H-13 => L+1, 17.1% H-15 => LUMO, 10.7% H-11 => L+2, 4.78% H-9 => L+3, 3.90% HOMO => L+11, 2.61% H-6 => L+4, 2.36% H-11 => LUMO
66	12826	780	0.00	45.3% HOMO => L+11, 18.3% H-13 => L+1, 14.9% H-1 => L+8, 7.53% H-3 => L+5, 3.58% H-6 => L+4
67	12856	778	0.00	36.3% H-16 => LUMO, 27.5% H-14 => L+1, 11.7% H-12 => L+2, 6.33% H-10 => L+3, 4.34% H-8 => L+4, 2.15% H-18 => L+1, 2.14% H-7 => L+5
68	12980	770	0.00	84.3% H-1 => L+6, 5.96% HOMO => L+7, 4.33% H-3 => L+7
69	13072	765	0.00	45.5% H-5 => L+4, 29.4% H-7 => L+3, 10.3% H-4 => L+5, 3.59% H-2 => L+8, 2.32% H-4 => L+3
70	13227	756	0.00	40.2% H-11 => L+2, 18.2% H-13 => L+1, 15.9% HOMO => L+11, 13.5% H-9 => L+3, 4.77% H-6 => L+4
71	13231	756	0.00	62.3% HOMO => L+12, 12.9% H-1 => L+7, 10.4% H-1 => L+10, 3.18% HOMO => L+9
72	13306	752	8.77	63.1% H-2 => L+6, 14.9% H-4 => L+7, 4.88% H-5 => L+9, 4.64% H-2 => L+9, 3.79% H-6 => L+3
73	13315	751	0.00	43.1% H-10 => L+2, 26.3% H-8 => L+3, 10.0% H-7 => L+4, 5.32% H-5 => L+5, 3.65% H-2 => L+5
74	13328	750	0.00	69.7% H-2 => L+5, 13.2% H-4 => L+4, 4.86% H-4 => L+8, 3.97% H-2 => L+3
75	13336	750	0.00	61.1% H-1 => L+7, 16.1% HOMO => L+12, 7.25% H-3 => L+6, 4.42% HOMO => L+9, 3.07% H-3 => L+9, 2.64% HOMO => L+6

76	13400	746	0.01	60.6% H-21 => LUMO, 13.3% H-18 => L+1, 6.27% H-16 => L+2, 3.42% H-28 => LUMO, 3.22% H-14 => L+3, 2.04% H-12 => L+4
77	13460	743	0.00	29.2% H-11 => L+2, 13.4% HOMO => L+11, 13.4% H-9 => L+3, 13.3% H-6 => L+4, 6.37% H-3 => L+5, 5.54% H-4 => L+6, 5.12% H-2 => L+7, 2.77% H-1 => L+8
78	13632	734	0.00	26.1% H-1 => L+8, 16.0% H-9 => L+3, 15.6% H-3 => L+5, 13.9% HOMO => L+11, 8.82% H-4 => L+6, 8.44% H-2 => L+7
79	13667	732	0.00	44.0% H-14 => L+1, 19.9% H-12 => L+2, 10.4% H-10 => L+3, 6.00% H-8 => L+4, 4.18% H-7 => L+5, 2.49% HOMO => L+12, 2.08% H-16 => L+2
80	13715	729	0.00	47.8% H-15 => L+1, 19.3% H-17 => LUMO, 8.78% H-13 => L+2, 3.62% H-11 => L+3, 2.96% H-13 => LUMO
81	13751	727	0.00	30.8% H-18 => LUMO, 23.9% H-16 => L+1, 10.7% H-14 => L+2, 5.78% H-12 => L+3, 4.45% H-10 => L+4, 3.18% HOMO => L+13, 2.42% H-8 => L+5, 2.25% H-22 => LUMO
82	13788	725	0.00	64.2% H-1 => L+9, 9.06% HOMO => L+10, 7.36% H-3 => L+7, 3.92% H-1 => L+12, 3.52% HOMO => L+13, 2.98% HOMO => L+7, 2.44% H-6 => L+6
83	13849	722	0.00	35.0% H-9 => L+3, 15.9% H-4 => L+6, 15.5% H-2 => L+7, 10.2% H-6 => L+4, 5.97% H-11 => L+2, 3.11% H-1 => L+8, 2.80% H-5 => L+7, 2.37% H-3 => L+5
84	13865	721	0.00	40.9% H-1 => L+8, 26.0% H-6 => L+4, 15.1% H-3 => L+5, 6.29% H-9 => L+3
85	13902	719	0.00	53.6% H-4 => L+5, 23.8% H-5 => L+4, 9.64% H-2 => L+8, 2.39% H-2 => L+4, 2.27% H-4 => L+3
86	13981	715	0.00	30.2% H-8 => L+3, 25.3% H-7 => L+4, 15.3% HOMO => L+13, 8.80% H-5 => L+5, 3.80% H-4 => L+8
87	13987	715	0.00	56.1% HOMO => L+13, 9.90% H-8 => L+3, 6.99% H-7 => L+4, 5.19% H-1 => L+9, 4.76% H-1 => L+12, 2.80% H-3 => L+10, 2.27% H-5 => L+5
88	13987	715	0.00	33.3% HOMO => L+14, 19.7% H-15 => L+1, 12.3% H-1 => L+11, 7.38% H-3 => L+8, 5.17% H-23 => LUMO, 4.89% H-6 => L+5, 3.23% H-19 => L+1, 2.94% H-9 => L+4
89	14019	713	0.00	42.1% H-3 => L+5, 30.7% H-6 => L+4, 7.86% H-2 => L+7, 7.23% H-4 => L+6, 2.64% H-1 => L+8
90	14138	707	0.32	83.0% H-22 => LUMO, 6.05% H-21 => L+1, 2.92% HOMO => L+22
91	14312	699	0.00	46.3% H-12 => L+2, 15.6% H-10 => L+3, 8.65% H-8 => L+4, 4.81% H-7 => L+5, 4.18% H-14 => L+3, 3.27% H-21 => LUMO, 2.99% H-5 => L+8
92	14404	694	0.00	61.3% H-1 => L+10, 11.1% HOMO => L+12, 9.62% H-3 => L+9, 4.07% H-1 => L+13, 3.03% HOMO => L+15, 2.01% HOMO => L+9

93	14414	694	1.03	24.7% H-2 => L+9, 21.7% H-4 => L+7, 17.1% H-5 => L+6, 16.6% H-13 => L+2, 3.34% H-15 => L+1, 2.49% H-7 => L+7
94	14429	693	0.00	44.7% H-17 => L+1, 16.2% H-19 => LUMO, 8.34% H-24 => LUMO, 5.29% H-15 => L+2, 3.38% H-19 => L+2, 3.33% H-15 => LUMO, 2.23% H-23 => L+1, 2.08% H-20 => L+1, 2.04% H-13 => L+3
95	14436	693	0.24	31.7% H-13 => L+2, 19.5% HOMO => L+14, 11.9% H-11 => L+3, 10.5% H-15 => L+1, 4.48% H-2 => L+9, 4.02% H-4 => L+7, 3.79% H-9 => L+4, 3.05% H-5 => L+6
96	14436	693	0.00	24.6% H-21 => LUMO, 14.5% H-18 => L+1, 9.36% H-22 => L+1, 7.58% H-16 => L+2, 5.53% H-28 => LUMO, 4.75% H-12 => L+4, 4.74% H-12 => L+2, 4.41% H-10 => L+3, 3.30% H-14 => L+3, 2.97% H-10 => L+5, 2.15% H-8 => L+8
97	14611	684	0.01	37.2% H-16 => L+1, 11.6% H-14 => L+2, 7.18% H-12 => L+3, 7.12% H-7 => L+4, 6.47% H-5 => L+5, 5.69% H-8 => L+5, 4.90% H-10 => L+4, 2.25% H-4 => L+8
98	14653	682	0.00	59.6% HOMO => L+15, 11.6% H-3 => L+6, 5.94% H-1 => L+13, 3.10% H-3 => L+12, 2.56% H-1 => L+10, 2.49% H-1 => L+7, 2.12% H-37 => LUMO
99	14670	682	0.00	33.1% H-5 => L+5, 28.6% H-7 => L+4, 8.09% H-4 => L+8, 7.45% H-16 => L+1, 4.21% H-14 => L+2, 2.87% H-2 => L+11, 2.61% H-7 => L+8
100	14704	680	0.00	41.3% H-24 => LUMO, 25.6% H-17 => L+1, 11.3% H-20 => L+1, 5.24% H-23 => L+1, 3.78% HOMO => L+17
101	14708	680	0.00	66.3% H-3 => L+6, 9.79% HOMO => L+15, 7.05% H-1 => L+7, 5.00% H-6 => L+7, 3.74% H-1 => L+10
102	14759	678	0.02	25.2% H-23 => LUMO, 23.3% HOMO => L+14, 14.2% H-19 => L+1, 12.5% H-13 => L+2, 3.26% H-20 => LUMO, 3.13% H-24 => L+1, 2.10% H-2 => L+9, 2.04% H-4 => L+7
103	14838	674	0.02	43.0% H-23 => LUMO, 16.3% H-19 => L+1, 6.60% H-13 => L+2, 6.37% H-11 => L+3, 4.70% H-24 => L+1, 4.45% H-9 => L+4, 2.98% H-6 => L+5, 2.02% H-3 => L+8
104	14844	674	0.00	49.0% H-20 => L+1, 20.9% H-24 => LUMO, 4.99% H-19 => LUMO, 4.53% H-26 => LUMO, 2.18% H-23 => L+1
105	14862	673	0.00	69.4% H-2 => L+8, 14.7% H-4 => L+5, 4.45% H-2 => L+4, 2.79% H-4 => L+11
106	14894	671	0.02	36.9% H-19 => L+1, 9.99% H-11 => L+3, 6.97% H-9 => L+4, 6.71% H-13 => L+2, 5.93% H-20 => LUMO, 5.26% H-6 => L+5, 4.70% H-3 => L+8, 3.76% HOMO => L+14, 2.91% H-1 => L+11, 2.27% H-17 => L+2

107	14945	669	0.00	48.8% H-10 => L+3, 21.5% H-8 => L+4, 9.11% H-7 => L+5, 4.63% H-5 => L+8, 3.55% H-4 => L+11
108	14967	668	0.00	58.6% H-3 => L+7, 10.1% H-1 => L+9, 8.11% H-1 => L+12, 7.73% H-6 => L+6, 4.73% H-3 => L+10, 4.40% H-1 => L+6, 2.45% HOMO => L+13
109	15031	665	0.00	68.9% H-25 => LUMO, 6.13% H-11 => L+3, 5.08% H-1 => L+11, 3.09% H-27 => L+1
110	15071	664	0.00	33.5% H-11 => L+3, 17.1% H-1 => L+11, 11.2% H-25 => LUMO, 10.4% H-3 => L+8, 9.89% HOMO => L+14, 4.31% H-6 => L+5, 3.02% H-13 => L+2
111	15076	663	0.00	64.9% H-26 => LUMO, 5.89% H-20 => L+1, 5.44% H-27 => LUMO
112	15100	662	0.00	40.2% H-1 => L+12, 11.6% HOMO => L+16, 9.41% HOMO => L+13, 7.73% H-3 => L+7, 6.24% H-1 => L+15, 5.35% H-3 => L+10, 3.96% H-6 => L+9, 2.24% HOMO => L+10
113	15214	657	0.00	40.3% H-18 => L+1, 19.0% H-28 => LUMO, 7.44% H-21 => L+2, 5.30% HOMO => L+18, 3.76% H-22 => L+1, 2.26% H-16 => LUMO
114	15225	657	0.00	20.6% H-4 => L+9, 16.6% H-2 => L+10, 13.3% H-27 => LUMO, 13.2% H-5 => L+7, 6.72% H-7 => L+6, 6.17% HOMO => L+17, 4.86% H-26 => LUMO, 2.26% H-20 => L+1, 2.10% H-33 => LUMO
115	15255	656	0.00	48.1% HOMO => L+16, 13.1% H-1 => L+12, 6.64% H-14 => L+2, 4.48% H-36 => LUMO, 3.20% H-1 => L+15, 3.15% H-3 => L+13, 2.27% H-3 => L+7
116	15269	655	0.02	34.8% H-1 => L+11, 28.3% H-9 => L+4, 15.3% H-11 => L+3, 10.6% H-6 => L+5
117	15299	654	0.01	47.3% H-14 => L+2, 7.04% H-12 => L+3, 5.96% HOMO => L+16, 5.11% H-10 => L+4, 3.74% H-7 => L+8, 3.58% H-8 => L+5, 3.21% H-31 => LUMO, 2.91% H-4 => L+8, 2.65% H-5 => L+5
118	15319	653	0.00	34.3% H-27 => LUMO, 16.8% H-15 => L+2, 4.73% H-5 => L+7, 4.72% H-4 => L+9, 4.62% H-2 => L+10, 4.40% H-25 => L+1, 4.02% HOMO => L+17, 3.62% H-17 => L+1
119	15354	651	0.00	43.4% H-2 => L+7, 39.9% H-4 => L+6, 8.04% H-4 => L+9, 3.85% H-5 => L+7
120	15387	650	0.00	25.4% HOMO => L+17, 12.7% H-20 => L+1, 8.40% H-26 => LUMO, 6.90% H-15 => L+2, 5.99% H-1 => L+14, 5.93% H-24 => LUMO, 3.85% H-13 => L+3, 3.25% H-3 => L+11, 2.83% H-11 => L+4, 2.64% H-6 => L+8, 2.62% H-17 => L+1, 2.53% H-9 => L+5
121	15412	649	0.06	28.8% H-3 => L+8, 28.0% H-9 => L+4, 14.1% H-1 => L+11, 6.17% H-6 => L+5, 5.54% H-29 => LUMO, 2.45% H-30 => LUMO
122	15446	647	0.00	46.3% H-4 => L+8, 24.5% H-5 => L+5, 9.32% H-2 => L+11, 2.86% H-14 => L+2, 2.79% H-5 => L+11,

				2.25% H-4 => L+4, 2.10% HOMO => L+16, 2.10% H-2 => L+5
123	15464	647	0.00	58.8% H-3 => L+9, 13.5% H-1 => L+10, 6.96% H-6 => L+7, 3.47% H-1 => L+7, 2.68% H-9 => L+6, 2.43% H-3 => L+12
124	15495	645	0.00	32.5% H-6 => L+5, 25.7% H-29 => LUMO, 8.89% H-30 => LUMO, 8.44% H-9 => L+4, 3.66% H-3 => L+8
125	15520	644	0.00	38.7% H-8 => L+4, 18.3% H-7 => L+5, 8.11% H-5 => L+8, 5.14% HOMO => L+18, 4.33% H-34 => LUMO, 4.24% H-4 => L+11, 2.59% H-3 => L+9, 2.23% H-2 => L+14
126	15526	644	0.05	40.9% H-21 => L+1, 14.3% HOMO => L+19, 7.60% H-31 => LUMO, 5.04% H-22 => LUMO, 4.56% H-22 => L+2, 3.64% H-18 => L+2, 3.24% H-18 => LUMO, 3.21% H-12 => L+3, 3.13% H-1 => L+18
127	15551	643	0.03	31.7% H-3 => L+8, 25.8% H-29 => LUMO, 20.3% H-6 => L+5, 3.06% H-1 => L+11, 2.61% H-30 => LUMO
128	15562	643	0.00	30.6% H-15 => L+2, 23.3% H-27 => LUMO, 18.0% HOMO => L+17, 6.13% H-13 => L+3, 3.34% H-17 => L+1, 2.50% H-1 => L+14
129	15628	640	0.00	22.1% HOMO => L+18, 15.5% H-34 => LUMO, 12.0% H-28 => LUMO, 7.99% H-7 => L+5, 5.42% HOMO => L+21, 5.07% H-1 => L+16, 4.70% H-8 => L+4, 3.38% HOMO => L+15, 3.33% H-1 => L+13
130	15665	638	0.39	45.0% H-2 => L+9, 15.7% H-2 => L+6, 11.9% H-4 => L+7, 11.8% H-5 => L+6, 3.90% H-4 => L+10, 2.65% H-9 => L+4
131	15709	637	0.01	48.9% H-30 => LUMO, 15.9% H-29 => LUMO, 4.68% H-27 => L+1, 2.29% H-33 => L+1, 2.16% H-32 => L+1, 2.08% H-26 => L+1, 2.02% H-4 => L+10
132	15725	636	0.00	21.6% H-16 => L+2, 18.4% H-18 => L+1, 16.2% H-28 => LUMO, 9.77% HOMO => L+18, 6.66% H-14 => L+3, 3.47% H-12 => L+4, 2.32% HOMO => L+21
133	15757	635	0.03	37.2% H-31 => LUMO, 17.7% H-21 => L+1, 13.7% H-12 => L+3, 5.07% HOMO => L+22, 4.31% H-28 => L+1, 3.92% HOMO => L+19, 3.59% H-22 => LUMO, 2.18% H-18 => L+2
134	15829	632	0.00	51.0% H-1 => L+13, 9.87% HOMO => L+15, 7.92% H-3 => L+12, 5.21% HOMO => L+18, 4.09% H-6 => L+10, 2.79% H-34 => LUMO, 2.67% H-3 => L+9, 2.22% HOMO => L+12
135	15839	631	0.00	50.0% H-32 => LUMO, 9.22% H-33 => LUMO, 8.26% H-15 => L+2, 6.19% H-29 => L+1, 6.14% H-13 => L+3
136	15959	627	0.00	48.7% H-33 => LUMO, 20.1% H-32 => LUMO, 7.27% H-30 => L+1, 3.02% H-13 => L+3

137	15966	626	0.01	46.8% H-12 => L+3, 14.2% H-10 => L+4, 8.54% H-8 => L+5, 5.90% H-31 => LUMO, 4.86% H-7 => L+8, 3.11% H-5 => L+11
138	15974	626	0.00	24.9% HOMO => L+20, 23.3% H-17 => L+2, 7.72% H-20 => L+2, 5.44% H-19 => L+1, 5.35% H-15 => L+3, 5.00% H-1 => L+17, 3.28% H-13 => L+4, 2.85% H-3 => L+14, 2.53% H-20 => LUMO, 2.42% H-11 => L+5, 2.24% H-6 => L+11, 2.14% H-9 => L+8
139	15982	626	0.00	45.1% H-22 => L+1, 29.4% H-28 => LUMO, 6.31% HOMO => L+21, 4.87% H-21 => LUMO, 3.91% H-21 => L+2
140	16013	625	0.14	47.0% H-5 => L+6, 22.9% H-4 => L+7, 10.8% H-2 => L+6, 4.35% H-5 => L+9, 4.26% H-7 => L+7, 3.03% H-35 => LUMO
141	16045	623	0.00	14.6% HOMO => L+17, 12.0% H-15 => L+2, 11.9% H-11 => L+4, 11.0% H-33 => LUMO, 9.47% H-13 => L+3, 7.95% H-9 => L+5, 6.66% H-32 => LUMO, 5.43% H-38 => LUMO, 3.91% H-6 => L+8, 3.35% H-3 => L+11, 2.34% H-2 => L+10
142	16071	622	0.00	50.1% H-3 => L+10, 16.4% H-1 => L+12, 9.90% H-6 => L+9, 3.16% H-6 => L+6, 2.50% H-3 => L+13, 2.04% H-1 => L+9
143	16124	620	0.16	47.5% H-35 => LUMO, 10.0% H-4 => L+10, 5.94% H-5 => L+9, 5.84% H-2 => L+12, 4.42% H-7 => L+7, 3.32% H-4 => L+7, 3.17% H-40 => LUMO, 2.65% H-33 => L+1
144	16154	619	0.00	47.1% H-2 => L+10, 14.7% H-5 => L+7, 7.45% H-7 => L+6, 6.39% H-4 => L+6, 5.11% H-2 => L+7, 4.35% H-4 => L+12, 2.99% H-13 => L+3
145	16184	618	0.00	36.6% H-7 => L+5, 30.1% H-5 => L+8, 10.2% H-4 => L+11, 4.40% H-2 => L+14, 4.32% H-16 => L+2, 3.49% H-8 => L+8, 2.30% H-5 => L+4
146	16224	616	0.00	67.1% H-6 => L+6, 10.0% H-3 => L+7, 6.14% H-9 => L+7, 3.35% H-42 => LUMO, 2.54% H-3 => L+10
147	16230	616	0.11	19.8% H-35 => LUMO, 17.7% H-4 => L+10, 13.4% H-5 => L+9, 8.40% H-2 => L+12, 6.85% H-40 => LUMO, 6.12% H-30 => LUMO, 3.92% HOMO => L+20, 3.76% H-7 => L+7, 3.13% H-29 => LUMO, 2.30% H-33 => L+1
148	16274	614	0.00	47.1% H-16 => L+2, 7.50% H-14 => L+3, 5.98% H-12 => L+4, 4.78% H-10 => L+5, 4.12% H-7 => L+11, 3.66% HOMO => L+18, 3.37% H-7 => L+5, 2.92% H-5 => L+8, 2.56% H-8 => L+8, 2.49% H-5 => L+14, 2.08% H-4 => L+17
149	16292	614	0.00	38.4% HOMO => L+20, 35.2% H-17 => L+2, 4.66% H-1 => L+17, 2.80% H-30 => LUMO
150	16307	613	0.00	31.1% H-13 => L+3, 20.3% H-1 => L+14, 13.8% HOMO => L+17, 10.3% H-3 => L+11, 6.19% H-6 => L+8

151	16326	613	0.00	63.5% H-2 => L+11, 17.0% H-4 => L+8, 4.75% H-2 => L+5, 3.34% H-4 => L+14
152	16367	611	0.01	22.5% H-1 => L+15, 18.5% H-36 => LUMO, 15.6% HOMO => L+16, 4.32% H-3 => L+13, 4.29% H-39 => LUMO, 3.38% H-2 => L+11, 2.84% H-31 => LUMO, 2.64% H-37 => L+1, 2.58% H-6 => L+12, 2.35% H-10 => L+4, 2.23% H-21 => L+1, 2.09% HOMO => L+13, 2.07% H-34 => L+1
153	16378	611	0.00	40.6% H-4 => L+9, 20.4% H-5 => L+7, 7.79% H-7 => L+6, 7.24% H-2 => L+7, 4.78% H-38 => LUMO, 3.47% H-4 => L+6, 3.18% H-5 => L+10, 2.03% H-2 => L+10
154	16396	610	0.00	45.6% H-38 => LUMO, 9.03% H-13 => L+3, 7.30% H-2 => L+10, 5.99% H-40 => L+1, 5.91% H-35 => L+1, 4.52% H-4 => L+9, 3.92% H-33 => LUMO, 2.28% H-11 => L+4
155	16438	608	1.08	63.7% H-40 => LUMO, 13.0% H-38 => L+1, 5.84% H-35 => LUMO, 2.98% H-35 => L+2
156	16468	607	0.00	46.9% H-34 => LUMO, 27.2% HOMO => L+18, 4.72% H-22 => L+1, 2.77% H-6 => L+7, 2.49% H-36 => L+1
157	16478	607	0.00	41.7% H-6 => L+7, 8.89% H-3 => L+9, 8.64% H-43 => LUMO, 7.67% H-9 => L+6, 6.66% H-37 => LUMO, 4.22% H-34 => LUMO, 3.43% H-3 => L+6, 3.13% H-41 => LUMO, 2.88% H-6 => L+10
158	16483	607	0.00	19.9% H-18 => L+2, 15.9% H-21 => L+1, 12.8% HOMO => L+22, 8.71% H-1 => L+15, 7.46% H-36 => LUMO, 5.78% H-16 => L+3, 5.48% HOMO => L+19, 2.73% H-39 => LUMO, 2.71% H-14 => L+4, 2.49% H-1 => L+21
159	16498	606	0.00	47.5% H-23 => L+1, 11.6% H-24 => LUMO, 10.4% H-19 => L+2, 9.25% H-24 => L+2, 3.14% H-38 => LUMO, 2.31% H-23 => L+3
160	16509	606	0.03	50.3% H-24 => L+1, 12.6% H-23 => LUMO, 9.81% H-23 => L+2, 9.23% H-20 => L+2, 2.31% H-24 => L+3
161	16515	606	0.00	51.3% H-10 => L+4, 11.5% H-8 => L+5, 9.28% H-7 => L+8, 5.69% H-5 => L+11, 4.07% H-4 => L+14, 3.97% H-31 => LUMO, 2.44% H-2 => L+17
162	16593	603	0.04	38.2% HOMO => L+19, 22.6% H-31 => LUMO, 8.20% HOMO => L+22, 4.57% H-18 => L+2, 4.07% H-1 => L+15, 3.31% H-10 => L+4, 2.53% H-22 => L+2, 2.19% H-39 => LUMO
163	16606	602	0.00	41.4% H-37 => LUMO, 8.67% H-41 => LUMO, 8.56% H-6 => L+7, 8.27% H-3 => L+12, 8.18% H-1 => L+13, 3.29% H-43 => LUMO, 2.70% H-9 => L+9, 2.11% HOMO => L+15
164	16610	602	0.00	33.0% H-1 => L+14, 22.3% H-11 => L+4, 10.9% H-13 => L+3, 10.7% H-38 => LUMO, 7.46% H-9 => L+5, 3.62% H-6 => L+8

165	16632	601	0.00	35.1% H-36 => LUMO, 26.2% H-39 => LUMO, 5.16% HOMO => L+19, 5.10% H-1 => L+15, 4.12% H-21 => L+1, 2.93% H-18 => L+2, 2.67% HOMO => L+16, 2.64% H-3 => L+10, 2.05% H-1 => L+18
166	16665	600	0.01	57.6% H-20 => L+2, 8.13% H-24 => L+1, 6.74% H-17 => L+2, 5.32% H-19 => L+3, 4.14% H-19 => L+1, 3.04% HOMO => L+20
167	16675	600	0.00	61.6% H-19 => L+2, 10.9% H-23 => L+1, 3.84% H-20 => L+3, 2.61% H-17 => L+1, 2.48% H-20 => L+1, 2.32% H-17 => L+3, 2.17% H-24 => LUMO
168	16744	597	0.26	35.8% H-2 => L+12, 20.2% H-5 => L+9, 12.0% H-7 => L+7, 6.11% H-8 => L+6, 5.60% H-4 => L+7, 5.28% H-4 => L+10, 2.03% H-4 => L+13
169	16746	597	0.00	21.4% H-41 => LUMO, 21.1% H-37 => LUMO, 15.3% H-3 => L+12, 12.2% H-43 => LUMO, 5.52% H-1 => L+16, 4.28% H-45 => LUMO, 2.32% H-39 => L+1, 2.30% H-3 => L+15
170	16780	596	0.00	37.4% H-11 => L+4, 17.1% H-1 => L+14, 12.8% H-3 => L+11, 11.9% H-6 => L+8, 6.81% H-9 => L+5
171	16826	594	0.00	17.1% H-14 => L+3, 15.0% H-41 => LUMO, 13.1% HOMO => L+21, 10.4% H-22 => L+1, 3.97% H-3 => L+12, 3.47% H-1 => L+13, 2.86% H-2 => L+20, 2.60% H-16 => L+4, 2.15% H-7 => L+11
172	16832	594	0.00	49.2% H-42 => LUMO, 19.0% H-39 => LUMO, 4.91% H-36 => LUMO, 4.72% H-6 => L+6, 4.12% H-1 => L+15, 3.50% H-3 => L+10, 2.70% H-3 => L+13, 2.24% H-43 => L+1
173	16862	593	0.00	26.1% H-43 => LUMO, 10.9% H-3 => L+12, 8.48% H-14 => L+3, 7.65% H-41 => LUMO, 5.56% H-1 => L+13, 3.85% H-45 => LUMO, 3.68% H-6 => L+10, 3.35% HOMO => L+21, 2.99% H-3 => L+9, 2.14% H-22 => L+1
174	16863	593	0.00	56.2% H-7 => L+6, 18.5% H-5 => L+7, 6.96% H-4 => L+6, 5.07% H-8 => L+7, 2.45% H-7 => L+9
175	16884	592	0.00	18.1% H-4 => L+11, 14.3% H-41 => LUMO, 13.6% H-5 => L+8, 13.3% H-43 => LUMO, 7.42% H-14 => L+3, 4.60% H-2 => L+14, 3.46% H-1 => L+13, 2.97% H-6 => L+7, 2.77% H-3 => L+12, 2.57% H-5 => L+14
176	16888	592	0.00	28.7% H-42 => LUMO, 15.4% H-39 => LUMO, 10.6% H-1 => L+15, 8.13% H-36 => LUMO, 6.87% H-44 => LUMO, 5.59% H-6 => L+9, 3.63% H-3 => L+10, 2.25% H-41 => L+1
177	16909	591	0.00	20.0% H-4 => L+11, 17.9% H-43 => LUMO, 15.0% H-5 => L+8, 13.0% H-41 => LUMO, 6.32% H-6 => L+7, 5.72% H-2 => L+14, 3.80% H-45 => LUMO, 2.93% H-1 => L+13, 2.26% H-42 => L+1
178	16925	591	0.00	33.9% H-9 => L+5, 32.2% H-3 => L+11, 5.40% H-11 => L+4, 4.77% H-4 => L+12, 4.33% H-5 => L+10, 2.55% H-1 => L+14, 2.34% H-2 => L+13

179	16947	590	0.01	32.0% H-14 => L+3, 31.7% HOMO => L+21, 10.4% H-22 => L+1, 2.48% H-12 => L+4, 2.39% H-10 => L+5, 2.05% H-34 => LUMO
180	16969	589	0.03	21.0% H-4 => L+10, 17.0% H-15 => L+3, 12.6% H-2 => L+12, 6.22% H-17 => L+2, 5.58% HOMO => L+20, 5.29% H-2 => L+9, 4.63% H-13 => L+4, 3.52% H-11 => L+5, 2.12% H-9 => L+8
181	16978	589	0.10	21.2% H-4 => L+10, 15.2% H-2 => L+12, 11.4% H-15 => L+3, 6.25% H-2 => L+9, 5.63% H-5 => L+9, 5.50% H-13 => L+4, 4.97% HOMO => L+20, 4.80% H-17 => L+2, 2.52% H-11 => L+5, 2.10% H-30 => LUMO, 2.10% H-9 => L+8
182	17001	588	0.00	22.0% H-4 => L+12, 18.0% H-5 => L+10, 10.2% H-2 => L+13, 9.44% H-9 => L+5, 7.56% H-3 => L+11, 6.13% H-7 => L+9, 5.96% H-27 => LUMO, 2.57% H-25 => L+1, 2.25% H-6 => L+8
183	17049	587	0.00	31.7% H-6 => L+9, 20.8% H-44 => LUMO, 11.2% H-3 => L+10, 8.63% H-8 => L+5, 3.63% H-45 => L+1, 3.36% H-3 => L+7, 3.16% H-39 => LUMO, 3.15% H-9 => L+7, 2.30% H-7 => L+8
184	17064	586	0.07	37.6% H-8 => L+5, 10.4% H-18 => L+2, 9.48% H-7 => L+8, 8.16% HOMO => L+22, 5.66% H-5 => L+11, 4.75% H-44 => LUMO, 3.68% H-6 => L+9, 3.43% H-4 => L+14, 2.86% H-10 => L+8
185	17068	586	0.00	55.1% H-6 => L+8, 16.1% H-3 => L+11, 15.3% H-9 => L+5, 2.35% H-7 => L+6
186	17084	585	0.21	38.7% H-18 => L+2, 17.2% HOMO => L+22, 10.5% H-8 => L+5, 3.03% HOMO => L+19, 2.85% H-7 => L+8, 2.31% H-21 => L+3, 2.25% H-6 => L+9
187	17176	582	0.00	50.0% H-45 => LUMO, 16.3% H-1 => L+16, 7.35% H-44 => L+1, 4.37% H-3 => L+15, 2.03% HOMO => L+18
188	17186	582	0.06	41.9% H-7 => L+7, 25.1% H-5 => L+9, 10.1% H-8 => L+6, 7.04% H-5 => L+6, 4.67% H-4 => L+7, 2.53% H-7 => L+10
189	17195	582	0.01	40.7% H-44 => LUMO, 16.6% H-6 => L+9, 10.8% H-39 => LUMO, 6.74% H-1 => L+15, 6.38% H-45 => L+1, 2.31% H-9 => L+7
190	17259	579	0.00	24.2% H-1 => L+16, 15.9% H-3 => L+12, 15.6% H-45 => LUMO, 9.46% H-37 => LUMO, 5.38% HOMO => L+18, 3.56% H-34 => LUMO, 3.00% H-43 => LUMO, 2.43% H-44 => L+1, 2.31% HOMO => L+21, 2.30% H-6 => L+13, 2.14% H-3 => L+15
191	17274	579	0.00	65.4% H-25 => L+1, 5.34% H-27 => LUMO, 4.56% H-5 => L+10, 3.55% H-17 => L+3, 2.67% H-29 => L+1, 2.14% H-27 => L+2, 2.02% H-7 => L+9
192	17293	578	0.00	45.3% H-26 => L+1, 12.1% H-15 => L+3, 7.02% H-1 => L+17, 6.43% H-29 => LUMO, 3.51% H-3 => L+14, 3.04% H-27 => L+1, 2.89% HOMO => L+20, 2.27% H-6 => L+11

193	17370	576	0.00	29.0% H-2 => L+13, 19.1% H-7 => L+9, 11.6% H-4 => L+12, 9.97% H-5 => L+10, 8.91% H-8 => L+7, 4.41% H-10 => L+6, 2.38% H-5 => L+7, 2.25% H-4 => L+9
194	17389	575	0.01	29.8% H-26 => L+1, 15.6% H-15 => L+3, 13.2% H-1 => L+17, 7.87% HOMO => L+20, 4.81% H-3 => L+14, 3.52% H-6 => L+11, 3.23% H-27 => L+1, 2.52% H-29 => LUMO, 2.21% H-9 => L+8
195	17454	573	0.03	14.8% H-28 => L+1, 13.1% H-1 => L+18, 11.0% H-3 => L+13, 9.22% HOMO => L+19, 7.16% H-22 => L+2, 6.30% H-1 => L+15, 6.04% H-3 => L+16, 4.78% H-7 => L+8, 4.61% H-44 => LUMO, 2.90% H-6 => L+12, 2.22% H-31 => LUMO
196	17459	573	0.00	67.1% H-12 => L+4, 4.27% H-7 => L+11, 4.25% H-5 => L+14, 3.74% H-2 => L+20, 3.57% H-4 => L+17, 3.29% H-8 => L+8, 2.61% H-14 => L+5, 2.57% H-10 => L+3, 2.25% HOMO => L+21
197	17487	572	0.01	38.4% H-27 => L+1, 7.67% H-15 => L+3, 6.45% H-30 => LUMO, 6.44% H-25 => LUMO, 6.24% H-5 => L+12, 6.16% H-4 => L+13, 3.16% H-7 => L+10, 2.88% H-2 => L+15, 2.78% H-30 => L+2
198	17514	571	0.01	55.9% H-21 => L+2, 12.1% HOMO => L+21, 5.46% H-1 => L+16, 3.76% H-1 => L+19, 3.58% H-22 => L+1, 2.50% H-18 => L+3, 2.19% H-22 => L+3
199	17575	569	0.00	18.4% H-29 => L+1, 9.99% H-17 => L+3, 8.86% H-32 => LUMO, 6.51% H-25 => L+1, 4.55% H-15 => L+4, 4.35% H-2 => L+22, 3.96% H-4 => L+21, 3.92% H-19 => L+2, 3.85% H-1 => L+20, 3.34% H-13 => L+5, 3.00% H-33 => LUMO, 2.77% H-30 => L+1, 2.62% H-11 => L+8, 2.42% H-5 => L+19, 2.40% H-3 => L+17, 2.26% H-26 => L+2, 2.24% H-9 => L+11, 2.12% H-6 => L+14
200	17589	569	0.07	35.7% H-28 => L+1, 24.2% H-3 => L+13, 6.91% H-1 => L+15, 4.01% H-6 => L+12, 2.91% H-22 => L+2, 2.35% H-44 => LUMO, 2.23% H-16 => L+3
201	17642	567	0.03	39.3% H-7 => L+8, 15.1% H-5 => L+11, 8.95% H-4 => L+14, 5.23% H-2 => L+17, 4.38% H-3 => L+13, 3.73% H-16 => L+3, 3.45% H-28 => L+1, 2.31% H-5 => L+5, 2.08% H-1 => L+15
202	17659	566	0.23	39.3% H-16 => L+3, 6.83% H-7 => L+8, 6.81% HOMO => L+22, 5.40% H-1 => L+18, 4.58% H-5 => L+11, 3.82% H-3 => L+13, 3.76% HOMO => L+19, 3.53% H-22 => L+2, 3.29% H-18 => L+2, 2.63% H-28 => L+1, 2.11% H-18 => L+4, 2.02% H-14 => L+4
203	17665	566	0.00	29.3% H-2 => L+14, 22.0% H-6 => L+10, 9.31% H-4 => L+11, 8.51% H-3 => L+12, 5.95% H-9 => L+9, 3.80% H-9 => L+6, 2.96% H-2 => L+8, 2.52% H-4 => L+17, 2.38% H-1 => L+16

204	17699	565	0.00	38.9% H-4 => L+12, 31.6% H-2 => L+13, 9.77% H-2 => L+10, 8.30% H-5 => L+10, 2.84% H-5 => L+13, 2.83% H-4 => L+15
205	17701	565	0.01	28.8% H-1 => L+17, 27.0% H-13 => L+4, 10.6% H-15 => L+3, 7.45% H-11 => L+5, 3.31% H-8 => L+6, 2.45% H-9 => L+8
206	17714	565	0.00	34.3% H-9 => L+6, 21.5% H-2 => L+14, 9.74% H-6 => L+10, 9.18% H-4 => L+11, 4.80% H-6 => L+7, 3.96% H-9 => L+9, 2.44% H-3 => L+12, 2.02% H-2 => L+8
207	17732	564	0.00	34.0% H-5 => L+10, 24.3% H-7 => L+9, 7.44% H-2 => L+13, 5.28% H-8 => L+7, 4.22% H-30 => L+1, 4.16% H-4 => L+9, 3.52% H-29 => L+1, 3.20% H-5 => L+7, 2.62% H-7 => L+12
208	17737	564	0.00	35.4% H-9 => L+6, 20.6% H-6 => L+10, 8.98% H-2 => L+14, 6.76% H-11 => L+7, 6.05% H-6 => L+7, 5.48% H-3 => L+12, 2.82% H-4 => L+11, 2.26% H-3 => L+9
209	17784	562	0.18	21.5% H-28 => L+1, 20.8% H-16 => L+3, 15.9% H-1 => L+18, 9.91% HOMO => L+22, 5.09% H-3 => L+13, 3.85% H-1 => L+21, 3.11% H-22 => L+2, 2.17% H-34 => L+1
210	17785	562	0.00	38.0% H-29 => L+1, 12.9% H-30 => L+1, 6.75% H-7 => L+9, 4.00% H-33 => LUMO, 2.61% H-15 => L+4, 2.52% H-20 => L+3, 2.32% H-17 => L+3, 2.22% H-27 => L+2, 2.01% H-5 => L+10
211	17832	561	0.00	22.4% H-4 => L+13, 17.7% H-27 => L+1, 17.7% H-2 => L+15, 11.6% H-5 => L+12, 3.41% H-24 => L+1, 2.73% H-15 => L+3, 2.28% H-25 => L+2, 2.09% H-23 => L+2
212	17835	561	0.01	59.5% H-8 => L+6, 14.9% H-7 => L+7, 4.81% H-10 => L+7, 4.71% H-5 => L+6, 2.63% H-8 => L+9, 2.02% H-1 => L+17
213	17895	559	0.00	35.3% H-30 => L+1, 15.2% H-17 => L+3, 10.8% H-20 => L+3, 3.06% H-33 => LUMO, 2.92% H-27 => L+2, 2.86% H-27 => LUMO, 2.85% H-29 => L+1, 2.57% H-1 => L+20, 2.34% H-26 => LUMO
214	17912	558	0.00	37.5% H-10 => L+5, 20.5% H-31 => L+1, 7.96% H-1 => L+19, 2.82% HOMO => L+21, 2.65% H-21 => L+2, 2.62% H-2 => L+20, 2.37% H-12 => L+8
215	17972	556	0.00	44.7% H-31 => L+1, 22.9% H-10 => L+5, 4.48% H-28 => L+2, 2.60% H-36 => L+1, 2.49% H-34 => LUMO, 2.30% H-4 => L+17
216	17984	556	0.00	52.1% H-22 => L+2, 12.0% H-1 => L+18, 4.94% H-1 => L+21, 4.70% H-28 => L+1, 3.43% H-34 => L+1, 2.71% H-5 => L+11, 2.61% H-21 => L+1
217	17993	556	0.03	25.0% H-13 => L+4, 17.6% H-1 => L+17, 8.80% H-32 => L+1, 6.95% H-9 => L+8, 6.18% H-6 => L+11, 5.39% H-3 => L+14, 4.37% H-11 => L+5
218	18012	555	0.00	56.4% H-9 => L+7, 13.8% H-6 => L+9, 10.1% H-11 => L+6, 4.63% H-6 => L+6

219	18038	554	0.18	13.9% H-19 => L+3, 12.6% H-33 => L+1, 12.0% H-7 => L+10, 5.91% H-2 => L+15, 5.80% H-27 => L+1, 5.58% H-32 => L+1, 5.29% H-5 => L+12, 4.66% H-8 => L+9, 3.02% H-20 => L+2, 2.87% H-26 => L+1, 2.31% H-17 => L+4, 2.26% H-10 => L+7
220	18059	554	0.09	15.3% H-32 => L+1, 10.3% H-7 => L+10, 8.38% H-2 => L+15, 6.97% H-19 => L+3, 6.57% H-13 => L+4, 5.59% H-5 => L+12, 4.97% H-8 => L+9, 3.25% H-6 => L+11, 3.04% H-3 => L+14, 2.94% H-26 => L+1, 2.93% H-1 => L+17, 2.59% H-10 => L+7, 2.58% H-4 => L+13, 2.26% H-9 => L+8
221	18079	553	0.00	39.7% H-17 => L+3, 20.3% H-1 => L+20, 5.35% H-3 => L+17, 4.03% H-24 => L+2, 3.19% H-19 => L+4, 2.79% H-6 => L+14, 2.76% H-25 => L+1, 2.27% H-19 => L+2
222	18081	553	0.00	16.5% H-1 => L+19, 15.5% H-3 => L+15, 14.0% H-1 => L+16, 8.66% H-10 => L+5, 6.93% H-3 => L+18, 4.55% H-6 => L+13, 4.32% H-21 => L+2, 3.71% H-1 => L+22, 2.59% H-9 => L+12, 2.11% H-18 => L+3, 2.09% H-8 => L+8
223	18136	551	0.00	31.6% H-8 => L+7, 13.3% H-24 => L+2, 12.9% H-7 => L+9, 7.40% H-23 => L+1, 7.04% H-10 => L+6, 4.18% H-7 => L+6, 3.09% H-23 => L+3, 2.25% H-1 => L+20, 2.20% H-5 => L+7, 2.09% H-2 => L+16
224	18138	551	0.06	34.8% H-33 => L+1, 17.7% H-32 => L+1, 6.19% H-13 => L+4, 5.41% H-35 => LUMO, 3.14% H-7 => L+10, 2.92% H-30 => L+2, 2.74% H-30 => LUMO, 2.26% H-2 => L+15, 2.25% H-23 => L+2
225	18161	551	0.00	23.7% H-24 => L+2, 17.7% H-8 => L+7, 13.0% H-23 => L+1, 6.52% H-1 => L+20, 5.72% H-7 => L+9, 5.16% H-23 => L+3, 2.99% H-10 => L+6, 2.75% H-7 => L+6
226	18180	550	0.18	34.4% H-14 => L+4, 11.8% H-16 => L+3, 10.5% HOMO => L+22, 8.60% H-1 => L+21, 8.30% H-12 => L+5, 3.16% H-3 => L+19, 3.15% H-10 => L+8, 2.77% H-34 => L+1
227	18215	549	0.03	19.6% H-3 => L+14, 16.0% H-23 => L+2, 15.9% H-11 => L+5, 11.8% H-5 => L+12, 5.77% H-24 => L+1, 5.14% H-1 => L+17, 3.10% H-24 => L+3, 2.86% H-6 => L+11, 2.29% H-4 => L+13, 2.16% H-13 => L+4
228	18235	548	0.11	26.8% H-23 => L+2, 17.4% H-11 => L+5, 12.5% H-3 => L+14, 9.57% H-24 => L+1, 5.32% H-24 => L+3, 5.25% H-19 => L+3, 2.82% H-13 => L+4, 2.40% H-33 => L+1, 2.02% H-9 => L+8
229	18259	548	0.00	33.4% H-5 => L+11, 22.9% H-4 => L+14, 11.4% H-2 => L+17, 11.0% H-34 => L+1, 3.30% H-4 => L+8
230	18279	547	0.00	44.5% H-20 => L+3, 8.85% H-29 => L+1, 8.30% H-30 => L+1, 4.51% H-35 => L+1, 3.91% H-19 => L+2, 3.46% H-19 => L+4

231	18290	547	0.03	33.3% H-34 => L+1, 12.0% H-3 => L+13, 10.0% H-6 => L+12, 6.71% H-5 => L+11, 3.49% H-4 => L+14, 3.10% H-1 => L+18, 2.80% H-9 => L+10, 2.74% H-31 => L+2, 2.19% H-22 => L+2
232	18297	547	0.00	23.4% H-3 => L+15, 15.2% H-18 => L+3, 9.10% H-21 => L+2, 7.34% H-1 => L+16, 5.52% H-8 => L+8, 4.37% H-1 => L+19, 3.88% H-36 => L+1, 3.54% H-16 => L+4, 3.52% H-31 => L+1, 3.26% H-6 => L+13, 2.05% HOMO => L+21
233	18344	545	0.00	30.3% H-19 => L+3, 25.8% H-32 => L+1, 14.9% H-33 => L+1, 3.12% H-20 => L+4
234	18372	544	0.00	64.3% H-35 => L+1, 4.94% H-33 => LUMO, 4.84% H-38 => LUMO, 4.02% H-33 => L+2, 3.59% H-20 => L+3, 3.52% H-40 => L+1
235	18373	544	0.00	35.9% H-1 => L+22, 14.6% H-18 => L+3, 11.1% H-36 => L+1, 7.10% H-1 => L+19, 3.64% H-3 => L+21, 2.43% HOMO => L+21, 2.24% H-16 => L+4, 2.02% H-8 => L+8, 2.02% H-3 => L+15
236	18376	544	0.01	28.9% H-6 => L+12, 16.6% H-34 => L+1, 11.3% H-3 => L+13, 10.3% H-37 => L+1, 6.75% H-9 => L+10, 4.01% H-1 => L+18, 2.73% H-11 => L+9
237	18393	544	0.20	21.3% H-9 => L+8, 18.6% H-3 => L+14, 13.2% H-5 => L+12, 9.07% H-7 => L+10, 6.96% H-4 => L+13, 6.34% H-6 => L+11, 6.20% H-11 => L+5, 2.51% H-4 => L+10
238	18432	543	0.05	35.6% H-2 => L+15, 32.7% H-4 => L+13, 8.18% H-2 => L+12, 4.75% H-7 => L+10, 3.16% H-3 => L+14, 3.01% H-4 => L+16, 2.60% H-5 => L+15
239	18439	542	0.00	83.5% H-46 => LUMO, 7.25% H-47 => L+1, 2.04% H-48 => L+2
240	18442	542	0.08	24.2% H-5 => L+12, 14.4% H-11 => L+5, 13.4% H-6 => L+11, 9.81% H-7 => L+10, 6.89% H-8 => L+9, 5.03% H-3 => L+14, 2.93% H-9 => L+8, 2.87% H-4 => L+10, 2.49% H-2 => L+15, 2.01% H-4 => L+13
241	18463	542	0.00	38.2% H-8 => L+8, 12.7% H-9 => L+9, 11.1% H-18 => L+3, 6.22% H-6 => L+10, 5.24% H-2 => L+20, 4.38% H-4 => L+17, 3.32% H-5 => L+14, 2.24% H-11 => L+7, 2.06% H-7 => L+5
242	18481	541	0.00	23.6% H-9 => L+9, 15.4% H-36 => L+1, 14.1% H-8 => L+8, 11.4% H-6 => L+10, 4.48% H-11 => L+7, 2.97% H-1 => L+22, 2.20% H-13 => L+6
243	18496	541	0.00	22.0% H-2 => L+16, 21.4% H-4 => L+15, 10.8% H-20 => L+3, 7.29% H-5 => L+13, 4.75% H-24 => L+2, 4.33% H-1 => L+20, 2.29% H-26 => L+2, 2.19% H-10 => L+9
244	18522	540	0.00	33.9% H-36 => L+1, 16.5% H-39 => L+1, 12.3% H-9 => L+9, 4.24% H-3 => L+15, 3.93% H-1 => L+22, 3.13% H-6 => L+10, 2.89% H-8 => L+8, 2.87% H-34 => L+2, 2.19% H-11 => L+7

245	18530	540	0.02	38.8% H-6 => L+11, 35.3% H-9 => L+8, 4.22% H-11 => L+5, 3.49% H-3 => L+14, 2.89% H-38 => L+1
246	18538	539	0.00	76.4% H-47 => LUMO, 9.22% H-46 => L+1, 4.99% H-48 => L+1
247	18558	539	0.09	32.8% H-14 => L+4, 14.1% H-1 => L+21, 12.3% H-1 => L+18, 4.99% H-3 => L+16, 3.69% H-37 => L+1, 3.62% H-3 => L+19, 2.88% H-12 => L+5, 2.72% H-10 => L+8
248	18625	537	0.25	53.3% H-38 => L+1, 11.5% H-40 => LUMO, 6.23% H-40 => L+2, 4.36% H-6 => L+11, 4.30% H-35 => LUMO, 4.18% H-11 => L+5, 3.73% H-35 => L+2, 2.69% H-8 => L+9
249	18635	537	0.00	50.0% H-40 => L+1, 9.82% H-38 => LUMO, 7.24% H-1 => L+20, 6.49% H-38 => L+2, 3.70% H-24 => L+2, 2.98% H-15 => L+4, 2.78% H-17 => L+3, 2.05% H-11 => L+8, 2.02% H-13 => L+5
250	18639	536	0.00	43.9% H-37 => L+1, 25.6% H-41 => L+1, 4.14% H-14 => L+4, 4.12% H-36 => L+2, 3.75% H-6 => L+12, 3.37% H-34 => L+1, 2.46% H-36 => LUMO
251	18675	535	0.00	19.3% H-15 => L+4, 17.8% H-1 => L+20, 17.7% H-40 => L+1, 8.20% H-17 => L+3, 4.58% H-13 => L+5, 4.02% H-38 => LUMO, 3.96% H-24 => L+2, 3.29% H-30 => L+1, 2.99% H-38 => L+2
252	18682	535	0.02	37.9% H-8 => L+9, 24.6% H-7 => L+10, 6.95% H-10 => L+7, 3.87% H-7 => L+7, 3.63% H-38 => L+1, 3.03% H-5 => L+9, 2.95% H-9 => L+8, 2.56% H-8 => L+12, 2.27% H-12 => L+6
253	18706	535	0.01	33.2% H-43 => L+1, 31.0% H-41 => L+1, 8.22% H-37 => L+1, 4.62% H-12 => L+5, 2.86% H-3 => L+16, 2.83% H-39 => L+2, 2.51% H-39 => LUMO
254	18710	534	0.00	42.6% H-39 => L+1, 26.6% H-42 => L+1, 6.80% H-36 => L+1, 4.19% H-37 => L+2, 3.24% H-37 => LUMO
255	18716	534	0.00	65.1% H-48 => LUMO, 7.69% H-47 => L+1, 4.46% H-49 => L+1, 3.10% H-7 => L+12, 2.72% H-46 => L+2
256	18738	534	0.01	24.6% H-18 => L+3, 17.5% H-1 => L+22, 14.4% H-1 => L+19, 7.60% H-7 => L+11, 5.88% H-8 => L+8, 4.69% H-3 => L+21, 4.10% H-3 => L+15, 2.79% H-42 => L+1
257	18760	533	0.00	19.2% H-7 => L+12, 14.7% H-5 => L+13, 9.57% H-48 => LUMO, 9.47% H-8 => L+10, 8.79% H-2 => L+16, 5.24% H-10 => L+6, 5.08% H-10 => L+9, 3.21% H-8 => L+7, 2.31% H-2 => L+19
258	18792	532	0.00	14.6% H-3 => L+16, 14.3% H-43 => L+1, 8.13% H-4 => L+14, 6.95% H-2 => L+17, 6.33% H-12 => L+5, 5.33% H-1 => L+18, 3.67% H-14 => L+4, 3.32% H-6 => L+15, 3.23% H-6 => L+12, 3.08% H-21 => L+3, 2.88% H-22 => L+2, 2.63% H-9 => L+13

259	18839	531	0.00	28.8% H-25 => L+2, 11.3% H-2 => L+18, 9.68% H-4 => L+16, 5.23% H-32 => L+1, 4.26% H-5 => L+15, 4.09% H-2 => L+21, 3.28% H-17 => L+4, 2.31% H-3 => L+20, 2.05% H-33 => L+1, 2.03% H-25 => LUMO
260	18858	530	0.17	22.9% H-43 => L+1, 14.1% H-2 => L+17, 13.4% H-4 => L+14, 8.55% H-41 => L+1, 5.86% H-12 => L+5, 3.77% H-42 => L+2, 3.20% H-1 => L+21, 3.06% H-2 => L+11, 2.83% H-4 => L+20, 2.71% H-42 => LUMO
261	18874	530	0.00	58.0% H-10 => L+6, 10.8% H-8 => L+7, 7.08% H-12 => L+7, 4.76% H-7 => L+12, 3.16% H-7 => L+6, 2.03% H-8 => L+10
262	18881	530	0.00	44.4% H-42 => L+1, 10.5% H-39 => L+1, 4.97% H-44 => L+1, 4.27% H-43 => L+2, 3.53% H-7 => L+11, 3.31% H-41 => LUMO, 3.05% H-41 => L+2, 2.87% H-9 => L+9, 2.80% H-43 => LUMO
263	18912	529	0.22	17.0% H-12 => L+5, 12.7% H-41 => L+1, 9.87% H-43 => L+1, 6.07% H-1 => L+21, 5.24% H-37 => L+1, 5.23% H-2 => L+17, 4.68% H-45 => L+1, 4.30% H-4 => L+14, 3.37% H-3 => L+16, 3.01% H-11 => L+6, 2.95% H-9 => L+7, 2.88% H-1 => L+18, 2.29% H-42 => L+2
264	18919	529	0.00	71.3% H-49 => LUMO, 10.7% H-48 => L+1, 4.11% H-50 => L+1, 3.38% H-47 => L+2, 2.18% H-51 => LUMO
265	18962	527	0.00	42.8% H-26 => L+2, 10.3% H-15 => L+4, 7.04% H-5 => L+13, 3.92% H-4 => L+15, 3.83% H-1 => L+20, 3.67% H-2 => L+16, 2.64% H-29 => L+1
266	18979	527	0.00	41.5% H-7 => L+11, 8.65% H-6 => L+13, 7.10% H-3 => L+15, 5.40% H-2 => L+20, 5.18% H-4 => L+17, 3.15% H-44 => L+1, 2.86% H-5 => L+14, 2.65% H-5 => L+8, 2.60% H-9 => L+12, 2.04% H-8 => L+14
267	19023	526	0.21	17.5% H-21 => L+3, 14.6% H-12 => L+5, 11.2% H-2 => L+17, 8.53% H-1 => L+21, 6.84% H-3 => L+16, 6.06% H-22 => L+2, 3.81% H-4 => L+14, 3.41% H-6 => L+12, 3.08% H-18 => L+4, 2.81% H-11 => L+6, 2.33% H-9 => L+10
268	19028	526	0.00	27.0% H-15 => L+4, 11.0% H-3 => L+17, 10.2% H-4 => L+15, 7.54% H-1 => L+20, 7.12% H-26 => L+2, 5.99% H-6 => L+14, 4.14% H-9 => L+11, 2.33% H-5 => L+16, 2.10% H-2 => L+19, 2.01% H-2 => L+13
269	19029	526	0.00	16.6% H-6 => L+13, 15.9% H-3 => L+15, 10.2% H-7 => L+11, 8.22% H-1 => L+19, 6.31% H-39 => L+1, 5.36% H-9 => L+12, 3.31% H-42 => L+1, 2.89% H-6 => L+16, 2.53% H-11 => L+10, 2.38% H-22 => L+3, 2.12% H-1 => L+22
270	19034	525	0.02	16.1% H-25 => L+2, 15.7% H-2 => L+18, 11.3% H-4 => L+16, 6.60% H-8 => L+9, 4.43% H-27 => L+1,

				4.06% H-10 => L+7, 3.80% H-17 => L+4, 3.27% H-10 => L+10, 2.68% H-5 => L+15, 2.68% H-19 => L+3, 2.63% H-23 => L+2
271	19061	525	0.01	56.8% H-11 => L+6, 8.41% H-9 => L+7, 3.85% H-11 => L+9, 3.34% H-41 => L+1, 2.89% H-13 => L+7, 2.52% H-6 => L+6, 2.36% H-9 => L+10, 2.16% H-2 => L+17, 2.16% H-6 => L+12, 2.03% H-4 => L+14
272	19132	523	0.00	25.2% H-50 => LUMO, 17.6% H-5 => L+13, 9.56% H-2 => L+16, 7.99% H-7 => L+12, 4.94% H-26 => L+2, 4.50% H-8 => L+10, 4.22% H-49 => L+1, 2.23% H-4 => L+12, 2.19% H-4 => L+18
273	19134	523	0.01	29.9% H-9 => L+10, 21.5% H-6 => L+12, 6.72% H-12 => L+5, 5.53% H-13 => L+7, 5.50% H-11 => L+9, 4.92% H-11 => L+6, 2.78% H-6 => L+9, 2.00% H-21 => L+3
274	19137	523	0.00	26.7% H-16 => L+4, 16.4% H-44 => L+1, 8.37% H-18 => L+3, 5.45% H-14 => L+5, 4.35% H-45 => LUMO, 3.37% H-1 => L+19, 2.95% H-45 => L+2, 2.54% H-3 => L+18, 2.42% H-7 => L+11, 2.07% H-4 => L+17
275	19145	522	0.00	25.0% H-4 => L+15, 23.0% H-5 => L+13, 14.8% H-50 => LUMO, 4.40% H-2 => L+16, 3.79% H-2 => L+13, 3.01% H-4 => L+12, 2.38% H-49 => L+1, 2.29% H-7 => L+12, 2.09% H-8 => L+10, 2.09% H-7 => L+15
276	19154	522	0.00	13.4% H-25 => L+2, 10.8% H-19 => L+3, 7.09% H-17 => L+4, 5.39% H-23 => L+2, 5.24% H-15 => L+5, 4.62% H-2 => L+21, 3.81% H-13 => L+8, 3.71% H-4 => L+22, 3.65% H-10 => L+7, 3.61% H-3 => L+20, 3.22% H-11 => L+11, 3.04% H-6 => L+17, 2.91% H-9 => L+14, 2.27% H-7 => L+13
277	19171	522	0.00	28.5% H-50 => LUMO, 15.4% H-2 => L+16, 10.1% H-26 => L+2, 8.25% H-4 => L+15, 4.48% H-49 => L+1, 4.26% H-4 => L+18, 4.22% H-7 => L+12, 2.47% H-10 => L+6
278	19190	521	0.00	56.5% H-45 => L+1, 13.4% H-44 => LUMO, 8.71% H-44 => L+2, 3.62% H-12 => L+5
279	19192	521	0.00	41.3% H-10 => L+7, 12.1% H-8 => L+9, 10.1% H-25 => L+2, 7.30% H-12 => L+6, 5.27% H-8 => L+6, 3.66% H-12 => L+9, 2.63% H-4 => L+16
280	19220	520	0.00	38.6% H-44 => L+1, 12.2% H-16 => L+4, 8.31% H-45 => LUMO, 5.59% H-45 => L+2, 4.83% H-6 => L+13, 3.75% H-1 => L+19, 2.64% H-3 => L+15, 2.35% H-18 => L+3, 2.05% H-3 => L+18
281	19240	520	0.00	33.3% H-21 => L+3, 15.5% H-3 => L+16, 9.79% H-12 => L+5, 7.91% H-10 => L+8, 7.34% H-9 => L+10, 2.66% H-8 => L+11
282	19265	519	0.00	20.3% H-7 => L+12, 9.84% H-2 => L+19, 5.23% H-4 => L+18, 4.15% H-10 => L+9, 3.90% H-20 => L+3, 3.77% H-19 => L+4, 3.35% H-8 => L+10,

				3.11% H-26 => L+2, 3.07% H-2 => L+22, 3.05% H-15 => L+4, 2.92% H-13 => L+5, 2.75% H-1 => L+20, 2.32% H-5 => L+10, 2.31% H-32 => L+2, 2.11% H-17 => L+5, 2.03% H-5 => L+16
283	19319	518	0.54	24.8% H-10 => L+8, 20.4% H-1 => L+21, 10.5% H-21 => L+3, 7.08% H-8 => L+11, 4.51% H-2 => L+17, 4.36% H-3 => L+16, 4.34% H-12 => L+5, 2.94% H-7 => L+14, 2.19% H-3 => L+19
284	19345	517	0.00	17.4% H-7 => L+12, 14.9% H-8 => L+10, 12.0% H-27 => L+2, 9.22% H-13 => L+5, 5.96% H-3 => L+17, 5.69% H-26 => L+2, 2.35% H-11 => L+8, 2.32% H-30 => L+1, 2.12% H-7 => L+9
285	19354	517	0.00	40.6% H-11 => L+7, 16.2% H-9 => L+9, 10.5% H-13 => L+6, 7.58% H-5 => L+14, 3.82% H-9 => L+6, 3.12% H-44 => L+1
286	19388	516	0.00	47.0% H-28 => L+2, 13.2% H-22 => L+3, 5.47% H-3 => L+18, 5.31% H-31 => L+1, 5.13% H-6 => L+13, 4.53% H-1 => L+19, 2.45% H-31 => L+3, 2.17% H-21 => L+4
287	19389	516	0.00	66.8% H-51 => LUMO, 11.4% H-50 => L+1, 4.26% H-53 => LUMO, 3.98% H-49 => L+2, 2.80% H-52 => L+1
288	19410	515	0.00	54.8% H-27 => L+2, 9.52% H-8 => L+10, 5.46% H-15 => L+4, 5.18% H-30 => L+1, 5.00% H-25 => L+3, 4.11% H-3 => L+17
289	19434	515	0.00	27.4% H-13 => L+5, 20.0% H-3 => L+17, 9.50% H-8 => L+10, 4.84% H-1 => L+20, 3.37% H-15 => L+4, 2.80% H-2 => L+16, 2.27% H-19 => L+4, 2.21% H-15 => L+8
290	19437	514	0.00	35.6% H-5 => L+14, 9.90% H-2 => L+20, 9.31% H-16 => L+4, 8.69% H-11 => L+7, 4.65% H-7 => L+17, 4.10% H-6 => L+13, 3.56% H-4 => L+11, 3.05% H-3 => L+18
291	19449	514	0.04	19.4% H-5 => L+15, 17.5% H-7 => L+13, 11.4% H-2 => L+18, 7.42% H-8 => L+12, 5.61% H-30 => L+2, 3.82% H-25 => L+2, 3.19% H-10 => L+7, 2.25% H-4 => L+16
292	19514	512	0.00	52.4% H-29 => L+2, 7.84% H-30 => L+2, 4.87% H-17 => L+4, 3.86% H-26 => L+3, 2.99% H-32 => L+1, 2.60% H-33 => L+1, 2.34% H-4 => L+16
293	19573	511	0.01	20.4% H-16 => L+4, 15.1% H-3 => L+18, 11.5% H-5 => L+14, 7.55% H-22 => L+3, 7.53% H-4 => L+17, 6.52% H-6 => L+13, 3.65% H-2 => L+20, 3.04% H-1 => L+22, 2.37% H-14 => L+5
294	19592	510	0.00	43.8% H-22 => L+3, 26.5% H-28 => L+2, 3.27% H-4 => L+17, 3.05% H-21 => L+2, 2.67% H-5 => L+14, 2.53% H-21 => L+4, 2.33% H-3 => L+18
295	19615	510	0.00	26.9% H-10 => L+8, 8.64% H-31 => L+2, 8.46% H-3 => L+16, 8.04% H-8 => L+11, 5.33% H-6 => L+15, 4.81% H-7 => L+14, 3.52% H-5 => L+17,

				3.50% H-3 => L+19, 2.93% H-2 => L+17, 2.61% H-6 => L+18, 2.34% H-12 => L+11
296	19621	510	0.00	18.3% H-3 => L+17, 17.0% H-52 => LUMO, 14.7% H-13 => L+5, 9.32% H-9 => L+11, 5.29% H-11 => L+8, 5.09% H-6 => L+14, 4.84% H-8 => L+10, 4.71% H-10 => L+9, 2.96% H-51 => L+1
297	19627	510	0.00	48.9% H-52 => LUMO, 8.78% H-51 => L+1, 5.67% H-13 => L+5, 5.63% H-3 => L+17, 4.01% H-54 => LUMO, 3.51% H-9 => L+11, 3.08% H-50 => L+2, 2.03% H-6 => L+14, 2.01% H-11 => L+8
298	19678	508	0.00	33.9% H-17 => L+4, 8.61% H-3 => L+20, 8.56% H-30 => L+2, 3.76% H-2 => L+21, 3.06% H-6 => L+17, 2.99% H-4 => L+19, 2.86% H-2 => L+18, 2.63% H-29 => L+2, 2.31% H-24 => L+3, 2.19% H-10 => L+7, 2.13% H-19 => L+5
299	19682	508	0.00	29.2% H-10 => L+9, 15.2% H-8 => L+10, 8.20% H-13 => L+5, 5.91% H-12 => L+7, 5.68% H-11 => L+8, 3.44% H-19 => L+4, 2.85% H-8 => L+7, 2.49% H-10 => L+12, 2.28% H-14 => L+6, 2.21% H-2 => L+19, 2.12% H-2 => L+16
300	19688	508	0.14	23.3% H-31 => L+2, 14.6% H-8 => L+11, 10.8% H-10 => L+8, 6.54% H-7 => L+14, 5.92% H-9 => L+10, 3.63% H-6 => L+15, 2.87% H-3 => L+16, 2.51% H-5 => L+17, 2.15% H-11 => L+12, 2.13% H-11 => L+9
301	19694	508	0.05	18.6% H-4 => L+16, 14.2% H-30 => L+2, 11.3% H-20 => L+4, 7.65% H-7 => L+13, 6.69% H-8 => L+12, 4.97% H-17 => L+4, 4.47% H-25 => L+2, 4.35% H-2 => L+15, 3.23% H-10 => L+10, 3.16% H-2 => L+18, 2.21% H-27 => L+1
302	19744	506	0.01	29.4% H-31 => L+2, 17.8% H-6 => L+15, 11.6% H-3 => L+16, 5.08% H-9 => L+13, 2.95% H-34 => L+1, 2.90% H-21 => L+3, 2.48% H-11 => L+12, 2.14% H-28 => L+1
303	19750	506	0.00	17.0% H-30 => L+2, 14.9% H-2 => L+18, 14.7% H-4 => L+16, 9.10% H-29 => L+2, 6.10% H-17 => L+4, 4.84% H-12 => L+6, 4.42% H-2 => L+15, 4.20% H-10 => L+7, 2.41% H-20 => L+4, 2.33% H-5 => L+15
304	19778	506	0.00	23.4% H-6 => L+13, 23.3% H-9 => L+12, 8.10% H-11 => L+10, 5.31% H-13 => L+9, 3.54% H-3 => L+18, 3.36% H-4 => L+17, 3.11% H-2 => L+20, 2.95% H-17 => L+6, 2.70% H-15 => L+7, 2.42% H-22 => L+3, 2.17% H-14 => L+5
305	19826	504	0.00	37.1% H-6 => L+14, 32.1% H-11 => L+8, 5.96% H-32 => L+2, 3.45% H-3 => L+17, 3.34% H-33 => L+2, 2.07% H-23 => L+3
306	19828	504	0.07	37.4% H-5 => L+15, 9.84% H-4 => L+16, 7.21% H-8 => L+12, 5.00% H-4 => L+13, 3.76% H-7 => L+13, 3.53% H-10 => L+10, 3.45% H-29 => L+2,

				3.09% H-30 => L+2, 3.08% H-24 => L+3, 2.84% H-7 => L+16
307	19836	504	0.00	20.5% H-32 => L+2, 9.54% H-4 => L+18, 9.19% H-23 => L+3, 9.12% H-19 => L+4, 8.47% H-5 => L+16, 5.88% H-24 => L+2, 3.27% H-7 => L+15, 2.47% H-9 => L+11, 2.26% H-2 => L+19, 2.25% H-6 => L+14, 2.22% H-10 => L+9, 2.19% H-29 => L+3
308	19844	504	0.03	36.7% H-11 => L+9, 23.1% H-9 => L+10, 8.85% H-13 => L+7, 5.30% H-15 => L+6, 3.15% H-9 => L+7, 2.67% H-31 => L+2, 2.56% H-8 => L+11
309	19848	504	0.00	62.6% H-53 => LUMO, 11.1% H-52 => L+1, 5.00% H-55 => LUMO, 3.92% H-51 => L+2, 2.52% H-54 => L+1, 2.47% H-57 => LUMO, 2.05% H-56 => L+1
310	19859	504	0.00	14.1% H-23 => L+3, 13.3% H-2 => L+19, 8.00% H-24 => L+2, 7.56% H-19 => L+4, 7.23% H-11 => L+8, 5.20% H-33 => L+2, 3.88% H-7 => L+15, 3.39% H-24 => L+4, 3.23% H-8 => L+13, 2.39% H-10 => L+9, 2.37% H-12 => L+10, 2.01% H-10 => L+12
311	19866	503	0.01	42.0% H-14 => L+5, 14.4% H-3 => L+18, 6.97% H-34 => L+2, 5.87% H-1 => L+22, 5.55% H-12 => L+8, 5.11% H-16 => L+4, 3.08% H-3 => L+21
312	19896	503	0.00	16.2% H-32 => L+2, 15.1% H-19 => L+4, 12.9% H-33 => L+2, 6.25% H-10 => L+9, 4.85% H-11 => L+8, 3.69% H-2 => L+19, 3.57% H-23 => L+3, 2.93% H-35 => L+1, 2.46% H-6 => L+14
313	19915	502	0.01	33.4% H-24 => L+3, 12.6% H-23 => L+2, 10.3% H-12 => L+6, 6.58% H-23 => L+4, 5.79% H-5 => L+15, 3.75% H-2 => L+21, 3.08% H-3 => L+20, 2.27% H-10 => L+7
314	19915	502	0.00	28.4% H-4 => L+17, 16.1% H-2 => L+20, 8.43% H-9 => L+12, 7.36% H-5 => L+20, 7.13% H-2 => L+14, 4.90% H-3 => L+18, 4.46% H-3 => L+21, 3.05% H-6 => L+13, 2.18% H-6 => L+19, 2.11% H-34 => L+2
315	19948	501	0.02	25.5% H-18 => L+4, 10.2% H-3 => L+19, 8.18% H-21 => L+3, 6.45% H-1 => L+21, 6.34% H-3 => L+22, 5.60% H-16 => L+5, 5.17% H-8 => L+11, 4.13% H-6 => L+21, 2.33% H-14 => L+8, 2.31% H-31 => L+2, 2.03% H-6 => L+15
316	19949	501	0.00	21.8% H-33 => L+2, 19.0% H-23 => L+3, 5.04% H-4 => L+18, 4.97% H-9 => L+11, 4.84% H-24 => L+2, 4.49% H-6 => L+14, 3.91% H-5 => L+16, 3.51% H-24 => L+4, 3.22% H-19 => L+4, 2.61% H-30 => L+3, 2.58% H-2 => L+22
317	19953	501	0.02	20.8% H-12 => L+6, 18.5% H-20 => L+4, 8.32% H-7 => L+13, 6.75% H-24 => L+3, 5.78% H-30 => L+2, 5.03% H-29 => L+2, 2.41% H-10 => L+7, 2.23% H-4 => L+16, 2.11% H-23 => L+2

318	19968	501	0.04	27.6% H-12 => L+6, 16.9% H-7 => L+13, 16.7% H-20 => L+4, 5.03% H-14 => L+7, 4.72% H-2 => L+18, 4.66% H-10 => L+7, 2.77% H-4 => L+16, 2.15% H-5 => L+12
319	19979	501	0.00	49.7% H-9 => L+11, 13.1% H-6 => L+14, 11.1% H-11 => L+8, 9.47% H-33 => L+2
320	20018	500	0.23	17.2% H-7 => L+13, 16.7% H-20 => L+4, 11.9% H-8 => L+12, 6.85% H-3 => L+20, 5.34% H-10 => L+10, 3.50% H-2 => L+18, 3.16% H-35 => L+2, 2.74% H-2 => L+21, 2.55% H-12 => L+9, 2.42% H-8 => L+15, 2.19% H-5 => L+12
321	20024	499	0.00	62.5% H-54 => LUMO, 10.5% H-53 => L+1, 10.4% H-56 => LUMO, 3.56% H-52 => L+2, 2.98% H-57 => L+1
322	20057	499	0.00	35.7% H-8 => L+11, 21.0% H-7 => L+14, 10.8% H-5 => L+17, 7.85% H-18 => L+4, 5.51% H-4 => L+20, 2.17% H-10 => L+14
323	20083	498	0.00	59.7% H-34 => L+2, 12.2% H-3 => L+18, 3.81% H-31 => L+3, 3.45% H-31 => L+1, 2.82% H-14 => L+5, 2.80% H-36 => L+1, 2.16% H-36 => L+3
324	20085	498	0.32	48.9% H-35 => L+2, 4.49% H-40 => L+2, 4.43% H-38 => L+1, 4.35% H-33 => L+3, 4.04% H-2 => L+21, 2.90% H-33 => L+1, 2.03% H-13 => L+8
325	20115	497	0.00	12.6% H-10 => L+9, 12.3% H-19 => L+4, 10.6% H-32 => L+2, 9.83% H-12 => L+7, 7.41% H-2 => L+19, 6.06% H-4 => L+18, 5.67% H-5 => L+16, 4.20% H-23 => L+3, 3.50% H-14 => L+6, 2.88% H-2 => L+16, 2.71% H-33 => L+2, 2.63% H-4 => L+21
326	20178	496	0.00	27.9% H-2 => L+22, 12.2% H-32 => L+2, 9.32% H-4 => L+21, 7.60% H-33 => L+2, 2.71% H-8 => L+13, 2.27% H-7 => L+15, 2.20% H-6 => L+14, 2.11% H-10 => L+12, 2.06% H-12 => L+7
327	20180	496	0.01	56.0% H-55 => LUMO, 17.3% H-57 => LUMO, 6.38% H-54 => L+1, 2.13% H-8 => L+12, 2.06% H-53 => L+2
328	20187	495	0.11	19.9% H-8 => L+12, 12.3% H-2 => L+21, 9.02% H-4 => L+19, 6.82% H-3 => L+20, 6.81% H-35 => L+2, 6.29% H-55 => LUMO, 3.24% H-7 => L+13, 3.06% H-5 => L+18
329	20192	495	0.00	29.2% H-3 => L+21, 9.99% H-1 => L+22, 7.89% H-22 => L+3, 7.86% H-6 => L+19, 6.34% H-2 => L+20, 6.16% H-4 => L+17, 3.80% H-6 => L+16, 3.39% H-3 => L+18, 2.31% H-9 => L+12
330	20224	494	0.41	26.1% H-3 => L+19, 19.6% H-18 => L+4, 19.2% H-36 => L+2, 6.70% H-6 => L+15, 3.13% H-31 => L+2, 2.28% H-6 => L+21
331	20245	494	0.00	38.9% H-13 => L+6, 11.1% H-11 => L+7, 8.25% H-14 => L+5, 5.72% H-12 => L+8, 4.11% H-15 => L+7, 3.16% H-37 => L+2, 2.85% H-9 => L+6, 2.11% H-13 => L+9, 2.05% H-10 => L+11

332	20261	494	0.22	45.4% H-36 => L+2, 10.5% H-3 => L+19, 8.64% H-6 => L+15, 5.85% H-39 => L+2, 3.43% H-34 => L+1, 3.35% H-34 => L+3, 2.47% H-18 => L+4, 2.19% H-3 => L+22
333	20281	493	0.00	21.4% H-12 => L+8, 17.6% H-14 => L+5, 17.3% H-13 => L+6, 6.88% H-10 => L+11, 5.55% H-2 => L+20, 4.14% H-11 => L+7, 3.33% H-3 => L+18, 2.90% H-8 => L+14, 2.32% H-6 => L+16
334	20292	493	0.00	36.4% H-12 => L+7, 15.9% H-2 => L+19, 10.0% H-4 => L+18, 4.64% H-10 => L+9, 4.44% H-10 => L+6, 4.37% H-14 => L+6, 2.81% H-2 => L+16, 2.31% H-4 => L+21
335	20299	493	0.00	25.2% H-3 => L+20, 22.3% H-15 => L+5, 8.29% H-17 => L+4, 4.80% H-13 => L+8, 4.45% H-24 => L+3, 3.76% H-30 => L+2, 3.31% H-40 => L+2, 2.94% H-11 => L+11
336	20312	492	0.04	16.3% H-8 => L+12, 11.8% H-10 => L+10, 10.0% H-4 => L+19, 9.06% H-5 => L+18, 6.58% H-4 => L+22, 4.82% H-2 => L+18, 4.65% H-7 => L+16, 4.22% H-12 => L+9, 3.56% H-10 => L+13, 2.45% HOMO => L+24
337	20345	492	0.00	25.4% H-4 => L+18, 8.71% H-2 => L+22, 8.69% H-7 => L+15, 8.07% H-5 => L+16, 5.09% H-19 => L+4, 4.49% H-23 => L+3, 4.24% H-2 => L+16, 4.12% H-5 => L+19, 3.55% H-12 => L+7, 3.33% HOMO => L+23, 2.97% H-8 => L+13
338	20379	491	0.01	21.5% H-7 => L+14, 16.2% H-6 => L+15, 7.84% H-4 => L+20, 5.01% H-36 => L+2, 4.88% H-9 => L+13, 4.42% H-18 => L+4, 3.67% H-2 => L+17, 3.62% H-5 => L+17, 3.41% H-13 => L+10, 3.17% H-11 => L+12, 2.96% H-8 => L+17, 2.91% H-19 => L+6
339	20381	491	0.00	24.4% H-9 => L+12, 19.9% H-37 => L+2, 12.9% H-11 => L+10, 5.65% H-15 => L+7, 5.35% H-13 => L+9, 4.36% H-43 => L+2, 3.79% H-17 => L+6
340	20397	490	0.01	17.5% H-10 => L+10, 14.1% HOMO => L+24, 7.74% H-2 => L+21, 5.20% H-8 => L+12, 5.19% H-15 => L+5, 5.10% H-3 => L+20, 4.20% H-20 => L+4, 3.25% H-4 => L+22, 3.17% H-12 => L+9, 2.79% H-12 => L+12, 2.73% H-1 => L+23, 2.71% H-24 => L+3, 2.61% H-7 => L+16, 2.31% H-5 => L+18
341	20416	490	0.00	56.9% H-38 => L+2, 10.00% H-40 => L+1, 6.52% H-40 => L+3, 5.86% H-5 => L+16, 4.53% H-35 => L+1, 3.33% H-35 => L+3
342	20428	490	0.00	43.1% H-37 => L+2, 7.72% H-11 => L+10, 7.67% H-9 => L+12, 6.42% H-12 => L+8, 6.13% H-41 => L+2, 3.18% H-13 => L+9, 2.40% H-36 => L+3, 2.06% H-6 => L+16
343	20441	489	0.24	20.6% H-3 => L+22, 11.0% H-3 => L+19, 10.7% H-7 => L+14, 9.16% H-6 => L+15, 7.16% H-9 =>

				L+13, 5.55% H-4 => L+20, 3.70% H-11 => L+12, 2.27% H-18 => L+4, 2.26% H-1 => L+21, 2.11% H-15 => L+9
344	20451	489	0.01	62.0% H-40 => L+2, 12.0% H-38 => L+1, 9.84% H-38 => L+3, 3.09% H-15 => L+5, 2.32% H-35 => L+2
345	20466	489	0.00	33.8% H-5 => L+16, 7.31% H-38 => L+2, 6.24% H-25 => L+3, 5.45% H-8 => L+13, 5.25% HOMO => L+23, 3.98% H-4 => L+15, 3.85% H-10 => L+12, 2.81% H-7 => L+15, 2.34% H-19 => L+4, 2.25% H-7 => L+18, 2.07% H-12 => L+10
346	20509	488	0.00	16.6% H-5 => L+17, 15.5% H-13 => L+7, 15.2% H-11 => L+9, 8.78% H-15 => L+6, 7.38% H-7 => L+14, 5.28% H-42 => L+2, 2.44% H-13 => L+10, 2.29% H-4 => L+14, 2.27% H-3 => L+22, 2.22% H-39 => L+2, 2.19% H-18 => L+4
347	20525	487	0.00	57.1% H-39 => L+2, 10.9% H-42 => L+2, 3.67% H-37 => L+1, 2.92% H-37 => L+3, 2.54% H-18 => L+4, 2.33% H-5 => L+17
348	20560	486	0.00	53.3% H-56 => LUMO, 14.7% H-57 => L+1, 5.86% H-54 => LUMO, 5.84% H-56 => L+2, 4.99% H-55 => L+1, 2.29% H-52 => LUMO, 2.03% H-54 => L+2
349	20561	486	0.00	45.7% H-57 => LUMO, 17.8% H-56 => L+1, 10.3% H-55 => LUMO, 4.42% H-57 => L+2, 3.82% H-53 => LUMO, 2.69% H-54 => L+1, 2.53% H-55 => L+2
350	20566	486	0.05	15.9% H-5 => L+17, 11.2% H-13 => L+7, 7.02% H-3 => L+22, 6.87% H-39 => L+2, 6.72% H-18 => L+4, 6.58% H-11 => L+9, 6.24% H-42 => L+2, 4.46% H-16 => L+5, 3.67% H-15 => L+6, 2.00% H-11 => L+6
351	20570	486	0.02	16.0% H-15 => L+5, 11.0% H-26 => L+3, 10.8% H-10 => L+10, 7.24% H-3 => L+20, 4.80% H-5 => L+21, 3.66% H-29 => L+2, 3.29% HOMO => L+24, 3.25% H-6 => L+17, 3.05% H-7 => L+19, 3.04% H-9 => L+14, 2.40% H-12 => L+12, 2.06% H-4 => L+22
352	20575	486	0.00	23.8% HOMO => L+23, 9.39% H-25 => L+3, 5.57% H-7 => L+15, 4.24% H-4 => L+21, 4.05% H-5 => L+19, 3.78% H-1 => L+24, 3.31% H-2 => L+19, 3.11% H-5 => L+22, 2.81% H-17 => L+5, 2.68% H-7 => L+21, 2.65% H-27 => L+2, 2.62% H-7 => L+18, 2.30% H-8 => L+19
353	20578	486	0.00	62.8% H-41 => L+2, 10.4% H-43 => L+2, 3.32% H-12 => L+8, 2.81% H-39 => L+1, 2.40% H-39 => L+3, 2.23% H-9 => L+12
354	20598	485	0.00	52.1% H-43 => L+2, 6.79% H-6 => L+16, 6.71% H-12 => L+8, 6.17% H-42 => L+1, 4.97% H-42 => L+3, 2.87% H-41 => L+2, 2.47% H-45 => L+2, 2.23% H-21 => L+4

355	20611	485	0.02	51.4% H-42 => L+2, 6.06% H-13 => L+7, 4.83% H-43 => L+1, 4.00% H-43 => L+3, 3.59% H-39 => L+2, 3.44% H-11 => L+9, 3.01% H-41 => L+1, 2.80% H-15 => L+6, 2.72% H-44 => L+2, 2.60% H-41 => L+3
356	20620	485	0.01	14.8% H-6 => L+16, 14.3% H-12 => L+8, 10.2% H-43 => L+2, 9.01% H-21 => L+4, 6.06% H-37 => L+2, 4.17% H-3 => L+21, 3.74% H-41 => L+2, 3.25% H-22 => L+3, 2.03% H-18 => L+5, 2.02% H-34 => L+2
357	20667	484	0.00	32.6% H-7 => L+15, 31.5% H-25 => L+3, 6.43% H-5 => L+16, 3.01% H-27 => L+2, 2.93% H-5 => L+13, 2.35% H-17 => L+5, 2.06% HOMO => L+23
358	20678	484	0.00	16.6% H-10 => L+10, 14.8% HOMO => L+24, 14.0% H-4 => L+19, 9.37% H-12 => L+9, 4.93% H-2 => L+18, 3.35% H-14 => L+7, 3.31% H-2 => L+21, 2.80% H-26 => L+3, 2.76% H-5 => L+21, 2.43% H-14 => L+10
359	20725	483	0.00	16.9% H-10 => L+11, 16.8% H-21 => L+4, 16.7% H-12 => L+8, 8.87% H-8 => L+14, 6.09% H-6 => L+16, 3.48% H-7 => L+17, 2.80% H-2 => L+20, 2.15% H-14 => L+11

Chapter 4 Supporting Information:

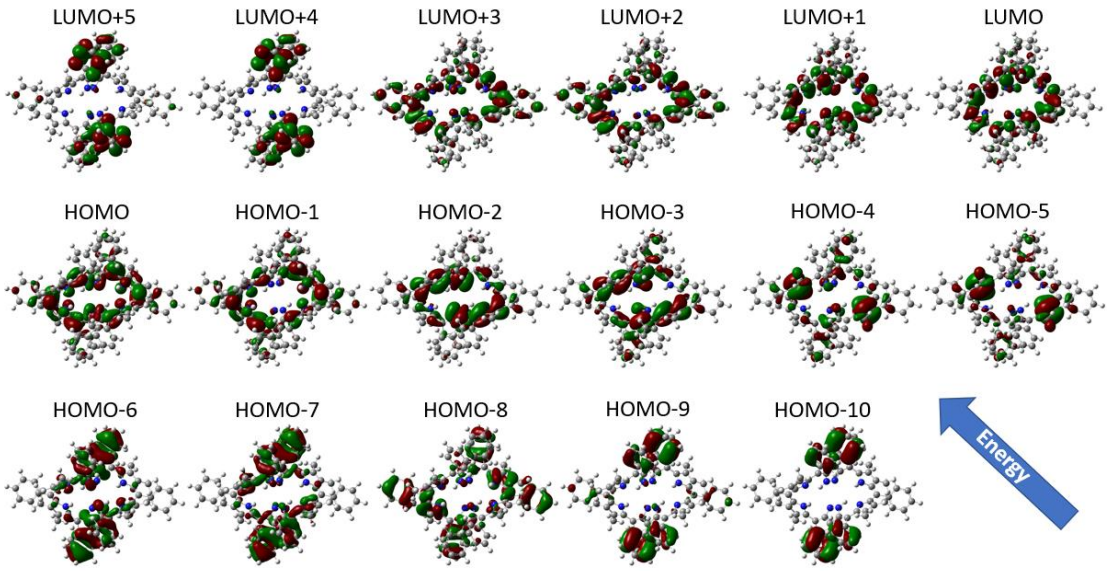


Figure S4.1. Select DFT-predicted molecular orbitals of **4.1**.

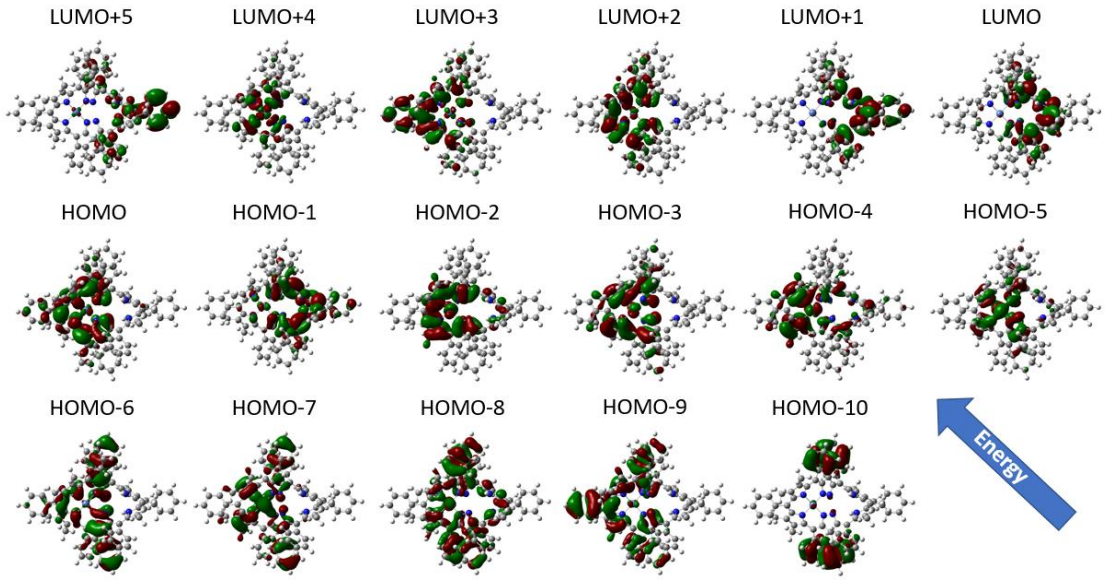


Figure S4.2. Select DFT-predicted molecular orbitals of **4.2**.

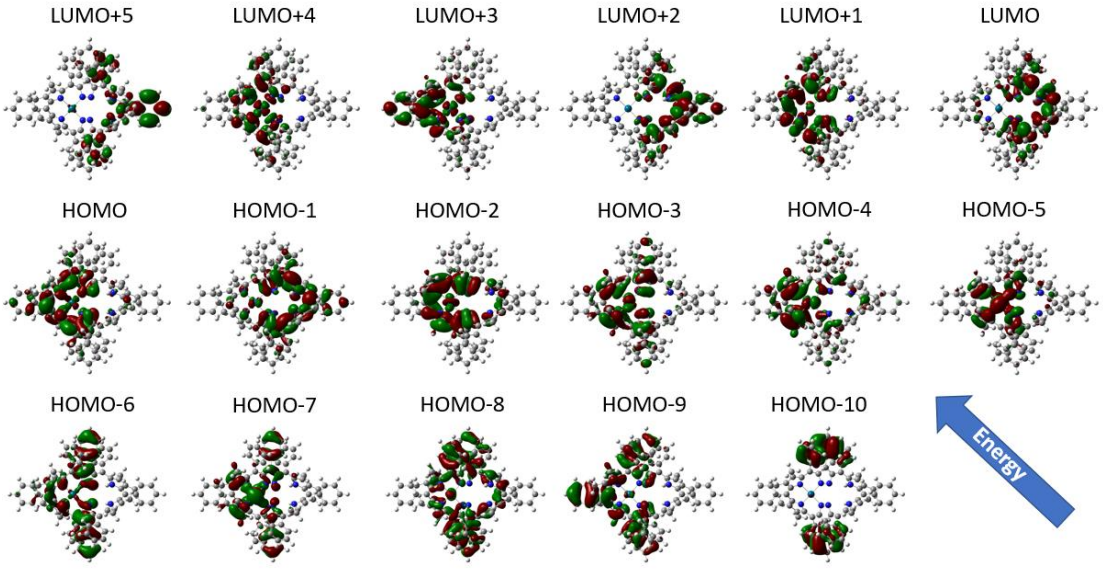


Figure S4.3. Select DFT-predicted molecular orbitals of **4.3**.

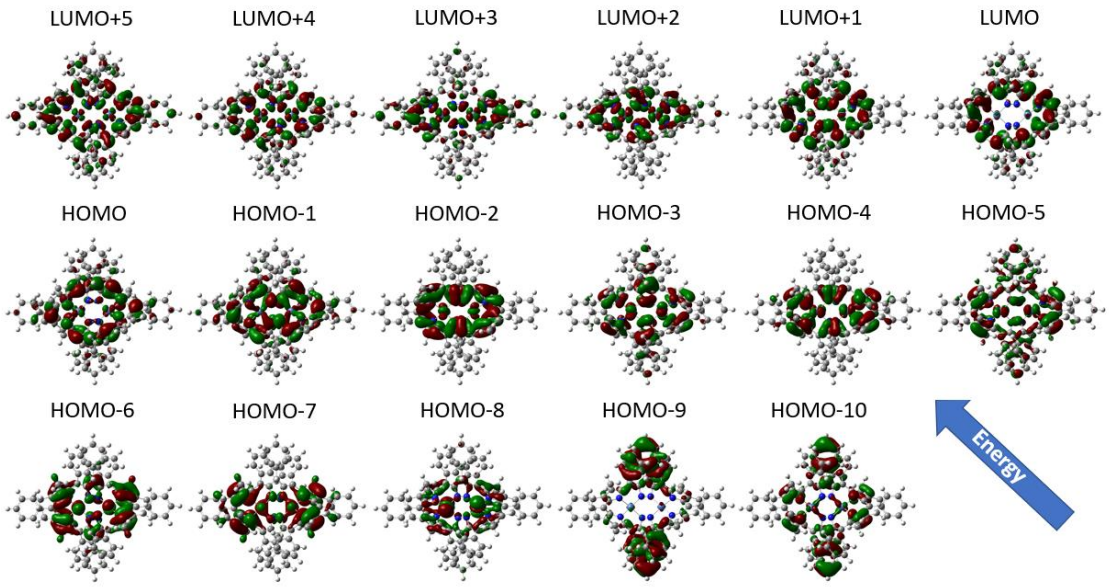


Figure S4.4. Select DFT-predicted molecular orbitals of **4.5**.

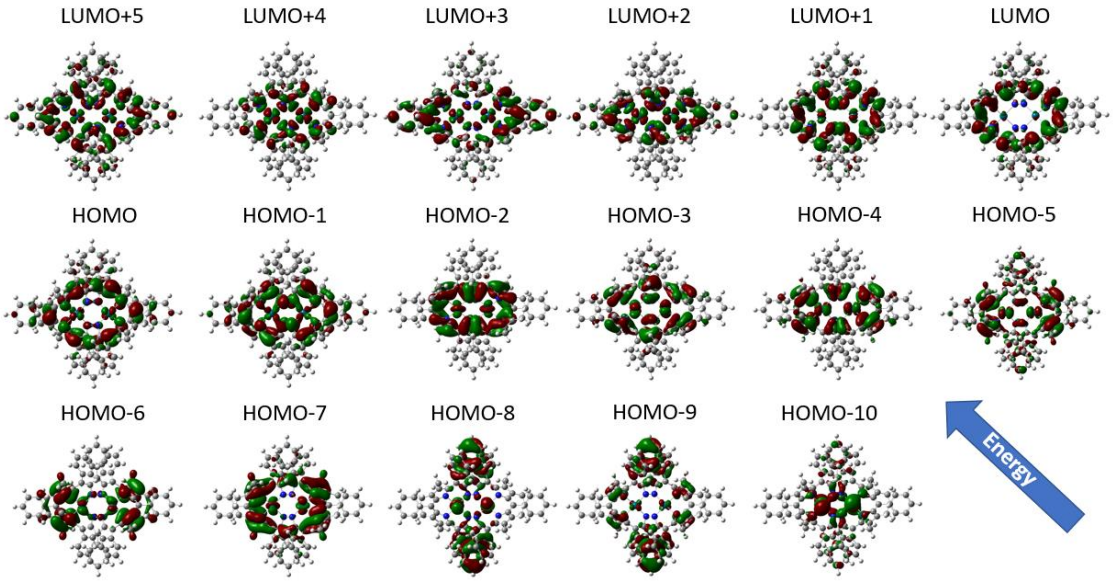


Figure S4.5. Select DFT-predicted molecular orbitals of **4.6**.

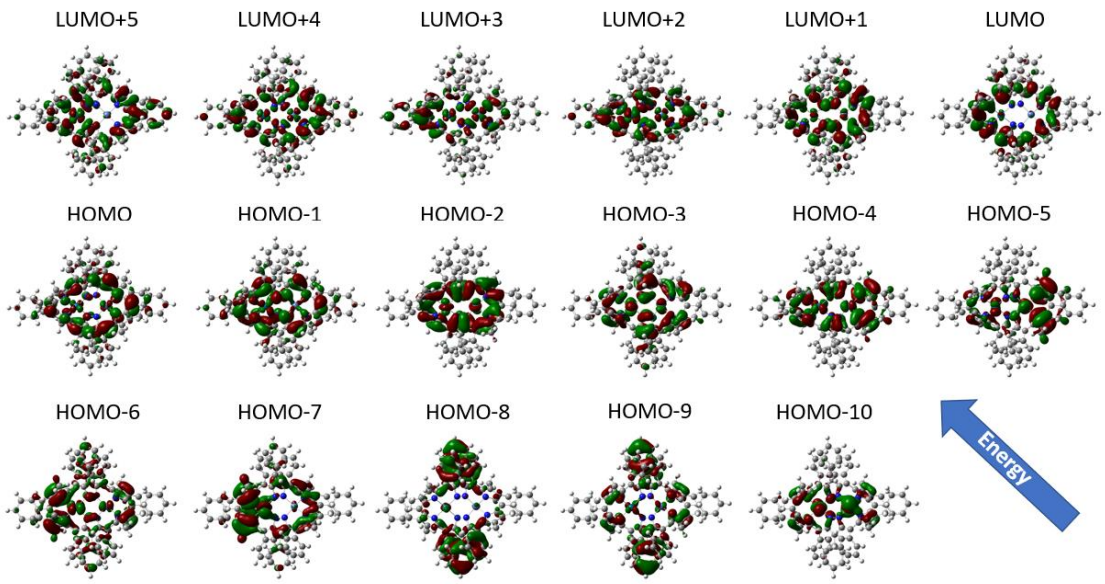


Figure S4.6. Select DFT-predicted molecular orbitals of **4.8**.

Table S4.1. Optimized coordinates of **4.1.**

N	3.76281	0.07339	-1.08445
N	2.65742	-2.27413	0.35775
N	0.86294	1.44835	-1.36241
N	0.10492	-1.7431	-0.4914
C	2.02935	-2.84565	1.47326
C	3.97021	-2.33548	0.58125
C	-0.23231	-2.71902	0.41228
C	1.88796	2.25637	-1.03489
C	4.75388	-0.8657	-1.26595
C	3.89702	1.15499	-1.95487
C	0.67404	-3.13837	1.48028
C	3.11146	2.27823	-1.87209
C	4.96744	-1.93963	-0.4055
C	5.48447	-0.43546	-2.46797
C	4.97557	0.77388	-2.87479
C	1.55821	3.08413	0.07651
C	0.23226	2.71903	0.41225
C	-1.88801	-2.25635	-1.03485
C	-1.55825	-3.08414	0.07653
C	3.0485	-3.14542	2.5058
C	4.25928	-2.85961	1.93476
H	1.05174	-1.38458	-0.60978
H	3.11146	0.04282	-0.31161
N	-0.10499	1.74314	-0.49145
N	-0.86302	-1.4483	-1.36235
C	-0.67406	3.13839	1.48026
C	-3.11152	-2.27822	-1.87204

C	-2.02937	2.84569	1.47328
C	-3.89709	-1.15498	-1.95481
C	-3.0485	3.14549	2.50584
N	-2.65747	2.27413	0.35782
C	-4.25929	2.85963	1.93486
C	-3.97025	2.33548	0.58134
C	-4.97563	-0.77383	-2.87473
C	-4.75392	0.86572	-1.26586
C	-5.48452	0.4355	-2.46789
N	-3.76283	-0.07336	-1.08441
C	-4.96749	1.93962	-0.40539
H	-1.05182	1.38465	-0.60985
H	-3.1116	-0.0429	-0.31147
C	2.48491	4.0894	0.65001
C	3.72161	3.683	1.18263
C	2.20164	5.46409	0.59743
C	4.64126	4.62018	1.6607
H	3.95901	2.62283	1.22915
C	3.1197	6.403	1.07434
H	1.26445	5.7987	0.16105
C	4.3432	5.98611	1.60933
H	5.58949	4.28336	2.07411
H	2.88137	7.46289	1.02128
H	5.05791	6.71792	1.97888
C	3.40444	3.552	-2.56987
C	4.67589	4.15423	-2.50911
C	2.3803	4.2285	-3.26437
C	4.92647	5.36943	-3.15011
H	5.46018	3.67745	-1.92745
C	2.63233	5.43981	-3.91086
H	1.38848	3.78582	-3.30912
C	3.90833	6.01562	-3.86018
H	5.91364	5.82116	-3.08126
H	1.83241	5.93602	-4.45591
H	4.10258	6.96288	-4.35781
C	-0.07824	3.94245	2.58874
C	-0.45746	5.28017	2.78518
C	0.87522	3.37883	3.45321
C	0.08886	6.03228	3.82817
H	-1.1831	5.7299	2.11188
C	1.41309	4.12511	4.50436
H	1.18551	2.34703	3.30739
C	1.0219	5.45538	4.69597
H	-0.21215	7.06894	3.96126
H	2.14292	3.67021	5.16981
H	1.44736	6.03868	5.5091
C	-2.48491	-4.08948	0.64995
C	-2.20155	-5.46416	0.59734
C	-3.72167	-3.68318	1.1825
C	-3.11957	-6.40314	1.07418
H	-1.26432	-5.79869	0.161
C	-4.64129	-4.62043	1.6605
H	-3.95915	-2.62303	1.22903
C	-4.34314	-5.98635	1.6091

H	-2.88118	-7.46301	1.02109
H	-5.58957	-4.28369	2.07385
H	-5.05782	-6.71821	1.9786
C	-3.4045	-3.55199	-2.56982
C	-4.67587	-4.15436	-2.50886
C	-2.38039	-4.22838	-3.26448
C	-4.92642	-5.36958	-3.14985
H	-5.46011	-3.67769	-1.92705
C	-2.6324	-5.4397	-3.91096
H	-1.38862	-3.7856	-3.30938
C	-3.90833	-6.01565	-3.8601
H	-5.91353	-5.82142	-3.08083
H	-1.83251	-5.93581	-4.45614
H	-4.10256	-6.96292	-4.35771
C	0.07828	-3.94245	2.58877
C	-0.87509	-3.37882	3.45334
C	0.4575	-5.28017	2.78516
C	-1.41287	-4.12511	4.50454
H	-1.18537	-2.34701	3.30757
C	-0.08873	-6.03228	3.8282
H	1.18306	-5.72991	2.1118
C	-1.02168	-5.45538	4.69609
H	-2.14263	-3.6702	5.17006
H	0.21227	-7.06895	3.96125
H	-1.44707	-6.03868	5.50926
C	-6.23548	2.71866	-0.44703
C	-7.49406	2.09648	-0.33539
C	-6.20299	4.12279	-0.56081
C	-8.67406	2.84396	-0.35229
H	-7.54122	1.01657	-0.21572
C	-7.38147	4.87372	-0.57759
H	-5.24198	4.62379	-0.6502
C	-8.62465	4.23782	-0.47514
H	-9.63339	2.3395	-0.25887
H	-7.33001	5.95594	-0.67479
H	-9.54242	4.82096	-0.48594
C	6.23544	-2.71865	-0.44709
C	6.20298	-4.12278	-0.56082
C	7.49401	-2.09644	-0.33545
C	7.38147	-4.87369	-0.57755
H	5.24197	-4.6238	-0.6502
C	8.67403	-2.84391	-0.3523
H	7.54115	-1.01653	-0.21581
C	8.62463	-4.23777	-0.47511
H	7.33002	-5.95592	-0.6747
H	9.63334	-2.33943	-0.25889
H	9.54242	-4.8209	-0.48586
C	6.50136	-1.25026	-3.221
C	5.34411	1.50225	-4.13791
C	-2.83653	3.55602	3.93954
C	-5.60869	2.9337	2.5952
C	-6.50138	1.25035	-3.22091
C	-5.34415	-1.50217	-4.13788
C	2.83661	-3.55583	3.93953

C	5.60869	-2.9337	2.59507
H	6.32456	-2.3209	-3.10253
H	6.46081	-1.01892	-4.28915
H	7.52507	-1.05526	-2.88477
H	6.15355	2.22275	-3.979
H	5.68228	0.79818	-4.90346
H	4.49515	2.05722	-4.54084
H	-3.66209	3.19932	4.56275
H	-1.91041	3.14747	4.34866
H	-2.78457	4.64288	4.06208
H	-6.22729	2.06794	2.34203
H	-5.5125	2.9684	3.68402
H	-6.17062	3.82259	2.28847
H	-6.46077	1.01911	-4.28907
H	-7.52511	1.05529	-2.88476
H	-6.32462	2.32098	-3.10233
H	-5.68266	-0.79811	-4.90329
H	-4.49508	-2.05682	-4.541
H	-6.15332	-2.22294	-3.97892
H	2.78492	-4.6427	4.06219
H	3.66208	-3.19886	4.56271
H	1.91039	-3.14747	4.34861
H	5.51254	-2.96801	3.68391
H	6.17043	-3.82282	2.28863
H	6.22746	-2.06817	2.34158

Table S4.2. Optimized coordinates of **4.2.**

N	1.24738	0.84899	-3.34043
N	-1.24738	-0.84899	-3.34043
N	1.32285	0.8177	-0.29141
N	-1.32285	-0.8177	-0.29141
C	-2.07295	-1.92411	-2.98576
C	-0.72856	-1.00732	-4.59685
C	-2.58441	-0.91747	-0.79495
C	2.58441	0.91747	-0.79495
C	0.72856	1.00732	-4.59685
C	2.07295	1.92411	-2.98576
C	-2.86706	-1.88706	-1.85044
C	2.86706	1.88706	-1.85044
C	0.	0.	-5.28762
C	1.1144	2.33897	-5.03116
C	1.91998	2.89576	-4.05253
C	3.47189	0.05246	-0.10136
C	2.64221	-0.57208	0.8565
C	-2.64221	0.57208	0.8565
C	-3.47189	-0.05246	-0.10136
C	-1.91998	-2.89576	-4.05253
C	-1.1144	-2.33897	-5.03116
H	1.22032	-0.0085	-2.79994
N	1.3723	-0.05568	0.7104
N	-1.3723	0.05568	0.7104
C	2.91566	-1.59636	1.84681

C	-2.91566	1.59636	1.84681
C	2.1417	-1.6756	2.99011
C	-2.1417	1.6756	2.99011
C	2.20786	-2.64521	4.09216
N	1.20261	-0.68801	3.32908
C	1.43635	-2.14761	5.10938
C	0.83133	-0.89874	4.62338
C	-2.20786	2.64521	4.09216
C	-0.83133	0.89874	4.62338
C	-1.43635	2.14761	5.10938
N	-1.20261	0.68801	3.32908
C	0.	0.	5.33414
C	4.91906	-0.103	-0.36933
C	5.37271	-0.49626	-1.6417
C	5.88048	0.18365	0.61564
C	6.73783	-0.60245	-1.92073
H	4.64462	-0.73507	-2.41373
C	7.2458	0.0795	0.33978
H	5.55039	0.50754	1.59936
C	7.68252	-0.31397	-0.93008
H	7.06379	-0.91587	-2.91036
H	7.97097	0.3106	1.11711
H	8.74575	-0.39497	-1.14439
C	4.013	2.80321	-1.66197
C	4.95624	3.03692	-2.68075
C	4.19035	3.44668	-0.42031
C	6.02753	3.90722	-2.47558
H	4.86131	2.50666	-3.62452
C	5.25191	4.33008	-0.22178
H	3.47649	3.26218	0.3778
C	6.17481	4.56482	-1.24859
H	6.75615	4.06299	-3.26781
H	5.36311	4.83231	0.73625
H	7.0096	5.2432	-1.08903
C	4.04915	-2.52978	1.59185
C	5.14921	-2.60636	2.46241
C	4.04257	-3.35251	0.45099
C	6.19802	-3.49631	2.21797
H	5.18081	-1.95701	3.33386
C	5.08474	-4.25055	0.20936
H	3.2033	-3.29657	-0.23799
C	6.16709	-4.32863	1.09416
H	7.04285	-3.53529	2.90217
H	5.05367	-4.88876	-0.67091
H	6.98214	-5.0229	0.90329
C	-4.91906	0.103	-0.36933
C	-5.37271	0.49626	-1.6417
C	-5.88048	-0.18365	0.61564
C	-6.73783	0.60245	-1.92073
H	-4.64462	0.73507	-2.41373
C	-7.2458	-0.0795	0.33978
H	-5.55039	-0.50754	1.59936
C	-7.68252	0.31397	-0.93008
H	-7.06379	0.91587	-2.91036

H	-7.97097	-0.3106	1.11711
H	-8.74575	0.39497	-1.14439
C	-4.04915	2.52978	1.59185
C	-5.14921	2.60636	2.46241
C	-4.04257	3.35251	0.45099
C	-6.19802	3.49631	2.21797
H	-5.18081	1.95701	3.33386
C	-5.08474	4.25055	0.20936
H	-3.2033	3.29657	-0.23799
C	-6.16709	4.32863	1.09416
H	-7.04285	3.53529	2.90217
H	-5.05367	4.88876	-0.67091
H	-6.98214	5.0229	0.90329
C	-4.013	-2.80321	-1.66197
C	-4.19035	-3.44668	-0.42031
C	-4.95624	-3.03692	-2.68075
C	-5.25191	-4.33008	-0.22178
H	-3.47649	-3.26218	0.3778
C	-6.02753	-3.90722	-2.47558
H	-4.86131	-2.50666	-3.62452
C	-6.17481	-4.56482	-1.24859
H	-5.36311	-4.83231	0.73625
H	-6.75615	-4.06299	-3.26781
H	-7.0096	-5.2432	-1.08903
C	0.	0.	6.82354
C	-1.18856	-0.20407	7.5502
C	1.18856	0.20407	7.5502
C	-1.1907	-0.20564	8.94771
H	-2.11538	-0.37502	7.00739
C	1.1907	0.20564	8.94771
H	2.11538	0.37502	7.00739
C	0.	0.	9.6549
H	-2.12142	-0.37259	9.48577
H	2.12142	0.37259	9.48577
H	0.	0.	10.74242
C	0.	0.	-6.77524
C	-1.20416	-0.08571	-7.50254
C	1.20416	0.08571	-7.50254
C	-1.2054	-0.08706	-8.89944
H	-2.14695	-0.13584	-6.96283
C	1.2054	0.08706	-8.89944
H	2.14695	0.13584	-6.96283
C	0.	0.	-9.60652
H	-2.14881	-0.14737	-9.43748
H	2.14881	0.14737	-9.43748
H	0.	0.	-10.69379
C	0.62071	3.04657	-6.26355
C	2.40213	4.32113	-4.0384
C	2.87542	-3.9957	4.08827
C	1.15641	-2.83575	6.41825
C	-1.15641	2.83575	6.41825
C	-2.87542	3.9957	4.08827
C	-2.40213	-4.32113	-4.0384
C	-0.62071	-3.04657	-6.26355

H	-0.36601	2.69034	-6.5659
H	0.5493	4.12346	-6.08403
H	1.28949	2.90239	-7.11927
H	2.63736	4.65874	-3.02885
H	3.30202	4.45734	-4.64812
H	1.63319	4.98511	-4.44629
H	2.2953	-4.7021	4.69005
H	2.95587	-4.40609	3.08071
H	3.88706	-3.9699	4.50708
H	0.12002	-2.69795	6.73468
H	1.34183	-3.91051	6.33554
H	1.7873	-2.45946	7.23066
H	-1.34183	3.91051	6.33554
H	-1.7873	2.45946	7.23066
H	-0.12002	2.69795	6.73468
H	-2.2953	4.7021	4.69005
H	-2.95587	4.40609	3.08071
H	-3.88706	3.9699	4.50708
H	-2.63736	-4.65874	-3.02885
H	-3.30202	-4.45734	-4.64812
H	-1.63319	-4.98511	-4.44629
H	-0.5493	-4.12346	-6.08403
H	-1.28949	-2.90239	-7.11927
H	0.36601	-2.69034	-6.5659
Ni	0.	0.	2.01425
H	-1.22032	0.0085	-2.79994

Table S4.3. Optimized coordinates of **4.3.**

N	1.36168	0.74419	-3.50177
N	-1.36168	-0.74419	-3.50177
N	1.50848	0.57654	-0.58307
N	-1.50848	-0.57654	-0.58307
C	-2.26358	-1.76184	-3.16555
C	-0.81496	-0.94563	-4.73958
C	-2.80479	-0.75671	-0.97163
C	2.80479	0.75671	-0.97163
C	0.81496	0.94563	-4.73958
C	2.26358	1.76184	-3.16555
C	-3.09137	-1.68933	-2.0522
C	3.09137	1.68933	-2.0522
C	0.	0.	-5.42239
C	1.28197	2.24689	-5.18449
C	2.14813	2.74559	-4.22714
C	3.67881	0.01272	-0.12812
C	2.80708	-0.60904	0.79278
C	-2.80708	0.60904	0.79278
C	-3.67881	-0.01272	-0.12812
C	-2.14813	-2.74559	-4.22714
C	-1.28197	-2.24689	-5.18449
H	1.23722	-0.0798	-2.92348
N	1.51756	-0.21765	0.47654
N	-1.51756	0.21765	0.47654

C	3.06909	-1.56729	1.85642
C	-3.06909	1.56729	1.85642
C	2.27909	-1.62363	2.99315
C	-2.27909	1.62363	2.99315
C	2.29494	-2.60566	4.0884
N	1.3457	-0.62372	3.31475
C	1.4722	-2.12316	5.07307
C	0.88754	-0.86755	4.57733
C	-2.29494	2.60566	4.0884
C	-0.88754	0.86755	4.57733
C	-1.4722	2.12316	5.07307
N	-1.3457	0.62372	3.31475
C	0.	0.	5.26726
C	5.15444	-0.05529	-0.20669
C	5.79514	-0.46997	-1.38793
C	5.95714	0.31968	0.88537
C	7.18886	-0.50951	-1.47625
H	5.19153	-0.77692	-2.23897
C	7.35063	0.2822	0.79979
H	5.47993	0.65859	1.8016
C	7.97465	-0.13291	-0.38183
H	7.66162	-0.83921	-2.39897
H	7.95099	0.58134	1.65636
H	9.05982	-0.16258	-0.44861
C	4.27364	2.57537	-1.92444
C	5.21511	2.70491	-2.96193
C	4.47804	3.30364	-0.73633
C	6.31514	3.55333	-2.82731
H	5.09099	2.11766	-3.8681
C	5.56899	4.16426	-0.608
H	3.76421	3.20356	0.07678
C	6.49253	4.2932	-1.6526
H	7.04026	3.62937	-3.6343
H	5.70225	4.7315	0.31009
H	7.34884	4.95503	-1.54689
C	4.21003	-2.5055	1.65408
C	5.28179	-2.57134	2.56005
C	4.23672	-3.34635	0.52618
C	6.33555	-3.46659	2.36127
H	5.28889	-1.90744	3.42085
C	5.28209	-4.25157	0.33193
H	3.41997	-3.29921	-0.18988
C	6.33676	-4.31708	1.25066
H	7.15969	-3.49522	3.07065
H	5.27566	-4.9048	-0.53776
H	7.1557	-5.01579	1.09612
C	-5.15444	0.05529	-0.20669
C	-5.79514	0.46997	-1.38793
C	-5.95714	-0.31968	0.88537
C	-7.18886	0.50951	-1.47625
H	-5.19153	0.77692	-2.23897
C	-7.35063	-0.2822	0.79979
H	-5.47993	-0.65859	1.8016
C	-7.97465	0.13291	-0.38183

H	-7.66162	0.83921	-2.39897
H	-7.95099	-0.58134	1.65636
H	-9.05982	0.16258	-0.44861
C	-4.21003	2.5055	1.65408
C	-5.28179	2.57134	2.56005
C	-4.23672	3.34635	0.52618
C	-6.33555	3.46659	2.36127
H	-5.28889	1.90744	3.42085
C	-5.28209	4.25157	0.33193
H	-3.41997	3.29921	-0.18988
C	-6.33676	4.31708	1.25066
H	-7.15969	3.49522	3.07065
H	-5.27566	4.9048	-0.53776
H	-7.1557	5.01579	1.09612
C	-4.27364	-2.57537	-1.92444
C	-4.47804	-3.30364	-0.73633
C	-5.21511	-2.70491	-2.96193
C	-5.56899	-4.16426	-0.608
H	-3.76421	-3.20356	0.07678
C	-6.31514	-3.55333	-2.82731
H	-5.09099	-2.11766	-3.8681
C	-6.49253	-4.2932	-1.6526
H	-5.70225	-4.7315	0.31009
H	-7.04026	-3.62937	-3.6343
H	-7.34884	-4.95503	-1.54689
C	0.	0.	6.75676
C	-1.19149	-0.18945	7.48356
C	1.19149	0.18945	7.48356
C	-1.19333	-0.19151	8.88075
H	-2.12039	-0.34976	6.94125
C	1.19333	0.19151	8.88075
H	2.12039	0.34976	6.94125
C	0.	0.	9.58789
H	-2.12582	-0.34799	9.4188
H	2.12582	0.34799	9.4188
H	0.	0.	10.67538
C	0.	0.	-6.90989
C	-1.20698	-0.014	-7.63812
C	1.20698	0.014	-7.63812
C	-1.2082	-0.01528	-9.03487
H	-2.15108	-0.00803	-7.09854
C	1.2082	0.01528	-9.03487
H	2.15108	0.00803	-7.09854
C	0.	0.	-9.74225
H	-2.15356	-0.01899	-9.57292
H	2.15356	0.01899	-9.57292
H	0.	0.	-10.82953
C	0.80264	2.99011	-6.40181
C	2.72017	4.13774	-4.23093
C	2.95633	-3.95918	4.10043
C	1.11498	-2.83843	6.34868
C	-1.11498	2.83843	6.34868
C	-2.95633	3.95918	4.10043
C	-2.72017	-4.13774	-4.23093

C	-0.80264	-2.99011	-6.40181
H	-0.20307	2.68169	-6.69302
H	0.78068	4.06698	-6.20917
H	1.45195	2.82777	-7.26924
H	2.96841	4.47781	-3.22535
H	3.63151	4.20913	-4.83431
H	1.99681	4.841	-4.65545
H	2.35879	-4.66402	4.6863
H	3.06213	-4.36893	3.09488
H	3.95691	-3.93702	4.54501
H	0.06799	-2.68408	6.61833
H	1.27874	-3.91493	6.24654
H	1.7146	-2.49862	7.19999
H	-1.27874	3.91493	6.24654
H	-1.7146	2.49862	7.19999
H	-0.06799	2.68408	6.61833
H	-2.35879	4.66402	4.6863
H	-3.06213	4.36893	3.09488
H	-3.95691	3.93702	4.54501
H	-2.96841	-4.47781	-3.22535
H	-3.63151	-4.20913	-4.83431
H	-1.99681	-4.841	-4.65545
H	-0.78068	-4.06698	-6.20917
H	-1.45195	-2.82777	-7.26924
H	0.20307	-2.68169	-6.69302
H	-1.23722	0.0798	-2.92348
Pd	0.	0.	1.86628

Table S4.4. Optimized coordinates of **4.5.**

N	-0.7846	1.12397	-3.26116
N	0.7846	-1.12397	-3.26116
N	-0.40447	1.30656	-0.54471
N	0.40447	-1.30656	-0.54471
C	1.79858	-2.0492	-2.9651
C	0.96351	-0.74612	-4.56094
C	0.71146	-2.60158	-0.85573
C	-0.71146	2.60158	-0.85573
C	-0.96351	0.74612	-4.56094
C	-1.79858	2.0492	-2.9651
C	1.71016	-2.88024	-1.87034
C	-1.71016	2.88024	-1.87034
C	0.	0.	-5.27277
C	-2.23374	1.28949	-5.06586
C	-2.76362	2.06387	-4.06951
C	0.	3.47037	0.
C	0.71146	2.60158	0.85573
C	-0.71146	-2.60158	0.85573
C	0.	-3.47037	0.
C	2.76362	-2.06387	-4.06951
C	2.23374	-1.28949	-5.06586
N	0.40447	1.30656	0.54471
N	-0.40447	-1.30656	0.54471

C	1.71016	2.88024	1.87034
C	-1.71016	-2.88024	1.87034
C	1.79858	2.0492	2.9651
C	-1.79858	-2.0492	2.9651
C	2.76362	2.06387	4.06951
N	0.7846	1.12397	3.26116
C	2.23374	1.28949	5.06586
C	0.96351	0.74612	4.56094
C	-2.76362	-2.06387	4.06951
C	-0.96351	-0.74612	4.56094
C	-2.23374	-1.28949	5.06586
N	-0.7846	-1.12397	3.26116
C	0.	0.	5.27277
C	0.	4.95074	0.
C	0.39608	5.67109	-1.13991
C	-0.39608	5.67109	1.13991
C	0.39752	7.06795	-1.14099
H	0.71682	5.12768	-2.02552
C	-0.39752	7.06795	1.14099
H	-0.71682	5.12768	2.02552
C	0.	7.77335	0.
H	0.71296	7.60643	-2.03204
H	-0.71296	7.60643	2.03204
H	0.	8.86098	0.
C	-2.62024	4.03848	-1.65472
C	-2.71919	5.08562	-2.58618
C	-3.40305	4.10397	-0.48729
C	-3.59255	6.15434	-2.37187
H	-2.09624	5.06427	-3.47676
C	-4.28514	5.16598	-0.27658
H	-3.32915	3.30676	0.24824
C	-4.38518	6.19567	-1.21974
H	-3.64812	6.95965	-3.10089
H	-4.89308	5.19114	0.62487
H	-5.06638	7.02683	-1.05311
C	2.62024	4.03848	1.65472
C	2.71919	5.08562	2.58618
C	3.40305	4.10397	0.48729
C	3.59255	6.15434	2.37187
H	2.09624	5.06427	3.47676
C	4.28514	5.16598	0.27658
H	3.32915	3.30676	-0.24824
C	4.38518	6.19567	1.21974
H	3.64812	6.95965	3.10089
H	4.89308	5.19114	-0.62487
H	5.06638	7.02683	1.05311
C	0.	-4.95074	0.
C	-0.39608	-5.67109	-1.13991
C	0.39608	-5.67109	1.13991
C	-0.39752	-7.06795	-1.14099
H	-0.71682	-5.12768	-2.02552
C	0.39752	-7.06795	1.14099
H	0.71682	-5.12768	2.02552
C	0.	-7.77335	0.

H	-0.71296	-7.60643	-2.03204
H	0.71296	-7.60643	2.03204
H	0.	-8.86098	0.
C	-2.62024	-4.03848	1.65472
C	-2.71919	-5.08562	2.58618
C	-3.40305	-4.10397	0.48729
C	-3.59255	-6.15434	2.37187
H	-2.09624	-5.06427	3.47676
C	-4.28514	-5.16598	0.27658
H	-3.32915	-3.30676	-0.24824
C	-4.38518	-6.19567	1.21974
H	-3.64812	-6.95965	3.10089
H	-4.89308	-5.19114	-0.62487
H	-5.06638	-7.02683	1.05311
C	2.62024	-4.03848	-1.65472
C	3.40305	-4.10397	-0.48729
C	2.71919	-5.08562	-2.58618
C	4.28514	-5.16598	-0.27658
H	3.32915	-3.30676	0.24824
C	3.59255	-6.15434	-2.37187
H	2.09624	-5.06427	-3.47676
C	4.38518	-6.19567	-1.21974
H	4.89308	-5.19114	0.62487
H	3.64812	-6.95965	-3.10089
H	5.06638	-7.02683	-1.05311
C	0.	0.	6.76396
C	0.15196	-1.19679	7.48822
C	-0.15196	1.19679	7.48822
C	0.15473	-1.19879	8.88592
H	0.28055	-2.13044	6.94545
C	-0.15473	1.19879	8.88592
H	-0.28055	2.13044	6.94545
C	0.	0.	9.59222
H	0.28151	-2.13552	9.42421
H	-0.28151	2.13552	9.42421
H	0.	0.	10.67966
C	0.	0.	-6.76396
C	-0.15196	-1.19679	-7.48822
C	0.15196	1.19679	-7.48822
C	-0.15473	-1.19879	-8.88592
H	-0.28055	-2.13044	-6.94545
C	0.15473	1.19879	-8.88592
H	0.28055	2.13044	-6.94545
C	0.	0.	-9.59222
H	-0.28151	-2.13552	-9.42421
H	0.28151	2.13552	-9.42421
H	0.	0.	-10.67966
C	-2.90451	0.95957	-6.37197
C	-4.12979	2.69702	-4.07809
C	4.12979	2.69702	4.07809
C	2.90451	0.95957	6.37197
C	-2.90451	-0.95957	6.37197
C	-4.12979	-2.69702	4.07809
C	4.12979	-2.69702	-4.07809

C	2.90451	-0.95957	-6.37197
H	-2.71832	-0.07306	-6.67525
H	-3.98674	1.0959	-6.29015
H	-2.55817	1.5978	-7.19172
H	-4.13405	3.68571	-4.54922
H	-4.83039	2.06954	-4.63817
H	-4.5257	2.81984	-3.06888
H	4.83039	2.06954	4.63817
H	4.5257	2.81984	3.06888
H	4.13405	3.68571	4.54922
H	2.71832	-0.07306	6.67525
H	3.98674	1.0959	6.29015
H	2.55817	1.5978	7.19172
H	-3.98674	-1.0959	6.29015
H	-2.55817	-1.5978	7.19172
H	-2.71832	0.07306	6.67525
H	-4.83039	-2.06954	4.63817
H	-4.5257	-2.81984	3.06888
H	-4.13405	-3.68571	4.54922
H	4.13405	-3.68571	-4.54922
H	4.83039	-2.06954	-4.63817
H	4.5257	-2.81984	-3.06888
H	3.98674	-1.0959	-6.29015
H	2.55817	-1.5978	-7.19172
H	2.71832	0.07306	-6.67525
Ni	0.	0.	1.91468
Ni	0.	0.	-1.91468

Table S4.5. Optimized coordinates of **4.6.**

N	-0.63859	1.32726	-3.44684
N	0.63859	-1.32726	-3.44684
N	-0.37956	1.47047	-0.55523
N	0.37956	-1.47047	-0.55523
C	1.6137	-2.29132	-3.14507
C	0.867	-0.88753	-4.71959
C	0.6484	-2.76646	-0.91137
C	-0.6484	2.76646	-0.91137
C	-0.867	0.88753	-4.71959
C	-1.6137	2.29132	-3.14507
C	1.55612	-3.07306	-2.00677
C	-1.55612	3.07306	-2.00677
C	0.	0.	-5.40656
C	-2.09575	1.51219	-5.23778
C	-2.56605	2.35309	-4.26407
C	0.	3.63146	0.
C	0.6484	2.76646	0.91137
C	-0.6484	-2.76646	0.91137
C	0.	-3.63146	0.
C	2.56605	-2.35309	-4.26407
C	2.09575	-1.51219	-5.23778
N	0.37956	1.47047	0.55523
N	-0.37956	-1.47047	0.55523

C	1.55612	3.07306	2.00677
C	-1.55612	-3.07306	2.00677
C	1.6137	2.29132	3.14507
C	-1.6137	-2.29132	3.14507
C	2.56605	2.35309	4.26407
N	0.63859	1.32726	3.44684
C	2.09575	1.51219	5.23778
C	0.867	0.88753	4.71959
C	-2.56605	-2.35309	4.26407
C	-0.867	-0.88753	4.71959
C	-2.09575	-1.51219	5.23778
N	-0.63859	-1.32726	3.44684
C	0.	0.	5.40656
C	0.	5.11515	0.
C	0.64671	5.83393	-1.01907
C	-0.64671	5.83393	1.01907
C	0.64975	7.2312	-1.01895
H	1.16088	5.28984	-1.80769
C	-0.64975	7.2312	1.01895
H	-1.16088	5.28984	1.80769
C	0.	7.93612	0.
H	1.16327	7.76967	-1.81255
H	-1.16327	7.76967	1.81255
H	0.	9.02381	0.
C	-2.46283	4.2412	-1.80318
C	-2.42099	5.36843	-2.63869
C	-3.3817	4.22745	-0.73779
C	-3.28633	6.44532	-2.42953
H	-1.69585	5.40369	-3.44758
C	-4.25929	5.29536	-0.53761
H	-3.41566	3.36563	-0.07567
C	-4.21494	6.40971	-1.38385
H	-3.2304	7.31553	-3.07953
H	-4.97456	5.25978	0.28096
H	-4.89105	7.24624	-1.22342
C	2.46283	4.2412	1.80318
C	2.42099	5.36843	2.63869
C	3.3817	4.22745	0.73779
C	3.28633	6.44532	2.42953
H	1.69585	5.40369	3.44758
C	4.25929	5.29536	0.53761
H	3.41566	3.36563	0.07567
C	4.21494	6.40971	1.38385
H	3.2304	7.31553	3.07953
H	4.97456	5.25978	-0.28096
H	4.89105	7.24624	1.22342
C	0.	-5.11515	0.
C	-0.64671	-5.83393	-1.01907
C	0.64671	-5.83393	1.01907
C	-0.64975	-7.2312	-1.01895
H	-1.16088	-5.28984	-1.80769
C	0.64975	-7.2312	1.01895
H	1.16088	-5.28984	1.80769
C	0.	-7.93612	0.

H	-1.16327	-7.76967	-1.81255
H	1.16327	-7.76967	1.81255
H	0.	-9.02381	0.
C	-2.46283	-4.2412	1.80318
C	-2.42099	-5.36843	2.63869
C	-3.3817	-4.22745	0.73779
C	-3.28633	-6.44532	2.42953
H	-1.69585	-5.40369	3.44758
C	-4.25929	-5.29536	0.53761
H	-3.41566	-3.36563	0.07567
C	-4.21494	-6.40971	1.38385
H	-3.2304	-7.31553	3.07953
H	-4.97456	-5.25978	-0.28096
H	-4.89105	-7.24624	1.22342
C	2.46283	-4.2412	-1.80318
C	3.3817	-4.22745	-0.73779
C	2.42099	-5.36843	-2.63869
C	4.25929	-5.29536	-0.53761
H	3.41566	-3.36563	-0.07567
C	3.28633	-6.44532	-2.42953
H	1.69585	-5.40369	-3.44758
C	4.21494	-6.40971	-1.38385
H	4.97456	-5.25978	0.28096
H	3.2304	-7.31553	-3.07953
H	4.89105	-7.24624	-1.22342
C	0.	0.	6.89817
C	0.24232	-1.18214	7.6228
C	-0.24232	1.18214	7.6228
C	0.24586	-1.18358	9.02011
H	0.44182	-2.10318	7.08006
C	-0.24586	1.18358	9.02011
H	-0.44182	2.10318	7.08006
C	0.	0.	9.72649
H	0.44393	-2.10784	9.55841
H	-0.44393	2.10784	9.55841
H	0.	0.	10.81392
C	0.	0.	-6.89817
C	-0.24232	-1.18214	-7.6228
C	0.24232	1.18214	-7.6228
C	-0.24586	-1.18358	-9.02011
H	-0.44182	-2.10318	-7.08006
C	0.24586	1.18358	-9.02011
H	0.44182	2.10318	-7.08006
C	0.	0.	-9.72649
H	-0.44393	-2.10784	-9.55841
H	0.44393	2.10784	-9.55841
H	0.	0.	-10.81392
C	-2.79956	1.18151	-6.52708
C	-3.87447	3.09604	-4.31007
C	3.87447	3.09604	4.31007
C	2.79956	1.18151	6.52708
C	-2.79956	-1.18151	6.52708
C	-3.87447	-3.09604	4.31007
C	3.87447	-3.09604	-4.31007

C	2.79956	-1.18151	-6.52708
H	-2.67533	0.13081	-6.79666
H	-3.87168	1.37851	-6.44121
H	-2.42692	1.77212	-7.37057
H	-3.76281	4.11511	-4.69487
H	-4.58164	2.57933	-4.96501
H	-4.3315	3.17707	-3.32244
H	4.58164	2.57933	4.96501
H	4.3315	3.17707	3.32244
H	3.76281	4.11511	4.69487
H	2.67533	0.13081	6.79666
H	3.87168	1.37851	6.44121
H	2.42692	1.77212	7.37057
H	-3.87168	-1.37851	6.44121
H	-2.42692	-1.77212	7.37057
H	-2.67533	-0.13081	6.79666
H	-4.58164	-2.57933	4.96501
H	-4.3315	-3.17707	3.32244
H	-3.76281	-4.11511	4.69487
H	3.76281	-4.11511	-4.69487
H	4.58164	-2.57933	-4.96501
H	4.3315	-3.17707	-3.32244
H	3.87168	-1.37851	-6.44121
H	2.42692	-1.77212	-7.37057
H	2.67533	-0.13081	-6.79666
Pd	0.	0.	1.98888
Pd	0.	0.	-1.98888

Table S4.6. Optimized coordinates of **4.8.**

N	1.16696	0.7284	-3.40085
N	-1.16696	-0.7284	-3.40085
N	1.3781	0.23924	-0.72802
N	-1.3781	-0.23924	-0.72802
C	-2.11954	-1.71405	-3.09758
C	-0.7896	-0.92821	-4.69826
C	-2.66573	-0.6199	-0.98228
C	2.66573	0.6199	-0.98228
C	0.7896	0.92821	-4.69826
C	2.11954	1.71405	-3.09758
C	-2.94477	-1.61438	-1.99727
C	2.94477	1.61438	-1.99727
C	0.	0.	-5.40986
C	1.37453	2.1798	-5.19916
C	2.16533	2.68128	-4.20076
C	3.52884	-0.02467	-0.06076
C	2.66289	-0.76288	0.76908
C	-2.66289	0.76288	0.76908
C	-3.52884	0.02467	-0.06076
C	-2.16533	-2.68128	-4.20076
C	-1.37453	-2.1798	-5.19916
N	1.36908	-0.56352	0.36049
N	-1.36908	0.56352	0.36049

C	2.96795	-1.69194	1.85286
C	-2.96795	1.69194	1.85286
C	2.19404	-1.73259	2.99666
C	-2.19404	1.73259	2.99666
C	2.21993	-2.68482	4.11627
N	1.27647	-0.71669	3.30277
C	1.41315	-2.17109	5.09743
C	0.8396	-0.91492	4.57985
C	-2.21993	2.68482	4.11627
C	-0.8396	0.91492	4.57985
C	-1.41315	2.17109	5.09743
N	-1.27647	0.71669	3.30277
C	0.	0.	5.2671
C	5.00504	0.05292	0.04037
C	5.82857	-0.39718	-1.00497
C	5.61562	0.55997	1.20042
C	7.22025	-0.34422	-0.89446
H	5.37147	-0.80601	-1.9029
C	7.00699	0.61791	1.31195
H	4.99055	0.92043	2.01397
C	7.81614	0.16441	0.26461
H	7.84026	-0.70459	-1.71245
H	7.45953	1.02044	2.21564
H	8.89957	0.20659	0.35066
C	4.10311	2.528	-1.78225
C	5.1858	2.57201	-2.67527
C	4.12408	3.37517	-0.65965
C	6.24927	3.45383	-2.46753
H	5.19416	1.90357	-3.5326
C	5.17999	4.26668	-0.45689
H	3.29741	3.34435	0.04596
C	6.2469	4.31115	-1.36203
H	7.08277	3.46747	-3.16619
H	5.17129	4.92489	0.40885
H	7.07299	4.99992	-1.20143
C	4.12577	-2.60284	1.6338
C	5.21199	-2.65117	2.52368
C	4.15399	-3.43103	0.49587
C	6.28377	-3.51779	2.29789
H	5.22025	-1.99146	3.38734
C	5.2175	-4.30898	0.27665
H	3.32637	-3.39537	-0.20825
C	6.28742	-4.35696	1.17837
H	7.12093	-3.53169	2.99211
H	5.21291	-4.9537	-0.59927
H	7.12076	-5.03357	1.00399
C	-5.00504	-0.05292	0.04037
C	-5.82857	0.39718	-1.00497
C	-5.61562	-0.55997	1.20042
C	-7.22025	0.34422	-0.89446
H	-5.37147	0.80601	-1.9029
C	-7.00699	-0.61791	1.31195
H	-4.99055	-0.92043	2.01397
C	-7.81614	-0.16441	0.26461

H	-7.84026	0.70459	-1.71245
H	-7.45953	-1.02044	2.21564
H	-8.89957	-0.20659	0.35066
C	-4.12577	2.60284	1.6338
C	-5.21199	2.65117	2.52368
C	-4.15399	3.43103	0.49587
C	-6.28377	3.51779	2.29789
H	-5.22025	1.99146	3.38734
C	-5.2175	4.30898	0.27665
H	-3.32637	3.39537	-0.20825
C	-6.28742	4.35696	1.17837
H	-7.12093	3.53169	2.99211
H	-5.21291	4.9537	-0.59927
H	-7.12076	5.03357	1.00399
C	-4.10311	-2.528	-1.78225
C	-4.12408	-3.37517	-0.65965
C	-5.1858	-2.57201	-2.67527
C	-5.17999	-4.26668	-0.45689
H	-3.29741	-3.34435	0.04596
C	-6.24927	-3.45383	-2.46753
H	-5.19416	-1.90357	-3.5326
C	-6.2469	-4.31115	-1.36203
H	-5.17129	-4.92489	0.40885
H	-7.08277	-3.46747	-3.16619
H	-7.07299	-4.99992	-1.20143
C	0.	0.	6.7591
C	-1.1896	-0.20196	7.48354
C	1.1896	0.20196	7.48354
C	-1.19125	-0.20559	8.88099
H	-2.117	-0.36969	6.94082
C	1.19125	0.20559	8.88099
H	2.117	0.36969	6.94082
C	0.	0.	9.5873
H	-2.12169	-0.37226	9.41926
H	2.12169	0.37226	9.41926
H	0.	0.	10.67473
C	0.	0.	-6.90065
C	-1.19092	0.19303	-7.6249
C	1.19092	-0.19303	-7.6249
C	-1.19278	0.19576	-9.02251
H	-2.1195	0.35378	-7.08202
C	1.19278	-0.19576	-9.02251
H	2.1195	-0.35378	-7.08202
C	0.	0.	-9.72884
H	-2.12462	0.3545	-9.56079
H	2.12462	-0.3545	-9.56079
H	0.	0.	-10.81628
C	1.06579	2.86297	-6.50416
C	2.84459	4.02498	-4.21208
C	2.88763	-4.03408	4.14646
C	1.06823	-2.85426	6.39372
C	-1.06823	2.85426	6.39372
C	-2.88763	4.03408	4.14646
C	-2.84459	-4.02498	-4.21208

C	-1.06579	-2.86297	-6.50416
H	0.02766	2.70982	-6.8068
H	1.23535	3.94028	-6.42141
H	1.69241	2.4979	-7.3247
H	3.84782	3.98642	-4.64938
H	2.26057	4.73547	-4.80514
H	2.94864	4.43605	-3.20691
H	2.30407	-4.73242	4.75367
H	2.98276	-4.46058	3.14655
H	3.89438	-3.99535	4.57589
H	0.02054	-2.70495	6.66364
H	1.24406	-3.93091	6.31884
H	1.66731	-2.48484	7.23258
H	-1.24406	3.93091	6.31884
H	-1.66731	2.48484	7.23258
H	-0.02054	2.70495	6.66364
H	-2.30407	4.73242	4.75367
H	-2.98276	4.46058	3.14655
H	-3.89438	3.99535	4.57589
H	-3.84782	-3.98642	-4.64938
H	-2.26057	-4.73547	-4.80514
H	-2.94864	-4.43605	-3.20691
H	-1.23535	-3.94028	-6.42141
H	-1.69241	-2.4979	-7.3247
H	-0.02766	-2.70982	-6.8068
Ni	0.	0.	-2.0601
Pd	0.	0.	1.84057

Table S4.7. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.1.**

```
Excited State   1:      Singlet-A      1.6113 eV  769.46 nm  f=0.0433
<S**2>=0.000
     314 -> 315        0.70553

 Excited State   2:      Singlet-A      1.7481 eV  709.26 nm  f=0.0007
<S**2>=0.000
     313 -> 315        0.48219
     314 -> 316        0.51600

 Excited State   3:      Singlet-A      1.8616 eV  666.02 nm  f=0.0647
<S**2>=0.000
     313 -> 316        0.70428

 Excited State   4:      Singlet-A      2.0471 eV  605.65 nm  f=0.7438
<S**2>=0.000
     313 -> 315        0.50791
     314 -> 316       -0.47659

 Excited State   5:      Singlet-A      2.6451 eV  468.74 nm  f=0.0047
<S**2>=0.000
     311 -> 315       -0.23828
     312 -> 316       -0.21756
     313 -> 317       -0.13333
```

```
     314 -> 318        0.60925

 Excited State   6:      Singlet-A      2.6574 eV  466.55 nm  f=0.2876
<S**2>=0.000
     311 -> 316       -0.12360
     312 -> 315       -0.14706
     314 -> 317        0.66677

 Excited State   7:      Singlet-A      2.7455 eV  451.60 nm  f=0.0016
<S**2>=0.000
     311 -> 315        0.12355
     312 -> 316        0.17350
     313 -> 317        0.61705
     314 -> 318        0.25310

 Excited State   8:      Singlet-A      2.7640 eV  448.56 nm  f=0.2028
<S**2>=0.000
     312 -> 315        0.33717
     313 -> 318        0.59395

 Excited State   9:      Singlet-A      2.9063 eV  426.60 nm  f=0.0010
<S**2>=0.000
     309 -> 316        0.32669
     310 -> 315        0.52648
     311 -> 315        0.17372
     312 -> 316        0.11905
     313 -> 317       -0.19505
     314 -> 318        0.10489

 Excited State  10:      Singlet-A      2.9100 eV  426.06 nm  f=0.1890
<S**2>=0.000
     309 -> 315        0.38628
     310 -> 316        0.35649
     312 -> 315        0.32670
     313 -> 318       -0.29030
     314 -> 317        0.10106

 Excited State  11:      Singlet-A      2.9738 eV  416.93 nm  f=0.0795
<S**2>=0.000
     309 -> 315        0.28787
     310 -> 316        0.13517
     311 -> 316        0.46510
     312 -> 315       -0.39739
     313 -> 318        0.12831

 Excited State  12:      Singlet-A      2.9798 eV  416.09 nm  f=0.0022
<S**2>=0.000
     310 -> 315       -0.10326
     311 -> 315        0.52465
     312 -> 316       -0.45444

 Excited State  13:      Singlet-A      3.1444 eV  394.30 nm  f=0.0035
<S**2>=0.000
     307 -> 315        0.37901
```

```
     308 -> 316       -0.15603
     310 -> 315       -0.35076
     311 -> 315        0.18211
     312 -> 316        0.33789
     313 -> 317       -0.15157
     314 -> 318        0.12198

 Excited State  14:      Singlet-A      3.1606 eV  392.28 nm  f=0.5500
<S**2>=0.000
     307 -> 316        0.21657
     308 -> 315       -0.35194
     309 -> 315       -0.18367
     310 -> 316       -0.24526
     311 -> 316        0.38127
     312 -> 315        0.21966
     313 -> 318       -0.11112
     314 -> 317        0.11277

 Excited State  15:      Singlet-A      3.2154 eV  385.60 nm  f=0.1053
<S**2>=0.000
     308 -> 315       -0.35631
     309 -> 315       -0.34178
     310 -> 316        0.47225
     312 -> 315       -0.11687

 Excited State  16:      Singlet-A      3.2627 eV  380.01 nm  f=0.3814
<S**2>=0.000
     308 -> 315        0.47038
     309 -> 315       -0.32066
     310 -> 316        0.21617
     311 -> 316        0.28948
     312 -> 315        0.10142
     313 -> 318       -0.10285

 Excited State  17:      Singlet-A      3.2645 eV  379.79 nm  f=0.0163
<S**2>=0.000
     307 -> 315       -0.20667
     308 -> 316        0.27298
     309 -> 316        0.54722
     310 -> 315       -0.25670

 Excited State  18:      Singlet-A      3.3396 eV  371.25 nm  f=0.0133
<S**2>=0.000
     307 -> 315        0.53555
     308 -> 316        0.17298
     309 -> 316        0.10572
     311 -> 315       -0.21510
     312 -> 316       -0.21671
     313 -> 317        0.13765
     314 -> 318       -0.13376

 Excited State  19:      Singlet-A      3.3622 eV  368.76 nm  f=0.0005
<S**2>=0.000
     308 -> 316        0.59037
```

```
     309 -> 316       -0.23223
     311 -> 315        0.15763
     312 -> 316        0.15598

 Excited State  20:      Singlet-A      3.4047 eV  364.16 nm  f=0.2216
<S**2>=0.000
     307 -> 316        0.64674
     308 -> 315        0.10406
     311 -> 316       -0.12904

 Excited State  21:      Singlet-A      3.5144 eV  352.79 nm  f=0.0851
<S**2>=0.000
     289 -> 315       -0.10858
     301 -> 315        0.23705
     302 -> 316       -0.21117
     303 -> 316       -0.16077
     306 -> 315        0.54130

 Excited State  22:      Singlet-A      3.5295 eV  351.28 nm  f=0.0074
<S**2>=0.000
     287 -> 315        0.11598
     289 -> 316       -0.10095
     301 -> 316        0.19076
     302 -> 315       -0.35815
     303 -> 315       -0.31039
     305 -> 315        0.17583
     306 -> 316        0.35993

 Excited State  23:      Singlet-A      3.5834 eV  346.00 nm  f=0.0030
<S**2>=0.000
     301 -> 316       -0.12804
     302 -> 315        0.13323
     303 -> 315        0.10753
     304 -> 316        0.15208
     305 -> 315        0.63512

 Excited State  24:      Singlet-A      3.5893 eV  345.42 nm  f=0.0031
<S**2>=0.000
     304 -> 315        0.66003
     305 -> 316        0.16558

 Excited State  25:      Singlet-A      3.6146 eV  343.01 nm  f=0.0388
<S**2>=0.000
     298 -> 315       -0.10820
     301 -> 316        0.17517
     302 -> 315       -0.32870
     303 -> 315        0.51325
     304 -> 316        0.13584

 Excited State  26:      Singlet-A      3.6252 eV  342.01 nm  f=0.0138
<S**2>=0.000
     301 -> 315        0.42605
     302 -> 316       -0.28142
     303 -> 316        0.13845
```

```
     305 -> 316       -0.18672
     306 -> 315       -0.26543
     314 -> 319        0.27033

 Excited State  27:      Singlet-A      3.6393 eV  340.68 nm  f=0.0005
<S**2>=0.000
     314 -> 319        0.14762
     314 -> 320        0.66102

 Excited State  28:      Singlet-A      3.6394 eV  340.68 nm  f=0.0093
<S**2>=0.000
     301 -> 315       -0.18426
     302 -> 316        0.12102
     306 -> 315        0.12487
     314 -> 319        0.60460
     314 -> 320       -0.16103

 Excited State  29:      Singlet-A      3.6667 eV  338.13 nm  f=0.0000
<S**2>=0.000
     298 -> 315       -0.16388
     300 -> 315       -0.11146
     302 -> 315        0.16135
     306 -> 316        0.20636
     313 -> 321        0.12773
     313 -> 324       -0.13626
     314 -> 322        0.51065
     314 -> 323        0.16336

 Excited State  30:      Singlet-A      3.6684 eV  337.98 nm  f=0.0029
<S**2>=0.000
     303 -> 316       -0.12082
     313 -> 320       -0.14173
     313 -> 322        0.15519
     313 -> 326        0.13149
     314 -> 321        0.59833

 Excited State  31:      Singlet-A      3.6856 eV  336.40 nm  f=0.0043
<S**2>=0.000
     298 -> 315       -0.17980
     300 -> 315       -0.18734
     301 -> 316       -0.11725
     302 -> 315        0.21794
     303 -> 315        0.14864
     304 -> 316       -0.12339
     306 -> 316        0.33893
     312 -> 317        0.10788
     313 -> 319       -0.11733
     313 -> 324        0.16464
     314 -> 322       -0.22997
     314 -> 323       -0.24517

 Excited State  32:      Singlet-A      3.7048 eV  334.65 nm  f=0.0100
<S**2>=0.000
     305 -> 316        0.19593
```

```
     306 -> 315       -0.10956
     313 -> 323       -0.34111
     314 -> 319        0.10864
     314 -> 324        0.48476
     314 -> 325       -0.15069

 Excited State  33:      Singlet-A      3.7114 eV  334.06 nm  f=0.0000
<S**2>=0.000
     303 -> 315        0.16859
     304 -> 316       -0.30573
     313 -> 324       -0.24571
     314 -> 322       -0.28370
     314 -> 323        0.42640

 Excited State  34:      Singlet-A      3.7152 eV  333.72 nm  f=0.0024
<S**2>=0.000
     299 -> 315        0.14590
     303 -> 316        0.13353
     304 -> 315       -0.18209
     305 -> 316        0.57473
     306 -> 315       -0.11107
     313 -> 323        0.10339
     314 -> 324       -0.15576

 Excited State  35:      Singlet-A      3.7212 eV  333.18 nm  f=0.0002
<S**2>=0.000
     302 -> 315        0.11280
     304 -> 316        0.54613
     305 -> 315       -0.16311
     306 -> 316        0.16151
     313 -> 324       -0.11350
     314 -> 322       -0.20585
     314 -> 323        0.18756

 Excited State  36:      Singlet-A      3.7369 eV  331.78 nm  f=0.0116
<S**2>=0.000
     289 -> 315       -0.12357
     292 -> 315       -0.11219
     297 -> 315       -0.15333
     298 -> 316       -0.16697
     301 -> 315       -0.11030
     303 -> 316        0.47652
     306 -> 315        0.10589
     313 -> 320       -0.17995
     314 -> 321        0.21933

 Excited State  37:      Singlet-A      3.7524 eV  330.41 nm  f=0.0006
<S**2>=0.000
     299 -> 315        0.11889
     313 -> 320        0.59504
     314 -> 321        0.18566
     314 -> 325       -0.15313
     314 -> 328        0.11902
```

```
 Excited State  38:      Singlet-A      3.7533 eV  330.33 nm  f=0.0101
<S**2>=0.000
     306 -> 316        0.10144
     313 -> 319        0.63774
     314 -> 323       -0.10753

 Excited State  39:      Singlet-A      3.7662 eV  329.20 nm  f=0.0137
<S**2>=0.000
     287 -> 315        0.17491
     289 -> 316       -0.15873
     291 -> 315       -0.12912
     303 -> 315       -0.12901
     306 -> 316       -0.15035
     313 -> 321        0.34676
     313 -> 325        0.15341
     314 -> 322       -0.17269
     314 -> 326        0.35618
     314 -> 327        0.10833

 Excited State  40:      Singlet-A      3.7766 eV  328.30 nm  f=0.0027
<S**2>=0.000
     287 -> 316       -0.22037
     288 -> 315       -0.12469
     289 -> 315        0.26905
     291 -> 316        0.14118
     297 -> 315        0.17241
     301 -> 315        0.19811
     303 -> 316        0.33133
     306 -> 315        0.20806
     311 -> 317       -0.10356
     313 -> 322        0.11304
     314 -> 325        0.12865

 Excited State  41:      Singlet-A      3.7871 eV  327.38 nm  f=0.0019
<S**2>=0.000
     287 -> 315       -0.10515
     298 -> 315        0.13275
     299 -> 316       -0.13208
     300 -> 315        0.44032
     303 -> 315        0.12763
     304 -> 316       -0.11244
     306 -> 316        0.28913
     312 -> 317        0.14068
     313 -> 319       -0.14112
     313 -> 321        0.19713
     314 -> 327        0.10291

 Excited State  42:      Singlet-A      3.7895 eV  327.18 nm  f=0.0013
<S**2>=0.000
     297 -> 315        0.11930
     299 -> 315        0.50241
     300 -> 316       -0.16934
     301 -> 315       -0.12721
     305 -> 316       -0.15949
```

```
     314 -> 325        0.28665
     314 -> 328        0.10999

 Excited State  43:      Singlet-A      3.8046 eV  325.88 nm  f=0.0017
<S**2>=0.000
     289 -> 315       -0.11995
     301 -> 315       -0.12481
     313 -> 322        0.58141
     314 -> 321       -0.10351
     314 -> 328       -0.19868

 Excited State  44:      Singlet-A      3.8096 eV  325.45 nm  f=0.0125
<S**2>=0.000
     297 -> 315       -0.18465
     298 -> 316       -0.14504
     299 -> 315       -0.24327
     306 -> 315       -0.12262
     312 -> 318        0.13198
     313 -> 320        0.19011
     313 -> 326        0.16730
     314 -> 324        0.20875
     314 -> 325        0.43111

 Excited State  45:      Singlet-A      3.8154 eV  324.95 nm  f=0.0076
<S**2>=0.000
     287 -> 315        0.14814
     289 -> 316       -0.11732
     306 -> 316       -0.10949
     309 -> 317        0.14146
     310 -> 318        0.17758
     311 -> 318        0.17791
     312 -> 317        0.48731
     313 -> 321       -0.25102

 Excited State  46:      Singlet-A      3.8184 eV  324.70 nm  f=0.0024
<S**2>=0.000
     287 -> 315        0.17394
     289 -> 316       -0.15440
     291 -> 315       -0.15394
     298 -> 315       -0.22578
     299 -> 316       -0.13474
     300 -> 315        0.33659
     312 -> 317       -0.24970
     313 -> 319       -0.11033
     313 -> 321       -0.23117
     314 -> 326       -0.10981

 Excited State  47:      Singlet-A      3.8298 eV  323.73 nm  f=0.0068
<S**2>=0.000
     287 -> 315        0.11911
     289 -> 316       -0.12752
     298 -> 315        0.32185
     299 -> 316        0.11797
     306 -> 316        0.14746
```

```
     312 -> 317       -0.15561
     313 -> 321       -0.17498
     313 -> 325        0.18584
     313 -> 328       -0.13279
     314 -> 326        0.26048
     314 -> 327       -0.29417

 Excited State  48:      Singlet-A      3.8361 eV  323.20 nm  f=0.0758
<S**2>=0.000
     297 -> 315        0.29460
     298 -> 316        0.13474
     300 -> 316        0.16793
     303 -> 316        0.15810
     309 -> 318        0.13291
     310 -> 317        0.19014
     311 -> 317        0.17709
     312 -> 318        0.44202
     313 -> 322       -0.12105

 Excited State  49:      Singlet-A      3.8556 eV  321.57 nm  f=0.0221
<S**2>=0.000
     287 -> 315        0.13990
     289 -> 316       -0.11237
     298 -> 315        0.20259
     299 -> 316        0.10615
     301 -> 316        0.39293
     302 -> 315        0.30499
     311 -> 318        0.10545
     313 -> 321        0.20493
     313 -> 325       -0.15914
     314 -> 326       -0.19512

 Excited State  50:      Singlet-A      3.8566 eV  321.48 nm  f=0.0364
<S**2>=0.000
     297 -> 315       -0.15222
     299 -> 315        0.11661
     301 -> 315        0.32757
     302 -> 316        0.48388
     311 -> 317        0.14355
     312 -> 318        0.15999
     313 -> 322        0.11851
     314 -> 328        0.10395

 Excited State  51:      Singlet-A      3.8660 eV  320.70 nm  f=0.0301
<S**2>=0.000
     287 -> 315       -0.10416
     299 -> 316       -0.12999
     300 -> 315       -0.16065
     301 -> 316        0.34526
     302 -> 315        0.14340
     313 -> 321       -0.25621
     313 -> 325        0.21974
     314 -> 323       -0.10036
     314 -> 326        0.19977
```

```
     314 -> 327        0.25429
     314 -> 331        0.10949

 Excited State  52:      Singlet-A      3.8858 eV  319.07 nm  f=0.0653
<S**2>=0.000
     287 -> 316        0.16115
     288 -> 315        0.13961
     289 -> 315       -0.20893
     291 -> 316       -0.11557
     297 -> 315        0.23974
     300 -> 316        0.13757
     301 -> 315        0.10514
     302 -> 316        0.28610
     311 -> 317       -0.10489
     312 -> 318       -0.20840
     313 -> 322       -0.11971
     313 -> 326        0.12421
     314 -> 325        0.13657
     314 -> 328       -0.22384

 Excited State  53:      Singlet-A      3.8990 eV  317.99 nm  f=0.0277
<S**2>=0.000
     291 -> 315       -0.13829
     298 -> 315        0.31152
     300 -> 315       -0.13269
     301 -> 316       -0.27262
     312 -> 317       -0.14151
     313 -> 328        0.14912
     314 -> 327        0.41354

 Excited State  54:      Singlet-A      3.9028 eV  317.68 nm  f=0.0138
<S**2>=0.000
     289 -> 315       -0.12008
     297 -> 315        0.28847
     299 -> 315       -0.24505
     313 -> 322        0.10871
     313 -> 327        0.21431
     314 -> 325        0.11852
     314 -> 328        0.41788

 Excited State  55:      Singlet-A      3.9239 eV  315.97 nm  f=0.0085
<S**2>=0.000
     293 -> 315        0.10876
     297 -> 315       -0.20845
     299 -> 315        0.12360
     300 -> 316        0.56015
     314 -> 325        0.11044
     314 -> 328        0.21360

 Excited State  56:      Singlet-A      3.9255 eV  315.84 nm  f=0.0036
<S**2>=0.000
     294 -> 315        0.12800
     298 -> 315       -0.16085
     299 -> 316        0.55081
```

```
     300 -> 315        0.17735
     314 -> 327        0.15551
     314 -> 329        0.16638

 Excited State  57:      Singlet-A      3.9325 eV  315.28 nm  f=0.0490
<S**2>=0.000
     309 -> 318        0.20885
     310 -> 317        0.16862
     311 -> 317        0.47219
     312 -> 318       -0.36379
     313 -> 323       -0.12204
     313 -> 327        0.10904

 Excited State  58:      Singlet-A      3.9429 eV  314.45 nm  f=0.0004
<S**2>=0.000
     298 -> 315       -0.12290
     309 -> 317        0.23308
     310 -> 318        0.13617
     311 -> 318        0.52740
     312 -> 317       -0.27063

 Excited State  59:      Singlet-A      3.9588 eV  313.18 nm  f=0.0106
<S**2>=0.000
     295 -> 316       -0.36046
     296 -> 315        0.55913
     298 -> 316       -0.14147

 Excited State  60:      Singlet-A      3.9608 eV  313.03 nm  f=0.0000
<S**2>=0.000
     295 -> 315        0.55599
     296 -> 316       -0.36520
```

Table S4.8. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.2.**

```
Excited State   1:      Singlet-B      0.7721 eV 1605.87 nm  f=0.0015
<S**2>=0.000
     327 -> 328        0.70583

 Excited State   2:      Singlet-B      1.4984 eV  827.43 nm  f=0.0997
<S**2>=0.000
     326 -> 328        0.61598
     327 -> 330       -0.32091

 Excited State   3:      Singlet-A      1.7735 eV  699.11 nm  f=0.0185
<S**2>=0.000
     327 -> 329        0.69615

 Excited State   4:      Singlet-B      1.9305 eV  642.24 nm  f=0.4850
<S**2>=0.000
     323 -> 328       -0.16079
     326 -> 328        0.30288
```

```
     327 -> 330        0.61385

 Excited State   5:      Singlet-A      1.9564 eV  633.73 nm  f=0.0135
<S**2>=0.000
     305 -> 332        0.10637
     306 -> 332        0.18218
     323 -> 332        0.30886
     324 -> 328        0.14053
     325 -> 328        0.19329
     326 -> 332       -0.20022
     327 -> 331        0.11743
     327 -> 332        0.43142

 Excited State   6:      Singlet-A      2.0300 eV  610.76 nm  f=0.0512
<S**2>=0.000
     322 -> 328        0.11546
     323 -> 332       -0.10156
     324 -> 328        0.18886
     325 -> 328        0.62118
     327 -> 332       -0.13359

 Excited State   7:      Singlet-A      2.0579 eV  602.48 nm  f=0.0091
<S**2>=0.000
     322 -> 328       -0.14612
     324 -> 328        0.64730
     325 -> 328       -0.20080

 Excited State   8:      Singlet-B      2.0963 eV  591.44 nm  f=0.0017
<S**2>=0.000
     319 -> 332        0.13933
     320 -> 332        0.28634
     322 -> 331        0.13291
     322 -> 332        0.52528
     324 -> 332        0.12813
     326 -> 330       -0.17405

 Excited State   9:      Singlet-A      2.1926 eV  565.46 nm  f=0.0234
<S**2>=0.000
     322 -> 328        0.66195
     324 -> 328        0.11858
     325 -> 328       -0.11230
     326 -> 329       -0.12516

 Excited State  10:      Singlet-B      2.2444 eV  552.41 nm  f=0.0016
<S**2>=0.000
     293 -> 332        0.10238
     295 -> 332        0.10438
     307 -> 332        0.22556
     312 -> 332       -0.10255
     314 -> 332        0.10642
     323 -> 328       -0.11185
     324 -> 332        0.32092
     325 -> 331        0.11798
     325 -> 332        0.46329
```

```
 Excited State  11:      Singlet-B      2.2857 eV  542.44 nm  f=0.2348
<S**2>=0.000
     321 -> 328       -0.12106
     323 -> 328        0.65331
     326 -> 328        0.14504
     327 -> 330        0.10223

 Excited State  12:      Singlet-B      2.3610 eV  525.14 nm  f=0.0319
<S**2>=0.000
     322 -> 332        0.14326
     323 -> 330       -0.10067
     326 -> 330        0.66140

 Excited State  13:      Singlet-B      2.4401 eV  508.11 nm  f=0.0230
<S**2>=0.000
     321 -> 328        0.68746
     323 -> 328        0.11529

 Excited State  14:      Singlet-A      2.5225 eV  491.52 nm  f=0.3073
<S**2>=0.000
     319 -> 328        0.19475
     320 -> 328        0.13459
     325 -> 328       -0.11125
     326 -> 329        0.60849
     327 -> 332       -0.15105

 Excited State  15:      Singlet-A      2.5735 eV  481.77 nm  f=0.0013
<S**2>=0.000
     306 -> 332       -0.14542
     320 -> 328        0.19860
     323 -> 332       -0.26196
     325 -> 330        0.22106
     326 -> 329        0.11343
     326 -> 332        0.22367
     327 -> 331        0.26820
     327 -> 332        0.35042

 Excited State  16:      Singlet-A      2.5975 eV  477.33 nm  f=0.0008
<S**2>=0.000
     320 -> 328        0.55606
     324 -> 330        0.16123
     326 -> 329       -0.10025
     327 -> 331       -0.34115

 Excited State  17:      Singlet-A      2.6236 eV  472.57 nm  f=0.2103
<S**2>=0.000
     320 -> 328        0.32586
     324 -> 330       -0.21923
     326 -> 329       -0.12214
     327 -> 331        0.43964
     327 -> 332       -0.28591
```

```
 Excited State  18:      Singlet-A      2.7494 eV  450.95 nm  f=0.0077
<S**2>=0.000
     320 -> 330        0.16707
     322 -> 330        0.61098
     324 -> 330        0.18802
     326 -> 332       -0.10028
     327 -> 332       -0.13191

 Excited State  19:      Singlet-A      2.8448 eV  435.83 nm  f=0.0220
<S**2>=0.000
     319 -> 328       -0.21980
     322 -> 330       -0.16664
     324 -> 330        0.33914
     325 -> 330        0.50110
     327 -> 332       -0.14520

 Excited State  20:      Singlet-B      2.8942 eV  428.39 nm  f=0.0152
<S**2>=0.000
     293 -> 332        0.18280
     295 -> 332        0.31208
     296 -> 332       -0.20058
     298 -> 332        0.17352
     307 -> 332       -0.18740
     314 -> 332       -0.10501
     323 -> 330        0.34238
     324 -> 332       -0.14206
     325 -> 329       -0.16506
     325 -> 332        0.13418

 Excited State  21:      Singlet-A      2.9033 eV  427.04 nm  f=0.3021
<S**2>=0.000
     319 -> 328        0.61731
     324 -> 330        0.16459
     326 -> 329       -0.18841

 Excited State  22:      Singlet-B      2.9323 eV  422.82 nm  f=0.0535
<S**2>=0.000
     313 -> 328       -0.13486
     318 -> 328        0.63490
     325 -> 329        0.18970

 Excited State  23:      Singlet-B      2.9487 eV  420.47 nm  f=0.0392
<S**2>=0.000
     293 -> 332       -0.11955
     295 -> 332       -0.21071
     296 -> 332        0.13013
     298 -> 332       -0.10924
     307 -> 332        0.12380
     323 -> 330        0.54491
     325 -> 329       -0.13991

 Excited State  24:      Singlet-B      2.9708 eV  417.34 nm  f=0.0337
<S**2>=0.000
     318 -> 328       -0.21939
```

```
     323 -> 330        0.18422
     325 -> 329        0.62554

 Excited State  25:      Singlet-B      3.0120 eV  411.63 nm  f=0.0022
<S**2>=0.000
     315 -> 328        0.14175
     316 -> 328        0.66242
     318 -> 328       -0.12409

 Excited State  26:      Singlet-A      3.0153 eV  411.19 nm  f=0.0581
<S**2>=0.000
     314 -> 328        0.10065
     317 -> 328        0.67406

 Excited State  27:      Singlet-B      3.0413 eV  407.68 nm  f=0.0018
<S**2>=0.000
     322 -> 329       -0.13317
     324 -> 329        0.67406

 Excited State  28:      Singlet-A      3.0778 eV  402.84 nm  f=0.4035
<S**2>=0.000
     314 -> 328       -0.23799
     317 -> 328        0.15449
     322 -> 330       -0.13789
     323 -> 329       -0.15152
     324 -> 330        0.40701
     325 -> 330       -0.32971
     327 -> 331        0.22249

 Excited State  29:      Singlet-B      3.0833 eV  402.11 nm  f=0.0039
<S**2>=0.000
     313 -> 328       -0.13205
     315 -> 328        0.62316
     316 -> 328       -0.18513
     322 -> 329        0.14675

 Excited State  30:      Singlet-A      3.1462 eV  394.07 nm  f=0.0144
<S**2>=0.000
     311 -> 328       -0.20100
     312 -> 328        0.17181
     314 -> 328        0.55610
     324 -> 330        0.18135
     325 -> 330       -0.14919
     327 -> 331        0.10718

 Excited State  31:      Singlet-A      3.1715 eV  390.93 nm  f=0.0007
<S**2>=0.000
     327 -> 333        0.68512

 Excited State  32:      Singlet-B      3.1812 eV  389.74 nm  f=0.0378
<S**2>=0.000
     315 -> 328       -0.16957
     322 -> 329        0.63146
     324 -> 329        0.13459
```

```
     327 -> 334       -0.16508

 Excited State  33:      Singlet-A      3.2067 eV  386.64 nm  f=0.0069
<S**2>=0.000
     311 -> 328       -0.11367
     314 -> 328       -0.10322
     323 -> 329        0.64041

 Excited State  34:      Singlet-B      3.2114 eV  386.07 nm  f=0.0085
<S**2>=0.000
     322 -> 329        0.18927
     327 -> 334        0.63168
     327 -> 335        0.19380
     327 -> 336        0.12530

 Excited State  35:      Singlet-B      3.2457 eV  381.99 nm  f=0.0582
<S**2>=0.000
     305 -> 328       -0.11546
     310 -> 328       -0.16259
     313 -> 328        0.61118
     315 -> 328        0.18102

 Excited State  36:      Singlet-A      3.2572 eV  380.65 nm  f=0.0006
<S**2>=0.000
     320 -> 330       -0.14425
     326 -> 331        0.66083

 Excited State  37:      Singlet-B      3.2945 eV  376.33 nm  f=0.0003
<S**2>=0.000
     321 -> 330        0.19940
     327 -> 334       -0.15328
     327 -> 335        0.61411
     327 -> 336       -0.19961

 Excited State  38:      Singlet-B      3.3178 eV  373.69 nm  f=0.0223
<S**2>=0.000
     321 -> 330        0.52656
     327 -> 334        0.15404
     327 -> 335       -0.23627
     327 -> 336       -0.32337

 Excited State  39:      Singlet-A      3.3272 eV  372.64 nm  f=0.0004
<S**2>=0.000
     327 -> 337        0.68736
     327 -> 340       -0.11187

 Excited State  40:      Singlet-B      3.3311 eV  372.20 nm  f=0.0352
<S**2>=0.000
     321 -> 330        0.36148
     327 -> 334       -0.12482
     327 -> 336        0.55571

 Excited State  41:      Singlet-A      3.3744 eV  367.42 nm  f=0.0002
<S**2>=0.000
```

```
     319 -> 330        0.14253
     320 -> 330        0.58086
     321 -> 329       -0.12936
     322 -> 330       -0.16453
     326 -> 331        0.17721
     326 -> 332        0.12189

 Excited State  42:      Singlet-A      3.4006 eV  364.60 nm  f=0.1190
<S**2>=0.000
     307 -> 328       -0.14044
     311 -> 328        0.43695
     312 -> 328       -0.26777
     314 -> 328        0.25790
     323 -> 329        0.14343
     326 -> 329        0.10106
     326 -> 332        0.11797
     326 -> 333        0.17311
     327 -> 338       -0.20257

 Excited State  43:      Singlet-B      3.4152 eV  363.03 nm  f=0.0584
<S**2>=0.000
     305 -> 328        0.23640
     306 -> 328       -0.11453
     308 -> 328        0.15192
     310 -> 328        0.57156
     313 -> 328        0.20192

 Excited State  44:      Singlet-A      3.4283 eV  361.65 nm  f=0.0057
<S**2>=0.000
     307 -> 328        0.13180
     309 -> 328       -0.15852
     320 -> 330        0.17927
     321 -> 329        0.55708
     326 -> 332       -0.16015
     327 -> 338       -0.21813

 Excited State  45:      Singlet-A      3.4332 eV  361.14 nm  f=0.0072
<S**2>=0.000
     306 -> 332        0.10245
     311 -> 328       -0.14361
     312 -> 328        0.16103
     320 -> 330       -0.12129
     321 -> 329        0.10246
     323 -> 332        0.19054
     326 -> 332        0.43684
     327 -> 338       -0.36546

 Excited State  46:      Singlet-A      3.4423 eV  360.18 nm  f=0.0064
<S**2>=0.000
     309 -> 328       -0.32657
     321 -> 329        0.16759
     323 -> 332        0.13810
     326 -> 332        0.30490
     327 -> 338        0.43363
```

```
     327 -> 342        0.10345

 Excited State  47:      Singlet-A      3.4490 eV  359.48 nm  f=0.0000
<S**2>=0.000
     303 -> 328       -0.10781
     307 -> 328        0.12300
     309 -> 328        0.55785
     311 -> 328        0.10311
     312 -> 328       -0.14458
     321 -> 329        0.23867
     326 -> 332        0.12680
     327 -> 338        0.16596

 Excited State  48:      Singlet-B      3.4588 eV  358.46 nm  f=0.0051
<S**2>=0.000
     308 -> 328        0.48405
     310 -> 328       -0.22656
     327 -> 339        0.40778

 Excited State  49:      Singlet-B      3.4652 eV  357.80 nm  f=0.0095
<S**2>=0.000
     308 -> 328       -0.17791
     327 -> 339        0.11755
     327 -> 341        0.61110
     327 -> 343        0.23470

 Excited State  50:      Singlet-A      3.4672 eV  357.59 nm  f=0.0073
<S**2>=0.000
     307 -> 328        0.50400
     311 -> 328       -0.12217
     312 -> 328       -0.29387
     321 -> 329       -0.17101
     327 -> 340        0.27263

 Excited State  51:      Singlet-B      3.4732 eV  356.97 nm  f=0.0301
<S**2>=0.000
     308 -> 328       -0.35711
     327 -> 339        0.53457
     327 -> 341       -0.18249
     327 -> 343       -0.10700

 Excited State  52:      Singlet-A      3.4824 eV  356.03 nm  f=0.0044
<S**2>=0.000
     307 -> 328       -0.17814
     321 -> 329        0.15087
     327 -> 338        0.15554
     327 -> 340        0.59880

 Excited State  53:      Singlet-B      3.4892 eV  355.34 nm  f=0.0077
<S**2>=0.000
     302 -> 328       -0.11079
     304 -> 328       -0.20570
     305 -> 328        0.10462
     306 -> 328        0.62523
```

```
     308 -> 328        0.10530

 Excited State  54:      Singlet-B      3.5377 eV  350.47 nm  f=0.0054
<S**2>=0.000
     302 -> 328        0.20995
     304 -> 328        0.50150
     305 -> 328        0.30250
     306 -> 328        0.19942
     308 -> 328       -0.10520
     310 -> 328       -0.10798
     327 -> 343       -0.13787

 Excited State  55:      Singlet-B      3.5476 eV  349.49 nm  f=0.0231
<S**2>=0.000
     304 -> 328        0.11661
     327 -> 341       -0.23104
     327 -> 343        0.62587

 Excited State  56:      Singlet-A      3.5483 eV  349.42 nm  f=0.0012
<S**2>=0.000
     307 -> 328        0.33897
     311 -> 328        0.38178
     312 -> 328        0.46684

 Excited State  57:      Singlet-A      3.5818 eV  346.15 nm  f=0.0000
<S**2>=0.000
     301 -> 328        0.61176
     303 -> 328       -0.28562
     326 -> 333       -0.10057

 Excited State  58:      Singlet-B      3.5982 eV  344.57 nm  f=0.0003
<S**2>=0.000
     304 -> 328       -0.15121
     305 -> 328        0.11387
     320 -> 329        0.63396
     325 -> 331        0.11764

 Excited State  59:      Singlet-A      3.6066 eV  343.77 nm  f=0.0002
<S**2>=0.000
     327 -> 338       -0.12922
     327 -> 342        0.66739

 Excited State  60:      Singlet-B      3.6094 eV  343.50 nm  f=0.0151
<S**2>=0.000
     302 -> 328       -0.14666
     304 -> 328       -0.23078
     305 -> 328        0.51081
     306 -> 328       -0.14806
     308 -> 328       -0.17487
     310 -> 328       -0.19923
     320 -> 329       -0.18272
```

Table S4.9. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.3.**

```
Excited State   1:      Singlet-B      0.9861 eV 1257.37 nm  f=0.0040
<S**2>=0.000
     336 -> 337        0.70525

 Excited State   2:      Singlet-B      1.5137 eV  819.07 nm  f=0.1155
<S**2>=0.000
     335 -> 337        0.63325
     336 -> 338       -0.29649

 Excited State   3:      Singlet-A      1.9783 eV  626.71 nm  f=0.0192
<S**2>=0.000
     336 -> 339        0.69425

 Excited State   4:      Singlet-B      1.9937 eV  621.87 nm  f=0.5904
<S**2>=0.000
     335 -> 337        0.29089
     336 -> 338        0.63311

 Excited State   5:      Singlet-A      2.1833 eV  567.89 nm  f=0.0324
<S**2>=0.000
     333 -> 337       -0.25831
     334 -> 337        0.62427
     335 -> 339       -0.16702

 Excited State   6:      Singlet-B      2.2049 eV  562.32 nm  f=0.0150
<S**2>=0.000
     335 -> 338        0.69759

 Excited State   7:      Singlet-A      2.2410 eV  553.25 nm  f=0.0279
<S**2>=0.000
     333 -> 337        0.63367
     334 -> 337        0.21240
     335 -> 339       -0.19149

 Excited State   8:      Singlet-A      2.3604 eV  525.27 nm  f=0.0729
<S**2>=0.000
     334 -> 338        0.16517
     336 -> 340        0.47554
     336 -> 341        0.45224

 Excited State   9:      Singlet-B      2.4527 eV  505.51 nm  f=0.1474
<S**2>=0.000
     330 -> 337        0.13907
     332 -> 337        0.67849

 Excited State  10:      Singlet-A      2.4910 eV  497.73 nm  f=0.1447
<S**2>=0.000
     329 -> 337       -0.18334
     331 -> 337        0.47644
     334 -> 337        0.10271
     335 -> 339        0.45037
```

```
 Excited State  11:      Singlet-A      2.5525 eV  485.74 nm  f=0.1847
<S**2>=0.000
     328 -> 337       -0.14867
     329 -> 337        0.46092
     331 -> 337       -0.26794
     334 -> 337        0.16539
     335 -> 339        0.37164

 Excited State  12:      Singlet-B      2.5953 eV  477.72 nm  f=0.0364
<S**2>=0.000
     330 -> 337        0.68443
     332 -> 337       -0.13464

 Excited State  13:      Singlet-A      2.6465 eV  468.48 nm  f=0.0106
<S**2>=0.000
     329 -> 337       -0.28410
     331 -> 337       -0.20223
     333 -> 338        0.17147
     334 -> 338       -0.17157
     336 -> 340       -0.36932
     336 -> 341        0.39623

 Excited State  14:      Singlet-A      2.6936 eV  460.29 nm  f=0.3046
<S**2>=0.000
     328 -> 337        0.15867
     329 -> 337        0.39491
     331 -> 337        0.36689
     335 -> 339       -0.17545
     336 -> 340       -0.21627
     336 -> 341        0.26135

 Excited State  15:      Singlet-A      2.8460 eV  435.65 nm  f=0.0001
<S**2>=0.000
     332 -> 340        0.14767
     332 -> 341        0.13476
     333 -> 338        0.22266
     335 -> 340        0.50542
     335 -> 341        0.34553

 Excited State  16:      Singlet-A      2.9103 eV  426.02 nm  f=0.0273
<S**2>=0.000
     328 -> 337       -0.20973
     331 -> 338        0.11453
     333 -> 338        0.45826
     334 -> 338        0.39671
     335 -> 341       -0.12807
     336 -> 341       -0.14240

 Excited State  17:      Singlet-A      2.9752 eV  416.73 nm  f=0.6584
<S**2>=0.000
     328 -> 337        0.53571
     333 -> 338        0.29100
     334 -> 338       -0.14196
     335 -> 339        0.16137
```

```
     335 -> 341       -0.13569
     336 -> 341       -0.12128

 Excited State  18:      Singlet-B      2.9807 eV  415.96 nm  f=0.0325
<S**2>=0.000
     330 -> 338       -0.13353
     331 -> 341       -0.14732
     332 -> 338        0.63506

 Excited State  19:      Singlet-A      3.0255 eV  409.80 nm  f=0.0234
<S**2>=0.000
     329 -> 338       -0.32925
     331 -> 338        0.57775
     333 -> 338       -0.14648

 Excited State  20:      Singlet-B      3.0279 eV  409.48 nm  f=0.0377
<S**2>=0.000
     323 -> 337        0.22400
     325 -> 337        0.19076
     327 -> 337        0.57442
     334 -> 339       -0.20903

 Excited State  21:      Singlet-B      3.0710 eV  403.73 nm  f=0.0045
<S**2>=0.000
     323 -> 337        0.12899
     325 -> 337        0.58526
     327 -> 337       -0.31720
     334 -> 339       -0.14687

 Excited State  22:      Singlet-A      3.0715 eV  403.66 nm  f=0.0703
<S**2>=0.000
     326 -> 337        0.38483
     328 -> 337       -0.23858
     333 -> 338        0.19033
     334 -> 338       -0.38245
     335 -> 341       -0.15389
     336 -> 340        0.17392

 Excited State  23:      Singlet-A      3.0879 eV  401.52 nm  f=0.0029
<S**2>=0.000
     326 -> 337        0.57659
     328 -> 337        0.16958
     333 -> 338       -0.12560
     334 -> 338        0.25736
     336 -> 340       -0.11369

 Excited State  24:      Singlet-A      3.1007 eV  399.85 nm  f=0.0471
<S**2>=0.000
     329 -> 338       -0.17885
     332 -> 341        0.12375
     333 -> 338        0.13844
     335 -> 340       -0.42995
     335 -> 341        0.47647
```

```
 Excited State  25:      Singlet-B      3.1042 eV  399.41 nm  f=0.0344
<S**2>=0.000
     325 -> 337        0.26867
     327 -> 337        0.17133
     334 -> 339        0.58317

 Excited State  26:      Singlet-B      3.1454 eV  394.18 nm  f=0.0337
<S**2>=0.000
     323 -> 337       -0.13227
     333 -> 339       -0.28596
     333 -> 340        0.28447
     333 -> 341        0.29071
     334 -> 339        0.15284
     334 -> 340        0.25504
     334 -> 341        0.28906

 Excited State  27:      Singlet-B      3.1849 eV  389.29 nm  f=0.0224
<S**2>=0.000
     323 -> 337        0.47881
     324 -> 337       -0.37465
     325 -> 337       -0.18659
     327 -> 337       -0.13177
     334 -> 339        0.17421

 Excited State  28:      Singlet-B      3.2047 eV  386.88 nm  f=0.0162
<S**2>=0.000
     323 -> 337       -0.15036
     333 -> 339        0.60844
     333 -> 340        0.10413
     333 -> 341        0.11386
     334 -> 340        0.12846
     334 -> 341        0.14112

 Excited State  29:      Singlet-B      3.2084 eV  386.44 nm  f=0.0414
<S**2>=0.000
     323 -> 337       -0.10105
     324 -> 337       -0.18930
     329 -> 340       -0.20793
     329 -> 341       -0.26399
     331 -> 340        0.30557
     331 -> 341        0.34416
     332 -> 338        0.21531
     333 -> 339       -0.10591

 Excited State  30:      Singlet-B      3.2831 eV  377.64 nm  f=0.0885
<S**2>=0.000
     323 -> 337        0.32101
     324 -> 337        0.51922
     331 -> 340        0.11769
     331 -> 341        0.12755
     334 -> 339        0.13551

 Excited State  31:      Singlet-A      3.3006 eV  375.64 nm  f=0.0000
<S**2>=0.000
```

```
     318 -> 337        0.14888
     321 -> 337        0.32720
     322 -> 337        0.44199
     329 -> 338        0.23542
     331 -> 338        0.20748
     332 -> 339       -0.18329

 Excited State  32:      Singlet-B      3.3025 eV  375.42 nm  f=0.0395
<S**2>=0.000
     330 -> 338        0.64075
     332 -> 338        0.11182
     333 -> 341        0.15710
     334 -> 340       -0.12587

 Excited State  33:      Singlet-A      3.3241 eV  372.98 nm  f=0.0000
<S**2>=0.000
     321 -> 337       -0.15211
     322 -> 337       -0.28875
     329 -> 338        0.50229
     331 -> 338        0.28026

 Excited State  34:      Singlet-A      3.3375 eV  371.48 nm  f=0.0009
<S**2>=0.000
     336 -> 342        0.67027

 Excited State  35:      Singlet-B      3.3651 eV  368.44 nm  f=0.0085
<S**2>=0.000
     336 -> 343        0.56283
     336 -> 344        0.32260
     336 -> 346       -0.20952

 Excited State  36:      Singlet-A      3.3923 eV  365.49 nm  f=0.0009
<S**2>=0.000
     322 -> 337        0.21146
     332 -> 339        0.63852

 Excited State  37:      Singlet-B      3.4111 eV  363.47 nm  f=0.0115
<S**2>=0.000
     336 -> 343       -0.22914
     336 -> 344        0.57436
     336 -> 346        0.26455

 Excited State  38:      Singlet-A      3.4356 eV  360.88 nm  f=0.0001
<S**2>=0.000
     336 -> 345        0.68618
     336 -> 350       -0.10531

 Excited State  39:      Singlet-B      3.4505 eV  359.32 nm  f=0.0208
<S**2>=0.000
     330 -> 338       -0.15247
     333 -> 340        0.37216
     333 -> 341        0.22695
     334 -> 340       -0.32188
     334 -> 341       -0.31051
```

```
     336 -> 344        0.11702

 Excited State  40:      Singlet-A      3.4555 eV  358.80 nm  f=0.0531
<S**2>=0.000
     314 -> 337        0.10130
     318 -> 337        0.17478
     319 -> 337       -0.14030
     321 -> 337        0.43966
     322 -> 337       -0.34960
     332 -> 340       -0.10269
     332 -> 341       -0.10653
     335 -> 342       -0.18295
     336 -> 347       -0.11956

 Excited State  41:      Singlet-B      3.4620 eV  358.13 nm  f=0.0300
<S**2>=0.000
     316 -> 337        0.26775
     317 -> 337        0.29329
     320 -> 337        0.34555
     335 -> 343        0.15480
     336 -> 343        0.12920
     336 -> 344       -0.11615
     336 -> 346        0.35254

 Excited State  42:      Singlet-B      3.4632 eV  358.01 nm  f=0.0443
<S**2>=0.000
     316 -> 337       -0.20804
     317 -> 337       -0.21856
     320 -> 337       -0.26519
     335 -> 343        0.12808
     336 -> 343        0.24894
     336 -> 344       -0.10019
     336 -> 346        0.45753

 Excited State  43:      Singlet-A      3.5042 eV  353.82 nm  f=0.0031
<S**2>=0.000
     321 -> 337        0.11865
     332 -> 339        0.13186
     332 -> 340        0.42444
     332 -> 341        0.35600
     335 -> 340       -0.12167
     335 -> 341       -0.22816

 Excited State  44:      Singlet-A      3.5143 eV  352.80 nm  f=0.0003
<S**2>=0.000
     314 -> 337        0.21781
     318 -> 337        0.57358
     319 -> 337       -0.10001
     321 -> 337       -0.29219

 Excited State  45:      Singlet-B      3.5180 eV  352.43 nm  f=0.0218
<S**2>=0.000
     315 -> 337        0.17448
     316 -> 337        0.23809
```

```
     317 -> 337       -0.18470
     320 -> 337       -0.17110
     323 -> 337        0.10228
     329 -> 339       -0.21711
     331 -> 339        0.51813

 Excited State  46:      Singlet-B      3.5290 eV  351.33 nm  f=0.0098
<S**2>=0.000
     312 -> 337       -0.12631
     317 -> 337        0.50383
     320 -> 337       -0.44329

 Excited State  47:      Singlet-B      3.5471 eV  349.54 nm  f=0.0038
<S**2>=0.000
     315 -> 337        0.24697
     316 -> 337        0.44829
     317 -> 337       -0.10491
     320 -> 337       -0.18083
     329 -> 339        0.28515
     331 -> 339       -0.27805

 Excited State  48:      Singlet-A      3.5605 eV  348.22 nm  f=0.0002
<S**2>=0.000
     330 -> 339        0.37074
     336 -> 347        0.54417

 Excited State  49:      Singlet-B      3.5688 eV  347.41 nm  f=0.0054
<S**2>=0.000
     336 -> 348        0.11407
     336 -> 349        0.65414
     336 -> 352        0.17621

 Excited State  50:      Singlet-A      3.5752 eV  346.79 nm  f=0.0070
<S**2>=0.000
     314 -> 337        0.26534
     330 -> 339        0.49286
     336 -> 347       -0.34544
     336 -> 350       -0.12672

 Excited State  51:      Singlet-A      3.5833 eV  346.00 nm  f=0.0034
<S**2>=0.000
     313 -> 337       -0.14487
     314 -> 337        0.55783
     318 -> 337       -0.18904
     328 -> 338        0.10804
     330 -> 339       -0.28358
     336 -> 350        0.10793

 Excited State  52:      Singlet-B      3.6108 eV  343.37 nm  f=0.0095
<S**2>=0.000
     329 -> 339        0.21346
     336 -> 348        0.62371
```

```
 Excited State  53:      Singlet-A      3.6122 eV  343.24 nm  f=0.0338
<S**2>=0.000
     314 -> 337       -0.10022
     328 -> 338        0.49183
     336 -> 350        0.40100
     336 -> 351        0.14828

 Excited State  54:      Singlet-B      3.6259 eV  341.94 nm  f=0.0087
<S**2>=0.000
     315 -> 337       -0.11819
     329 -> 339        0.51832
     331 -> 339        0.30318
     335 -> 343        0.17133
     336 -> 348       -0.20775

 Excited State  55:      Singlet-A      3.6462 eV  340.04 nm  f=0.0041
<S**2>=0.000
     311 -> 337        0.12169
     319 -> 337        0.46534
     328 -> 338       -0.16358
     335 -> 342       -0.37486
     336 -> 350        0.24392

 Excited State  56:      Singlet-A      3.6545 eV  339.27 nm  f=0.0000
<S**2>=0.000
     318 -> 337        0.13936
     319 -> 337        0.47761
     321 -> 337        0.17229
     328 -> 338        0.14859
     335 -> 342        0.34256
     336 -> 350       -0.23306

 Excited State  57:      Singlet-B      3.6591 eV  338.84 nm  f=0.0010
<S**2>=0.000
     329 -> 339       -0.10859
     335 -> 343        0.61173
     336 -> 343       -0.18992
     336 -> 346       -0.11793

 Excited State  58:      Singlet-A      3.6628 eV  338.50 nm  f=0.0054
<S**2>=0.000
     328 -> 338        0.38450
     335 -> 342       -0.36285
     336 -> 347        0.14757
     336 -> 350       -0.34798
     336 -> 351       -0.18113

 Excited State  59:      Singlet-B      3.6685 eV  337.97 nm  f=0.0101
<S**2>=0.000
     327 -> 338        0.23931
     336 -> 349       -0.15525
     336 -> 352        0.59889
```

```
 Excited State  60:      Singlet-B      3.6833 eV  336.61 nm  f=0.0495
<S**2>=0.000
     312 -> 337        0.11082
     315 -> 337       -0.27144
     316 -> 337        0.12291
     327 -> 338        0.37963
     333 -> 340       -0.13622
     334 -> 340       -0.25478
     334 -> 341        0.27829
     336 -> 352       -0.16424
```

Table S4.10. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.5.**

```
Excited State   1:      Singlet-B1     1.6889 eV  734.13 nm  f=0.0327
<S**2>=0.000
     310 -> 344       -0.10569
     319 -> 343       -0.10154
     335 -> 343       -0.22049
     336 -> 344       -0.18753
     336 -> 345       -0.15229
     340 -> 343        0.53059
     340 -> 346        0.14365
 Excited State   2:      Singlet-B2     1.7346 eV  714.77 nm  f=0.1330
<S**2>=0.000
     339 -> 342       -0.19680
     340 -> 341        0.66916

 Excited State   3:      Singlet-B3     1.7605 eV  704.26 nm  f=0.0349
<S**2>=0.000
     329 -> 344       -0.10261
     332 -> 343       -0.13318
     340 -> 342        0.66305

 Excited State   4:      Singlet-A      1.8196 eV  681.40 nm  f=0.0000
<S**2>=0.000
     310 -> 343       -0.15858
     313 -> 343       -0.11983
     335 -> 344       -0.19420
     335 -> 345       -0.16963
     336 -> 343       -0.30879
     336 -> 346       -0.11554
     339 -> 343       -0.10244
     340 -> 344        0.34289
     340 -> 345        0.29481

 Excited State   5:      Singlet-B3     1.8364 eV  675.16 nm  f=0.0403
<S**2>=0.000
     339 -> 341        0.69685

 Excited State   6:      Singlet-B2     1.9546 eV  634.34 nm  f=0.0028
<S**2>=0.000
```

```
     329 -> 343        0.43993
     329 -> 346        0.17992
     332 -> 344        0.29252
     332 -> 345        0.26430
     333 -> 343       -0.13840
     334 -> 344       -0.19911
     334 -> 345       -0.16613

 Excited State   7:      Singlet-B3     1.9588 eV  632.97 nm  f=0.0116
<S**2>=0.000
     329 -> 344        0.31257
     329 -> 345        0.27613
     332 -> 343        0.37830
     332 -> 346        0.16055
     334 -> 343       -0.25192
     340 -> 342        0.22084

 Excited State   8:      Singlet-B3     2.0467 eV  605.77 nm  f=0.0019
<S**2>=0.000
     308 -> 343        0.13223
     311 -> 344        0.16016
     311 -> 345        0.14356
     320 -> 343        0.14804
     322 -> 343        0.13487
     333 -> 344        0.13886
     333 -> 345        0.11713
     334 -> 343        0.17060
     337 -> 343        0.38834
     337 -> 346        0.14114
     338 -> 344        0.24168
     338 -> 345        0.19950

 Excited State   9:      Singlet-B2     2.0548 eV  603.39 nm  f=0.0129
<S**2>=0.000
     308 -> 344        0.10673
     311 -> 343        0.20524
     320 -> 344        0.11411
     320 -> 345        0.10273
     322 -> 344        0.10219
     333 -> 343        0.17947
     334 -> 344        0.10690
     337 -> 344        0.26860
     337 -> 345        0.23702
     338 -> 343        0.35302
     338 -> 346        0.13290

 Excited State  10:      Singlet-B2     2.1928 eV  565.41 nm  f=0.3803
<S**2>=0.000
     338 -> 343        0.10730
     339 -> 342        0.66960
     340 -> 341        0.17883

 Excited State  11:      Singlet-A      2.2902 eV  541.37 nm  f=0.0000
<S**2>=0.000
```

```
     338 -> 342       -0.20502
     339 -> 343        0.64117
     339 -> 346        0.10251

 Excited State  12:      Singlet-B1     2.4432 eV  507.46 nm  f=0.0210
<S**2>=0.000
     309 -> 343        0.10354
     310 -> 344        0.10549
     319 -> 343        0.11224
     335 -> 343        0.23420
     336 -> 344        0.18254
     336 -> 345        0.18183
     338 -> 341       -0.30110
     339 -> 344       -0.15237
     339 -> 345       -0.10595
     340 -> 343        0.36268
     340 -> 346       -0.13458

 Excited State  13:      Singlet-B1     2.6105 eV  474.95 nm  f=0.0434
<S**2>=0.000
     333 -> 341        0.14281
     337 -> 342       -0.36004
     338 -> 341        0.17027
     339 -> 344        0.38083
     339 -> 345        0.27197
     340 -> 343        0.23374
     340 -> 346       -0.10592

 Excited State  14:      Singlet-A      2.6404 eV  469.57 nm  f=0.0000
<S**2>=0.000
     333 -> 342       -0.11357
     337 -> 341        0.61764
     340 -> 345       -0.25592

 Excited State  15:      Singlet-B1     2.6850 eV  461.76 nm  f=0.1493
<S**2>=0.000
     338 -> 341        0.55259
     339 -> 344       -0.12796
     339 -> 345       -0.28134
     340 -> 343        0.12480
     340 -> 346        0.18611

 Excited State  16:      Singlet-A      2.6976 eV  459.61 nm  f=0.0000
<S**2>=0.000
     336 -> 343        0.23177
     338 -> 342        0.20491
     339 -> 343        0.14689
     340 -> 344        0.55788

 Excited State  17:      Singlet-B2     2.7370 eV  452.99 nm  f=0.0104
<S**2>=0.000
     301 -> 344        0.10056
     304 -> 343        0.19913
     306 -> 344        0.26207
```

```
     306 -> 345        0.23473
     307 -> 343        0.32876
     307 -> 346        0.14309
     308 -> 344       -0.10113
     311 -> 343       -0.10110
     333 -> 343       -0.13917
     335 -> 341        0.11566
     337 -> 344       -0.11754
     338 -> 343        0.21820

 Excited State  18:      Singlet-B3     2.7374 eV  452.92 nm  f=0.0004
<S**2>=0.000
     335 -> 342       -0.20493
     336 -> 341        0.64348

 Excited State  19:      Singlet-B3     2.7580 eV  449.54 nm  f=0.0002
<S**2>=0.000
     301 -> 343       -0.13403
     304 -> 344       -0.16867
     304 -> 345       -0.14723
     306 -> 343       -0.33959
     306 -> 346       -0.15043
     307 -> 344       -0.26163
     307 -> 345       -0.23889
     308 -> 343        0.11581
     336 -> 341        0.15166
     337 -> 343        0.15568
     338 -> 344       -0.16227
     338 -> 345       -0.14244

 Excited State  20:      Singlet-A      2.7594 eV  449.31 nm  f=0.0000
<S**2>=0.000
     329 -> 342       -0.13633
     332 -> 341        0.20346
     333 -> 342        0.11295
     334 -> 341       -0.16592
     336 -> 343        0.14375
     337 -> 341        0.26162
     338 -> 342       -0.11220
     340 -> 345        0.50637

 Excited State  21:      Singlet-B1     2.7942 eV  443.72 nm  f=0.0926
<S**2>=0.000
     329 -> 341        0.12351
     332 -> 342       -0.15279
     333 -> 341       -0.26588
     334 -> 342        0.20223
     338 -> 341       -0.12805
     339 -> 344        0.23847
     339 -> 345        0.11709
     340 -> 346        0.48085

 Excited State  22:      Singlet-B2     2.8286 eV  438.33 nm  f=0.0488
<S**2>=0.000
```

```
     330 -> 341       -0.10772
     335 -> 341       -0.36793
     336 -> 342        0.55778

 Excited State  23:      Singlet-A      2.8387 eV  436.77 nm  f=0.0000
<S**2>=0.000
     329 -> 342        0.25934
     332 -> 341       -0.32178
     333 -> 342       -0.15680
     334 -> 341        0.44236
     336 -> 343        0.11723
     340 -> 345        0.24893

 Excited State  24:      Singlet-B1     2.8401 eV  436.54 nm  f=0.0005
<S**2>=0.000
     329 -> 341       -0.28509
     332 -> 342        0.29700
     333 -> 341        0.12311
     334 -> 342       -0.30495
     337 -> 342        0.32350
     339 -> 344        0.27432
     340 -> 346        0.14656

 Excited State  25:      Singlet-A      2.8938 eV  428.45 nm  f=0.0000
<S**2>=0.000
     338 -> 342        0.57457
     339 -> 343        0.10453
     339 -> 346        0.29806
     340 -> 344       -0.19476
     340 -> 345        0.10993

 Excited State  26:      Singlet-B1     2.9039 eV  426.96 nm  f=0.0001
<S**2>=0.000
     329 -> 341        0.14300
     332 -> 342       -0.15993
     333 -> 341       -0.14168
     337 -> 342        0.24654
     339 -> 344        0.38291
     339 -> 345       -0.29778
     340 -> 346       -0.33366

 Excited State  27:      Singlet-A      3.0349 eV  408.53 nm  f=0.0000
<S**2>=0.000
     332 -> 341       -0.22576
     334 -> 341       -0.28514
     338 -> 342       -0.20967
     339 -> 343       -0.11523
     339 -> 346        0.52652

 Excited State  28:      Singlet-B1     3.0462 eV  407.01 nm  f=0.2201
<S**2>=0.000
     329 -> 341        0.19695
     332 -> 342       -0.18400
     333 -> 341        0.35314
```

```
     337 -> 342        0.39813
     338 -> 341        0.11076
     339 -> 345        0.31214

 Excited State  29:      Singlet-B2     3.0528 eV  406.14 nm  f=0.0369
<S**2>=0.000
     335 -> 341        0.56104
     336 -> 342        0.36654
     338 -> 343        0.12618

 Excited State  30:      Singlet-B1     3.0901 eV  401.23 nm  f=0.4489
<S**2>=0.000
     329 -> 341        0.11568
     332 -> 342       -0.26168
     333 -> 341        0.39537
     334 -> 342       -0.17808
     337 -> 342       -0.13814
     338 -> 341       -0.17359
     339 -> 345       -0.32242
     340 -> 346        0.19984

 Excited State  31:      Singlet-A      3.0954 eV  400.55 nm  f=0.0000
<S**2>=0.000
     329 -> 342       -0.23131
     331 -> 341       -0.19651
     332 -> 341        0.35728
     333 -> 342       -0.28499
     334 -> 341        0.30577
     337 -> 341       -0.14796
     339 -> 346        0.23318

 Excited State  32:      Singlet-B3     3.1542 eV  393.07 nm  f=0.0492
<S**2>=0.000
     335 -> 342        0.63161
     336 -> 341        0.20110
     337 -> 343        0.11352

 Excited State  33:      Singlet-B1     3.2064 eV  386.68 nm  f=0.0817
<S**2>=0.000
     329 -> 341       -0.45324
     333 -> 341        0.21689
     334 -> 342        0.47756

 Excited State  34:      Singlet-A      3.2295 eV  383.91 nm  f=0.0000
<S**2>=0.000
     329 -> 342        0.41801
     332 -> 341        0.26338
     333 -> 342       -0.41672
     334 -> 341       -0.22726
     339 -> 346       -0.11327

 Excited State  35:      Singlet-B2     3.2635 eV  379.91 nm  f=0.1406
<S**2>=0.000
     304 -> 343       -0.10849
```

```
     306 -> 344       -0.12061
     306 -> 345       -0.10996
     307 -> 343       -0.14592
     330 -> 341        0.24746
     333 -> 343       -0.14468
     335 -> 341       -0.13957
     337 -> 344       -0.23109
     337 -> 345       -0.15781
     338 -> 343        0.46580

 Excited State  36:      Singlet-B3     3.2900 eV  376.85 nm  f=0.0249
<S**2>=0.000
     306 -> 343        0.12800
     307 -> 344        0.10919
     334 -> 343       -0.13860
     335 -> 342       -0.17057
     337 -> 343        0.46662
     338 -> 344       -0.24214
     338 -> 345       -0.28038

 Excited State  37:      Singlet-B2     3.2951 eV  376.27 nm  f=0.0926
<S**2>=0.000
     330 -> 341        0.63825
     336 -> 342        0.16617
     337 -> 345        0.10837
     338 -> 343       -0.16499

 Excited State  38:      Singlet-A      3.3084 eV  374.75 nm  f=0.0000
<S**2>=0.000
     329 -> 342       -0.26681
     331 -> 341        0.60571
     333 -> 342       -0.20680

 Excited State  39:      Singlet-B1     3.3252 eV  372.86 nm  f=0.2101
<S**2>=0.000
     329 -> 341        0.34450
     331 -> 342       -0.13444
     332 -> 342        0.47743
     333 -> 341        0.18295
     334 -> 342        0.27217

 Excited State  40:      Singlet-A      3.3632 eV  368.65 nm  f=0.0000
<S**2>=0.000
     329 -> 342        0.29960
     331 -> 341        0.26519
     332 -> 341        0.30579
     333 -> 342        0.35589
     334 -> 341        0.18260
     339 -> 346        0.18078

 Excited State  41:      Singlet-B3     3.4370 eV  360.73 nm  f=0.0005
<S**2>=0.000
     327 -> 341        0.10585
     330 -> 342        0.65745
```

```
     337 -> 346       -0.11375

 Excited State  42:      Singlet-B1     3.4859 eV  355.67 nm  f=0.0797
<S**2>=0.000
     328 -> 341        0.23674
     331 -> 342        0.62124
     332 -> 342        0.10414
     340 -> 348        0.10224

 Excited State  43:      Singlet-B3     3.5079 eV  353.44 nm  f=0.0249
<S**2>=0.000
     332 -> 343        0.21810
     333 -> 344        0.12558
     334 -> 343        0.52340
     338 -> 344       -0.21089
     338 -> 345       -0.20003

 Excited State  44:      Singlet-A      3.5140 eV  352.83 nm  f=0.0000
<S**2>=0.000
     310 -> 343       -0.12810
     319 -> 344       -0.10764
     335 -> 344       -0.21294
     335 -> 345       -0.25567
     336 -> 343        0.52281
     340 -> 349        0.10825

 Excited State  45:      Singlet-B2     3.5207 eV  352.15 nm  f=0.0000
<S**2>=0.000
     326 -> 341        0.10859
     329 -> 343        0.13613
     333 -> 343        0.55767
     334 -> 344        0.12237
     337 -> 345       -0.26340
     338 -> 346       -0.14784

 Excited State  46:      Singlet-B3     3.5457 eV  349.67 nm  f=0.0000
<S**2>=0.000
     327 -> 341        0.62047
     338 -> 344       -0.14158
     340 -> 347        0.21292
     340 -> 353       -0.10341

 Excited State  47:      Singlet-B1     3.5489 eV  349.36 nm  f=0.0084
<S**2>=0.000
     328 -> 341        0.65090
     331 -> 342       -0.21649
     340 -> 348       -0.12638

 Excited State  48:      Singlet-B3     3.5555 eV  348.71 nm  f=0.0002
<S**2>=0.000
     327 -> 341       -0.27913
     338 -> 344       -0.17061
     338 -> 345        0.10877
     340 -> 347        0.57294
```

```
     340 -> 353       -0.12258

 Excited State  49:      Singlet-B2     3.5751 eV  346.80 nm  f=0.0294
<S**2>=0.000
     326 -> 341        0.19336
     339 -> 351       -0.11602
     340 -> 350        0.64840

 Excited State  50:      Singlet-B1     3.5794 eV  346.38 nm  f=0.0073
<S**2>=0.000
     331 -> 342       -0.13914
     339 -> 349       -0.12028
     340 -> 348        0.65517

 Excited State  51:      Singlet-A      3.5917 eV  345.20 nm  f=0.0000
<S**2>=0.000
     339 -> 348       -0.15160
     339 -> 355       -0.10287
     340 -> 349        0.65569

 Excited State  52:      Singlet-B1     3.6090 eV  343.54 nm  f=0.0431
<S**2>=0.000
     330 -> 343       -0.10491
     335 -> 343        0.51540
     336 -> 344       -0.32337
     336 -> 345       -0.29552

 Excited State  53:      Singlet-B3     3.6208 eV  342.42 nm  f=0.0026
<S**2>=0.000
     323 -> 341        0.10327
     326 -> 342       -0.18864
     333 -> 345       -0.10293
     337 -> 346       -0.14402
     338 -> 344        0.28244
     338 -> 345       -0.17447
     340 -> 347        0.28087
     340 -> 351        0.12368
     340 -> 353        0.39504

 Excited State  54:      Singlet-B2     3.6253 eV  342.00 nm  f=0.0717
<S**2>=0.000
     326 -> 341        0.54164
     333 -> 343       -0.10647
     334 -> 345       -0.11769
     337 -> 344        0.20734
     338 -> 346       -0.26272
     340 -> 350       -0.15108

 Excited State  55:      Singlet-B3     3.6508 eV  339.61 nm  f=0.0603
<S**2>=0.000
     326 -> 342        0.10408
     330 -> 342        0.11369
     337 -> 346        0.19253
     338 -> 344       -0.25688
```

```
     338 -> 345        0.10389
     340 -> 351       -0.16679
     340 -> 353        0.52013

 Excited State  56:      Singlet-B2     3.6611 eV  338.65 nm  f=0.0094
<S**2>=0.000
     339 -> 347       -0.22807
     339 -> 351       -0.17877
     340 -> 352        0.62735

 Excited State  57:      Singlet-B3     3.6634 eV  338.44 nm  f=0.0211
<S**2>=0.000
     338 -> 344       -0.11906
     339 -> 350       -0.23328
     339 -> 352       -0.14240
     340 -> 351        0.59799

 Excited State  58:      Singlet-B2     3.6914 eV  335.87 nm  f=0.0063
<S**2>=0.000
     326 -> 341        0.29905
     329 -> 343        0.18873
     334 -> 344        0.16562
     334 -> 345        0.23758
     337 -> 344       -0.26432
     338 -> 343       -0.13938
     338 -> 346        0.33128
     339 -> 347       -0.13556
     340 -> 350       -0.15117
     340 -> 356        0.10463

 Excited State  59:      Singlet-A      3.7058 eV  334.57 nm  f=0.0000
<S**2>=0.000
     320 -> 341       -0.12606
     328 -> 342        0.29960
     339 -> 348       -0.28300
     340 -> 354        0.54170

 Excited State  60:      Singlet-B3     3.7179 eV  333.48 nm  f=0.0083
<S**2>=0.000
     325 -> 341       -0.11865
     329 -> 344       -0.16227
     329 -> 345       -0.22307
     332 -> 343        0.31312
     333 -> 344        0.16783
     333 -> 345        0.22404
     334 -> 343       -0.21519
     337 -> 343       -0.14931
     337 -> 346        0.10934
     338 -> 345       -0.29644
```

Table S4.11. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.6.**

```
Excited State   1:      Singlet-B2     1.7805 eV  696.35 nm  f=0.1612
<S**2>=0.000
     357 -> 360       -0.16639
     358 -> 359        0.68237

 Excited State   2:      Singlet-B3     1.8663 eV  664.34 nm  f=0.0461
<S**2>=0.000
     358 -> 360        0.69549

 Excited State   3:      Singlet-B3     1.8902 eV  655.94 nm  f=0.0299
<S**2>=0.000
     357 -> 359        0.69773

 Excited State   4:      Singlet-B1     2.0698 eV  599.02 nm  f=0.1065
<S**2>=0.000
     356 -> 359       -0.12650
     358 -> 361        0.66745
     358 -> 364        0.11154

 Excited State   5:      Singlet-B2     2.2718 eV  545.75 nm  f=0.3580
<S**2>=0.000
     356 -> 361        0.13061
     357 -> 360        0.67325
     358 -> 359        0.14863

 Excited State   6:      Singlet-A      2.3486 eV  527.92 nm  f=0.0000
<S**2>=0.000
     356 -> 360       -0.20914
     357 -> 361        0.56601
     358 -> 362       -0.20341
     358 -> 363       -0.24502

 Excited State   7:      Singlet-A      2.4892 eV  498.08 nm  f=0.0000
<S**2>=0.000
     354 -> 361        0.13270
     357 -> 361        0.35006
     358 -> 362        0.33231
     358 -> 363        0.47685

 Excited State   8:      Singlet-B1     2.6512 eV  467.66 nm  f=0.1281
<S**2>=0.000
     355 -> 360       -0.13269
     356 -> 359        0.62283
     357 -> 362        0.13211
     358 -> 364        0.24628

 Excited State   9:      Singlet-A      2.7043 eV  458.47 nm  f=0.0000
<S**2>=0.000
     352 -> 360       -0.11887
     355 -> 359        0.51785
     358 -> 362        0.35322
     358 -> 363       -0.26192
```

```
 Excited State  10:      Singlet-B1     2.7597 eV  449.27 nm  f=0.0129
<S**2>=0.000
     352 -> 359        0.21239
     355 -> 360       -0.35027
     357 -> 362        0.21657
     357 -> 363        0.37562
     358 -> 361        0.11288
     358 -> 364       -0.34307

 Excited State  11:      Singlet-A      2.7899 eV  444.41 nm  f=0.0000
<S**2>=0.000
     355 -> 359        0.42207
     356 -> 360       -0.23527
     357 -> 361       -0.12617
     358 -> 362       -0.37947
     358 -> 363        0.29221

 Excited State  12:      Singlet-B3     2.8082 eV  441.51 nm  f=0.0003
<S**2>=0.000
     353 -> 360       -0.19752
     354 -> 359        0.65056

 Excited State  13:      Singlet-B1     2.8443 eV  435.90 nm  f=0.2644
<S**2>=0.000
     356 -> 359       -0.23168
     357 -> 362        0.24741
     357 -> 363        0.35974
     358 -> 364        0.47448

 Excited State  14:      Singlet-B2     2.8708 eV  431.89 nm  f=0.0180
<S**2>=0.000
     345 -> 361        0.11474
     353 -> 359       -0.37195
     354 -> 360        0.25503
     355 -> 363        0.10538
     356 -> 361        0.45361

 Excited State  15:      Singlet-B2     2.9266 eV  423.64 nm  f=0.1688
<S**2>=0.000
     352 -> 361       -0.11237
     353 -> 359       -0.26791
     354 -> 360        0.41030
     356 -> 361       -0.38112
     356 -> 364       -0.10539

 Excited State  16:      Singlet-B3     2.9406 eV  421.63 nm  f=0.0000
<S**2>=0.000
     338 -> 361        0.12305
     351 -> 361        0.15638
     352 -> 363        0.10939
     355 -> 361        0.55700
     355 -> 364        0.12112
     356 -> 362        0.15859
```

```
     356 -> 363        0.22655

 Excited State  17:      Singlet-A      2.9424 eV  421.36 nm  f=0.0000
<S**2>=0.000
     356 -> 360        0.57046
     357 -> 361        0.10714
     357 -> 364        0.27545
     358 -> 362       -0.21870
     358 -> 363        0.10062

 Excited State  18:      Singlet-B1     2.9472 eV  420.69 nm  f=0.0123
<S**2>=0.000
     352 -> 359       -0.12093
     355 -> 360        0.30578
     357 -> 362        0.56987
     357 -> 363       -0.15823
     358 -> 364       -0.17257

 Excited State  19:      Singlet-A      3.0554 eV  405.79 nm  f=0.0000
<S**2>=0.000
     345 -> 360       -0.21562
     348 -> 359        0.40785
     350 -> 359       -0.33888
     351 -> 359       -0.29679
     357 -> 364        0.27160

 Excited State  20:      Singlet-B3     3.0679 eV  404.14 nm  f=0.0066
<S**2>=0.000
     345 -> 362        0.18183
     345 -> 363        0.26307
     348 -> 361        0.46671
     348 -> 364        0.13725
     350 -> 361       -0.28271
     354 -> 359        0.16667

 Excited State  21:      Singlet-B1     3.0951 eV  400.58 nm  f=0.0524
<S**2>=0.000
     345 -> 359       -0.18207
     348 -> 360        0.15035
     350 -> 360       -0.13980
     351 -> 360       -0.25350
     352 -> 359        0.54214
     355 -> 360        0.11074
     357 -> 363       -0.13377
     358 -> 364        0.13695

 Excited State  22:      Singlet-A      3.0970 eV  400.33 nm  f=0.0000
<S**2>=0.000
     348 -> 359       -0.24456
     350 -> 359        0.27626
     351 -> 359       -0.26481
     356 -> 360       -0.20469
     357 -> 364        0.46946
```

```
 Excited State  23:      Singlet-B2     3.1139 eV  398.17 nm  f=0.1001
<S**2>=0.000
     345 -> 361        0.30318
     348 -> 362        0.13734
     348 -> 363        0.17960
     350 -> 363       -0.11664
     353 -> 359        0.48273
     354 -> 360        0.24094

 Excited State  24:      Singlet-B1     3.1247 eV  396.79 nm  f=0.1933
<S**2>=0.000
     345 -> 359        0.24304
     348 -> 360       -0.30882
     350 -> 360        0.13314
     352 -> 359        0.23476
     355 -> 360        0.41081
     357 -> 363        0.27606

 Excited State  25:      Singlet-A      3.1522 eV  393.33 nm  f=0.0000
<S**2>=0.000
     351 -> 359        0.15298
     352 -> 360       -0.15536
     353 -> 362        0.14039
     353 -> 363        0.12415
     354 -> 361        0.55830
     358 -> 363       -0.15714

 Excited State  26:      Singlet-A      3.1586 eV  392.53 nm  f=0.0000
<S**2>=0.000
     348 -> 359        0.23598
     351 -> 359        0.40850
     352 -> 360       -0.30474
     354 -> 361       -0.21024
     355 -> 359       -0.13912
     357 -> 364        0.23199
     358 -> 363        0.11320

 Excited State  27:      Singlet-B1     3.1675 eV  391.42 nm  f=0.4873
<S**2>=0.000
     345 -> 359       -0.26965
     348 -> 360        0.29899
     350 -> 360       -0.25523
     352 -> 359       -0.12600
     355 -> 360        0.26279
     356 -> 359        0.14955
     357 -> 362       -0.14474
     357 -> 363        0.29381
     358 -> 364       -0.10054

 Excited State  28:      Singlet-B2     3.1892 eV  388.76 nm  f=0.0003
<S**2>=0.000
     345 -> 361       -0.31717
     348 -> 362       -0.13262
     348 -> 363       -0.19997
```

```
     349 -> 359        0.15897
     351 -> 363        0.10733
     352 -> 361        0.19401
     353 -> 359        0.18502
     354 -> 360        0.37321
     355 -> 363        0.14933

 Excited State  29:      Singlet-B1     3.2151 eV  385.63 nm  f=0.0034
<S**2>=0.000
     328 -> 361        0.10360
     349 -> 361       -0.13925
     353 -> 361        0.49552
     353 -> 364        0.10438
     354 -> 362        0.22317
     354 -> 363        0.28233
     358 -> 361       -0.10436
     358 -> 364       -0.12444

 Excited State  30:      Singlet-B3     3.2243 eV  384.53 nm  f=0.0069
<S**2>=0.000
     351 -> 361        0.22635
     353 -> 360        0.45576
     354 -> 359        0.10273
     355 -> 361       -0.23655
     356 -> 362        0.21578
     356 -> 363        0.29658

 Excited State  31:      Singlet-A      3.2740 eV  378.69 nm  f=0.0000
<S**2>=0.000
     348 -> 359        0.37173
     350 -> 359        0.52788
     351 -> 359       -0.13065
     352 -> 360        0.12962
     357 -> 364       -0.12021

 Excited State  32:      Singlet-B2     3.2904 eV  376.80 nm  f=0.0390
<S**2>=0.000
     345 -> 361        0.16727
     349 -> 359       -0.19263
     352 -> 361        0.38209
     355 -> 362        0.27160
     355 -> 363        0.29825
     356 -> 361       -0.23117

 Excited State  33:      Singlet-B3     3.2972 eV  376.03 nm  f=0.0505
<S**2>=0.000
     353 -> 360        0.47666
     354 -> 359        0.15346
     355 -> 361        0.24943
     356 -> 362       -0.17953
     356 -> 363       -0.34793

 Excited State  34:      Singlet-B2     3.3216 eV  373.27 nm  f=0.0311
<S**2>=0.000
```

```
     349 -> 359        0.63633
     354 -> 360       -0.22932

 Excited State  35:      Singlet-B1     3.3813 eV  366.67 nm  f=0.1572
<S**2>=0.000
     345 -> 359       -0.20068
     350 -> 360        0.15608
     351 -> 360        0.60360
     352 -> 359        0.22233

 Excited State  36:      Singlet-A      3.3905 eV  365.68 nm  f=0.0000
<S**2>=0.000
     345 -> 360       -0.15867
     351 -> 359        0.32746
     352 -> 360        0.56011
     357 -> 364        0.15363

 Excited State  37:      Singlet-B1     3.4561 eV  358.74 nm  f=0.0907
<S**2>=0.000
     345 -> 359       -0.41916
     350 -> 360        0.49582
     351 -> 360       -0.21420

 Excited State  38:      Singlet-B1     3.5042 eV  353.82 nm  f=0.0000
<S**2>=0.000
     345 -> 359        0.25711
     346 -> 359        0.37202
     348 -> 360        0.46523
     350 -> 360        0.25084

 Excited State  39:      Singlet-B3     3.5053 eV  353.71 nm  f=0.0014
<S**2>=0.000
     343 -> 359        0.10711
     347 -> 359        0.41477
     349 -> 360        0.53931

 Excited State  40:      Singlet-B1     3.5433 eV  349.91 nm  f=0.0047
<S**2>=0.000
     345 -> 359       -0.20251
     346 -> 359        0.58758
     348 -> 360       -0.23568
     350 -> 360       -0.21592

 Excited State  41:      Singlet-B3     3.5458 eV  349.67 nm  f=0.0001
<S**2>=0.000
     347 -> 359        0.56197
     349 -> 360       -0.39702

 Excited State  42:      Singlet-B2     3.5536 eV  348.90 nm  f=0.0260
<S**2>=0.000
     344 -> 359        0.61265
     352 -> 361        0.17551
     355 -> 363       -0.15432
     356 -> 364       -0.17804
```

```
 Excited State  43:      Singlet-A      3.5552 eV  348.74 nm  f=0.0000
<S**2>=0.000
     345 -> 360        0.61866
     346 -> 360        0.10899
     348 -> 359        0.24926
     352 -> 360        0.14152

 Excited State  44:      Singlet-B3     3.5994 eV  344.46 nm  f=0.0236
<S**2>=0.000
     343 -> 359       -0.15959
     344 -> 360       -0.19300
     348 -> 361        0.16255
     351 -> 361        0.52283
     352 -> 362        0.13842
     355 -> 364       -0.10325
     356 -> 362       -0.11653
     356 -> 363       -0.23386

 Excited State  45:      Singlet-B3     3.6201 eV  342.49 nm  f=0.0046
<S**2>=0.000
     356 -> 362        0.32714
     356 -> 363       -0.17048
     358 -> 365        0.55177

 Excited State  46:      Singlet-B2     3.6488 eV  339.79 nm  f=0.0201
<S**2>=0.000
     344 -> 359       -0.22175
     352 -> 361        0.37365
     355 -> 363       -0.33756
     356 -> 364       -0.17073
     358 -> 368       -0.34461

 Excited State  47:      Singlet-B1     3.6550 eV  339.22 nm  f=0.0023
<S**2>=0.000
     358 -> 366        0.68251

 Excited State  48:      Singlet-B3     3.6617 eV  338.60 nm  f=0.0128
<S**2>=0.000
     341 -> 359        0.10617
     343 -> 359       -0.14970
     344 -> 360       -0.30627
     351 -> 361       -0.10577
     355 -> 364       -0.10359
     356 -> 362        0.37363
     356 -> 363       -0.17943
     358 -> 365       -0.37244

 Excited State  49:      Singlet-A      3.6623 eV  338.55 nm  f=0.0000
<S**2>=0.000
     357 -> 366       -0.11422
     358 -> 367        0.67523
```

```
 Excited State  50:      Singlet-B2     3.6637 eV  338.41 nm  f=0.0325
<S**2>=0.000
     344 -> 359       -0.16920
     352 -> 361        0.23714
     355 -> 362       -0.12150
     355 -> 363       -0.21050
     357 -> 369       -0.10352
     358 -> 368        0.56422

 Excited State  51:      Singlet-B3     3.7094 eV  334.25 nm  f=0.0259
<S**2>=0.000
     335 -> 360        0.11375
     341 -> 359        0.17479
     343 -> 359        0.58534
     349 -> 360       -0.12874
     351 -> 361        0.12051
     355 -> 364       -0.11239
     358 -> 369        0.14147

 Excited State  52:      Singlet-B3     3.7358 eV  331.88 nm  f=0.0096
<S**2>=0.000
     343 -> 359       -0.11412
     344 -> 360        0.10368
     357 -> 368       -0.19647
     357 -> 370       -0.17796
     358 -> 369        0.61917

 Excited State  53:      Singlet-B2     3.7367 eV  331.80 nm  f=0.0048
<S**2>=0.000
     347 -> 360       -0.19376
     357 -> 365        0.17682
     357 -> 369       -0.18818
     358 -> 370        0.60532

 Excited State  54:      Singlet-B1     3.7403 eV  331.48 nm  f=0.0482
<S**2>=0.000
     344 -> 361       -0.12081
     349 -> 361        0.18846
     353 -> 361        0.43576
     354 -> 362       -0.26588
     354 -> 363       -0.40460

 Excited State  55:      Singlet-B2     3.7423 eV  331.31 nm  f=0.0131
<S**2>=0.000
     344 -> 359        0.13003
     347 -> 360       -0.13400
     351 -> 363        0.14159
     352 -> 361        0.11386
     355 -> 362       -0.17784
     356 -> 361       -0.14497
     356 -> 364        0.54441
     358 -> 368       -0.14381
```

```
 Excited State  56:      Singlet-B3     3.7492 eV  330.69 nm  f=0.0503
<S**2>=0.000
     341 -> 359        0.10258
     356 -> 362       -0.14094
     358 -> 371        0.64237

 Excited State  57:      Singlet-A      3.7563 eV  330.07 nm  f=0.0000
<S**2>=0.000
     339 -> 359        0.20394
     345 -> 360       -0.11815
     346 -> 360        0.63270
     358 -> 372        0.14265

 Excited State  58:      Singlet-B2     3.7582 eV  329.90 nm  f=0.0046
<S**2>=0.000
     340 -> 359        0.19481
     347 -> 360        0.61437
     358 -> 370        0.20376

 Excited State  59:      Singlet-B3     3.7809 eV  327.93 nm  f=0.0173
<S**2>=0.000
     341 -> 359       -0.23183
     344 -> 360        0.41841
     350 -> 361        0.11276
     351 -> 361        0.13546
     356 -> 362        0.26470
     356 -> 363       -0.23721
     358 -> 365       -0.13875
     358 -> 371        0.17610

 Excited State  60:      Singlet-A      3.7959 eV  326.62 nm  f=0.0000
<S**2>=0.000
     327 -> 361        0.11541
     346 -> 360        0.12541
     353 -> 362        0.19000
     353 -> 363        0.40023
     354 -> 361       -0.27028
     354 -> 364        0.19452
     357 -> 366        0.12695
     358 -> 372       -0.26514
```

Table S4.12. Vertical excitation energies, oscillator strengths, and expansion coefficients for **4.8.**

```
Excited State   1:      Singlet-B      1.7279 eV  717.54 nm  f=0.1185
<S**2>=0.000
     348 -> 350        0.12623
     348 -> 351        0.13719
     349 -> 350        0.66443
     349 -> 351        0.13152
```

```
 Excited State   2:      Singlet-A      1.7651 eV  702.42 nm  f=0.0217
<S**2>=0.000
     319 -> 352        0.10333
     319 -> 353        0.15103
     319 -> 354        0.10139
     343 -> 352        0.11456
     343 -> 353        0.12416
     345 -> 352        0.15792
     345 -> 353        0.22004
     345 -> 354        0.13681
     349 -> 352        0.39885
     349 -> 353        0.29867
     349 -> 354        0.18291

 Excited State   3:      Singlet-B      1.7986 eV  689.34 nm  f=0.0522
<S**2>=0.000
     349 -> 351        0.65552

 Excited State   4:      Singlet-B      1.8984 eV  653.10 nm  f=0.0656
<S**2>=0.000
     348 -> 350        0.68136
     349 -> 350       -0.11534

 Excited State   5:      Singlet-B      1.9602 eV  632.50 nm  f=0.0110
<S**2>=0.000
     338 -> 352        0.13414
     338 -> 353        0.18219
     338 -> 354        0.12224
     339 -> 352        0.25937
     339 -> 353        0.35454
     339 -> 354        0.23699
     344 -> 352        0.18905
     344 -> 353        0.23352
     344 -> 354        0.14921
     349 -> 351       -0.19502

 Excited State   6:      Singlet-B      2.0621 eV  601.24 nm  f=0.0045
<S**2>=0.000
     320 -> 352        0.10040
     320 -> 353        0.14048
     321 -> 353        0.10742
     329 -> 352       -0.10608
     329 -> 353       -0.15145
     329 -> 354       -0.10237
     344 -> 352       -0.12906
     344 -> 353       -0.16875
     344 -> 354       -0.10962
     346 -> 352       -0.19334
     346 -> 353       -0.23474
     346 -> 354       -0.15458
     347 -> 352        0.21756
     347 -> 353        0.27098
     347 -> 354        0.17079
```

```
 Excited State   7:      Singlet-A      2.1383 eV  579.84 nm  f=0.0802
<S**2>=0.000
     345 -> 352       -0.14896
     347 -> 350        0.12604
     348 -> 352       -0.14457
     349 -> 352        0.51555
     349 -> 353       -0.24963
     349 -> 354       -0.17422
     349 -> 355        0.13645

 Excited State   8:      Singlet-B      2.2433 eV  552.69 nm  f=0.3551
<S**2>=0.000
     347 -> 352        0.11708
     348 -> 351        0.66999
     349 -> 350       -0.14674

 Excited State   9:      Singlet-A      2.3446 eV  528.80 nm  f=0.0017
<S**2>=0.000
     347 -> 351       -0.20309
     348 -> 352        0.60822
     348 -> 353        0.13613
     349 -> 352        0.12116

 Excited State  10:      Singlet-A      2.5835 eV  479.91 nm  f=0.0178
<S**2>=0.000
     344 -> 350       -0.10422
     345 -> 353       -0.11945
     346 -> 351        0.24094
     347 -> 350        0.26322
     348 -> 352       -0.19027
     348 -> 353        0.33466
     348 -> 354        0.16028
     349 -> 353        0.25644
     349 -> 354        0.16382

 Excited State  11:      Singlet-A      2.6432 eV  469.07 nm  f=0.0939
<S**2>=0.000
     347 -> 350        0.54603
     348 -> 354       -0.14852
     349 -> 353       -0.27630
     349 -> 355       -0.19259

 Excited State  12:      Singlet-A      2.6675 eV  464.79 nm  f=0.0061
<S**2>=0.000
     344 -> 351       -0.10285
     346 -> 350        0.54271
     347 -> 350        0.10186
     349 -> 353        0.20601
     349 -> 354       -0.32629

 Excited State  13:      Singlet-A      2.7254 eV  454.92 nm  f=0.0044
<S**2>=0.000
     346 -> 350       -0.28867
     346 -> 351       -0.13977
```

```
     347 -> 350        0.11547
     347 -> 351       -0.18037
     348 -> 352       -0.11770
     348 -> 353       -0.27457
     348 -> 354       -0.22247
     349 -> 353        0.32497
     349 -> 354       -0.15016
     349 -> 355       -0.13183

 Excited State  14:      Singlet-B      2.7537 eV  450.25 nm  f=0.0120
<S**2>=0.000
     313 -> 352        0.19233
     313 -> 353        0.26473
     313 -> 354        0.17872
     315 -> 352        0.12890
     315 -> 353        0.19686
     315 -> 354        0.13254
     317 -> 352        0.13488
     317 -> 353        0.16889
     317 -> 354        0.11162
     320 -> 353        0.12365
     345 -> 350       -0.13855
     345 -> 351        0.11019
     346 -> 352       -0.15407
     347 -> 352       -0.19852
     347 -> 353       -0.11466

 Excited State  15:      Singlet-A      2.7558 eV  449.91 nm  f=0.0335
<S**2>=0.000
     345 -> 353       -0.11887
     345 -> 354       -0.10134
     346 -> 350        0.24933
     346 -> 351       -0.12674
     347 -> 350       -0.10372
     348 -> 353       -0.17142
     349 -> 352        0.15100
     349 -> 354        0.41245
     349 -> 355       -0.30231

 Excited State  16:      Singlet-B      2.7670 eV  448.09 nm  f=0.0011
<S**2>=0.000
     343 -> 350       -0.12910
     343 -> 351       -0.17628
     345 -> 350        0.63074

 Excited State  17:      Singlet-A      2.7975 eV  443.20 nm  f=0.1176
<S**2>=0.000
     339 -> 351        0.11459
     344 -> 350       -0.30710
     344 -> 351        0.19573
     347 -> 350        0.15593
     348 -> 353       -0.28403
     348 -> 354       -0.10373
     349 -> 354        0.15527
```

```
     349 -> 355        0.39012

 Excited State  18:      Singlet-B      2.8535 eV  434.50 nm  f=0.0152
<S**2>=0.000
     338 -> 352        0.12388
     340 -> 350        0.10552
     343 -> 350       -0.37827
     345 -> 351        0.45118
     347 -> 352       -0.13225

 Excited State  19:      Singlet-A      2.8540 eV  434.43 nm  f=0.0064
<S**2>=0.000
     339 -> 350        0.20682
     339 -> 351       -0.21249
     344 -> 350        0.22767
     344 -> 351       -0.26685
     346 -> 351        0.31294
     347 -> 351       -0.20811
     348 -> 353       -0.23295
     349 -> 354        0.18123
     349 -> 355        0.14200

 Excited State  20:      Singlet-A      2.8686 eV  432.21 nm  f=0.0204
<S**2>=0.000
     339 -> 350        0.10173
     344 -> 350        0.28905
     344 -> 351       -0.13540
     346 -> 351       -0.14227
     347 -> 351        0.42667
     348 -> 353        0.12019
     348 -> 354       -0.12265
     348 -> 355        0.13862
     349 -> 353        0.18173
     349 -> 355        0.22061

 Excited State  21:      Singlet-B      2.8925 eV  428.63 nm  f=0.0818
<S**2>=0.000
     342 -> 352        0.21796
     345 -> 351        0.25857
     346 -> 352        0.34862
     346 -> 355        0.10768
     347 -> 352        0.34059
     347 -> 355        0.11880

 Excited State  22:      Singlet-A      2.9461 eV  420.84 nm  f=0.0007
<S**2>=0.000
     338 -> 350       -0.11509
     342 -> 350       -0.27021
     342 -> 351       -0.11129
     346 -> 351        0.25651
     347 -> 351        0.25822
     348 -> 353       -0.24340
     348 -> 354        0.34320
     349 -> 354       -0.15732
```

```
     349 -> 355       -0.14066

 Excited State  23:      Singlet-A      2.9744 eV  416.84 nm  f=0.0000
<S**2>=0.000
     338 -> 350        0.18916
     339 -> 351       -0.10998
     341 -> 350        0.10732
     342 -> 350        0.37873
     342 -> 351        0.15504
     344 -> 350       -0.23032
     344 -> 351       -0.25429
     346 -> 350       -0.12476
     347 -> 351        0.22630
     348 -> 353       -0.11090
     348 -> 354        0.13517
     349 -> 355       -0.12370

 Excited State  24:      Singlet-B      3.0428 eV  407.47 nm  f=0.0499
<S**2>=0.000
     338 -> 352        0.37888
     338 -> 353       -0.10471
     338 -> 355        0.16209
     339 -> 352       -0.18779
     342 -> 352        0.25108
     342 -> 355        0.11021
     343 -> 350        0.33984
     344 -> 352       -0.14753

 Excited State  25:      Singlet-B      3.0502 eV  406.47 nm  f=0.0061
<S**2>=0.000
     338 -> 352       -0.12780
     342 -> 352       -0.11314
     343 -> 350        0.29550
     343 -> 351        0.13156
     344 -> 352        0.16780
     345 -> 350        0.15319
     345 -> 351        0.32106
     346 -> 352       -0.28215
     347 -> 352        0.23248
     347 -> 353       -0.10831

 Excited State  26:      Singlet-A      3.0870 eV  401.63 nm  f=0.2162
<S**2>=0.000
     338 -> 350       -0.11376
     339 -> 351        0.19813
     342 -> 350        0.30452
     344 -> 350        0.24240
     344 -> 351        0.14600
     345 -> 352        0.12640
     346 -> 351       -0.14915
     347 -> 351       -0.16011
     348 -> 354        0.29488
     348 -> 355        0.26907
```

```
 Excited State  27:      Singlet-A      3.0988 eV  400.10 nm  f=0.3924
<S**2>=0.000
     339 -> 350       -0.16683
     342 -> 350        0.12619
     343 -> 352       -0.10105
     344 -> 350        0.12455
     344 -> 351        0.10238
     345 -> 352        0.10157
     346 -> 351        0.40573
     347 -> 350       -0.13381
     348 -> 354       -0.30219
     348 -> 355        0.26608

 Excited State  28:      Singlet-A      3.1215 eV  397.19 nm  f=0.0119
<S**2>=0.000
     340 -> 352        0.10028
     342 -> 350       -0.11923
     343 -> 352       -0.35754
     343 -> 355       -0.10716
     344 -> 350       -0.11747
     345 -> 352        0.40399
     345 -> 353       -0.10346
     345 -> 355        0.12655
     348 -> 355       -0.13560
     349 -> 355        0.16145

 Excited State  29:      Singlet-A      3.1401 eV  394.84 nm  f=0.0221
<S**2>=0.000
     338 -> 350        0.16851
     339 -> 350       -0.19150
     339 -> 351       -0.23502
     341 -> 350       -0.13988
     342 -> 350       -0.22968
     342 -> 351       -0.15687
     344 -> 350       -0.14828
     344 -> 351       -0.13861
     346 -> 350        0.10846
     348 -> 354        0.11054
     348 -> 355        0.40698

 Excited State  30:      Singlet-B      3.1431 eV  394.46 nm  f=0.1344
<S**2>=0.000
     343 -> 350        0.32479
     345 -> 350        0.10384
     345 -> 351        0.24930
     346 -> 352        0.29663
     347 -> 352       -0.32077
     347 -> 353        0.12643
     347 -> 354        0.12456
     347 -> 355       -0.10377

 Excited State  31:      Singlet-A      3.1604 eV  392.31 nm  f=0.0540
<S**2>=0.000
     338 -> 350       -0.11246
```

```
     338 -> 351       -0.16160
     339 -> 350        0.45654
     339 -> 351       -0.16327
     341 -> 350       -0.19356
     342 -> 351        0.13600
     344 -> 350       -0.17672
     344 -> 351        0.16134
     348 -> 355        0.24423
     349 -> 355       -0.10030

 Excited State  32:      Singlet-B      3.2159 eV  385.54 nm  f=0.0475
<S**2>=0.000
     340 -> 350       -0.12252
     342 -> 352        0.13305
     343 -> 351        0.62447
     345 -> 350        0.16420
     347 -> 352       -0.10172

 Excited State  33:      Singlet-A      3.2339 eV  383.38 nm  f=0.0789
<S**2>=0.000
     338 -> 350        0.38714
     338 -> 351        0.13545
     339 -> 351       -0.18864
     341 -> 350        0.19151
     342 -> 351        0.20667
     344 -> 350        0.17635
     344 -> 351        0.36530

 Excited State  34:      Singlet-A      3.2760 eV  378.46 nm  f=0.0780
<S**2>=0.000
     338 -> 351        0.14664
     341 -> 350       -0.41225
     341 -> 351        0.10119
     342 -> 350       -0.13132
     342 -> 351        0.46272
     344 -> 350        0.12097
     344 -> 351       -0.12584

 Excited State  35:      Singlet-B      3.2887 eV  377.00 nm  f=0.0183
<S**2>=0.000
     340 -> 350        0.66418
     343 -> 351        0.10067
     345 -> 351       -0.16372

 Excited State  36:      Singlet-A      3.3176 eV  373.72 nm  f=0.0053
<S**2>=0.000
     338 -> 350       -0.32599
     341 -> 350        0.44137
     342 -> 350       -0.14649
     342 -> 351        0.31912
     344 -> 351       -0.10124
     348 -> 355        0.17547
```

```
 Excited State  37:      Singlet-B      3.3473 eV  370.40 nm  f=0.0484
<S**2>=0.000
     313 -> 353        0.12375
     338 -> 352        0.10914
     342 -> 352       -0.16227
     343 -> 351        0.13974
     346 -> 352        0.19171
     346 -> 353        0.30968
     346 -> 354        0.15533
     347 -> 352        0.16738
     347 -> 353        0.31259
     347 -> 354        0.20640

 Excited State  38:      Singlet-A      3.4006 eV  364.60 nm  f=0.0352
<S**2>=0.000
     338 -> 350        0.20958
     338 -> 351        0.26630
     339 -> 350        0.34709
     339 -> 351        0.39672
     341 -> 350        0.10012
     342 -> 350       -0.11709
     344 -> 351       -0.17392

 Excited State  39:      Singlet-B      3.4513 eV  359.24 nm  f=0.0013
<S**2>=0.000
     337 -> 350       -0.14273
     340 -> 351        0.61861
     344 -> 352        0.18750

 Excited State  40:      Singlet-A      3.4719 eV  357.11 nm  f=0.0963
<S**2>=0.000
     336 -> 350       -0.23596
     341 -> 351        0.61426
     342 -> 351       -0.10351

 Excited State  41:      Singlet-B      3.4918 eV  355.07 nm  f=0.0223
<S**2>=0.000
     337 -> 350        0.15918
     339 -> 353       -0.10709
     340 -> 351       -0.20337
     342 -> 352        0.24433
     344 -> 352        0.49021
     346 -> 354       -0.10709
     347 -> 353        0.10234

 Excited State  42:      Singlet-A      3.5206 eV  352.17 nm  f=0.0000
<S**2>=0.000
     336 -> 350        0.45745
     338 -> 350       -0.20418
     338 -> 351        0.27673
     339 -> 351       -0.17093
     343 -> 352        0.20214
     345 -> 352        0.20414
```

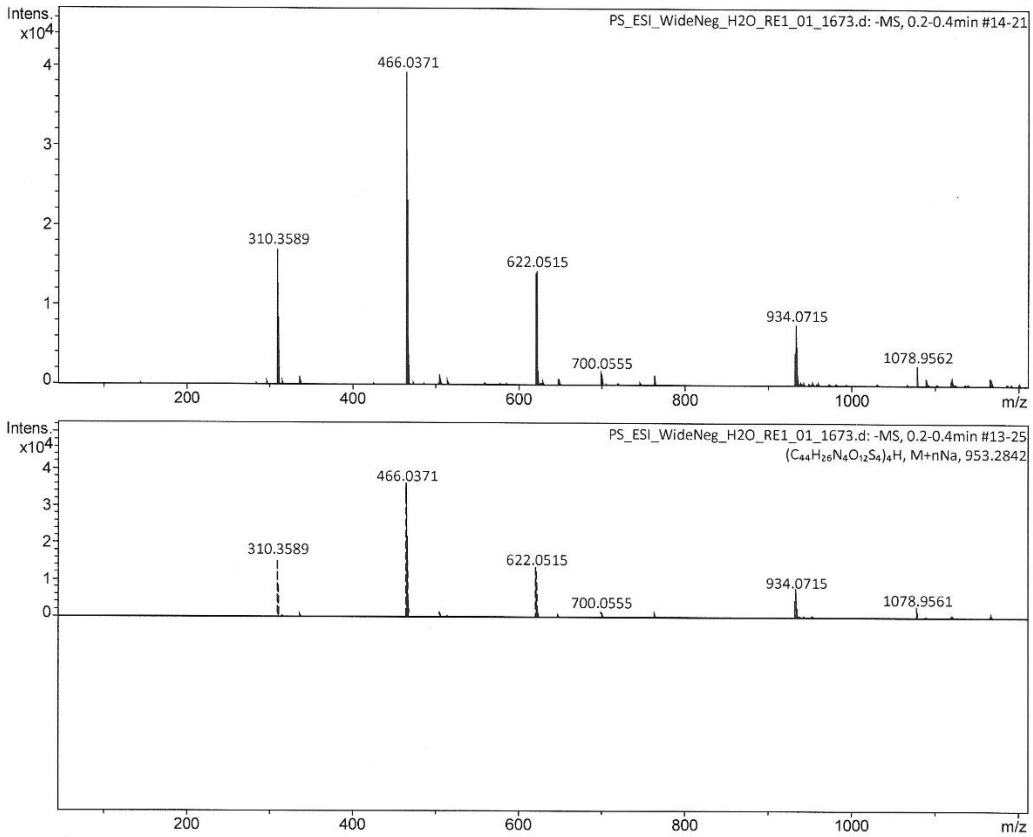
```
 Excited State  43:      Singlet-B      3.5277 eV  351.46 nm  f=0.0009
<S**2>=0.000
     337 -> 350        0.66066
     340 -> 351        0.17794

 Excited State  44:      Singlet-A      3.5369 eV  350.55 nm  f=0.0666
<S**2>=0.000
     336 -> 350        0.41884
     341 -> 351        0.19821
     343 -> 352       -0.31547
     345 -> 352       -0.30562
     345 -> 353        0.10695
     345 -> 354        0.11430

 Excited State  45:      Singlet-A      3.5458 eV  349.66 nm  f=0.0260
<S**2>=0.000
     336 -> 350       -0.21218
     338 -> 350       -0.17793
     338 -> 351        0.47232
     339 -> 351       -0.15430
     341 -> 351       -0.15287
     342 -> 351       -0.12283
     343 -> 352       -0.21218
     345 -> 352       -0.19005

 Excited State  46:      Singlet-B      3.5607 eV  348.20 nm  f=0.0108
<S**2>=0.000
     335 -> 350        0.17941
     338 -> 352       -0.20227
     339 -> 352        0.22785
     342 -> 352        0.37581
     346 -> 352       -0.12649
     346 -> 353        0.11409
     346 -> 354        0.19358
     347 -> 353        0.21524
     347 -> 355       -0.10572
     349 -> 359        0.14046

 Excited State  47:      Singlet-B      3.5799 eV  346.33 nm  f=0.0028
<S**2>=0.000
     335 -> 350        0.28669
     347 -> 353       -0.15677
     347 -> 354        0.17336
     349 -> 356        0.50973
     349 -> 359        0.22701

 Excited State  48:      Singlet-A      3.5974 eV  344.65 nm  f=0.0009
<S**2>=0.000
     349 -> 357        0.58999
     349 -> 358        0.32229

 Excited State  49:      Singlet-B      3.5981 eV  344.58 nm  f=0.0016
<S**2>=0.000
     335 -> 350        0.42945
```

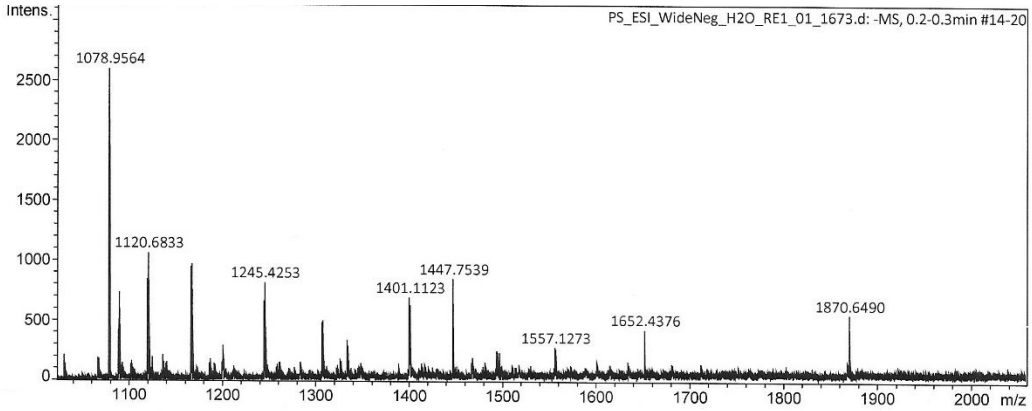
```
     342 -> 352       -0.13389
     344 -> 352        0.10399
     349 -> 356       -0.37642
     349 -> 359        0.23511

 Excited State  50:      Singlet-B      3.6139 eV  343.08 nm  f=0.0666
<S**2>=0.000
     335 -> 350       -0.26605
     347 -> 353        0.10109
     347 -> 354       -0.11184
     347 -> 355        0.14580
     349 -> 359        0.54989
     349 -> 360       -0.11541

 Excited State  51:      Singlet-A      3.6254 eV  341.99 nm  f=0.0008
<S**2>=0.000
     349 -> 357       -0.33242
     349 -> 358        0.58726

 Excited State  52:      Singlet-B      3.6535 eV  339.35 nm  f=0.0424
<S**2>=0.000
     332 -> 350        0.10690
     334 -> 350       -0.12220
     335 -> 350       -0.19523
     335 -> 351        0.26265
     344 -> 354       -0.10395
     346 -> 355       -0.10008
     347 -> 353       -0.26118
     347 -> 354        0.36424
     349 -> 356       -0.20181
     349 -> 359        0.11602
     349 -> 362       -0.13923

 Excited State  53:      Singlet-B      3.6745 eV  337.42 nm  f=0.0165
<S**2>=0.000
     338 -> 352        0.21990
     339 -> 352        0.35921
     344 -> 352        0.10365
     344 -> 353       -0.27305
     344 -> 354       -0.23237
     346 -> 353        0.11827
     347 -> 354       -0.22644
     349 -> 361        0.16631
     349 -> 362       -0.13626

 Excited State  54:      Singlet-B      3.6792 eV  336.99 nm  f=0.0079
<S**2>=0.000
     339 -> 352       -0.12838
     344 -> 353        0.12143
     348 -> 356        0.11510
     348 -> 361        0.12831
     349 -> 360        0.18829
     349 -> 361        0.55573
     349 -> 362       -0.17974
```

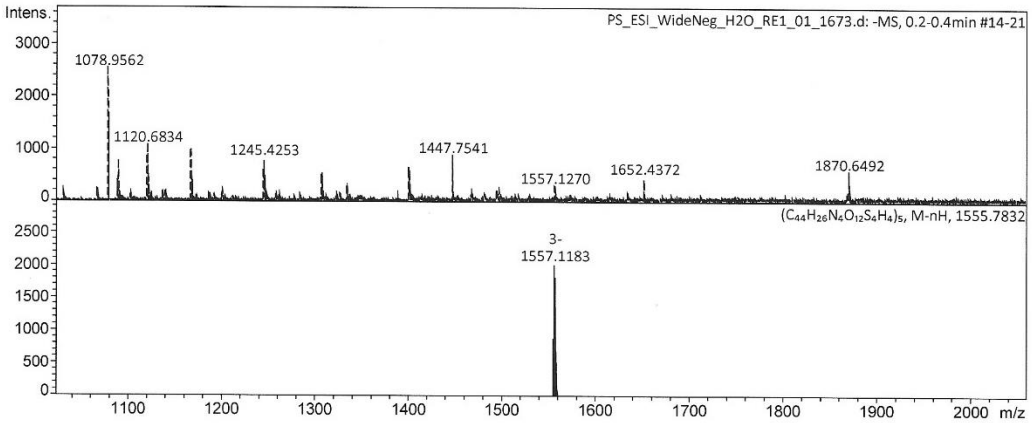
```
 Excited State  55:      Singlet-B      3.6920 eV  335.82 nm  f=0.0107
<S**2>=0.000
     347 -> 355        0.10081
     348 -> 359       -0.18844
     348 -> 360       -0.13658
     349 -> 360        0.53782
     349 -> 361       -0.27294
     349 -> 362       -0.10942

 Excited State  56:      Singlet-B      3.7059 eV  334.56 nm  f=0.0208
<S**2>=0.000
     334 -> 350        0.34187
     335 -> 350       -0.16666
     339 -> 353       -0.10360
     341 -> 352        0.15869
     346 -> 353       -0.20912
     346 -> 354        0.12674
     347 -> 352        0.10721
     347 -> 353       -0.10154
     347 -> 355       -0.30397
     349 -> 359        0.10754
     349 -> 360        0.10195
     349 -> 362        0.13218

 Excited State  57:      Singlet-B      3.7157 eV  333.67 nm  f=0.0040
<S**2>=0.000
     332 -> 350       -0.13663
     334 -> 350       -0.30747
     337 -> 351       -0.24472
     348 -> 356        0.10999
     349 -> 360        0.18038
     349 -> 362        0.46695

 Excited State  58:      Singlet-A      3.7194 eV  333.35 nm  f=0.0006
<S**2>=0.000
     335 -> 352       -0.14139
     336 -> 351       -0.10843
     340 -> 352       -0.30108
     343 -> 352       -0.20552
     343 -> 353       -0.28523
     343 -> 354       -0.16673
     345 -> 352        0.12417
     345 -> 353        0.31909
     345 -> 355       -0.11990
     349 -> 363       -0.13994

 Excited State  59:      Singlet-A      3.7267 eV  332.69 nm  f=0.0002
<S**2>=0.000
     330 -> 350       -0.14470
     336 -> 351        0.63040
     349 -> 363        0.15333
```

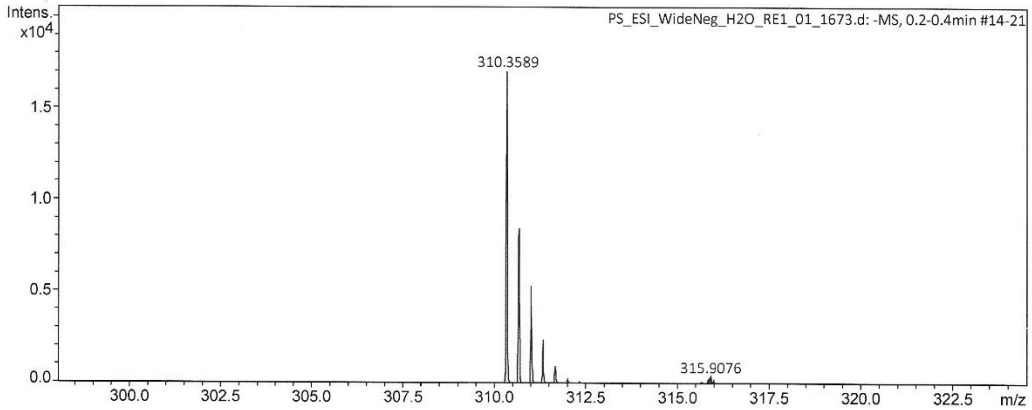
```
 Excited State  60:      Singlet-B      3.7310 eV  332.31 nm  f=0.0160
<S**2>=0.000
     331 -> 350        0.16939
     334 -> 350       -0.17294
     337 -> 351        0.60558
     347 -> 355       -0.11820
     349 -> 360        0.11010
     349 -> 362        0.11685
```

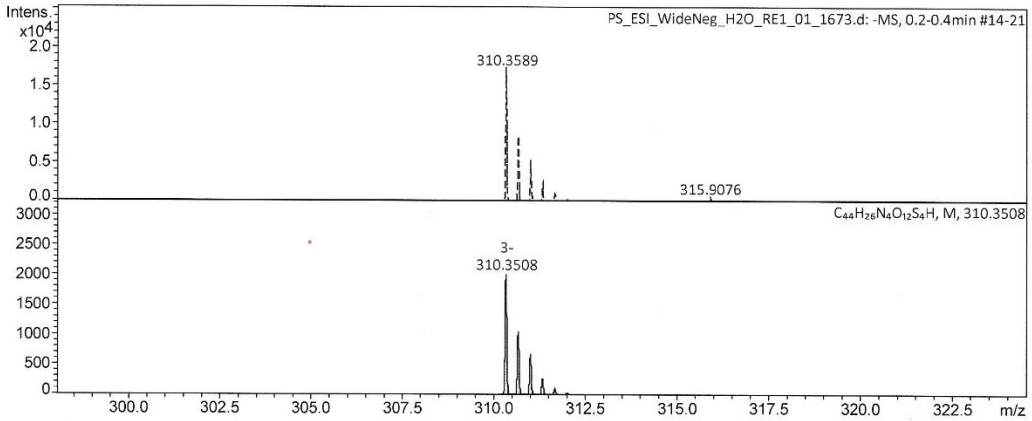
Chapter 5 Supporting Information:

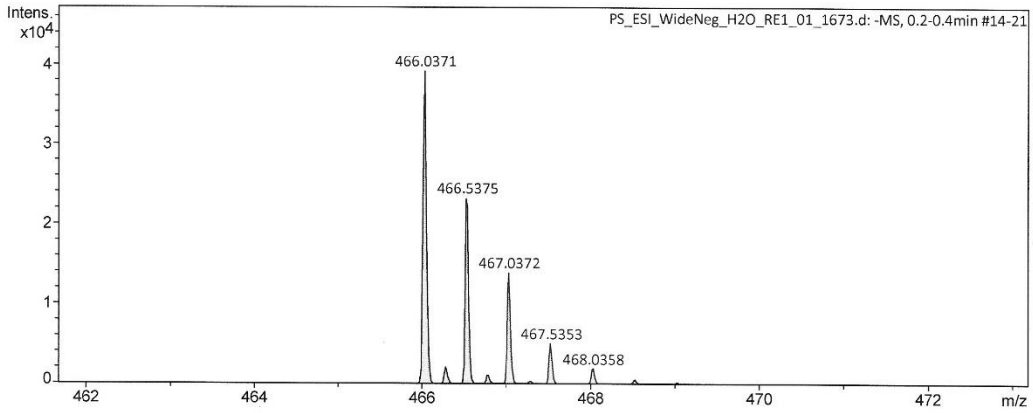


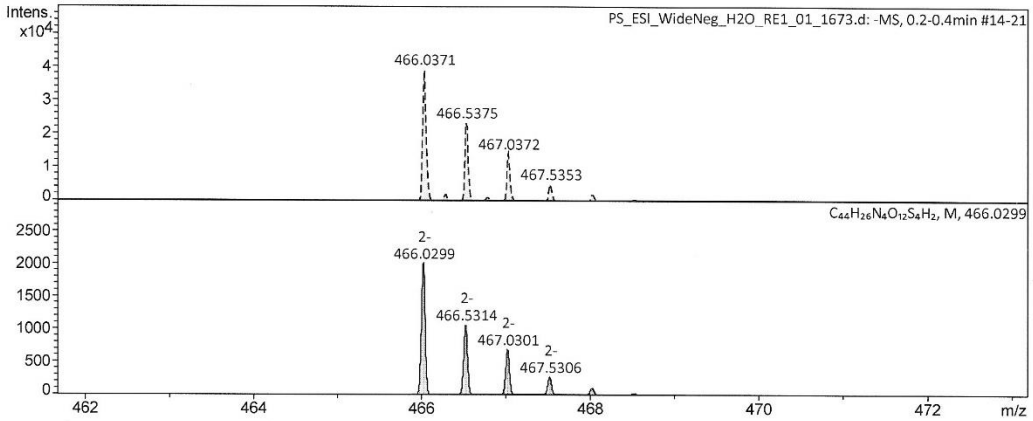

Intens.
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.3min #14-20
1078.9564
1120.6833
1245.4253
1401.1123
1447.7539
1557.1273
1652.4376
1870.6490
m/z

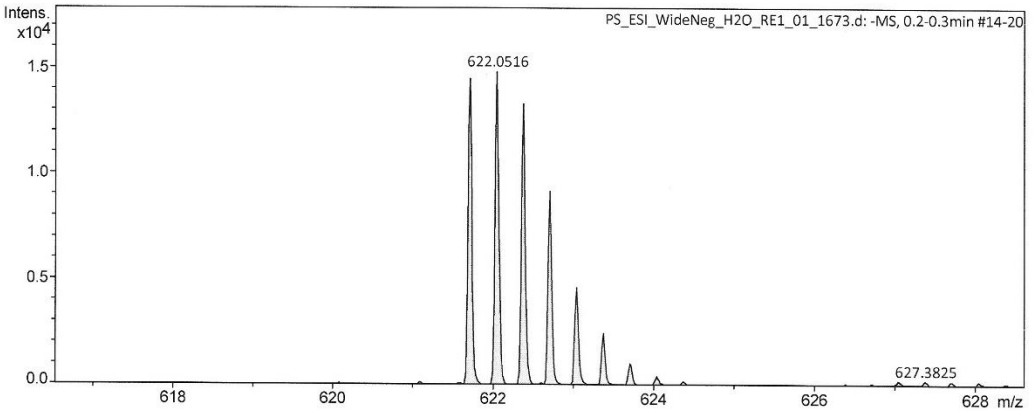

Intens.
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
1078.9562
1120.6834
1245.4253
1447.7541
1557.1270
1652.4372
1870.6492
(C44H26N4O12S4H4)5, M-nH, 1555.7832
3-
1557.1183
m/z

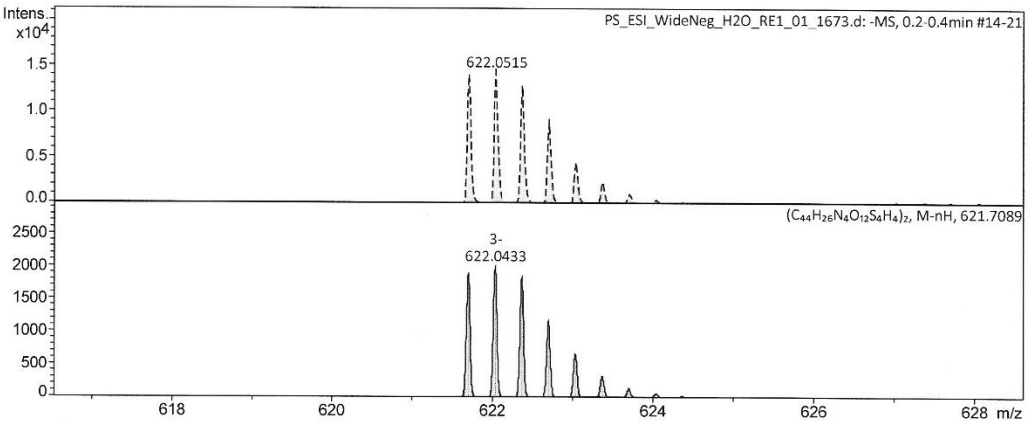

Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
310.3589
315.9076
m/z


Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
310.3589
315.9076
C44H26N4O12S4H, M, 310.3508
3-
310.3508
m/z


Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
466.0371
466.5375
467.0372
467.5353
468.0358
m/z


Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
466.0371
466.5375
467.0372
467.5353
C44H26N4O12S4H2, M, 466.0299
2-
466.0299
2-
466.5314
2-
467.0301
2-
467.5306
m/z


Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.3min #14-20
622.0516
627.3825
m/z


Intens.
x10^4
PS_ESI_WideNeg_H2O_RE1_01_1673.d: -MS, 0.2-0.4min #14-21
622.0515
(C44H26N4O12S4H4)2, M-nH, 621.7089
3-
622.0433
m/z

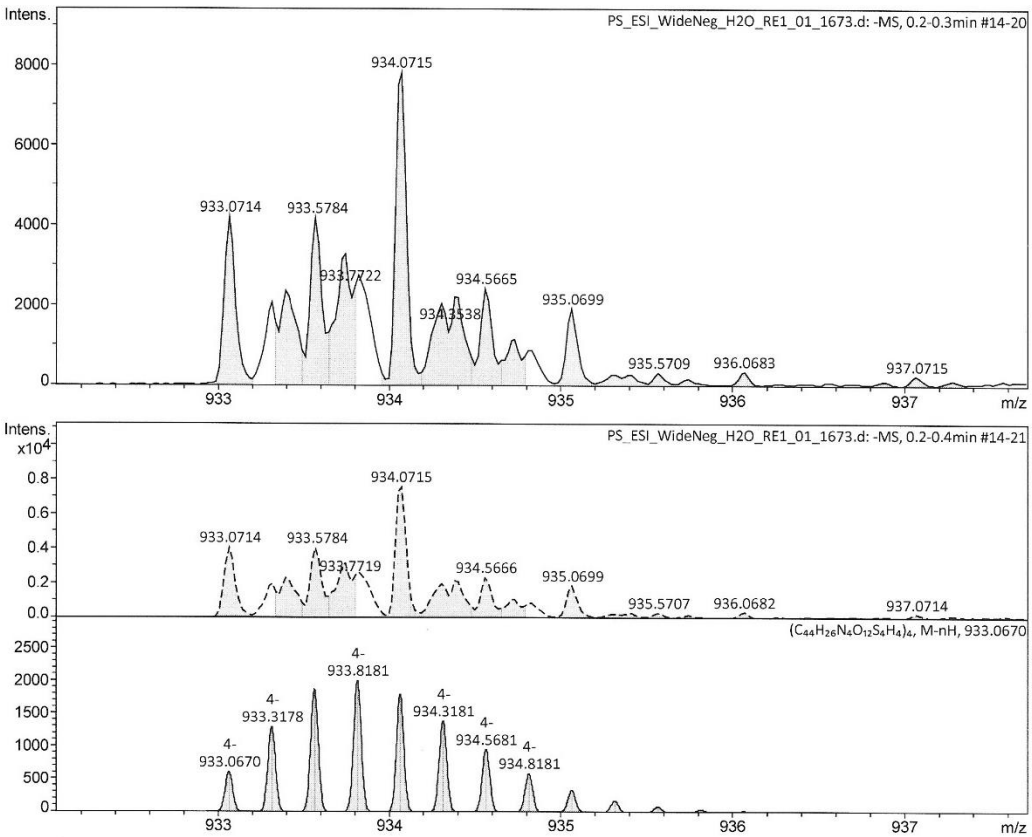
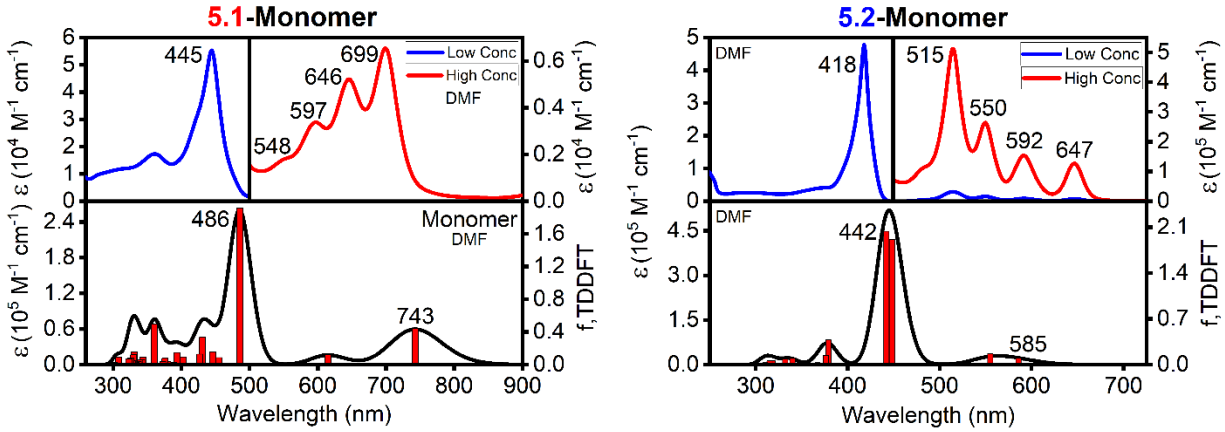


Figure S5.1. Select high-resolution ESI mass spectra of the **5.1** assemblies.



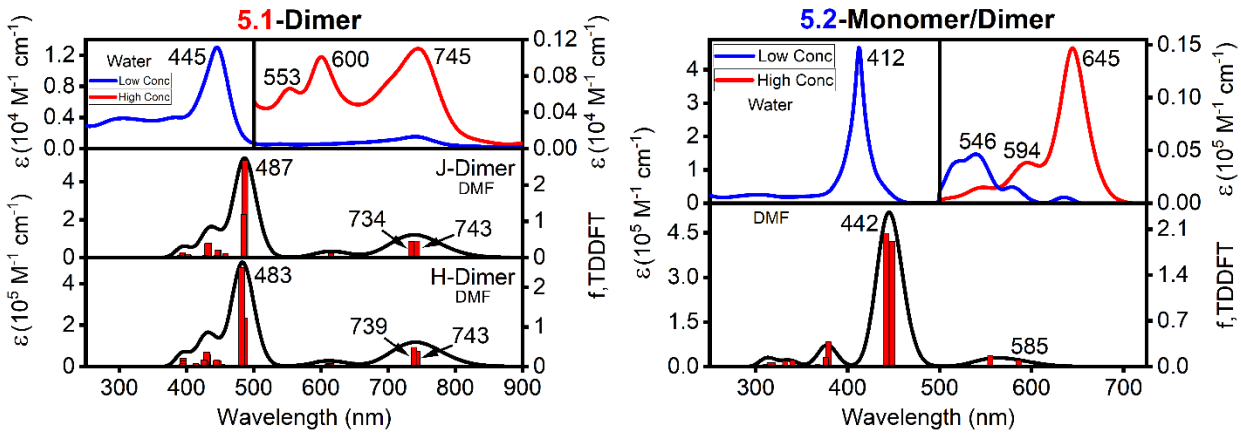
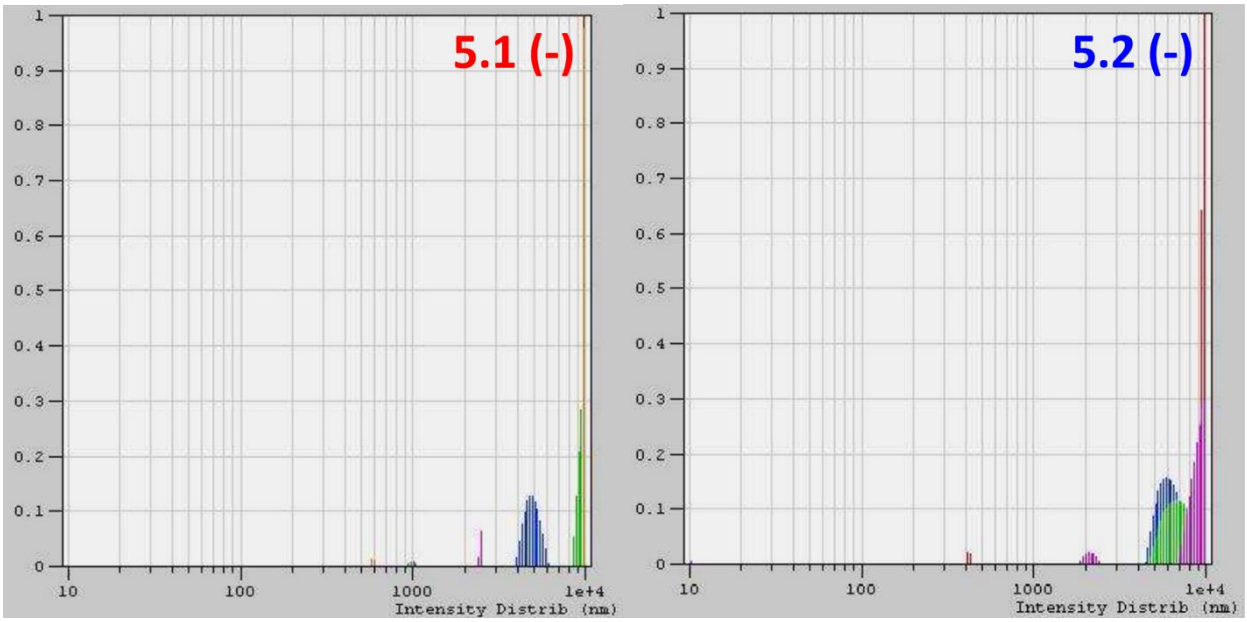


Figure S5.2. TDDFT-predicted UV-vis spectra of the monomer and dimer for **5.1** and **5.2** using the TPSSh exchange correlation functional.



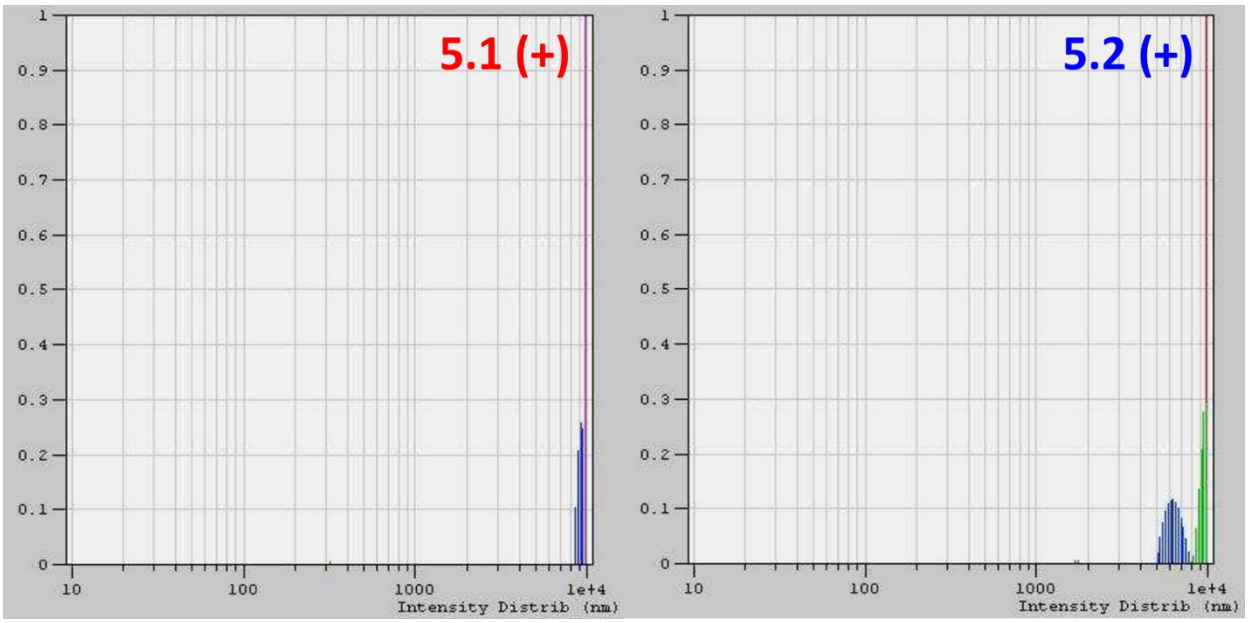


Figure S5.3. Additional DLS size distribution profiles for **5.1** and **5.2** (the – and + refer to the tartaric acid enantiomer used for particle preparation).

Table S5.1. Optimized coordinates for the monomer of **5.1** using the CAM-B3LYP exchange correlation functional.

N	0.19338	-2.13843	-0.11478
N	2.08224	0.10755	0.05727
N	-0.12768	2.08914	-0.05867
C	-0.84215	-3.04752	-0.14983
C	1.32592	-2.87937	-0.15003
C	-2.64486	-1.34973	-0.16331
C	-2.84898	0.92283	-0.16915
C	2.95362	-0.96677	-0.00326
C	2.78192	1.30235	0.06289
C	-1.27774	2.85604	-0.1132
C	0.89481	2.97269	-0.02867
C	-2.20458	-2.70434	-0.12781
C	-0.32764	-4.41016	-0.22734
C	1.02814	-4.30798	-0.21931
C	-2.57705	2.33361	-0.14429
C	-4.09825	0.34087	0.17932
C	2.63948	-2.33044	-0.08591
C	4.28151	-0.40866	-0.03355
C	4.17902	0.95105	0.00901
C	-0.94175	4.27706	-0.13746
C	2.27223	2.60747	0.04591
C	0.41277	4.35246	-0.06845
H	-0.91837	-5.31335	-0.29825
H	1.74889	-5.11364	-0.24929

H	-5.03085	0.80661	0.46163
H	5.18862	-0.98984	-0.10898
H	4.98904	1.66443	-0.02568
H	-1.64112	5.0986	-0.21163
H	1.0221	5.24564	-0.04651
C	3.27881	3.71309	0.09116
C	3.44342	4.57797	-1.00677
C	4.07958	3.90117	1.2324
C	4.38138	5.60835	-0.97156
H	2.84299	4.43093	-1.89909
C	5.02194	4.92753	1.28526
H	3.95771	3.24137	2.08577
C	5.15628	5.77258	0.18052
H	4.51951	6.26272	-1.82539
H	5.64155	5.06941	2.16397
C	3.79169	-3.28251	-0.11416
C	4.03161	-4.08167	-1.24734
C	4.64668	-3.40219	0.99687
C	5.10006	-4.97642	-1.27843
H	3.38128	-3.99426	-2.11205
C	5.71959	-4.2923	0.98308
H	4.45927	-2.80314	1.88257
C	5.93461	-5.06609	-0.16072
H	5.28365	-5.5929	-2.15161
H	6.36819	-4.39403	1.84632
C	-3.23006	-3.77438	-0.01729
C	-3.15948	-4.72932	1.01612
C	-4.30146	-3.84089	-0.93245
C	-4.12148	-5.7304	1.13261
H	-2.35326	-4.67475	1.74018
C	-5.26845	-4.83879	-0.82952
H	-4.35719	-3.12664	-1.74848
C	-5.1676	-5.77313	0.20631
H	-4.06295	-6.46631	1.92697
H	-6.07566	-4.90133	-1.55114
C	-3.74388	3.25264	-0.12396
C	-3.88528	4.24098	0.86991
C	-4.75577	3.12152	-1.09767
C	-4.99165	5.0885	0.88425
H	-3.13674	4.32585	1.6509
C	-5.86513	3.96322	-1.09823
H	-4.65889	2.36671	-1.87182
C	-5.96817	4.94345	-0.10566
H	-5.1066	5.83643	1.66112
H	-6.63808	3.85927	-1.85191
H	1.06777	0.02579	0.08731

C	-1.96206	-0.1577	-0.39314
H	-0.93242	-0.08455	-0.68487
N	-3.96511	-0.98886	0.17256
H	-4.69416	-1.64187	0.43621
S	6.36216	7.07412	0.23334
S	7.28992	-6.2121	-0.18752
S	-6.40432	-7.04594	0.34784
S	-7.37748	6.02918	-0.10132
O	5.38115	8.26012	0.81162
O	7.3843	6.77055	1.24174
O	6.78138	7.42985	-1.12745
O	8.43322	-5.18731	-0.77611
O	7.03934	-7.26315	-1.18061
O	7.65631	-6.59246	1.18175
O	-8.51665	5.33989	-0.70471
O	-7.48099	6.66767	1.21458
O	-6.99	7.1788	-1.20504
O	-7.65521	-6.29614	1.09774
O	-6.92941	-7.35093	-0.98166
O	-5.89942	-8.1012	1.23141
H	5.90965	9.08407	0.89523
H	-6.41976	7.85177	-0.77657
H	-7.49994	-6.30804	2.06598
H	9.27972	-5.68016	-0.85185

Table S5.2. Optimized coordinates for the J-dimer of **5.1** using the CAM-B3LYP exchange correlation functional.

N	7.8971	1.96536	1.14811
N	10.3727	0.53711	0.42839
N	8.83512	-1.66786	-0.82184
C	6.64174	2.48895	1.37316
C	8.75913	2.82295	1.74415
C	5.41296	0.65677	0.2449
C	5.89057	-1.29937	-0.82655
C	10.88126	1.6097	1.14156
C	11.38694	-0.33631	0.07285
C	7.95771	-2.5744	-1.38744
C	10.06714	-2.19472	-1.00451
C	5.44233	1.90726	0.92614
C	6.73079	3.71874	2.15222
C	8.05451	3.93624	2.37468
C	6.56561	-2.4137	-1.42751
C	4.55604	-0.90681	-1.12976
C	10.17592	2.66751	1.73339
C	12.30311	1.39604	1.23202

C	12.60632	0.23035	0.59089
C	8.68461	-3.71952	-1.92632
C	11.27946	-1.56658	-0.59045
C	10.00263	-3.47884	-1.70011
H	5.89993	4.32081	2.49402
H	8.50505	4.7648	2.90378
H	3.82474	-1.35342	-1.78834
H	12.98858	2.0472	1.7539
H	13.58029	-0.22784	0.50292
H	8.24785	-4.59056	-2.39541
H	10.84211	-4.10183	-1.97698
C	12.55856	-2.29033	-0.86536
C	12.8181	-3.53176	-0.25534
C	13.52073	-1.7451	-1.73529
C	14.00483	-4.21838	-0.50566
H	12.09056	-3.95321	0.43126
C	14.71366	-2.41798	-1.99657
H	13.32816	-0.79042	-2.21484
C	14.93688	-3.65224	-1.38023
H	14.21138	-5.16688	-0.02209
H	15.45604	-1.99443	-2.66419
C	10.9932	3.70479	2.43358
C	10.86557	3.896	3.8222
C	11.89783	4.50953	1.71638
C	11.62299	4.85981	4.48535
H	10.17452	3.27734	4.38608
C	12.66421	5.47754	2.36381
H	11.99045	4.38321	0.64216
C	12.51933	5.63599	3.7447
H	11.52288	5.00617	5.55528
H	13.35169	6.10591	1.80818
C	4.15561	2.61801	1.14914
C	3.97649	3.94692	0.71779
C	3.08948	1.96385	1.79918
C	2.77376	4.61457	0.93965
H	4.78232	4.45326	0.19658
C	1.88278	2.61994	2.03127
H	3.21962	0.94552	2.15239
C	1.73931	3.94149	1.59682
H	2.64091	5.64005	0.61283
H	1.07447	2.12246	2.55588
C	5.7341	-3.4098	-2.1516
C	6.00314	-3.74423	-3.49366
C	4.6327	-4.01347	-1.51106
C	5.20965	-4.66404	-4.17607
H	6.82312	-3.2576	-4.01169

C	3.83353	-4.93878	-2.17834
H	4.4151	-3.76815	-0.47622
C	4.13403	-5.25642	-3.5069
H	5.40734	-4.90257	-5.21542
H	2.98888	-5.40157	-1.67984
H	9.38734	0.40518	0.20791
C	6.39849	-0.30831	0.04704
H	7.37669	-0.2893	0.48683
N	4.2862	0.23213	-0.48921
H	3.4102	0.74465	-0.61377
S	16.45651	-4.5134	-1.69629
S	13.48966	6.86739	4.57693
S	0.2024	4.78771	1.89397
S	3.11626	-6.43556	-4.36634
O	15.95797	-5.36624	-3.01071
O	17.49577	-3.56528	-2.11521
O	16.7401	-5.4505	-0.60301
O	14.78263	5.91797	4.93886
O	12.83366	7.26867	5.82705
O	13.91323	7.90168	3.62567
O	1.78232	-6.44179	-3.7682
O	3.30541	-6.26311	-5.81028
O	3.74397	-7.88908	-3.93592
O	-0.75678	4.32287	0.6414
O	-0.44688	4.20221	3.06494
O	0.42407	6.23243	1.78224
H	16.714	-5.90363	-3.33468
H	4.50026	-8.09556	-4.52512
H	-0.58199	4.90886	-0.12551
H	15.43699	6.46075	5.4312
N	-6.60266	-1.39106	0.17176
N	-7.08308	1.23777	-1.06462
N	-9.99818	1.05533	-0.53124
C	-6.57769	-2.61249	0.81122
C	-5.32984	-1.16766	-0.23092
C	-9.00478	-2.66429	1.29871
C	-10.85032	-1.37262	0.9373
C	-5.72791	1.07756	-1.29781
C	-7.54692	2.39699	-1.66413
C	-11.31221	0.80626	-0.17847
C	-10.01831	2.23571	-1.18941
C	-7.69895	-3.229	1.39025
C	-5.23245	-3.1757	0.79102
C	-4.4477	-2.26821	0.15177
C	-11.74087	-0.31868	0.53816
C	-11.13774	-2.32668	1.95088

C	-4.90472	0.00796	-0.91639
C	-5.31859	2.20844	-2.09143
C	-6.40814	2.99974	-2.3098
C	-12.18119	1.87545	-0.66159
C	-8.86037	2.88233	-1.71658
C	-11.374	2.7764	-1.27942
H	-4.93384	-4.1345	1.19254
H	-3.38458	-2.33526	-0.03441
H	-12.02715	-2.46598	2.54739
H	-4.31822	2.36372	-2.46733
H	-6.44456	3.90797	-2.89288
H	-13.2565	1.92218	-0.55664
H	-11.66454	3.7078	-1.74579
C	-9.05809	4.19533	-2.40454
C	-9.81244	4.27496	-3.59016
C	-8.49489	5.37086	-1.8755
C	-10.00871	5.49595	-4.23259
H	-10.23524	3.37116	-4.01756
C	-8.68159	6.60109	-2.50507
H	-7.9144	5.32037	-0.95959
C	-9.44396	6.64711	-3.675
H	-10.57711	5.55324	-5.15454
H	-8.24616	7.50673	-2.09724
C	-3.4599	0.11483	-1.28241
C	-2.87574	-0.81216	-2.16678
C	-2.65881	1.13837	-0.74333
C	-1.52868	-0.723	-2.51144
H	-3.48488	-1.60234	-2.59405
C	-1.30979	1.24607	-1.07778
H	-3.09229	1.8478	-0.04537
C	-0.76481	0.31219	-1.96299
H	-1.08085	-1.43939	-3.19152
H	-0.69535	2.02931	-0.64845
C	-7.54122	-4.49479	2.15291
C	-6.6067	-4.60164	3.20188
C	-8.34959	-5.60972	1.84698
C	-6.47298	-5.78689	3.92222
H	-5.99566	-3.74414	3.46371
C	-8.22638	-6.80075	2.55903
H	-9.05744	-5.55065	1.02569
C	-7.28832	-6.87441	3.59346
H	-5.74988	-5.86686	4.72656
H	-8.83405	-7.66229	2.30497
C	-13.16552	-0.43568	0.94187
C	-13.81293	0.59987	1.64436
C	-13.8874	-1.61216	0.65213

C	-15.14611	0.47853	2.03154
H	-13.25812	1.49338	1.91129
C	-15.22077	-1.74706	1.03075
H	-13.40337	-2.41658	0.10719
C	-15.83776	-0.69432	1.71485
H	-15.63681	1.27057	2.58643
H	-15.7715	-2.653	0.802
H	-7.65725	0.58836	-0.5304
C	-9.51317	-1.61472	0.53824
H	-8.97091	-1.0837	-0.21977
N	-10.05176	-3.08072	2.14539
H	-9.97191	-3.80406	2.85104
S	-9.68982	8.20797	-4.48444
S	0.94947	0.43225	-2.39102
S	-7.13832	-8.38805	4.51891
S	-17.54431	-0.85299	2.19124
O	-11.10763	8.61023	-3.7558
O	-8.65269	9.15821	-4.06659
O	-9.93986	8.00355	-5.91632
O	1.66037	1.21677	-1.36459
O	0.79716	1.35241	-3.73677
O	1.48566	-0.88207	-2.76469
O	-17.85334	-2.26477	2.411
O	-17.85197	0.16214	3.2035
O	-18.368	-0.48564	0.82106
O	-8.32125	-8.27598	5.64952
O	-7.56517	-9.50511	3.67873
O	-5.84261	-8.39762	5.20488
H	-11.43552	9.44431	-4.15808
H	-18.42582	0.48964	0.73545
H	-7.98939	-7.75012	6.40807
H	1.68435	1.4583	-4.14697

Table S5.3. Optimized coordinates for the H-dimer of **5.1** using the CAM-B3LYP exchange correlation functional.

N	5.07057	1.69153	1.03063
N	5.07707	-1.24241	1.29269
N	2.24507	-1.26091	2.16808
C	4.86311	3.05268	0.94901
C	6.36906	1.50373	0.69826
C	2.48995	2.96898	1.65157
C	0.93938	1.40404	2.24521
C	6.39601	-1.00111	0.94221
C	4.88409	-2.58677	1.56839
C	0.9217	-1.0727	2.52697

C	2.46694	-2.59008	2.28526
C	3.63983	3.68843	1.21553
C	6.09063	3.73722	0.55941
C	7.02993	2.76948	0.3876
C	0.272	0.16851	2.5466
C	0.27798	2.62071	1.92404
C	7.00093	0.22689	0.64114
C	7.06836	-2.27337	1.00445
C	6.16367	-3.22274	1.38139
C	0.30945	-2.34497	2.896
C	3.71106	-3.22607	1.99294
C	1.26688	-3.29483	2.73227
H	6.21835	4.80518	0.446
H	8.05793	2.8982	0.07792
H	-0.77586	2.85239	1.8819
H	8.12119	-2.41943	0.81359
H	6.35599	-4.27195	1.54946
H	-0.70317	-2.48851	3.24722
H	1.17086	-4.35934	2.8961
C	3.78431	-4.71075	2.15225
C	3.60052	-5.30769	3.41331
C	4.03834	-5.53442	1.03922
C	3.66142	-6.69189	3.56591
H	3.42401	-4.68089	4.28175
C	4.10401	-6.92024	1.17472
H	4.17977	-5.08591	0.06053
C	3.90747	-7.48191	2.43937
H	3.53491	-7.15008	4.54069
H	4.30394	-7.55311	0.31694
C	8.43791	0.17911	0.23218
C	9.42769	0.80249	1.01462
C	8.81762	-0.48031	-0.95202
C	10.76731	0.77151	0.63111
H	9.14531	1.3079	1.93284
C	10.15357	-0.52062	-1.34927
H	8.05965	-0.95031	-1.57144
C	11.11288	0.10446	-0.54793
H	11.52915	1.25494	1.2329
H	10.44484	-1.0148	-2.26972
C	3.5114	5.1577	1.0209
C	3.81235	5.76002	-0.21492
C	3.06546	5.97108	2.0838
C	3.69089	7.13913	-0.38495
H	4.12631	5.14168	-1.04969
C	2.95354	7.35095	1.93053
H	2.83645	5.52047	3.04491

C	3.26731	7.92194	0.69206
H	3.91088	7.60229	-1.34039
H	2.62595	7.96939	2.75941
C	-1.1779	0.23208	2.86337
C	-2.11272	-0.54968	2.15849
C	-1.64542	1.10814	3.86602
C	-3.4739	-0.48003	2.45399
H	-1.77349	-1.19584	1.35563
C	-3.00134	1.19308	4.1684
H	-0.9355	1.70904	4.42575
C	-3.90243	0.38928	3.46006
H	-4.19246	-1.07435	1.90075
H	-3.34868	1.86336	4.94759
H	4.35564	-0.52621	1.35109
C	2.32307	1.65513	2.08027
H	3.11912	0.95713	2.24985
N	1.19854	3.53043	1.59011
H	0.98917	4.46894	1.26892
S	3.99501	-9.24526	2.6233
S	12.81391	0.07282	-1.05427
S	3.19772	9.69352	0.49225
S	-5.64219	0.51003	3.81418
O	2.41372	-9.57646	2.31745
O	4.81215	-9.82672	1.55144
O	4.29257	-9.58952	4.0183
O	13.25114	-1.30872	-0.2769
O	13.53916	1.20025	-0.45658
O	12.90325	-0.14987	-2.50213
O	-6.05218	1.91477	3.79704
O	-6.36096	-0.49632	3.02771
O	-5.73134	0.10922	5.40057
O	1.75077	10.07821	1.10335
O	4.15107	10.32911	1.40451
O	3.23756	9.99955	-0.94235
H	2.2994	-10.55213	2.30264
H	-5.68572	-0.86678	5.48812
H	1.01425	9.80523	0.48564
H	14.20717	-1.46556	-0.44064
N	-1.69507	0.71372	-1.84487
N	-2.68441	-2.05533	-1.96455
N	-5.41784	-1.19971	-1.17912
C	-1.43281	2.06497	-1.76971
C	-0.50867	0.13091	-2.13855
C	-3.74233	2.7238	-1.15854
C	-5.76185	1.72368	-0.8008
C	-1.3362	-2.24461	-2.2176

C	-3.33945	-3.2725	-1.87452
C	-6.62829	-0.61276	-0.85497
C	-5.66698	-2.52672	-1.25019
C	-2.39141	3.04856	-1.47453
C	-0.01992	2.32907	-2.01918
C	0.55731	1.12286	-2.26266
C	-6.82353	0.76396	-0.68508
C	-5.95475	3.12211	-0.96927
C	-0.33158	-1.27142	-2.3241
C	-1.13521	-3.66946	-2.28695
C	-2.33525	-4.28534	-2.08197
C	-7.66375	-1.63058	-0.70495
C	-4.68834	-3.513	-1.57848
C	-7.06991	-2.82427	-0.96555
H	0.46519	3.29529	-1.99389
H	1.59265	0.9276	-2.50532
H	-6.86394	3.70451	-0.99114
H	-0.17913	-4.14673	-2.44299
H	-2.52024	-5.3485	-2.04232
H	-8.69443	-1.45725	-0.42736
H	-7.5319	-3.80193	-0.9686
C	-5.12924	-4.94139	-1.59397
C	-5.59556	-5.55686	-0.41729
C	-5.08487	-5.69266	-2.78307
C	-6.01159	-6.88712	-0.42171
H	-5.61763	-4.99237	0.50962
C	-5.49623	-7.02445	-2.80531
H	-4.73212	-5.22592	-3.69748
C	-5.96112	-7.60326	-1.62108
H	-6.35557	-7.36506	0.48903
H	-5.45724	-7.60242	-3.72221
C	1.04636	-1.75837	-2.63463
C	2.09497	-1.55289	-1.71732
C	1.32225	-2.41399	-3.84844
C	3.38692	-1.98807	-2.00165
H	1.89685	-1.06054	-0.77031
C	2.60914	-2.86396	-4.1447
H	0.52545	-2.55962	-4.57119
C	3.6258	-2.64621	-3.21187
H	4.19261	-1.81947	-1.29635
H	2.82337	-3.36163	-5.08406
C	-2.00612	4.48369	-1.51625
C	-1.41159	5.0399	-2.66564
C	-2.24458	5.31541	-0.40176
C	-1.04687	6.38404	-2.70294
H	-1.2467	4.41648	-3.53807

C	-1.88238	6.66025	-0.42176
H	-2.6887	4.89719	0.49646
C	-1.28508	7.17735	-1.57647
H	-0.58426	6.80882	-3.58689
H	-2.04467	7.28895	0.44668
C	-8.18866	1.28282	-0.40738
C	-9.26714	0.98265	-1.262
C	-8.41559	2.11742	0.70625
C	-10.54183	1.48693	-1.01058
H	-9.0981	0.37226	-2.14315
C	-9.68482	2.62666	0.97096
H	-7.59742	2.34601	1.38202
C	-10.73705	2.3024	0.10794
H	-11.36677	1.26931	-1.68002
H	-9.85422	3.26646	1.83025
H	-3.12806	-1.14528	-1.85713
C	-4.36695	1.50505	-0.9089
H	-3.8648	0.56172	-0.82358
N	-4.76397	3.69508	-1.16953
H	-4.62666	4.67951	-1.36788
S	-6.48292	-9.30002	-1.63597
S	5.27079	-3.20561	-3.57255
S	-0.81418	8.88922	-1.61661
S	-12.36112	2.94873	0.43964
O	-8.05302	-9.04346	-2.05074
O	-5.82142	-10.0241	-2.72791
O	-6.43325	-9.85099	-0.27683
O	5.23568	-4.60103	-2.69935
O	6.2647	-2.3142	-2.9606
O	5.38161	-3.53393	-4.99711
O	-12.23536	4.23605	1.12093
O	-13.18688	2.79849	-0.76276
O	-12.95264	1.95216	1.60026
O	-2.2031	9.70236	-1.88101
O	-0.47002	9.30204	-0.24527
O	0.10657	9.11755	-2.72863
H	-8.48495	-9.91667	-2.17762
H	-13.32122	1.15034	1.17264
H	-2.41243	9.68609	-2.83993
H	6.16195	-4.89263	-2.55162

Table S5.4. Optimized coordinates for the monomer of **5.2** using the CAM-B3LYP exchange correlation functional.

N	2.07914	-0.00873	0.01203
N	0.04782	-2.12905	-0.09882

N	-1.98989	-0.02944	0.00467
C	2.91071	1.07952	0.05568
C	2.91701	-1.09276	-0.00997
C	1.16367	2.87878	0.08465
C	-1.09781	2.86876	0.03119
C	1.18416	-2.90597	-0.08022
C	-1.07751	-2.92024	-0.03536
C	-2.82843	1.05423	-0.01238
C	-2.82094	-1.11849	0.01929
C	2.49728	2.43064	0.08813
C	4.31123	0.67462	0.07243
C	4.31543	-0.68114	0.01528
C	-2.42586	2.40838	-0.01102
C	-0.65657	4.23109	-0.0443
C	2.51276	-2.44561	-0.06112
C	0.74815	-4.27069	-0.0121
C	-0.62221	-4.27925	0.01988
C	-4.22649	0.64185	-0.00478
C	-2.40886	-2.47071	0.01347
C	-4.22206	-0.71512	0.00798
H	5.16487	1.3358	0.12359
H	5.1733	-1.33847	-0.00779
H	-1.30991	5.0862	-0.13564
H	1.40666	-5.12559	0.03332
H	-1.26651	-5.14292	0.09432
H	-5.08411	1.3	-0.00303
H	-5.07566	-1.37838	0.00217
C	-3.46793	-3.52468	0.07937
C	-4.27758	-3.64014	1.22388
C	-3.66941	-4.4106	-0.9943
C	-5.27768	-4.60854	1.29634
H	-4.115	-2.9729	2.06447
C	-4.66599	-5.38443	-0.93803
H	-3.05075	-4.32742	-1.88243
C	-5.46318	-5.46428	0.20705
H	-5.89566	-4.70501	2.18227
H	-4.82284	-6.06658	-1.76647
C	3.5739	-3.50056	-0.0814
C	4.40787	-3.70088	1.03212
C	3.74687	-4.307	-1.22139
C	5.39549	-4.68607	1.01535
H	4.2765	-3.08785	1.91821
C	4.73432	-5.28963	-1.25753
H	3.11432	-4.15032	-2.08949
C	5.54324	-5.46988	-0.13112
H	6.03899	-4.84554	1.87334

H	4.87805	-5.89644	-2.14507
C	3.54666	3.49582	0.10942
C	4.42691	3.65989	-0.97474
C	3.66022	4.35565	1.21771
C	5.39775	4.66128	-0.96108
H	4.34428	3.00579	-1.83717
C	4.6269	5.35887	1.24828
H	2.99519	4.2271	2.06603
C	5.48397	5.50191	0.15221
H	6.07689	4.78715	-1.79716
H	4.72202	6.00912	2.1112
C	-3.48743	3.46056	-0.07207
C	-4.29074	3.59412	-1.21883
C	-3.68525	4.34018	1.0071
C	-5.27005	4.58346	-1.29314
H	-4.13417	2.93054	-2.0635
C	-4.66571	5.33014	0.95142
H	-3.07138	4.24363	1.89722
C	-5.44848	5.43957	-0.20156
H	-5.87195	4.69902	-2.18807
H	-4.81532	6.0102	1.78274
H	0.03948	-1.11135	-0.11876
S	-6.74097	-6.6962	0.2858
S	6.81955	-6.70533	-0.16992
S	6.70802	6.79386	0.17304
S	-6.69442	6.70908	-0.28257
O	-7.93813	-5.80767	-0.40705
O	-6.41373	-7.82037	-0.59883
O	-7.0964	-6.96379	1.68409
O	5.85795	-8.01858	0.05714
O	7.70197	-6.54355	0.99069
O	7.40887	-6.78902	-1.51214
O	-6.38837	7.74022	0.70724
O	-6.93538	7.04745	-1.68895
O	-8.04266	5.98506	0.30814
O	5.86753	8.13532	-0.25741
O	7.10189	7.05825	1.55605
O	7.7056	6.52232	-0.86656
H	-8.74714	-6.36296	-0.45733
H	-8.48557	5.49761	-0.41858
H	5.82669	8.18333	-1.23627
H	6.40001	-8.82631	-0.07983
C	0.71363	4.23749	-0.00892
H	1.36217	5.09905	-0.06762
N	0.03538	2.09035	0.10865
H	0.03953	1.07298	0.14145

Table S5.5. Optimized coordinates for the monomer of **5.1** using the TPSSh exchange correlation functional.

N	0.19338	-2.13843	-0.11478
N	2.08224	0.10755	0.05727
N	-0.12768	2.08914	-0.05867
C	-0.84215	-3.04752	-0.14983
C	1.32592	-2.87937	-0.15003
C	-2.64486	-1.34973	-0.16331
C	-2.84898	0.92283	-0.16915
C	2.95362	-0.96677	-0.00326
C	2.78192	1.30235	0.06289
C	-1.27774	2.85604	-0.1132
C	0.89481	2.97269	-0.02867
C	-2.20458	-2.70434	-0.12781
C	-0.32764	-4.41016	-0.22734
C	1.02814	-4.30798	-0.21931
C	-2.57705	2.33361	-0.14429
C	-4.09825	0.34087	0.17932
C	2.63948	-2.33044	-0.08591
C	4.28151	-0.40866	-0.03355
C	4.17902	0.95105	0.00901
C	-0.94175	4.27706	-0.13746
C	2.27223	2.60747	0.04591
C	0.41277	4.35246	-0.06845
H	-0.91837	-5.31335	-0.29825
H	1.74889	-5.11364	-0.24929
H	-5.03085	0.80661	0.46163
H	5.18862	-0.98984	-0.10898
H	4.98904	1.66443	-0.02568
H	-1.64112	5.0986	-0.21163
H	1.0221	5.24564	-0.04651
C	3.27881	3.71309	0.09116
C	3.44342	4.57797	-1.00677
C	4.07958	3.90117	1.2324
C	4.38138	5.60835	-0.97156
H	2.84299	4.43093	-1.89909
C	5.02194	4.92753	1.28526
H	3.95771	3.24137	2.08577
C	5.15628	5.77258	0.18052
H	4.51951	6.26272	-1.82539
H	5.64155	5.06941	2.16397
C	3.79169	-3.28251	-0.11416
C	4.03161	-4.08167	-1.24734
C	4.64668	-3.40219	0.99687
C	5.10006	-4.97642	-1.27843
H	3.38128	-3.99426	-2.11205

C	5.71959	-4.2923	0.98308
H	4.45927	-2.80314	1.88257
C	5.93461	-5.06609	-0.16072
H	5.28365	-5.5929	-2.15161
H	6.36819	-4.39403	1.84632
C	-3.23006	-3.77438	-0.01729
C	-3.15948	-4.72932	1.01612
C	-4.30146	-3.84089	-0.93245
C	-4.12148	-5.7304	1.13261
H	-2.35326	-4.67475	1.74018
C	-5.26845	-4.83879	-0.82952
H	-4.35719	-3.12664	-1.74848
C	-5.1676	-5.77313	0.20631
H	-4.06295	-6.46631	1.92697
H	-6.07566	-4.90133	-1.55114
C	-3.74388	3.25264	-0.12396
C	-3.88528	4.24098	0.86991
C	-4.75577	3.12152	-1.09767
C	-4.99165	5.0885	0.88425
H	-3.13674	4.32585	1.6509
C	-5.86513	3.96322	-1.09823
H	-4.65889	2.36671	-1.87182
C	-5.96817	4.94345	-0.10566
H	-5.1066	5.83643	1.66112
H	-6.63808	3.85927	-1.85191
H	1.06777	0.02579	0.08731
C	-1.96206	-0.1577	-0.39314
H	-0.93242	-0.08455	-0.68487
N	-3.96511	-0.98886	0.17256
H	-4.69416	-1.64187	0.43621
S	6.36216	7.07412	0.23334
S	7.28992	-6.2121	-0.18752
S	-6.40432	-7.04594	0.34784
S	-7.37748	6.02918	-0.10132
O	5.38115	8.26012	0.81162
O	7.3843	6.77055	1.24174
O	6.78138	7.42985	-1.12745
O	8.43322	-5.18731	-0.77611
O	7.03934	-7.26315	-1.18061
O	7.65631	-6.59246	1.18175
O	-8.51665	5.33989	-0.70471
O	-7.48099	6.66767	1.21458
O	-6.99	7.1788	-1.20504
O	-7.65521	-6.29614	1.09774
O	-6.92941	-7.35093	-0.98166
O	-5.89942	-8.1012	1.23141

H	5.90965	9.08407	0.89523
H	-6.41976	7.85177	-0.77657
H	-7.49994	-6.30804	2.06598
H	9.27972	-5.68016	-0.85185

Table S5.6. Optimized coordinates for the J-dimer of **5.1** using the TPSSh exchange correlation functional.

N	7.8971	1.96536	1.14811
N	10.3727	0.53711	0.42839
N	8.83512	-1.66786	-0.82184
C	6.64174	2.48895	1.37316
C	8.75913	2.82295	1.74415
C	5.41296	0.65677	0.2449
C	5.89057	-1.29937	-0.82655
C	10.88126	1.6097	1.14156
C	11.38694	-0.33631	0.07285
C	7.95771	-2.5744	-1.38744
C	10.06714	-2.19472	-1.00451
C	5.44233	1.90726	0.92614
C	6.73079	3.71874	2.15222
C	8.05451	3.93624	2.37468
C	6.56561	-2.4137	-1.42751
C	4.55604	-0.90681	-1.12976
C	10.17592	2.66751	1.73339
C	12.30311	1.39604	1.23202
C	12.60632	0.23035	0.59089
C	8.68461	-3.71952	-1.92632
C	11.27946	-1.56658	-0.59045
C	10.00263	-3.47884	-1.70011
H	5.89993	4.32081	2.49402
H	8.50505	4.7648	2.90378
H	3.82474	-1.35342	-1.78834
H	12.98858	2.0472	1.7539
H	13.58029	-0.22784	0.50292
H	8.24785	-4.59056	-2.39541
H	10.84211	-4.10183	-1.97698
C	12.55856	-2.29033	-0.86536
C	12.8181	-3.53176	-0.25534
C	13.52073	-1.7451	-1.73529
C	14.00483	-4.21838	-0.50566
H	12.09056	-3.95321	0.43126
C	14.71366	-2.41798	-1.99657
H	13.32816	-0.79042	-2.21484
C	14.93688	-3.65224	-1.38023
H	14.21138	-5.16688	-0.02209

H	15.45604	-1.99443	-2.66419
C	10.9932	3.70479	2.43358
C	10.86557	3.896	3.8222
C	11.89783	4.50953	1.71638
C	11.62299	4.85981	4.48535
H	10.17452	3.27734	4.38608
C	12.66421	5.47754	2.36381
H	11.99045	4.38321	0.64216
C	12.51933	5.63599	3.7447
H	11.52288	5.00617	5.55528
H	13.35169	6.10591	1.80818
C	4.15561	2.61801	1.14914
C	3.97649	3.94692	0.71779
C	3.08948	1.96385	1.79918
C	2.77376	4.61457	0.93965
H	4.78232	4.45326	0.19658
C	1.88278	2.61994	2.03127
H	3.21962	0.94552	2.15239
C	1.73931	3.94149	1.59682
H	2.64091	5.64005	0.61283
H	1.07447	2.12246	2.55588
C	5.7341	-3.4098	-2.1516
C	6.00314	-3.74423	-3.49366
C	4.6327	-4.01347	-1.51106
C	5.20965	-4.66404	-4.17607
H	6.82312	-3.2576	-4.01169
C	3.83353	-4.93878	-2.17834
H	4.4151	-3.76815	-0.47622
C	4.13403	-5.25642	-3.5069
H	5.40734	-4.90257	-5.21542
H	2.98888	-5.40157	-1.67984
H	9.38734	0.40518	0.20791
C	6.39849	-0.30831	0.04704
H	7.37669	-0.2893	0.48683
N	4.2862	0.23213	-0.48921
H	3.4102	0.74465	-0.61377
S	16.45651	-4.5134	-1.69629
S	13.48966	6.86739	4.57693
S	0.2024	4.78771	1.89397
S	3.11626	-6.43556	-4.36634
O	15.95797	-5.36624	-3.01071
O	17.49577	-3.56528	-2.11521
O	16.7401	-5.4505	-0.60301
O	14.78263	5.91797	4.93886
O	12.83366	7.26867	5.82705
O	13.91323	7.90168	3.62567

O	1.78232	-6.44179	-3.7682
O	3.30541	-6.26311	-5.81028
O	3.74397	-7.88908	-3.93592
O	-0.75678	4.32287	0.6414
O	-0.44688	4.20221	3.06494
O	0.42407	6.23243	1.78224
H	16.714	-5.90363	-3.33468
H	4.50026	-8.09556	-4.52512
H	-0.58199	4.90886	-0.12551
H	15.43699	6.46075	5.4312
N	-6.60266	-1.39106	0.17176
N	-7.08308	1.23777	-1.06462
N	-9.99818	1.05533	-0.53124
C	-6.57769	-2.61249	0.81122
C	-5.32984	-1.16766	-0.23092
C	-9.00478	-2.66429	1.29871
C	-10.85032	-1.37262	0.9373
C	-5.72791	1.07756	-1.29781
C	-7.54692	2.39699	-1.66413
C	-11.31221	0.80626	-0.17847
C	-10.01831	2.23571	-1.18941
C	-7.69895	-3.229	1.39025
C	-5.23245	-3.1757	0.79102
C	-4.4477	-2.26821	0.15177
C	-11.74087	-0.31868	0.53816
C	-11.13774	-2.32668	1.95088
C	-4.90472	0.00796	-0.91639
C	-5.31859	2.20844	-2.09143
C	-6.40814	2.99974	-2.3098
C	-12.18119	1.87545	-0.66159
C	-8.86037	2.88233	-1.71658
C	-11.374	2.7764	-1.27942
H	-4.93384	-4.1345	1.19254
H	-3.38458	-2.33526	-0.03441
H	-12.02715	-2.46598	2.54739
H	-4.31822	2.36372	-2.46733
H	-6.44456	3.90797	-2.89288
H	-13.2565	1.92218	-0.55664
H	-11.66454	3.7078	-1.74579
C	-9.05809	4.19533	-2.40454
C	-9.81244	4.27496	-3.59016
C	-8.49489	5.37086	-1.8755
C	-10.00871	5.49595	-4.23259
H	-10.23524	3.37116	-4.01756
C	-8.68159	6.60109	-2.50507
H	-7.9144	5.32037	-0.95959

C	-9.44396	6.64711	-3.675
H	-10.57711	5.55324	-5.15454
H	-8.24616	7.50673	-2.09724
C	-3.4599	0.11483	-1.28241
C	-2.87574	-0.81216	-2.16678
C	-2.65881	1.13837	-0.74333
C	-1.52868	-0.723	-2.51144
H	-3.48488	-1.60234	-2.59405
C	-1.30979	1.24607	-1.07778
H	-3.09229	1.8478	-0.04537
C	-0.76481	0.31219	-1.96299
H	-1.08085	-1.43939	-3.19152
H	-0.69535	2.02931	-0.64845
C	-7.54122	-4.49479	2.15291
C	-6.6067	-4.60164	3.20188
C	-8.34959	-5.60972	1.84698
C	-6.47298	-5.78689	3.92222
H	-5.99566	-3.74414	3.46371
C	-8.22638	-6.80075	2.55903
H	-9.05744	-5.55065	1.02569
C	-7.28832	-6.87441	3.59346
H	-5.74988	-5.86686	4.72656
H	-8.83405	-7.66229	2.30497
C	-13.16552	-0.43568	0.94187
C	-13.81293	0.59987	1.64436
C	-13.8874	-1.61216	0.65213
C	-15.14611	0.47853	2.03154
H	-13.25812	1.49338	1.91129
C	-15.22077	-1.74706	1.03075
H	-13.40337	-2.41658	0.10719
C	-15.83776	-0.69432	1.71485
H	-15.63681	1.27057	2.58643
H	-15.7715	-2.653	0.802
H	-7.65725	0.58836	-0.5304
C	-9.51317	-1.61472	0.53824
H	-8.97091	-1.0837	-0.21977
N	-10.05176	-3.08072	2.14539
H	-9.97191	-3.80406	2.85104
S	-9.68982	8.20797	-4.48444
S	0.94947	0.43225	-2.39102
S	-7.13832	-8.38805	4.51891
S	-17.54431	-0.85299	2.19124
O	-11.10763	8.61023	-3.7558
O	-8.65269	9.15821	-4.06659
O	-9.93986	8.00355	-5.91632
O	1.66037	1.21677	-1.36459

O	0.79716	1.35241	-3.73677
O	1.48566	-0.88207	-2.76469
O	-17.85334	-2.26477	2.411
O	-17.85197	0.16214	3.2035
O	-18.368	-0.48564	0.82106
O	-8.32125	-8.27598	5.64952
O	-7.56517	-9.50511	3.67873
O	-5.84261	-8.39762	5.20488
H	-11.43552	9.44431	-4.15808
H	-18.42582	0.48964	0.73545
H	-7.98939	-7.75012	6.40807
H	1.68435	1.4583	-4.14697

Table S5.7. Optimized coordinates for the H-dimer of **5.1** using the TPSSh exchange correlation functional.

N	5.07057	1.69153	1.03063
N	5.07707	-1.24241	1.29269
N	2.24507	-1.26091	2.16808
C	4.86311	3.05268	0.94901
C	6.36906	1.50373	0.69826
C	2.48995	2.96898	1.65157
C	0.93938	1.40404	2.24521
C	6.39601	-1.00111	0.94221
C	4.88409	-2.58677	1.56839
C	0.9217	-1.0727	2.52697
C	2.46694	-2.59008	2.28526
C	3.63983	3.68843	1.21553
C	6.09063	3.73722	0.55941
C	7.02993	2.76948	0.3876
C	0.272	0.16851	2.5466
C	0.27798	2.62071	1.92404
C	7.00093	0.22689	0.64114
C	7.06836	-2.27337	1.00445
C	6.16367	-3.22274	1.38139
C	0.30945	-2.34497	2.896
C	3.71106	-3.22607	1.99294
C	1.26688	-3.29483	2.73227
H	6.21835	4.80518	0.446
H	8.05793	2.8982	0.07792
H	-0.77586	2.85239	1.8819
H	8.12119	-2.41943	0.81359
H	6.35599	-4.27195	1.54946
H	-0.70317	-2.48851	3.24722
H	1.17086	-4.35934	2.8961
C	3.78431	-4.71075	2.15225

C	3.60052	-5.30769	3.41331
C	4.03834	-5.53442	1.03922
C	3.66142	-6.69189	3.56591
H	3.42401	-4.68089	4.28175
C	4.10401	-6.92024	1.17472
H	4.17977	-5.08591	0.06053
C	3.90747	-7.48191	2.43937
H	3.53491	-7.15008	4.54069
H	4.30394	-7.55311	0.31694
C	8.43791	0.17911	0.23218
C	9.42769	0.80249	1.01462
C	8.81762	-0.48031	-0.95202
C	10.76731	0.77151	0.63111
H	9.14531	1.3079	1.93284
C	10.15357	-0.52062	-1.34927
H	8.05965	-0.95031	-1.57144
C	11.11288	0.10446	-0.54793
H	11.52915	1.25494	1.2329
H	10.44484	-1.0148	-2.26972
C	3.5114	5.1577	1.0209
C	3.81235	5.76002	-0.21492
C	3.06546	5.97108	2.0838
C	3.69089	7.13913	-0.38495
H	4.12631	5.14168	-1.04969
C	2.95354	7.35095	1.93053
H	2.83645	5.52047	3.04491
C	3.26731	7.92194	0.69206
H	3.91088	7.60229	-1.34039
H	2.62595	7.96939	2.75941
C	-1.1779	0.23208	2.86337
C	-2.11272	-0.54968	2.15849
C	-1.64542	1.10814	3.86602
C	-3.4739	-0.48003	2.45399
H	-1.77349	-1.19584	1.35563
C	-3.00134	1.19308	4.1684
H	-0.9355	1.70904	4.42575
C	-3.90243	0.38928	3.46006
H	-4.19246	-1.07435	1.90075
H	-3.34868	1.86336	4.94759
H	4.35564	-0.52621	1.35109
C	2.32307	1.65513	2.08027
H	3.11912	0.95713	2.24985
N	1.19854	3.53043	1.59011
H	0.98917	4.46894	1.26892
S	3.99501	-9.24526	2.6233
S	12.81391	0.07282	-1.05427

S	3.19772	9.69352	0.49225
S	-5.64219	0.51003	3.81418
O	2.41372	-9.57646	2.31745
O	4.81215	-9.82672	1.55144
O	4.29257	-9.58952	4.0183
O	13.25114	-1.30872	-0.2769
O	13.53916	1.20025	-0.45658
O	12.90325	-0.14987	-2.50213
O	-6.05218	1.91477	3.79704
O	-6.36096	-0.49632	3.02771
O	-5.73134	0.10922	5.40057
O	1.75077	10.07821	1.10335
O	4.15107	10.32911	1.40451
O	3.23756	9.99955	-0.94235
H	2.2994	-10.55213	2.30264
H	-5.68572	-0.86678	5.48812
H	1.01425	9.80523	0.48564
H	14.20717	-1.46556	-0.44064
N	-1.69507	0.71372	-1.84487
N	-2.68441	-2.05533	-1.96455
N	-5.41784	-1.19971	-1.17912
C	-1.43281	2.06497	-1.76971
C	-0.50867	0.13091	-2.13855
C	-3.74233	2.7238	-1.15854
C	-5.76185	1.72368	-0.8008
C	-1.3362	-2.24461	-2.2176
C	-3.33945	-3.2725	-1.87452
C	-6.62829	-0.61276	-0.85497
C	-5.66698	-2.52672	-1.25019
C	-2.39141	3.04856	-1.47453
C	-0.01992	2.32907	-2.01918
C	0.55731	1.12286	-2.26266
C	-6.82353	0.76396	-0.68508
C	-5.95475	3.12211	-0.96927
C	-0.33158	-1.27142	-2.3241
C	-1.13521	-3.66946	-2.28695
C	-2.33525	-4.28534	-2.08197
C	-7.66375	-1.63058	-0.70495
C	-4.68834	-3.513	-1.57848
C	-7.06991	-2.82427	-0.96555
H	0.46519	3.29529	-1.99389
H	1.59265	0.9276	-2.50532
H	-6.86394	3.70451	-0.99114
H	-0.17913	-4.14673	-2.44299
H	-2.52024	-5.3485	-2.04232
H	-8.69443	-1.45725	-0.42736

H	-7.5319	-3.80193	-0.9686
C	-5.12924	-4.94139	-1.59397
C	-5.59556	-5.55686	-0.41729
C	-5.08487	-5.69266	-2.78307
C	-6.01159	-6.88712	-0.42171
H	-5.61763	-4.99237	0.50962
C	-5.49623	-7.02445	-2.80531
H	-4.73212	-5.22592	-3.69748
C	-5.96112	-7.60326	-1.62108
H	-6.35557	-7.36506	0.48903
H	-5.45724	-7.60242	-3.72221
C	1.04636	-1.75837	-2.63463
C	2.09497	-1.55289	-1.71732
C	1.32225	-2.41399	-3.84844
C	3.38692	-1.98807	-2.00165
H	1.89685	-1.06054	-0.77031
C	2.60914	-2.86396	-4.1447
H	0.52545	-2.55962	-4.57119
C	3.6258	-2.64621	-3.21187
H	4.19261	-1.81947	-1.29635
H	2.82337	-3.36163	-5.08406
C	-2.00612	4.48369	-1.51625
C	-1.41159	5.0399	-2.66564
C	-2.24458	5.31541	-0.40176
C	-1.04687	6.38404	-2.70294
H	-1.2467	4.41648	-3.53807
C	-1.88238	6.66025	-0.42176
H	-2.6887	4.89719	0.49646
C	-1.28508	7.17735	-1.57647
H	-0.58426	6.80882	-3.58689
H	-2.04467	7.28895	0.44668
C	-8.18866	1.28282	-0.40738
C	-9.26714	0.98265	-1.262
C	-8.41559	2.11742	0.70625
C	-10.54183	1.48693	-1.01058
H	-9.0981	0.37226	-2.14315
C	-9.68482	2.62666	0.97096
H	-7.59742	2.34601	1.38202
C	-10.73705	2.3024	0.10794
H	-11.36677	1.26931	-1.68002
H	-9.85422	3.26646	1.83025
H	-3.12806	-1.14528	-1.85713
C	-4.36695	1.50505	-0.9089
H	-3.8648	0.56172	-0.82358
N	-4.76397	3.69508	-1.16953
H	-4.62666	4.67951	-1.36788

S	-6.48292	-9.30002	-1.63597
S	5.27079	-3.20561	-3.57255
S	-0.81418	8.88922	-1.61661
S	-12.36112	2.94873	0.43964
O	-8.05302	-9.04346	-2.05074
O	-5.82142	-10.0241	-2.72791
O	-6.43325	-9.85099	-0.27683
O	5.23568	-4.60103	-2.69935
O	6.2647	-2.3142	-2.9606
O	5.38161	-3.53393	-4.99711
O	-12.23536	4.23605	1.12093
O	-13.18688	2.79849	-0.76276
O	-12.95264	1.95216	1.60026
O	-2.2031	9.70236	-1.88101
O	-0.47002	9.30204	-0.24527
O	0.10657	9.11755	-2.72863
H	-8.48495	-9.91667	-2.17762
H	-13.32122	1.15034	1.17264
H	-2.41243	9.68609	-2.83993
H	6.16195	-4.89263	-2.55162

Table S5.8. Optimized coordinates for the monomer of **5.2** using the TPSSh exchange correlation functional.

N	2.07914	-0.00873	0.01203
N	0.04782	-2.12905	-0.09882
N	-1.98989	-0.02944	0.00467
C	2.91071	1.07952	0.05568
C	2.91701	-1.09276	-0.00997
C	1.16367	2.87878	0.08465
C	-1.09781	2.86876	0.03119
C	1.18416	-2.90597	-0.08022
C	-1.07751	-2.92024	-0.03536
C	-2.82843	1.05423	-0.01238
C	-2.82094	-1.11849	0.01929
C	2.49728	2.43064	0.08813
C	4.31123	0.67462	0.07243
C	4.31543	-0.68114	0.01528
C	-2.42586	2.40838	-0.01102
C	-0.65657	4.23109	-0.0443
C	2.51276	-2.44561	-0.06112
C	0.74815	-4.27069	-0.0121
C	-0.62221	-4.27925	0.01988
C	-4.22649	0.64185	-0.00478
C	-2.40886	-2.47071	0.01347
C	-4.22206	-0.71512	0.00798

H	5.16487	1.3358	0.12359
H	5.1733	-1.33847	-0.00779
H	-1.30991	5.0862	-0.13564
H	1.40666	-5.12559	0.03332
H	-1.26651	-5.14292	0.09432
H	-5.08411	1.3	-0.00303
H	-5.07566	-1.37838	0.00217
C	-3.46793	-3.52468	0.07937
C	-4.27758	-3.64014	1.22388
C	-3.66941	-4.4106	-0.9943
C	-5.27768	-4.60854	1.29634
H	-4.115	-2.9729	2.06447
C	-4.66599	-5.38443	-0.93803
H	-3.05075	-4.32742	-1.88243
C	-5.46318	-5.46428	0.20705
H	-5.89566	-4.70501	2.18227
H	-4.82284	-6.06658	-1.76647
C	3.5739	-3.50056	-0.0814
C	4.40787	-3.70088	1.03212
C	3.74687	-4.307	-1.22139
C	5.39549	-4.68607	1.01535
H	4.2765	-3.08785	1.91821
C	4.73432	-5.28963	-1.25753
H	3.11432	-4.15032	-2.08949
C	5.54324	-5.46988	-0.13112
H	6.03899	-4.84554	1.87334
H	4.87805	-5.89644	-2.14507
C	3.54666	3.49582	0.10942
C	4.42691	3.65989	-0.97474
C	3.66022	4.35565	1.21771
C	5.39775	4.66128	-0.96108
H	4.34428	3.00579	-1.83717
C	4.6269	5.35887	1.24828
H	2.99519	4.2271	2.06603
C	5.48397	5.50191	0.15221
H	6.07689	4.78715	-1.79716
H	4.72202	6.00912	2.1112
C	-3.48743	3.46056	-0.07207
C	-4.29074	3.59412	-1.21883
C	-3.68525	4.34018	1.0071
C	-5.27005	4.58346	-1.29314
H	-4.13417	2.93054	-2.0635
C	-4.66571	5.33014	0.95142
H	-3.07138	4.24363	1.89722
C	-5.44848	5.43957	-0.20156
H	-5.87195	4.69902	-2.18807

H	-4.81532	6.0102	1.78274
H	0.03948	-1.11135	-0.11876
S	-6.74097	-6.6962	0.2858
S	6.81955	-6.70533	-0.16992
S	6.70802	6.79386	0.17304
S	-6.69442	6.70908	-0.28257
O	-7.93813	-5.80767	-0.40705
O	-6.41373	-7.82037	-0.59883
O	-7.0964	-6.96379	1.68409
O	5.85795	-8.01858	0.05714
O	7.70197	-6.54355	0.99069
O	7.40887	-6.78902	-1.51214
O	-6.38837	7.74022	0.70724
O	-6.93538	7.04745	-1.68895
O	-8.04266	5.98506	0.30814
O	5.86753	8.13532	-0.25741
O	7.10189	7.05825	1.55605
O	7.7056	6.52232	-0.86656
H	-8.74714	-6.36296	-0.45733
H	-8.48557	5.49761	-0.41858
H	5.82669	8.18333	-1.23627
H	6.40001	-8.82631	-0.07983
C	0.71363	4.23749	-0.00892
H	1.36217	5.09905	-0.06762
N	0.03538	2.09035	0.10865
H	0.03953	1.07298	0.14145

Chapter 6 Supporting Information:

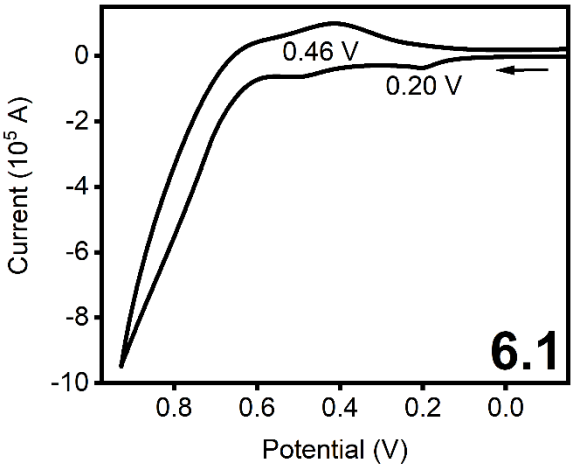


Figure S6.1. Oxidation CV scan of **6.1** to high potential shows solvent discharge and the absence of a multielectron oxidation event (measured in a DCM/0.1M TBAP system).

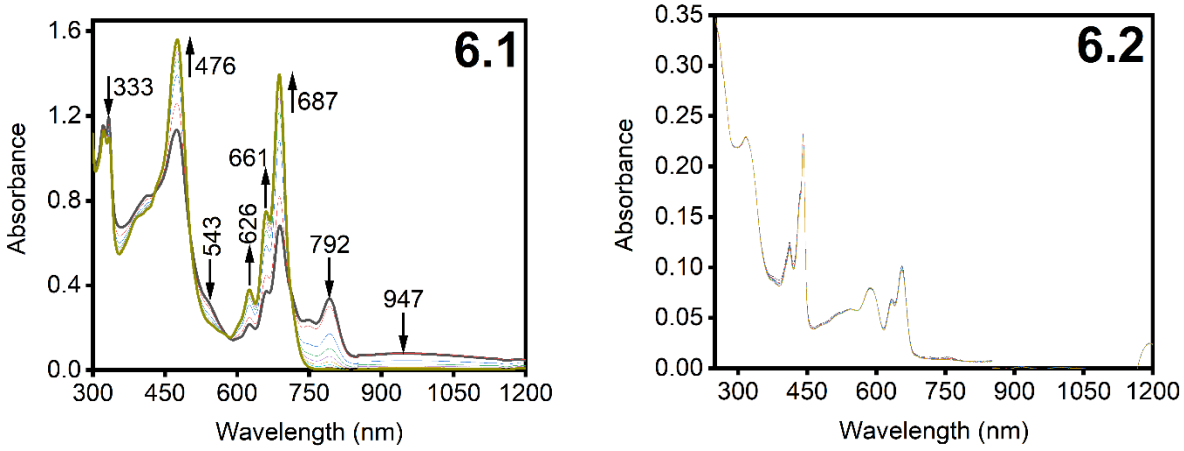


Figure S6.2. Spectro-electrochemical reduction of oxidized solutions of **6.1** and **6.2** in a DCM/0.3M TBAP system.

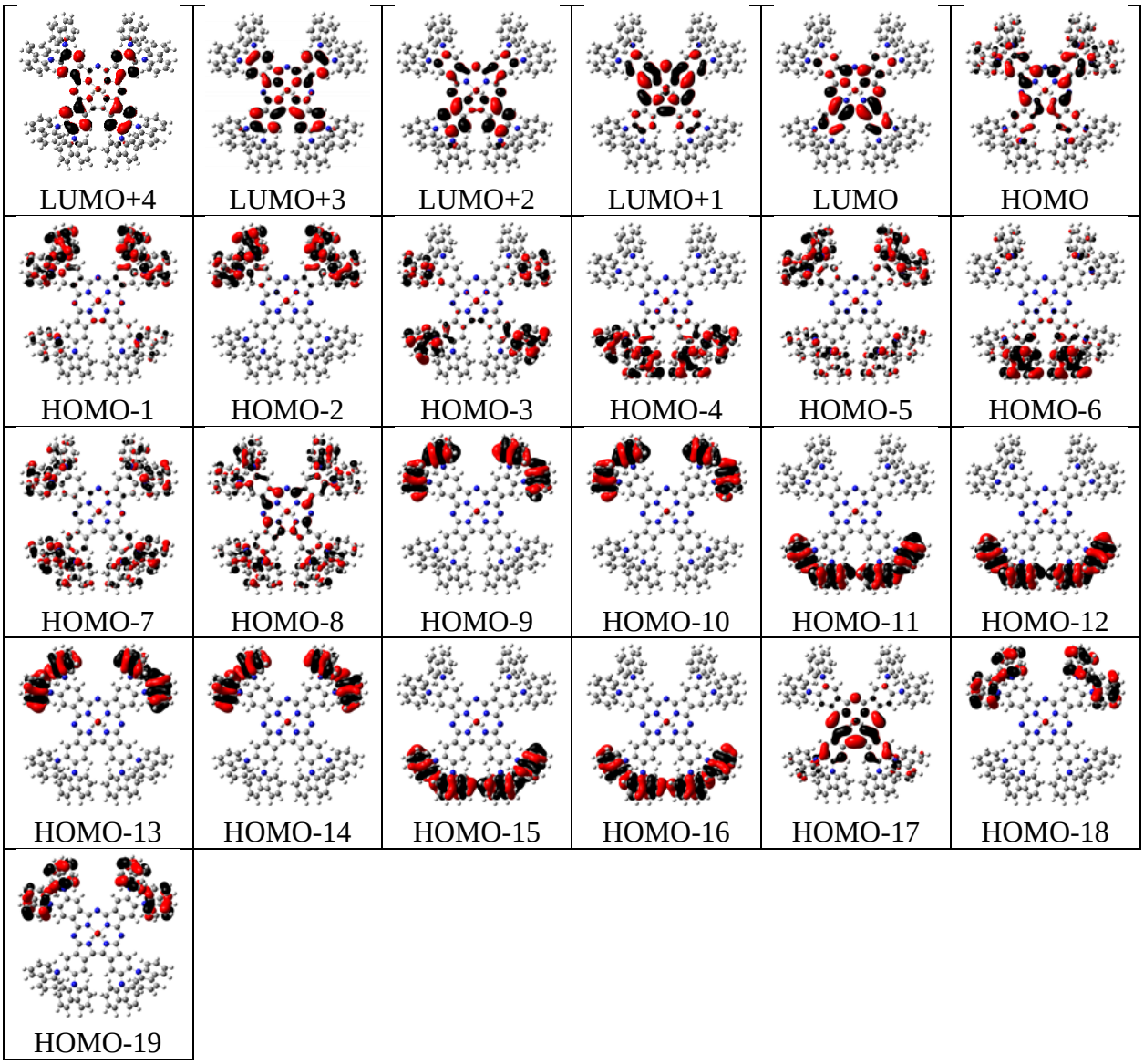


Figure S6.3. Select DFT-predicted molecular orbitals of **6.1**.

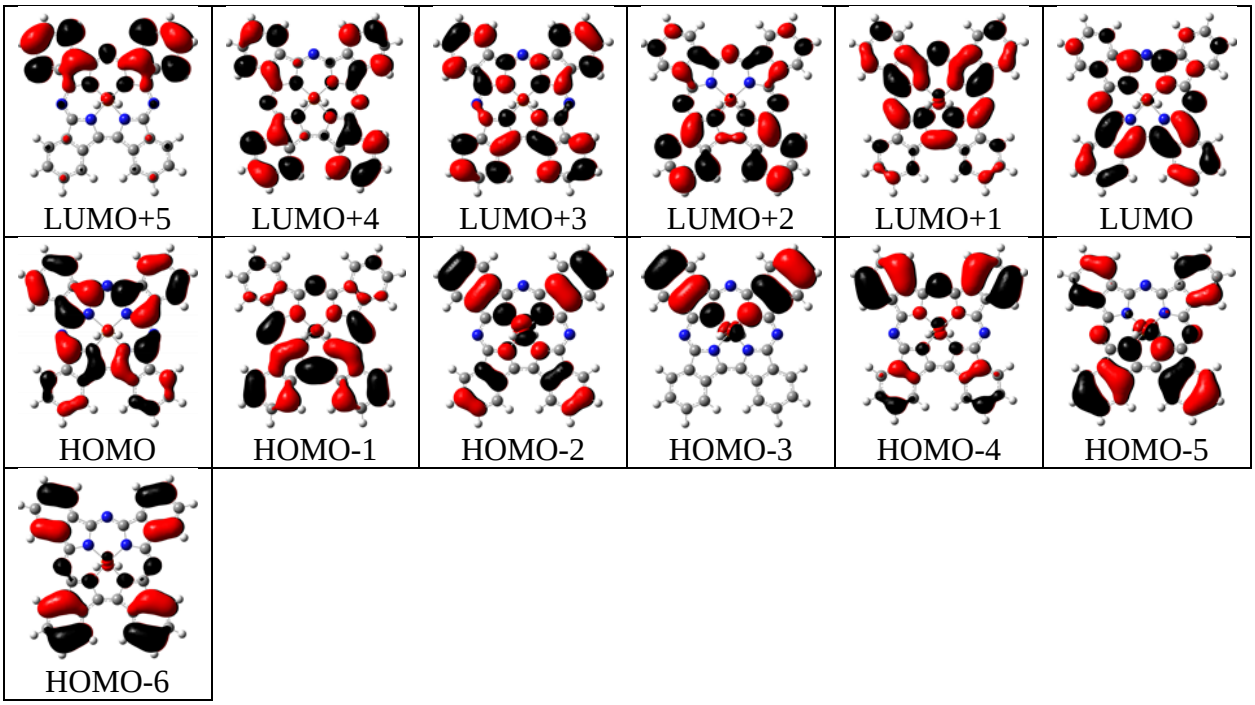
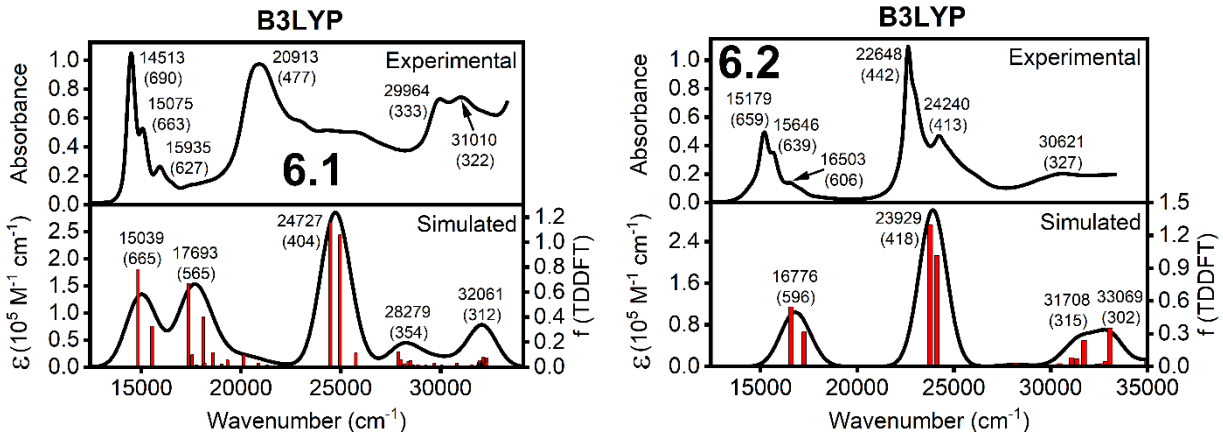


Figure S6.4. Select DFT-predicted molecular orbitals of **6.2**.



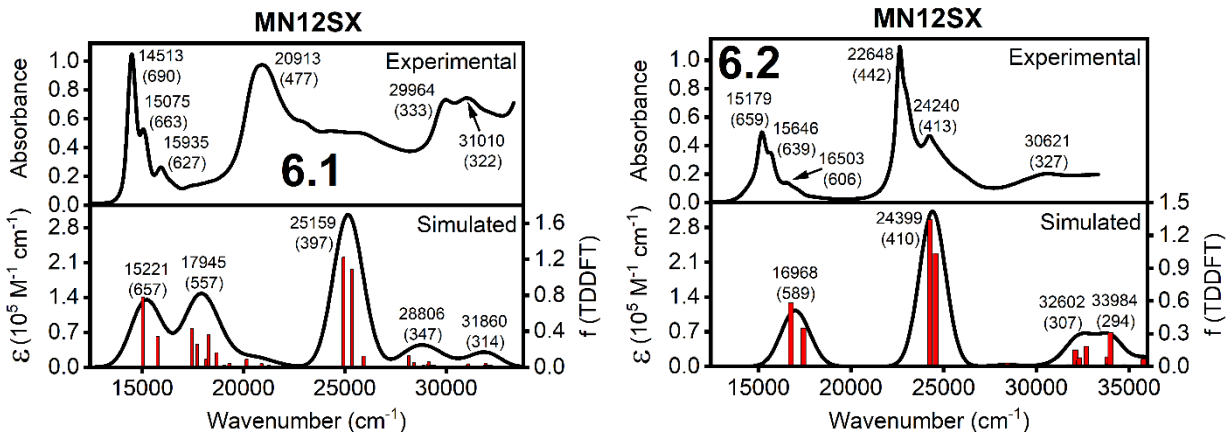


Figure S6.5. Experimental and TDDFT-predicted UV-vis spectra of **6.1** and **6.2** using the B3LYP/LANL2DZ (upper) and MN12SX/LANL2DZ (lower) methods.

Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

Figure S6.6. Full citation for Gaussian 16.

Table S6.1. Major TDDFT-predicted excited state contributions for **6.1** and **6.2** using the HSEHS1PBE/LANL2DZ method.

6.1

Excited State	*Wavelength (nm)*	*Wavenumber (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
1	680	14702	0.7336	H→L (95%)
2	647	15465	0.2828	H→L+1 (85%), H-1→L (10%), H-3→L (3%)
3	600	16680	0.3699	H-1→L (84%), H-3→L (8%), H→L+1 (6%)
5	589	16977	0.3078	H-3→L (85%), H→L+1 (5%), H-1→L (5%)

9	571	17525	0.3237	H-1→L+1 (93%)
12	558	17931	0.1744	H-3→L+1 (76%), H-7→L (16%), H-5→L+1 (5%)
35	407	24597	1.2360	H-17→L (85%), H-8→L+1 (6%), H→L+1 (3%)
36	399	25052	1.1120	H-17→L+1 (85%), H-8→L (4%)
37	391	25588	0.1028	H→L+2 (98%)
41	359	27891	0.1306	H→L+4 (66%), H-19→L (17%), H-1→L+2 (10%), H-6→L+2 (2%)

6.2

Excited State	*Wavelength (nm)*	*Wavenumber (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
1	596	16769	0.5654	H→L (93%), H-1→L+1 (7%)
2	572	17487	0.3344	H→L+1 (90%), H-1→L (10%)
3	416	24037	1.3030	H-1→L (88%), H→L+1 (10%)
4	410	24368	1.0120	H-1→L+1 (92%), H→L (7%)
11	318	31431	0.1326	H-4→L (57%), H-3→L+1 (38%)
14	312	32047	0.1969	H-3→L+1 (39%), H-4→L (34%), H→L+5 (11%), H-2→L (8%), H-6→L (4%)
21	300	33320	0.3651	H-6→L+1 (89%), H-1→L+2 (7%)

Table S6.2. Optimized coordinates for **6.1** using the B3LYP/LANL2DZ-PCM method.

N	0.74507	0.95725	-0.95461
N	-0.74507	-0.95725	-0.95461
N	-0.89028	-1.04584	1.66114
N	0.89028	1.04584	1.66114
C	-0.76558	-0.88823	3.04606
C	-1.62652	-1.86445	3.6679
C	-2.26337	-2.59014	2.63829
C	-1.7981	-2.0692	1.37322
C	1.7981	2.0692	1.37322
C	2.26337	2.59014	2.63829
C	1.62652	1.86445	3.6679
C	0.76558	0.88823	3.04606
C	0.43666	0.54069	-2.2489
C	1.20383	1.37933	-3.1439
C	1.97172	2.2618	-2.33008
C	1.67895	1.96285	-0.94114
C	-1.67895	-1.96285	-0.94114
C	-1.97172	-2.2618	-2.33008

C	-1.20383	-1.37933	-3.1439
C	-0.43666	-0.54069	-2.2489
C	-1.89707	-2.14242	5.01152
C	-2.80044	-3.15963	5.3206
C	-3.42147	-3.92038	4.27395
C	-3.157	-3.62343	2.93665
C	3.157	3.62343	2.93665
C	3.42147	3.92038	4.27395
C	2.80044	3.15963	5.3206
C	1.89707	2.14242	5.01152
C	1.30681	1.45788	-4.53742
C	2.16578	2.39765	-5.11341
C	2.95407	3.26158	-4.28882
C	2.84223	3.19225	-2.89868
C	-2.84223	-3.19225	-2.89868
C	-2.95407	-3.26158	-4.28882
C	-1.30681	-1.45788	-4.53742
N	-2.17545	-2.50538	0.1674
N	0.	0.	3.66654
N	2.17545	2.50538	0.1674
H	-1.43677	-1.56288	5.80332
H	-3.61947	-4.20438	2.14711
H	3.61947	4.20438	2.14711
H	1.43677	1.56288	5.80332
H	0.71799	0.82705	-5.19145
H	3.44977	3.83548	-2.27236
H	-3.44977	-3.83548	-2.27236
H	-0.71799	-0.82705	-5.19145
C	-2.16578	-2.39765	-5.11341
C	-2.11429	-3.71363	7.67452
C	-4.33801	-3.32659	7.32147
C	-0.73334	-3.90237	7.53699
C	-2.75898	-3.8322	8.93116
C	-5.58367	-2.99163	6.77953
C	-4.17511	-3.58056	8.70711
C	0.	-4.20947	8.6888
H	-0.23798	-3.81595	6.57597
C	-2.00855	-4.14216	10.07454
C	-6.67872	-2.93682	7.64867
H	-5.70875	-2.77528	5.72547
C	-5.28451	-3.52565	9.56335
C	-0.62751	-4.32839	9.94843
H	1.0729	-4.35836	8.6108
H	-2.48961	-4.23813	11.04342
C	-6.53676	-3.20685	9.02765
H	-7.65727	-2.68287	7.25211

H	-5.17411	-3.72013	10.62603
C	-4.02015	-6.15712	5.2907
C	-5.63684	-5.0926	4.07774
C	-2.82463	-6.54345	5.90643
C	-5.158	-7.00338	5.28209
C	-6.37739	-4.18626	3.30846
C	-6.18968	-6.32312	4.51291
C	-2.79125	-7.79056	6.53977
H	-1.94672	-5.90894	5.89778
C	-5.10856	-8.24843	5.92579
C	-7.69099	-4.53593	2.97529
H	-5.95805	-3.24263	2.97663
C	-7.50817	-6.65644	4.17076
C	-3.9223	-8.63623	6.5576
H	-1.87649	-8.1117	7.02906
H	-5.97385	-8.9046	5.92927
C	-8.25514	-5.75923	3.39949
H	-8.28688	-3.8519	2.37831
H	-7.9452	-7.59473	4.49947
C	-3.85728	-5.58762	-4.5854
C	-4.96892	-3.91126	-5.67133
C	-2.95919	-6.34726	-3.82548
C	-4.95115	-6.18532	-5.25949
C	-5.42919	-2.67724	-6.14286
C	-5.66208	-5.11699	-5.94673
C	-3.17864	-7.72736	-3.74552
H	-2.11817	-5.89407	-3.31196
C	-5.15477	-7.56975	-5.16983
C	-6.59143	-2.67017	-6.92193
H	-4.91629	-1.75053	-5.91584
C	-6.82306	-5.09234	-6.73291
C	-4.26578	-8.33713	-4.40909
H	-2.49872	-8.33992	-3.16089
H	-5.98748	-8.04132	-5.68318
C	-7.28169	-3.86489	-7.22258
H	-6.96757	-1.7256	-7.30339
H	-7.36224	-6.00886	-6.95298
C	-1.91098	-3.58104	-7.33256
C	-2.52476	-1.37939	-7.38378
C	-1.49399	-4.8609	-6.95149
C	-2.0177	-3.21003	-8.69674
C	-2.90063	-0.06972	-7.06004
C	-2.41381	-1.80957	-8.72929
C	-1.20362	-5.78009	-7.96577
H	-1.39254	-5.14357	-5.91062
C	-1.72671	-4.14507	-9.70047

C	-3.15905	0.81331	-8.11492
H	-2.99627	0.26062	-6.03126
C	-2.67875	-0.91203	-9.77336
C	-1.32331	-5.432	-9.32905
H	-0.88236	-6.78188	-7.69659
H	-1.80599	-3.87445	-10.74913
C	-3.049	0.40056	-9.46069
H	-3.45028	1.83555	-7.89252
H	-2.59978	-1.22872	-10.80903
C	2.52476	1.37939	-7.38378
C	1.91098	3.58104	-7.33256
C	2.90063	0.06972	-7.06004
C	2.41381	1.80957	-8.72929
C	1.49399	4.8609	-6.95149
C	2.0177	3.21003	-8.69674
C	3.15905	-0.81331	-8.11492
H	2.99627	-0.26062	-6.03126
C	2.67875	0.91203	-9.77336
C	1.20362	5.78009	-7.96577
H	1.39254	5.14357	-5.91062
C	1.72671	4.14507	-9.70047
C	3.049	-0.40056	-9.46069
H	3.45028	-1.83555	-7.89252
H	2.59978	1.22872	-10.80903
C	1.32331	5.432	-9.32905
H	0.88236	6.78188	-7.69659
H	1.80599	3.87445	-10.74913
C	4.96892	3.91126	-5.67133
C	3.85728	5.58762	-4.5854
C	5.42919	2.67724	-6.14286
C	5.66208	5.11699	-5.94673
C	2.95919	6.34726	-3.82548
C	4.95115	6.18532	-5.25949
C	6.59143	2.67017	-6.92193
H	4.91629	1.75053	-5.91584
C	6.82306	5.09234	-6.73291
C	3.17864	7.72736	-3.74552
H	2.11817	5.89407	-3.31196
C	5.15477	7.56975	-5.16983
C	7.28169	3.86489	-7.22258
H	6.96757	1.7256	-7.30339
H	7.36224	6.00886	-6.95298
C	4.26578	8.33713	-4.40909
H	2.49872	8.33992	-3.16089
H	5.98748	8.04132	-5.68318
C	2.11429	3.71363	7.67452

C	4.33801	3.32659	7.32147
C	0.73334	3.90237	7.53699
C	2.75898	3.8322	8.93116
C	5.58367	2.99163	6.77953
C	4.17511	3.58056	8.70711
C	0.	4.20947	8.6888
H	0.23798	3.81595	6.57597
C	2.00855	4.14216	10.07454
C	6.67872	2.93682	7.64867
H	5.70875	2.77528	5.72547
C	5.28451	3.52565	9.56335
C	0.62751	4.32839	9.94843
H	-1.0729	4.35836	8.6108
H	2.48961	4.23813	11.04342
C	6.53676	3.20685	9.02765
H	7.65727	2.68287	7.25211
H	5.17411	3.72013	10.62603
C	4.02015	6.15712	5.2907
C	5.63684	5.0926	4.07774
C	2.82463	6.54345	5.90643
C	5.158	7.00338	5.28209
C	6.37739	4.18626	3.30846
C	6.18968	6.32312	4.51291
C	2.79125	7.79056	6.53977
H	1.94672	5.90894	5.89778
C	5.10856	8.24843	5.92579
C	7.69099	4.53593	2.97529
H	5.95805	3.24263	2.97663
C	7.50817	6.65644	4.17076
C	3.9223	8.63623	6.5576
H	1.87649	8.1117	7.02906
H	5.97385	8.9046	5.92927
C	8.25514	5.75923	3.39949
H	8.28688	3.8519	2.37831
H	7.9452	7.59473	4.49947
N	3.08156	3.42686	6.68893
N	4.32005	4.98237	4.57065
N	3.85565	4.20238	-4.85457
N	2.23713	2.46645	-6.53084
N	-2.23713	-2.46645	-6.53084
N	-3.85565	-4.20238	-4.85457
N	-4.32005	-4.98237	4.57065
N	-3.08156	-3.42686	6.68893
H	3.25505	-1.1103	-10.25568
H	1.09415	6.17005	-10.09141
H	8.17848	3.82507	-7.833

H	4.40861	9.41001	-4.32643
H	-1.09415	-6.17005	-10.09141
H	-4.40861	-9.41001	-4.32643
H	-3.86446	-9.59598	7.06162
H	-0.03001	-4.56678	10.82282
H	-9.27689	-6.00073	3.12355
H	-7.40752	-3.15937	9.67421
H	-8.17848	-3.82507	-7.833
H	-3.25505	1.1103	-10.25568
H	9.27689	6.00073	3.12355
H	3.86446	9.59598	7.06162
H	7.40752	3.15937	9.67421
H	0.03001	4.56678	10.82282
P	0.	0.	0.42707
O	-1.41752	1.05499	0.49437
H	-1.32213	1.93584	0.08014
O	1.41752	-1.05499	0.49437
H	1.32213	-1.93584	0.08014

Table S6.3. Optimized coordinates for **6.1** using the HSEH1PBE/LANL2DZ-PCM method.

N	0.74507	0.95725	-0.95461
N	-0.74507	-0.95725	-0.95461
N	-0.89028	-1.04584	1.66114
N	0.89028	1.04584	1.66114
C	-0.76558	-0.88823	3.04606
C	-1.62652	-1.86445	3.6679
C	-2.26337	-2.59014	2.63829
C	-1.7981	-2.0692	1.37322
C	1.7981	2.0692	1.37322
C	2.26337	2.59014	2.63829
C	1.62652	1.86445	3.6679
C	0.76558	0.88823	3.04606
C	0.43666	0.54069	-2.2489
C	1.20383	1.37933	-3.1439
C	1.97172	2.2618	-2.33008
C	1.67895	1.96285	-0.94114
C	-1.67895	-1.96285	-0.94114
C	-1.97172	-2.2618	-2.33008
C	-1.20383	-1.37933	-3.1439
C	-0.43666	-0.54069	-2.2489
C	-1.89707	-2.14242	5.01152
C	-2.80044	-3.15963	5.3206
C	-3.42147	-3.92038	4.27395
C	-3.157	-3.62343	2.93665
C	3.157	3.62343	2.93665

C	3.42147	3.92038	4.27395
C	2.80044	3.15963	5.3206
C	1.89707	2.14242	5.01152
C	1.30681	1.45788	-4.53742
C	2.16578	2.39765	-5.11341
C	2.95407	3.26158	-4.28882
C	2.84223	3.19225	-2.89868
C	-2.84223	-3.19225	-2.89868
C	-2.95407	-3.26158	-4.28882
C	-1.30681	-1.45788	-4.53742
N	-2.17545	-2.50538	0.1674
N	0.	0.	3.66654
N	2.17545	2.50538	0.1674
H	-1.43677	-1.56288	5.80332
H	-3.61947	-4.20438	2.14711
H	3.61947	4.20438	2.14711
H	1.43677	1.56288	5.80332
H	0.71799	0.82705	-5.19145
H	3.44977	3.83548	-2.27236
H	-3.44977	-3.83548	-2.27236
H	-0.71799	-0.82705	-5.19145
C	-2.16578	-2.39765	-5.11341
C	-2.11429	-3.71363	7.67452
C	-4.33801	-3.32659	7.32147
C	-0.73334	-3.90237	7.53699
C	-2.75898	-3.8322	8.93116
C	-5.58367	-2.99163	6.77953
C	-4.17511	-3.58056	8.70711
C	0.	-4.20947	8.6888
H	-0.23798	-3.81595	6.57597
C	-2.00855	-4.14216	10.07454
C	-6.67872	-2.93682	7.64867
H	-5.70875	-2.77528	5.72547
C	-5.28451	-3.52565	9.56335
C	-0.62751	-4.32839	9.94843
H	1.0729	-4.35836	8.6108
H	-2.48961	-4.23813	11.04342
C	-6.53676	-3.20685	9.02765
H	-7.65727	-2.68287	7.25211
H	-5.17411	-3.72013	10.62603
C	-4.02015	-6.15712	5.2907
C	-5.63684	-5.0926	4.07774
C	-2.82463	-6.54345	5.90643
C	-5.158	-7.00338	5.28209
C	-6.37739	-4.18626	3.30846
C	-6.18968	-6.32312	4.51291

C	-2.79125	-7.79056	6.53977
H	-1.94672	-5.90894	5.89778
C	-5.10856	-8.24843	5.92579
C	-7.69099	-4.53593	2.97529
H	-5.95805	-3.24263	2.97663
C	-7.50817	-6.65644	4.17076
C	-3.9223	-8.63623	6.5576
H	-1.87649	-8.1117	7.02906
H	-5.97385	-8.9046	5.92927
C	-8.25514	-5.75923	3.39949
H	-8.28688	-3.8519	2.37831
H	-7.9452	-7.59473	4.49947
C	-3.85728	-5.58762	-4.5854
C	-4.96892	-3.91126	-5.67133
C	-2.95919	-6.34726	-3.82548
C	-4.95115	-6.18532	-5.25949
C	-5.42919	-2.67724	-6.14286
C	-5.66208	-5.11699	-5.94673
C	-3.17864	-7.72736	-3.74552
H	-2.11817	-5.89407	-3.31196
C	-5.15477	-7.56975	-5.16983
C	-6.59143	-2.67017	-6.92193
H	-4.91629	-1.75053	-5.91584
C	-6.82306	-5.09234	-6.73291
C	-4.26578	-8.33713	-4.40909
H	-2.49872	-8.33992	-3.16089
H	-5.98748	-8.04132	-5.68318
C	-7.28169	-3.86489	-7.22258
H	-6.96757	-1.7256	-7.30339
H	-7.36224	-6.00886	-6.95298
C	-1.91098	-3.58104	-7.33256
C	-2.52476	-1.37939	-7.38378
C	-1.49399	-4.8609	-6.95149
C	-2.0177	-3.21003	-8.69674
C	-2.90063	-0.06972	-7.06004
C	-2.41381	-1.80957	-8.72929
C	-1.20362	-5.78009	-7.96577
H	-1.39254	-5.14357	-5.91062
C	-1.72671	-4.14507	-9.70047
C	-3.15905	0.81331	-8.11492
H	-2.99627	0.26062	-6.03126
C	-2.67875	-0.91203	-9.77336
C	-1.32331	-5.432	-9.32905
H	-0.88236	-6.78188	-7.69659
H	-1.80599	-3.87445	-10.74913
C	-3.049	0.40056	-9.46069

H	-3.45028	1.83555	-7.89252
H	-2.59978	-1.22872	-10.80903
C	2.52476	1.37939	-7.38378
C	1.91098	3.58104	-7.33256
C	2.90063	0.06972	-7.06004
C	2.41381	1.80957	-8.72929
C	1.49399	4.8609	-6.95149
C	2.0177	3.21003	-8.69674
C	3.15905	-0.81331	-8.11492
H	2.99627	-0.26062	-6.03126
C	2.67875	0.91203	-9.77336
C	1.20362	5.78009	-7.96577
H	1.39254	5.14357	-5.91062
C	1.72671	4.14507	-9.70047
C	3.049	-0.40056	-9.46069
H	3.45028	-1.83555	-7.89252
H	2.59978	1.22872	-10.80903
C	1.32331	5.432	-9.32905
H	0.88236	6.78188	-7.69659
H	1.80599	3.87445	-10.74913
C	4.96892	3.91126	-5.67133
C	3.85728	5.58762	-4.5854
C	5.42919	2.67724	-6.14286
C	5.66208	5.11699	-5.94673
C	2.95919	6.34726	-3.82548
C	4.95115	6.18532	-5.25949
C	6.59143	2.67017	-6.92193
H	4.91629	1.75053	-5.91584
C	6.82306	5.09234	-6.73291
C	3.17864	7.72736	-3.74552
H	2.11817	5.89407	-3.31196
C	5.15477	7.56975	-5.16983
C	7.28169	3.86489	-7.22258
H	6.96757	1.7256	-7.30339
H	7.36224	6.00886	-6.95298
C	4.26578	8.33713	-4.40909
H	2.49872	8.33992	-3.16089
H	5.98748	8.04132	-5.68318
C	2.11429	3.71363	7.67452
C	4.33801	3.32659	7.32147
C	0.73334	3.90237	7.53699
C	2.75898	3.8322	8.93116
C	5.58367	2.99163	6.77953
C	4.17511	3.58056	8.70711
C	0.	4.20947	8.6888
H	0.23798	3.81595	6.57597

C	2.00855	4.14216	10.07454
C	6.67872	2.93682	7.64867
H	5.70875	2.77528	5.72547
C	5.28451	3.52565	9.56335
C	0.62751	4.32839	9.94843
H	-1.0729	4.35836	8.6108
H	2.48961	4.23813	11.04342
C	6.53676	3.20685	9.02765
H	7.65727	2.68287	7.25211
H	5.17411	3.72013	10.62603
C	4.02015	6.15712	5.2907
C	5.63684	5.0926	4.07774
C	2.82463	6.54345	5.90643
C	5.158	7.00338	5.28209
C	6.37739	4.18626	3.30846
C	6.18968	6.32312	4.51291
C	2.79125	7.79056	6.53977
H	1.94672	5.90894	5.89778
C	5.10856	8.24843	5.92579
C	7.69099	4.53593	2.97529
H	5.95805	3.24263	2.97663
C	7.50817	6.65644	4.17076
C	3.9223	8.63623	6.5576
H	1.87649	8.1117	7.02906
H	5.97385	8.9046	5.92927
C	8.25514	5.75923	3.39949
H	8.28688	3.8519	2.37831
H	7.9452	7.59473	4.49947
N	3.08156	3.42686	6.68893
N	4.32005	4.98237	4.57065
N	3.85565	4.20238	-4.85457
N	2.23713	2.46645	-6.53084
N	-2.23713	-2.46645	-6.53084
N	-3.85565	-4.20238	-4.85457
N	-4.32005	-4.98237	4.57065
N	-3.08156	-3.42686	6.68893
H	3.25505	-1.1103	-10.25568
H	1.09415	6.17005	-10.09141
H	8.17848	3.82507	-7.833
H	4.40861	9.41001	-4.32643
H	-1.09415	-6.17005	-10.09141
H	-4.40861	-9.41001	-4.32643
H	-3.86446	-9.59598	7.06162
H	-0.03001	-4.56678	10.82282
H	-9.27689	-6.00073	3.12355
H	-7.40752	-3.15937	9.67421

H	-8.17848	-3.82507	-7.833
H	-3.25505	1.1103	-10.25568
H	9.27689	6.00073	3.12355
H	3.86446	9.59598	7.06162
H	7.40752	3.15937	9.67421
H	0.03001	4.56678	10.82282
P	0.	0.	0.42707
O	-1.41752	1.05499	0.49437
H	-1.32213	1.93584	0.08014
O	1.41752	-1.05499	0.49437
H	1.32213	-1.93584	0.08014

Table S6.4. Optimized coordinates for **6.1** using the MN12SX/LANL2DZ-PCM method.

N	0.74507	0.95725	-0.95461
N	-0.74507	-0.95725	-0.95461
N	-0.89028	-1.04584	1.66114
N	0.89028	1.04584	1.66114
C	-0.76558	-0.88823	3.04606
C	-1.62652	-1.86445	3.6679
C	-2.26337	-2.59014	2.63829
C	-1.7981	-2.0692	1.37322
C	1.7981	2.0692	1.37322
C	2.26337	2.59014	2.63829
C	1.62652	1.86445	3.6679
C	0.76558	0.88823	3.04606
C	0.43666	0.54069	-2.2489
C	1.20383	1.37933	-3.1439
C	1.97172	2.2618	-2.33008
C	1.67895	1.96285	-0.94114
C	-1.67895	-1.96285	-0.94114
C	-1.97172	-2.2618	-2.33008
C	-1.20383	-1.37933	-3.1439
C	-0.43666	-0.54069	-2.2489
C	-1.89707	-2.14242	5.01152
C	-2.80044	-3.15963	5.3206
C	-3.42147	-3.92038	4.27395
C	-3.157	-3.62343	2.93665
C	3.157	3.62343	2.93665
C	3.42147	3.92038	4.27395
C	2.80044	3.15963	5.3206
C	1.89707	2.14242	5.01152
C	1.30681	1.45788	-4.53742
C	2.16578	2.39765	-5.11341
C	2.95407	3.26158	-4.28882
C	2.84223	3.19225	-2.89868

C	-2.84223	-3.19225	-2.89868
C	-2.95407	-3.26158	-4.28882
C	-1.30681	-1.45788	-4.53742
N	-2.17545	-2.50538	0.1674
N	0.	0.	3.66654
N	2.17545	2.50538	0.1674
H	-1.43677	-1.56288	5.80332
H	-3.61947	-4.20438	2.14711
H	3.61947	4.20438	2.14711
H	1.43677	1.56288	5.80332
H	0.71799	0.82705	-5.19145
H	3.44977	3.83548	-2.27236
H	-3.44977	-3.83548	-2.27236
H	-0.71799	-0.82705	-5.19145
C	-2.16578	-2.39765	-5.11341
C	-2.11429	-3.71363	7.67452
C	-4.33801	-3.32659	7.32147
C	-0.73334	-3.90237	7.53699
C	-2.75898	-3.8322	8.93116
C	-5.58367	-2.99163	6.77953
C	-4.17511	-3.58056	8.70711
C	0.	-4.20947	8.6888
H	-0.23798	-3.81595	6.57597
C	-2.00855	-4.14216	10.07454
C	-6.67872	-2.93682	7.64867
H	-5.70875	-2.77528	5.72547
C	-5.28451	-3.52565	9.56335
C	-0.62751	-4.32839	9.94843
H	1.0729	-4.35836	8.6108
H	-2.48961	-4.23813	11.04342
C	-6.53676	-3.20685	9.02765
H	-7.65727	-2.68287	7.25211
H	-5.17411	-3.72013	10.62603
C	-4.02015	-6.15712	5.2907
C	-5.63684	-5.0926	4.07774
C	-2.82463	-6.54345	5.90643
C	-5.158	-7.00338	5.28209
C	-6.37739	-4.18626	3.30846
C	-6.18968	-6.32312	4.51291
C	-2.79125	-7.79056	6.53977
H	-1.94672	-5.90894	5.89778
C	-5.10856	-8.24843	5.92579
C	-7.69099	-4.53593	2.97529
H	-5.95805	-3.24263	2.97663
C	-7.50817	-6.65644	4.17076
C	-3.9223	-8.63623	6.5576

H	-1.87649	-8.1117	7.02906
H	-5.97385	-8.9046	5.92927
C	-8.25514	-5.75923	3.39949
H	-8.28688	-3.8519	2.37831
H	-7.9452	-7.59473	4.49947
C	-3.85728	-5.58762	-4.5854
C	-4.96892	-3.91126	-5.67133
C	-2.95919	-6.34726	-3.82548
C	-4.95115	-6.18532	-5.25949
C	-5.42919	-2.67724	-6.14286
C	-5.66208	-5.11699	-5.94673
C	-3.17864	-7.72736	-3.74552
H	-2.11817	-5.89407	-3.31196
C	-5.15477	-7.56975	-5.16983
C	-6.59143	-2.67017	-6.92193
H	-4.91629	-1.75053	-5.91584
C	-6.82306	-5.09234	-6.73291
C	-4.26578	-8.33713	-4.40909
H	-2.49872	-8.33992	-3.16089
H	-5.98748	-8.04132	-5.68318
C	-7.28169	-3.86489	-7.22258
H	-6.96757	-1.7256	-7.30339
H	-7.36224	-6.00886	-6.95298
C	-1.91098	-3.58104	-7.33256
C	-2.52476	-1.37939	-7.38378
C	-1.49399	-4.8609	-6.95149
C	-2.0177	-3.21003	-8.69674
C	-2.90063	-0.06972	-7.06004
C	-2.41381	-1.80957	-8.72929
C	-1.20362	-5.78009	-7.96577
H	-1.39254	-5.14357	-5.91062
C	-1.72671	-4.14507	-9.70047
C	-3.15905	0.81331	-8.11492
H	-2.99627	0.26062	-6.03126
C	-2.67875	-0.91203	-9.77336
C	-1.32331	-5.432	-9.32905
H	-0.88236	-6.78188	-7.69659
H	-1.80599	-3.87445	-10.74913
C	-3.049	0.40056	-9.46069
H	-3.45028	1.83555	-7.89252
H	-2.59978	-1.22872	-10.80903
C	2.52476	1.37939	-7.38378
C	1.91098	3.58104	-7.33256
C	2.90063	0.06972	-7.06004
C	2.41381	1.80957	-8.72929
C	1.49399	4.8609	-6.95149

C	2.0177	3.21003	-8.69674
C	3.15905	-0.81331	-8.11492
H	2.99627	-0.26062	-6.03126
C	2.67875	0.91203	-9.77336
C	1.20362	5.78009	-7.96577
H	1.39254	5.14357	-5.91062
C	1.72671	4.14507	-9.70047
C	3.049	-0.40056	-9.46069
H	3.45028	-1.83555	-7.89252
H	2.59978	1.22872	-10.80903
C	1.32331	5.432	-9.32905
H	0.88236	6.78188	-7.69659
H	1.80599	3.87445	-10.74913
C	4.96892	3.91126	-5.67133
C	3.85728	5.58762	-4.5854
C	5.42919	2.67724	-6.14286
C	5.66208	5.11699	-5.94673
C	2.95919	6.34726	-3.82548
C	4.95115	6.18532	-5.25949
C	6.59143	2.67017	-6.92193
H	4.91629	1.75053	-5.91584
C	6.82306	5.09234	-6.73291
C	3.17864	7.72736	-3.74552
H	2.11817	5.89407	-3.31196
C	5.15477	7.56975	-5.16983
C	7.28169	3.86489	-7.22258
H	6.96757	1.7256	-7.30339
H	7.36224	6.00886	-6.95298
C	4.26578	8.33713	-4.40909
H	2.49872	8.33992	-3.16089
H	5.98748	8.04132	-5.68318
C	2.11429	3.71363	7.67452
C	4.33801	3.32659	7.32147
C	0.73334	3.90237	7.53699
C	2.75898	3.8322	8.93116
C	5.58367	2.99163	6.77953
C	4.17511	3.58056	8.70711
C	0.	4.20947	8.6888
H	0.23798	3.81595	6.57597
C	2.00855	4.14216	10.07454
C	6.67872	2.93682	7.64867
H	5.70875	2.77528	5.72547
C	5.28451	3.52565	9.56335
C	0.62751	4.32839	9.94843
H	-1.0729	4.35836	8.6108
H	2.48961	4.23813	11.04342

C	6.53676	3.20685	9.02765
H	7.65727	2.68287	7.25211
H	5.17411	3.72013	10.62603
C	4.02015	6.15712	5.2907
C	5.63684	5.0926	4.07774
C	2.82463	6.54345	5.90643
C	5.158	7.00338	5.28209
C	6.37739	4.18626	3.30846
C	6.18968	6.32312	4.51291
C	2.79125	7.79056	6.53977
H	1.94672	5.90894	5.89778
C	5.10856	8.24843	5.92579
C	7.69099	4.53593	2.97529
H	5.95805	3.24263	2.97663
C	7.50817	6.65644	4.17076
C	3.9223	8.63623	6.5576
H	1.87649	8.1117	7.02906
H	5.97385	8.9046	5.92927
C	8.25514	5.75923	3.39949
H	8.28688	3.8519	2.37831
H	7.9452	7.59473	4.49947
N	3.08156	3.42686	6.68893
N	4.32005	4.98237	4.57065
N	3.85565	4.20238	-4.85457
N	2.23713	2.46645	-6.53084
N	-2.23713	-2.46645	-6.53084
N	-3.85565	-4.20238	-4.85457
N	-4.32005	-4.98237	4.57065
N	-3.08156	-3.42686	6.68893
H	3.25505	-1.1103	-10.25568
H	1.09415	6.17005	-10.09141
H	8.17848	3.82507	-7.833
H	4.40861	9.41001	-4.32643
H	-1.09415	-6.17005	-10.09141
H	-4.40861	-9.41001	-4.32643
H	-3.86446	-9.59598	7.06162
H	-0.03001	-4.56678	10.82282
H	-9.27689	-6.00073	3.12355
H	-7.40752	-3.15937	9.67421
H	-8.17848	-3.82507	-7.833
H	-3.25505	1.1103	-10.25568
H	9.27689	6.00073	3.12355
H	3.86446	9.59598	7.06162
H	7.40752	3.15937	9.67421
H	0.03001	4.56678	10.82282
P	0.	0.	0.42707

O	-1.41752	1.05499	0.49437
H	-1.32213	1.93584	0.08014
O	1.41752	-1.05499	0.49437
H	1.32213	-1.93584	0.08014

Table S6.5. Optimized coordinates for **6.2** using the B3LYP/LANL2DZ-PCM method.

N	-1.21271	0.02464	-1.24906
N	1.21271	-0.02464	-1.24906
N	1.3707	-0.08752	1.36286
N	-1.3707	0.08752	1.36286
C	1.17112	-0.08399	2.74874
C	2.46809	-0.19565	3.37288
C	3.43214	-0.27217	2.34128
C	2.73457	-0.20582	1.07638
C	-2.73457	0.20582	1.07638
C	-3.43214	0.27217	2.34128
C	-2.46809	0.19565	3.37288
C	-1.17112	0.08399	2.74874
C	-0.69441	0.02343	-2.5434
C	-1.82358	0.12611	-3.44312
C	-2.99293	0.21993	-2.63043
C	-2.57757	0.17026	-1.2398
C	2.57757	-0.17026	-1.2398
C	2.99293	-0.21993	-2.63043
C	1.82358	-0.12611	-3.44312
C	0.69441	-0.02343	-2.5434
C	2.84952	-0.23682	4.72472
C	4.20871	-0.35527	5.01314
C	5.17712	-0.43275	3.97655
C	4.80106	-0.39202	2.63434
C	-4.80106	0.39202	2.63434
C	-5.17712	0.43275	3.97655
C	-4.20871	0.35527	5.01314
C	-2.84952	0.23682	4.72472
C	-1.93668	0.15482	-4.84412
C	-3.2093	0.27523	-5.40432
C	-4.36608	0.36854	-4.59205
C	-4.268	0.34241	-3.20017
C	4.268	-0.34241	-3.20017
C	4.36608	-0.36854	-4.59205
C	1.93668	-0.15482	-4.84412
N	3.31003	-0.24558	-0.13078
N	0.	0.	3.36818
N	-3.31003	0.24558	-0.13078
H	2.1062	-0.17859	5.51219

H	5.53446	-0.45211	1.83775
H	-5.53446	0.45211	1.83775
H	-2.1062	0.17859	5.51219
H	-1.06569	0.08493	-5.48476
H	-5.14759	0.41524	-2.56994
H	5.14759	-0.41524	-2.56994
H	1.06569	-0.08493	-5.48476
C	3.2093	-0.27523	-5.40432
P	0.	0.	0.13107
O	0.	-1.77063	0.19548
H	-0.78045	-2.21214	-0.19464
O	0.	1.77063	0.19548
H	0.78045	2.21214	-0.19464
H	-6.22603	0.52598	4.24044
H	-4.53927	0.3904	6.04669
H	-5.33891	0.46235	-5.06406
H	-3.31883	0.29849	-6.48401
H	3.31883	-0.29849	-6.48401
H	5.33891	-0.46235	-5.06406
H	6.22603	-0.52598	4.24044
H	4.53927	-0.3904	6.04669

Table S6.6. Optimized coordinates for **6.2** using the HSEH1PBE/LANL2DZ-PCM method.

N	-1.21271	0.02464	-1.24906
N	1.21271	-0.02464	-1.24906
N	1.3707	-0.08752	1.36286
N	-1.3707	0.08752	1.36286
C	1.17112	-0.08399	2.74874
C	2.46809	-0.19565	3.37288
C	3.43214	-0.27217	2.34128
C	2.73457	-0.20582	1.07638
C	-2.73457	0.20582	1.07638
C	-3.43214	0.27217	2.34128
C	-2.46809	0.19565	3.37288
C	-1.17112	0.08399	2.74874
C	-0.69441	0.02343	-2.5434
C	-1.82358	0.12611	-3.44312
C	-2.99293	0.21993	-2.63043
C	-2.57757	0.17026	-1.2398
C	2.57757	-0.17026	-1.2398
C	2.99293	-0.21993	-2.63043
C	1.82358	-0.12611	-3.44312
C	0.69441	-0.02343	-2.5434
C	2.84952	-0.23682	4.72472
C	4.20871	-0.35527	5.01314

C	5.17712	-0.43275	3.97655
C	4.80106	-0.39202	2.63434
C	-4.80106	0.39202	2.63434
C	-5.17712	0.43275	3.97655
C	-4.20871	0.35527	5.01314
C	-2.84952	0.23682	4.72472
C	-1.93668	0.15482	-4.84412
C	-3.2093	0.27523	-5.40432
C	-4.36608	0.36854	-4.59205
C	-4.268	0.34241	-3.20017
C	4.268	-0.34241	-3.20017
C	4.36608	-0.36854	-4.59205
C	1.93668	-0.15482	-4.84412
N	3.31003	-0.24558	-0.13078
N	0.	0.	3.36818
N	-3.31003	0.24558	-0.13078
H	2.1062	-0.17859	5.51219
H	5.53446	-0.45211	1.83775
H	-5.53446	0.45211	1.83775
H	-2.1062	0.17859	5.51219
H	-1.06569	0.08493	-5.48476
H	-5.14759	0.41524	-2.56994
H	5.14759	-0.41524	-2.56994
H	1.06569	-0.08493	-5.48476
C	3.2093	-0.27523	-5.40432
P	0.	0.	0.13107
O	0.	-1.77063	0.19548
H	-0.78045	-2.21214	-0.19464
O	0.	1.77063	0.19548
H	0.78045	2.21214	-0.19464
H	-6.22603	0.52598	4.24044
H	-4.53927	0.3904	6.04669
H	-5.33891	0.46235	-5.06406
H	-3.31883	0.29849	-6.48401
H	3.31883	-0.29849	-6.48401
H	5.33891	-0.46235	-5.06406
H	6.22603	-0.52598	4.24044
H	4.53927	-0.3904	6.04669

Table S6.7. Optimized coordinates for **6.2** using the MN12SX/LANL2DZ-PCM method.

N	-1.21271	0.02464	-1.24906
N	1.21271	-0.02464	-1.24906
N	1.3707	-0.08752	1.36286
N	-1.3707	0.08752	1.36286
C	1.17112	-0.08399	2.74874

C	2.46809	-0.19565	3.37288
C	3.43214	-0.27217	2.34128
C	2.73457	-0.20582	1.07638
C	-2.73457	0.20582	1.07638
C	-3.43214	0.27217	2.34128
C	-2.46809	0.19565	3.37288
C	-1.17112	0.08399	2.74874
C	-0.69441	0.02343	-2.5434
C	-1.82358	0.12611	-3.44312
C	-2.99293	0.21993	-2.63043
C	-2.57757	0.17026	-1.2398
C	2.57757	-0.17026	-1.2398
C	2.99293	-0.21993	-2.63043
C	1.82358	-0.12611	-3.44312
C	0.69441	-0.02343	-2.5434
C	2.84952	-0.23682	4.72472
C	4.20871	-0.35527	5.01314
C	5.17712	-0.43275	3.97655
C	4.80106	-0.39202	2.63434
C	-4.80106	0.39202	2.63434
C	-5.17712	0.43275	3.97655
C	-4.20871	0.35527	5.01314
C	-2.84952	0.23682	4.72472
C	-1.93668	0.15482	-4.84412
C	-3.2093	0.27523	-5.40432
C	-4.36608	0.36854	-4.59205
C	-4.268	0.34241	-3.20017
C	4.268	-0.34241	-3.20017
C	4.36608	-0.36854	-4.59205
C	1.93668	-0.15482	-4.84412
N	3.31003	-0.24558	-0.13078
N	0.	0.	3.36818
N	-3.31003	0.24558	-0.13078
H	2.1062	-0.17859	5.51219
H	5.53446	-0.45211	1.83775
H	-5.53446	0.45211	1.83775
H	-2.1062	0.17859	5.51219
H	-1.06569	0.08493	-5.48476
H	-5.14759	0.41524	-2.56994
H	5.14759	-0.41524	-2.56994
H	1.06569	-0.08493	-5.48476
C	3.2093	-0.27523	-5.40432
P	0.	0.	0.13107
O	0.	-1.77063	0.19548
H	-0.78045	-2.21214	-0.19464
O	0.	1.77063	0.19548

H	0.78045	2.21214	-0.19464
H	-6.22603	0.52598	4.24044
H	-4.53927	0.3904	6.04669
H	-5.33891	0.46235	-5.06406
H	-3.31883	0.29849	-6.48401
H	3.31883	-0.29849	-6.48401
H	5.33891	-0.46235	-5.06406
H	6.22603	-0.52598	4.24044
H	4.53927	-0.3904	6.04669

Chapter 7 Supporting Information:

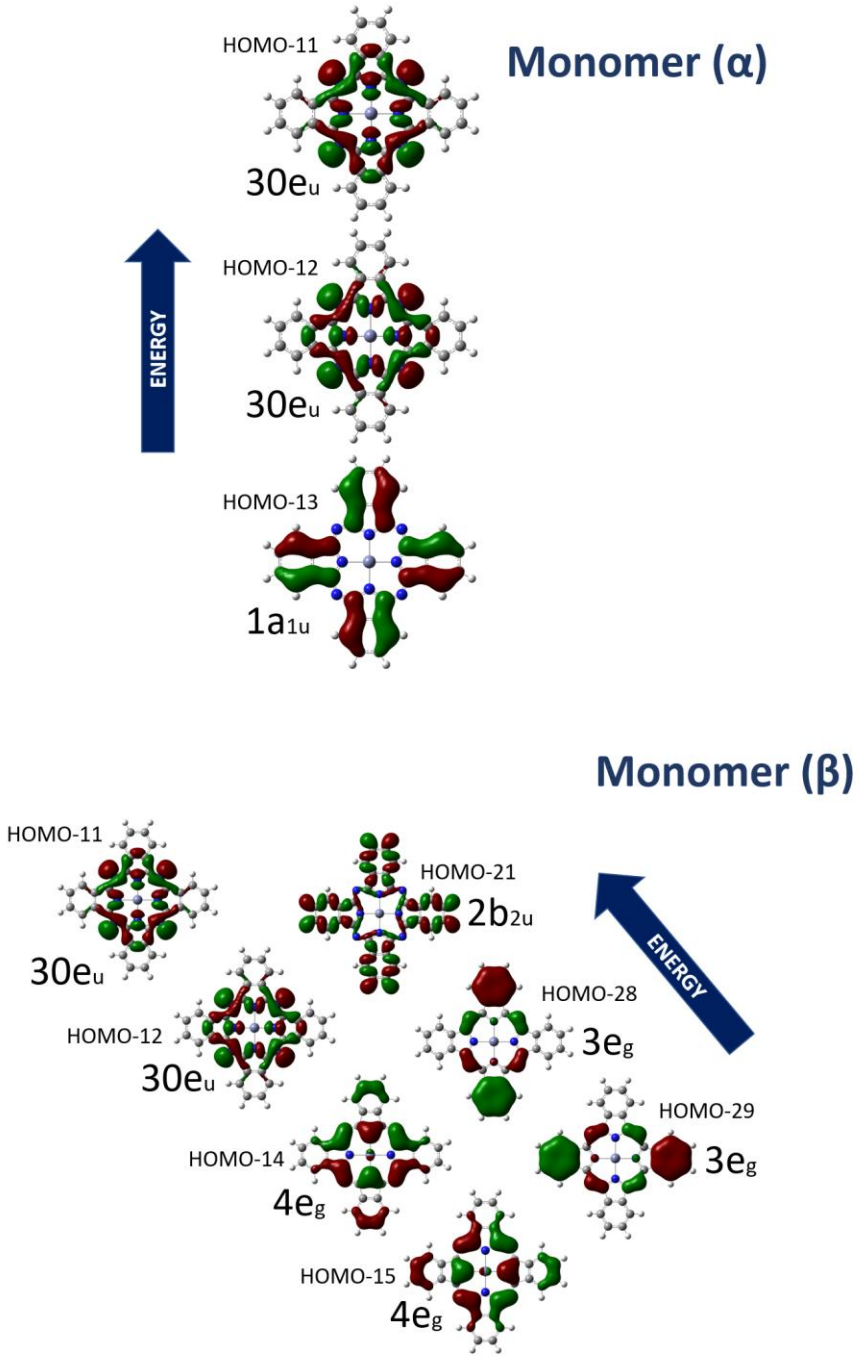
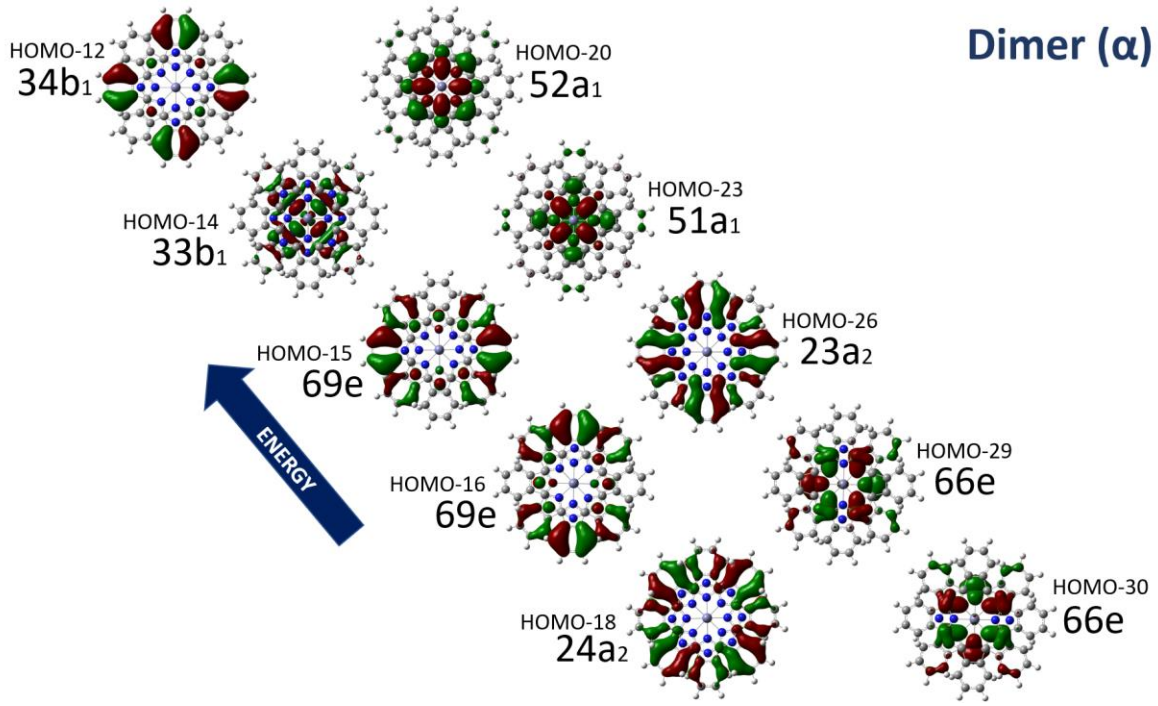
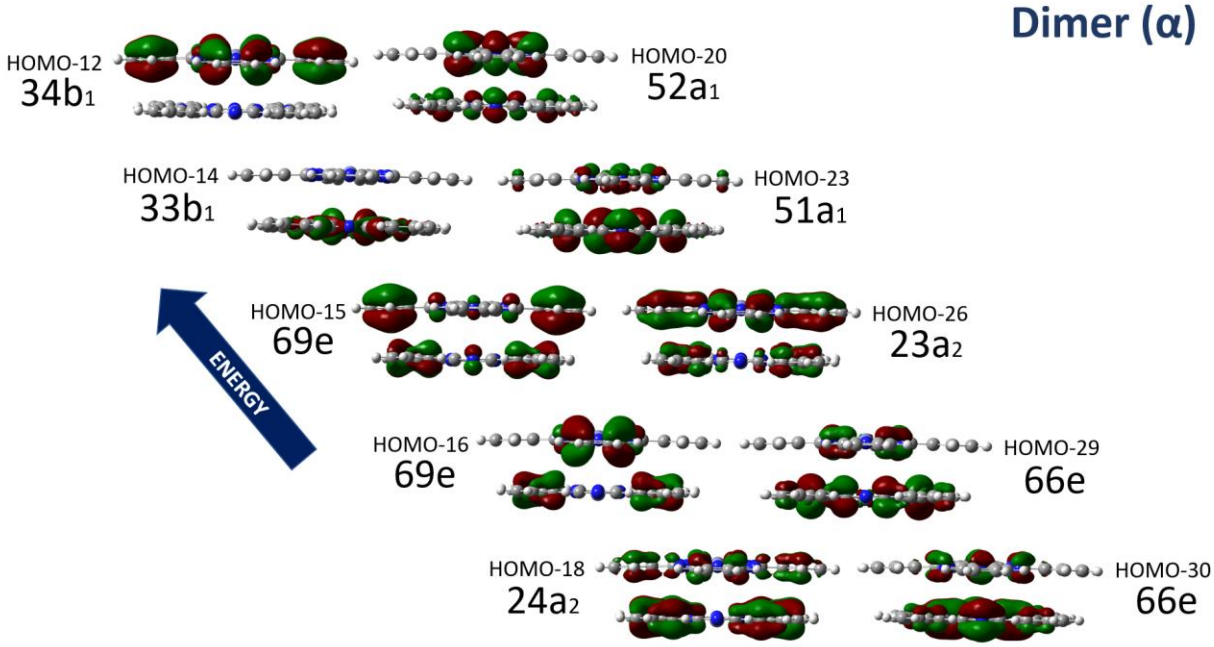


Figure S7.1. Additional DFT-predicted (M05 exchange-correlation functional) MOs that significantly contribute into degenerate excited states of [**7.1**]$^{+\bullet}$.


Dimer (α)
HOMO-12
34b1
HOMO-20
52a1
HOMO-14
33b1
HOMO-23
51a1
HOMO-15
69e
HOMO-26
23a2
ENERGY
HOMO-16
69e
HOMO-29
66e
HOMO-18
24a2
HOMO-30
66e


Dimer (α)
HOMO-12
34b1
HOMO-20
52a1
HOMO-14
33b1
HOMO-23
51a1
HOMO-15
69e
HOMO-26
23a2
ENERGY
HOMO-16
69e
HOMO-29
66e
HOMO-18
24a2
HOMO-30
66e

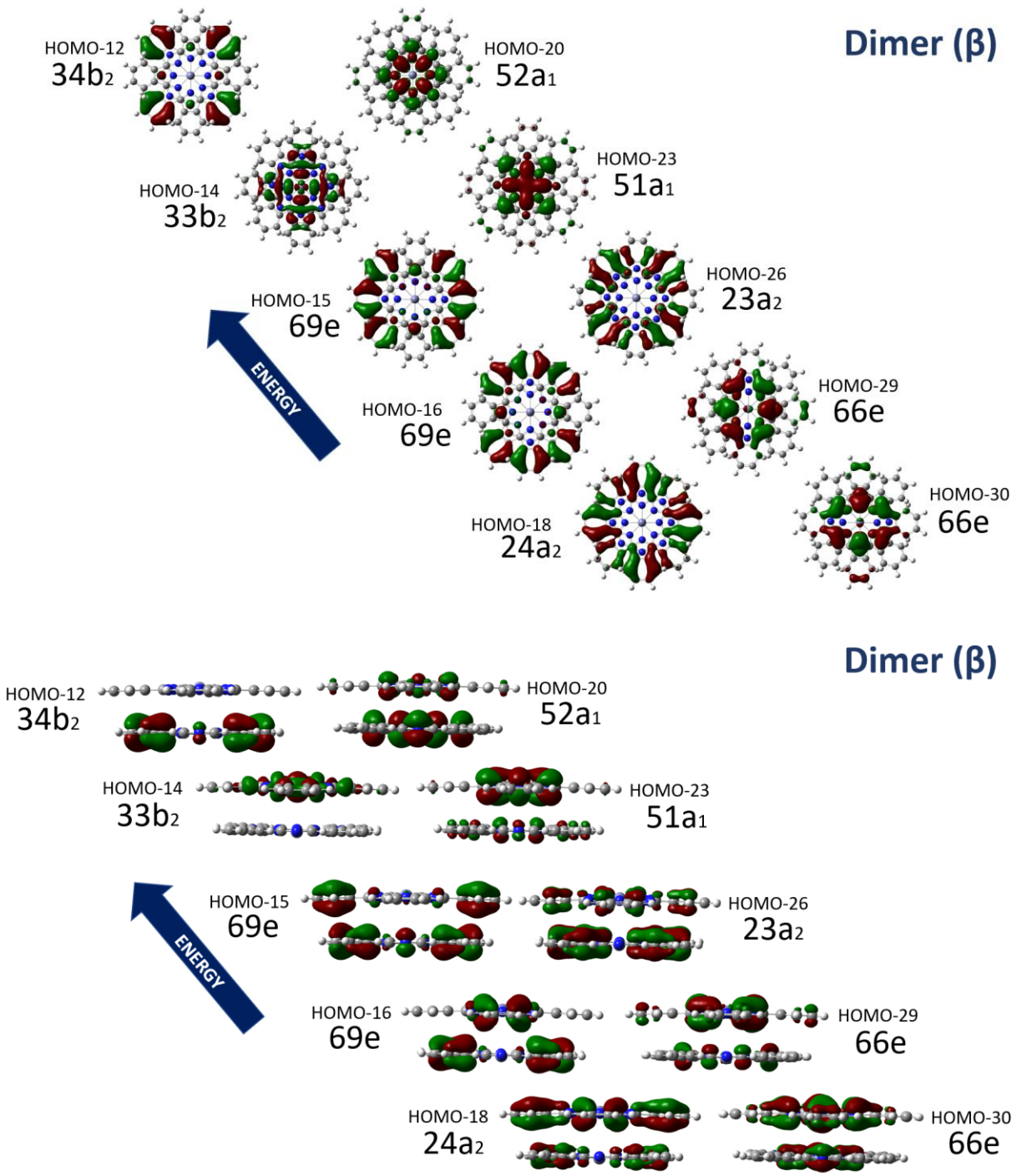


Figure S7.2. Additional DFT-predicted (M05 exchange-correlation functional) MOs that significantly contribute into degenerate excited states of [**7.1**]$_2^{2+}$.

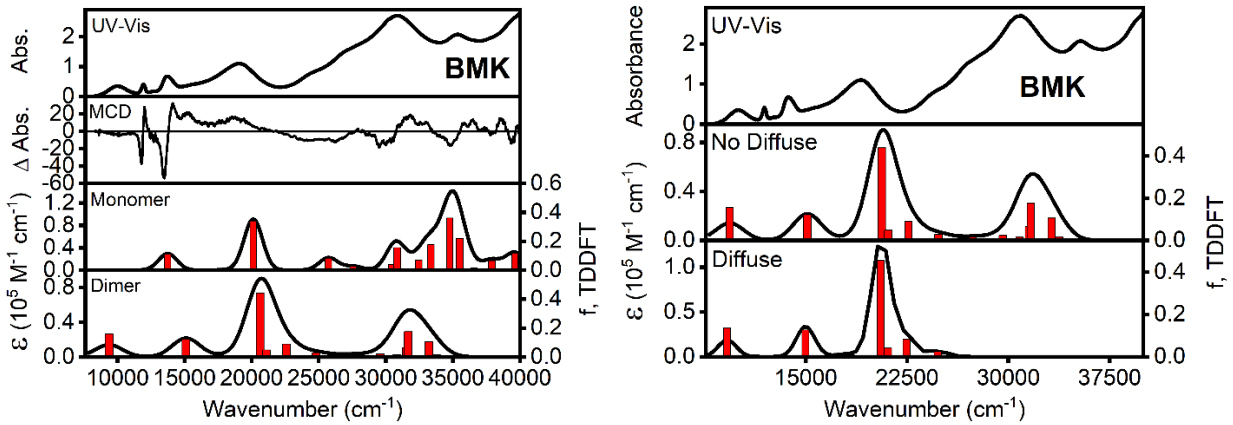


Figure S7.3. Comparison between experimental UV-vis and MCD and TDDFT-predicted (BMK exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer") and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

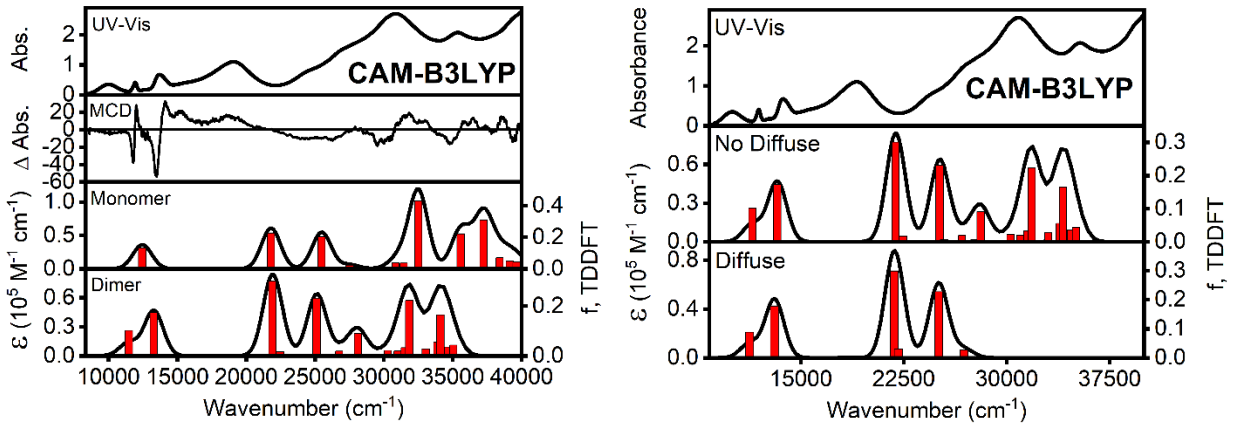


Figure S7.4. Comparison between experimental UV-vis and MCD and TDDFT-predicted (CAM-B3LYP exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer") and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

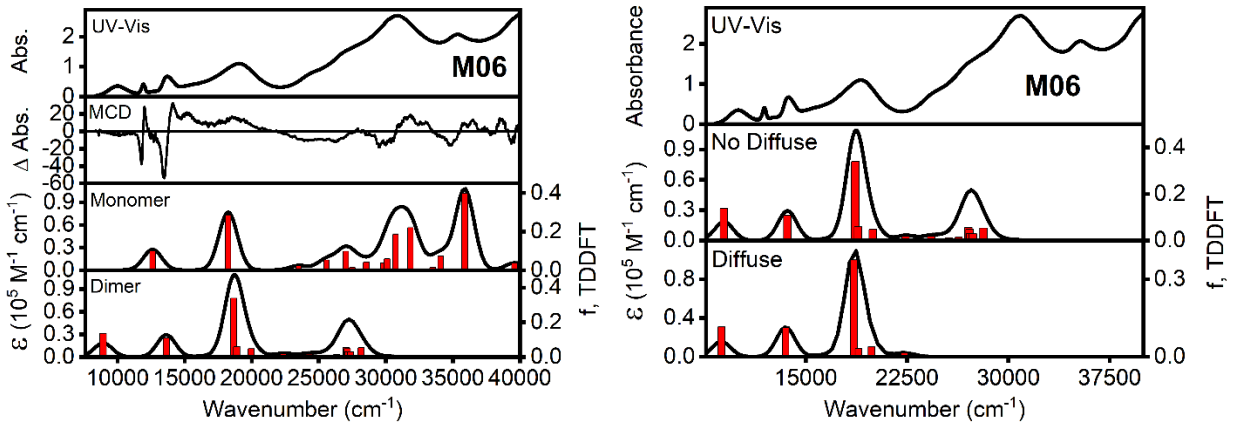


Figure S7.5. Comparison between experimental UV-vis and MCD and TDDFT-predicted (M06 exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer") and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

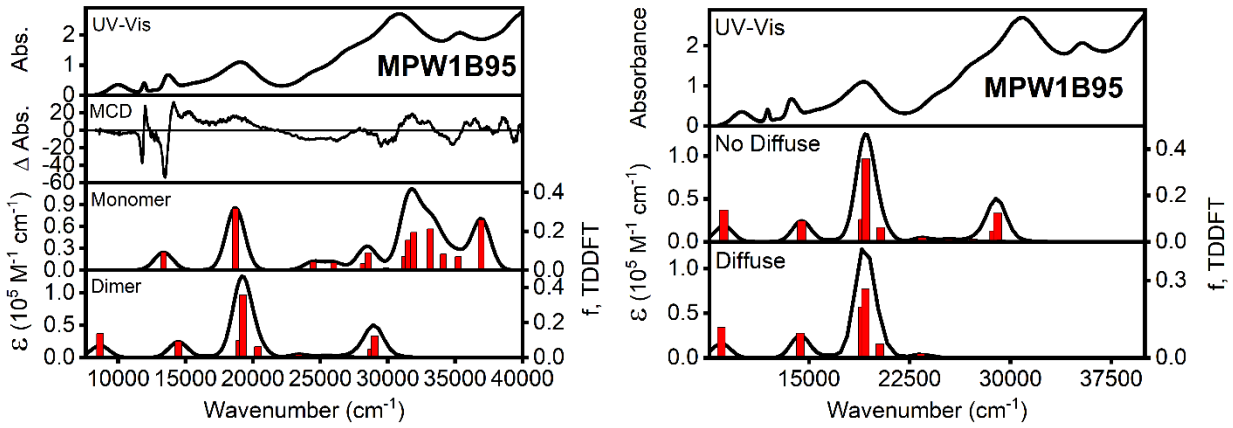


Figure S7.6. Comparison between experimental UV-vis and MCD and TDDFT-predicted (MPW1B95 exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer") and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

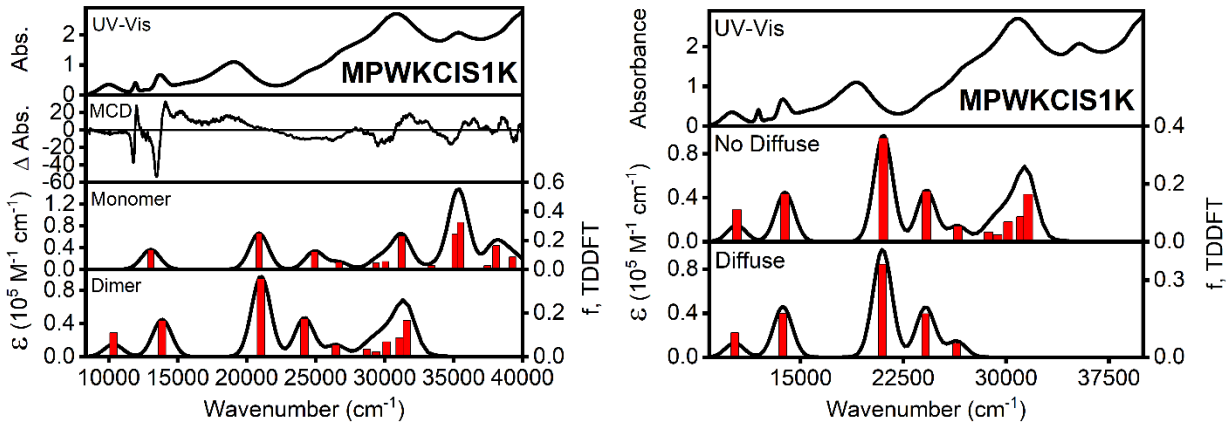


Figure S7.7. Comparison between experimental UV-vis and MCD and TDDFT-predicted (MPWKCIS1K exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer") and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

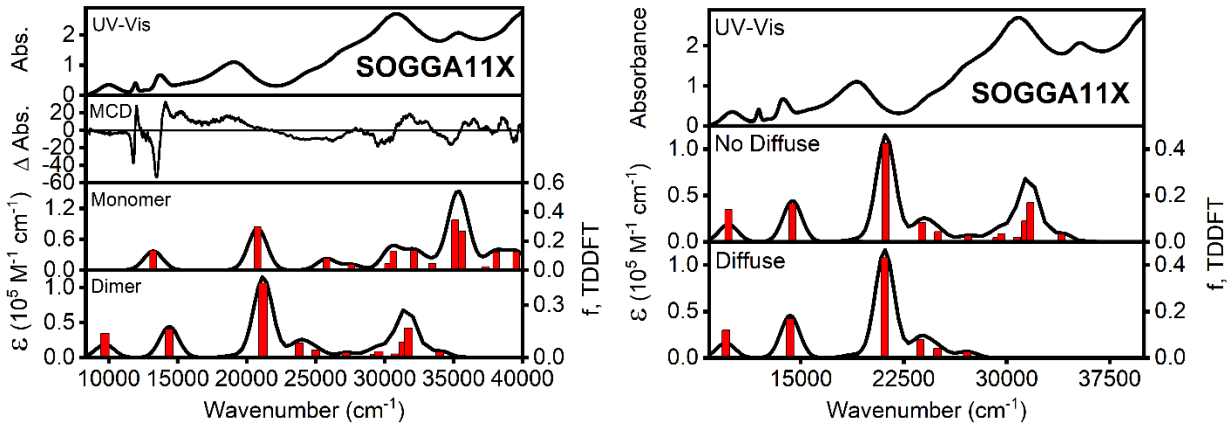


Figure S7.8. Comparison between experimental UV-vis and MCD and TDDFT-predicted (SOGGA11X exchange-correlation functional) UV-vis spectra of [**7.1**]$^{+\bullet}$ (labeled as "Monomer")

and [**7.1**]$_2^{2+}$ (labeled as "Dimer"). The right panel compares TDDFT-predicted UV-vis spectra of the [**7.1**]$_2^{2+}$ using 6-31G(d) (labeled as "No Diffuse") and 6-31+G(d) (labeled as "Diffuse") basis sets.

Table S7.1. Analysis of TDDFT-predicted selected excited state energies and oscillator strengths for monomeric [**7.1**]$^{+\bullet}$ (M05 exchange-correlation functional) as a function of the basis set.[a]

	6-31G(Zn)/6-31G(d) (C, N, H)			W+(Zn)/6-311G(d) (C, N, H)		
State	Energy/cm^{-1}	λ/nm	f [b]	Energy/cm^{-1}	λ/nm	f [b]
1E$_g$	12620	792	0.1159	12565	796	0.1198
2E$_g$	16238	616	0.0004	16234	616	0.0002
3E$_g$	18897	529	0.2345	18945	528	0.2301
4E$_g$	22604	442	0.0348	22551	443	0.0335
5E$_g$	25363	394	0.0735	25354	394	0.0757
6E$_g$	26525	377	0.0455	26402	379	0.0411
7E$_g$	27223	367	0.0348	27181	368	0.0366
8E$_g$	28008	357	0.1509	27876	359	0.1561
1A$_{2g}$	28435	352	0.0011	28518	351	0.0010
9E$_g$	29853	335	0.0033	29805	335	0.0027
10E$_g$	30577	327	0.0060	30499	328	0.0029
11E$_g$	31572	317	0.0314	31562	317	0.0232
12E$_g$	32040	312	0.3688	31975	313	0.3704

[a]E$_g$ states have x,y-polarization and A$_{2g}$ states have z-polarization; [b]f is the TDDFT-predicted oscillator strength.

Table S7.2. B3LYP optimized coordinates for the [**7.1**]$^{+\bullet}$ cationic-radical monomer.

Zn	0.	0.	0.
N	0.	1.99105	0.
N	1.99105	0.	0.
N	-1.99105	0.	0.
N	0.	-1.99105	0.
C	1.11974	2.78671	0.
C	-1.11974	2.78671	0.
C	2.78671	1.11974	0.
C	2.78671	-1.11974	0.
C	-2.78671	1.11974	0.

C	-2.78671	-1.11974	0.
C	1.11974	-2.78671	0.
C	-1.11974	-2.78671	0.
N	2.39112	2.39112	0.
C	0.70495	4.19282	0.
C	-0.70495	4.19282	0.
C	4.19282	0.70495	0.
N	2.39112	-2.39112	0.
C	4.19282	-0.70495	0.
N	-2.39112	2.39112	0.
C	-4.19282	0.70495	0.
C	-4.19282	-0.70495	0.
C	0.70495	-4.19282	0.
N	-2.39112	-2.39112	0.
C	-0.70495	-4.19282	0.
C	1.42852	5.38191	0.
C	-1.42852	5.38191	0.
C	5.38191	1.42852	0.
C	5.38191	-1.42852	0.
C	-5.38191	1.42852	0.
C	-5.38191	-1.42852	0.
C	1.42852	-5.38191	0.
C	-1.42852	-5.38191	0.
C	0.70176	6.58207	0.
C	-0.70176	6.58207	0.
C	6.58207	0.70176	0.
C	6.58207	-0.70176	0.
C	-6.58207	0.70176	0.
C	-6.58207	-0.70176	0.
C	0.70176	-6.58207	0.
C	-0.70176	-6.58207	0.
H	2.514	5.37763	0.
H	-2.514	5.37763	0.
H	5.37763	2.514	0.
H	5.37763	-2.514	0.
H	-5.37763	2.514	0.
H	-5.37763	-2.514	0.
H	2.514	-5.37763	0.
H	-2.514	-5.37763	0.
H	1.23333	7.52925	0.
H	-1.23333	7.52925	0.
H	7.52925	1.23333	0.
H	7.52925	-1.23333	0.
H	-7.52925	1.23333	0.

H	-7.52925	-1.23333	0.
H	1.23333	-7.52925	0.
H	-1.23333	-7.52925	0.

Table S7.3. B3LYP-D3 optimized coordinates for the [**7.1**]$_2^{2+}$ cationic radical dimer.

Zn,0,0.,0.,1.767995
N,0,0.,3.381708,1.647293
C,0,-1.177703,2.763069,1.652678
N,0,-1.407016,1.407016,1.654306
C,0,-2.46384,3.461087,1.64182
C,0,-2.791102,4.812321,1.622346
H,0,-2.018071,5.573953,1.62284
N,0,-3.381708,0.,1.647293
C,0,-4.154357,5.147051,1.603648
H,0,-4.448676,6.192549,1.596004
N,0,-1.407016,-1.407016,1.654306
C,0,-5.147051,4.154357,1.603648
H,0,-6.192549,4.448676,1.596004
N,0,0.,-3.381708,1.647293
C,0,-4.812321,2.791102,1.622346
H,0,-5.573953,2.018071,1.62284
N,0,1.407016,-1.407016,1.654306
C,0,-3.461087,2.46384,1.64182
N,0,3.381708,0.,1.647293
C,0,-2.763069,1.177703,1.652678
N,0,1.407016,1.407016,1.654306
C,0,-2.763069,-1.177703,1.652678
C,0,-3.461087,-2.46384,1.64182
C,0,-4.812321,-2.791102,1.622346
H,0,-5.573953,-2.018071,1.62284
C,0,-5.147051,-4.154357,1.603648
H,0,-6.192549,-4.448676,1.596004
C,0,-4.154357,-5.147051,1.603648
H,0,-4.448676,-6.192549,1.596004
C,0,-2.791102,-4.812321,1.622346
H,0,-2.018071,-5.573953,1.62284
C,0,-2.46384,-3.461087,1.64182
C,0,-1.177703,-2.763069,1.652678
C,0,1.177703,-2.763069,1.652678
C,0,2.46384,-3.461087,1.64182
C,0,2.791102,-4.812321,1.622346

H,0,2.018071,-5.573953,1.62284
C,0,5.147051,-4.154357,1.603648
H,0,6.192549,-4.448676,1.596004
C,0,4.154357,-5.147051,1.603648
H,0,4.448676,-6.192549,1.596004
C,0,4.812321,-2.791102,1.622346
H,0,5.573953,-2.018071,1.62284
C,0,3.461087,-2.46384,1.64182
C,0,2.763069,-1.177703,1.652678
C,0,2.763069,1.177703,1.652678
C,0,4.812321,2.791102,1.622346
H,0,5.573953,2.018071,1.62284
C,0,3.461087,2.46384,1.64182
C,0,5.147051,4.154357,1.603648
H,0,6.192549,4.448676,1.596004
C,0,4.154357,5.147051,1.603648
H,0,4.448676,6.192549,1.596004
C,0,2.791102,4.812321,1.622346
H,0,2.018071,5.573953,1.62284
C,0,2.46384,3.461087,1.64182
C,0,1.177703,2.763069,1.652678
Zn,0,0.,0.,-1.812433
N,0,-2.391114,-2.391114,-1.664568
N,0,0.,-1.989733,-1.693109
N,0,2.391114,-2.391114,-1.664568
N,0,1.989733,0.,-1.693109
N,0,2.391114,2.391114,-1.664568
N,0,0.,1.989733,-1.693109
N,0,-2.391114,2.391114,-1.664568
N,0,-1.989733,0.,-1.693109
C,0,-0.705069,-4.188819,-1.640595
C,0,-1.120893,-2.786242,-1.674195
C,0,-1.429066,-5.374888,-1.599739
H,0,-2.514218,-5.366161,-1.599438
C,0,0.701931,-6.575203,-1.559555
H,0,1.233297,-7.522178,-1.534936
C,0,-0.701931,-6.575203,-1.559555
H,0,-1.233297,-7.522178,-1.534936
C,0,1.429066,-5.374888,-1.599739
H,0,2.514218,-5.366161,-1.599438
C,0,0.705069,-4.188819,-1.640595
C,0,2.786242,-1.120893,-1.674195
C,0,1.120893,-2.786242,-1.674195
C,0,4.188819,-0.705069,-1.640595

C,0,5.374888,-1.429066,-1.599739
H,0,5.366161,-2.514218,-1.599438
C,0,6.575203,-0.701931,-1.559555
H,0,7.522178,-1.233297,-1.534936
C,0,5.374888,1.429066,-1.599739
H,0,5.366161,2.514218,-1.599438
C,0,6.575203,0.701931,-1.559555
H,0,7.522178,1.233297,-1.534936
C,0,4.188819,0.705069,-1.640595
C,0,1.120893,2.786242,-1.674195
C,0,2.786242,1.120893,-1.674195
C,0,0.705069,4.188819,-1.640595
C,0,1.429066,5.374888,-1.599739
H,0,2.514218,5.366161,-1.599438
C,0,-0.705069,4.188819,-1.640595
C,0,-1.120893,2.786242,-1.674195
C,0,-4.188819,0.705069,-1.640595
C,0,-2.786242,1.120893,-1.674195
C,0,-5.374888,1.429066,-1.599739
H,0,-5.366161,2.514218,-1.599438
C,0,-6.575203,0.701931,-1.559555
H,0,-7.522178,1.233297,-1.534936
C,0,-6.575203,-0.701931,-1.559555
H,0,-7.522178,-1.233297,-1.534936
C,0,-5.374888,-1.429066,-1.599739
H,0,-5.366161,-2.514218,-1.599438
C,0,-4.188819,-0.705069,-1.640595
C,0,-2.786242,-1.120893,-1.674195
C,0,-1.429066,5.374888,-1.599739
H,0,-2.514218,5.366161,-1.599438
C,0,-0.701931,6.575203,-1.559555
H,0,-1.233297,7.522178,-1.534936
C,0,0.701931,6.575203,-1.559555
H,0,1.233297,7.522178,-1.534936

Chapter 8 Supporting Information:

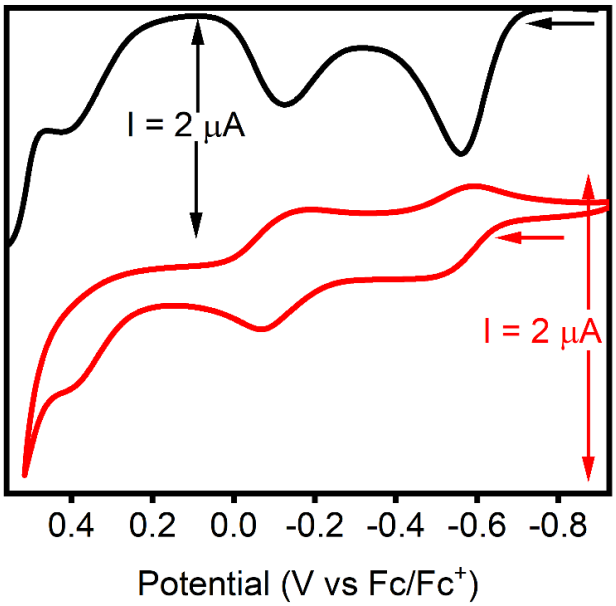


Figure S8.1. CV/DPV voltammogram for **8.2** in a DMF/0.1M TBAP system.

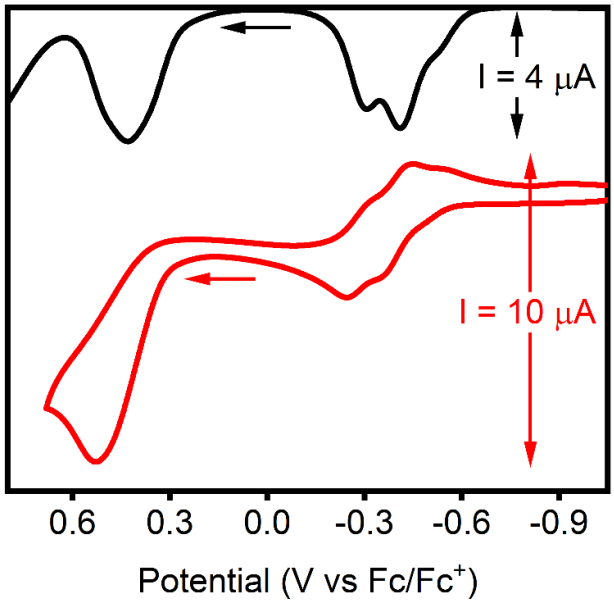


Figure S8.2. CV/DPV voltammogram for **8.3** in a DMF/0.1M TBAP system.

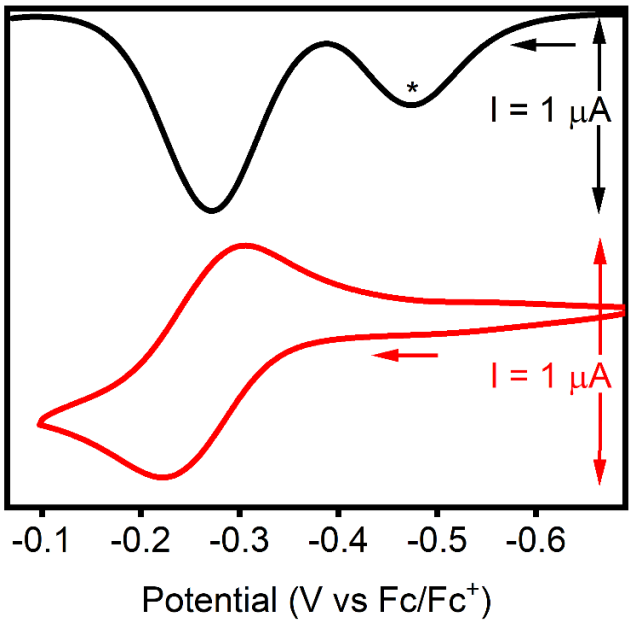


Figure S8.3. CV/DPV voltammogram for **8.4** in a DMF/0.1M KSCN system. Asterisk (*) in DPV curve is the reference decamethylferrocene compound.

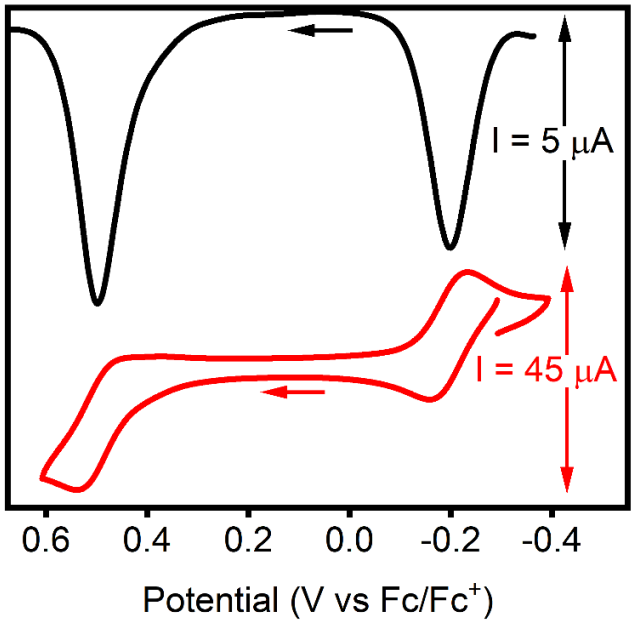


Figure S8.4. CV/DPV voltammogram for **8.5** in a DMF/0.1M TBAP system.

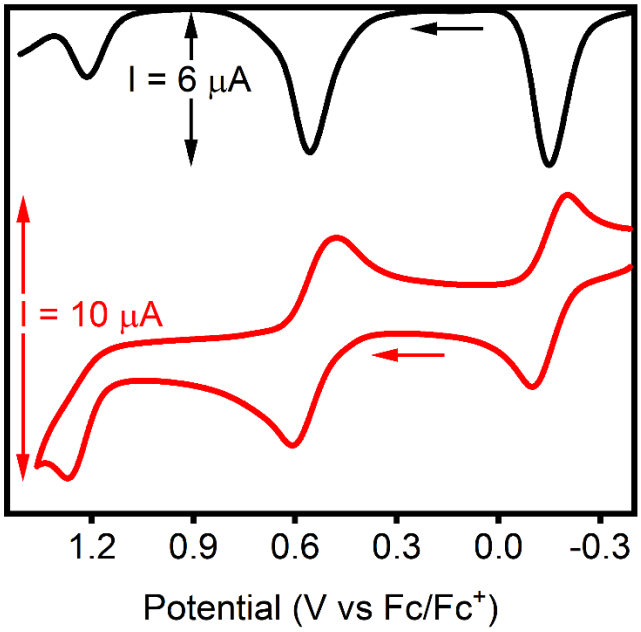


Figure S8.5. CV/DPV voltammogram for **8.6** in a DCM/0.1M TBAP system.

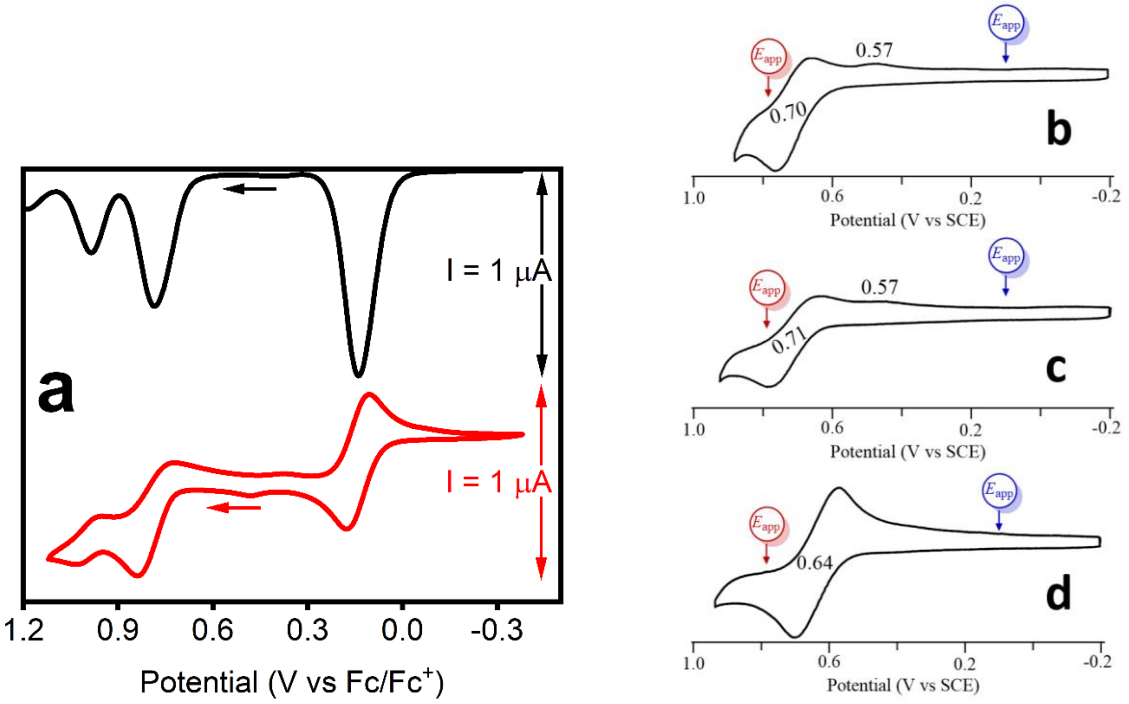


Figure S8.6. CV/DPV voltammogram for **8.8** in a DCM/0.1M TFAB (5% Py) system (a), and CV voltammograms for **8.8** in a DMF/0.05M TFAB (5% Py) system (b), pyridine/0.1M TBAP system (c), or DCM/0.1M TBAP (5% Py) system (d).

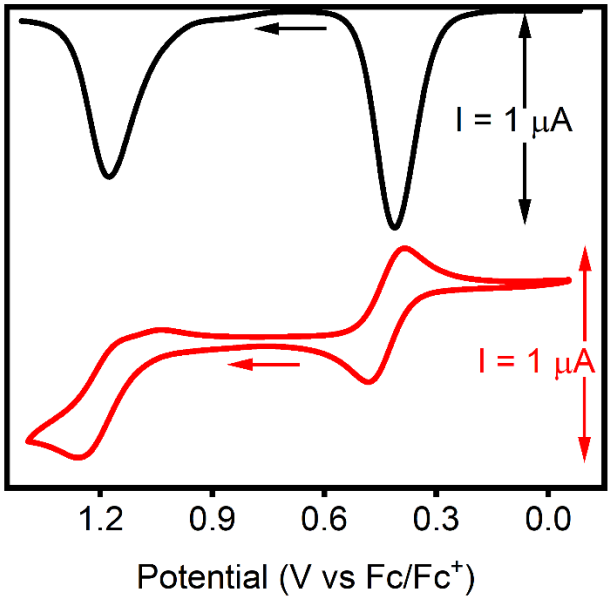


Figure S8.7. CV/DPV voltammogram for **8.9** in a DCM/0.1M TBAP system.

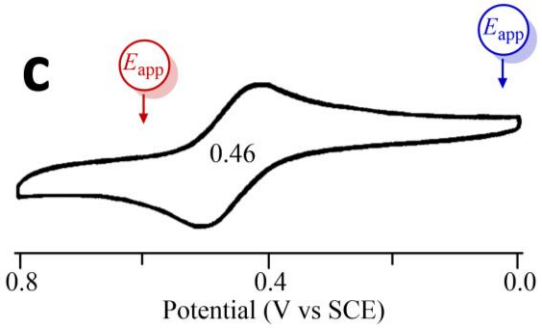


Figure S8.8. CV voltammogram for **8.12** in a DMSO/0.1M TBAP system (vs SCE).

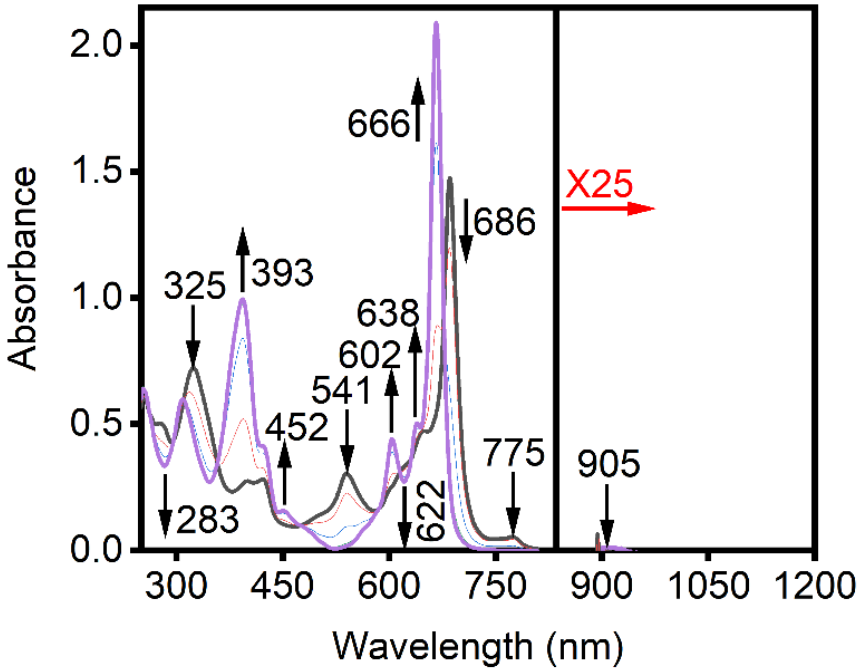


Figure S8.9. Spectroelectrochemical reduction of **8.5** in a DMSO/0.3M TBAP system.

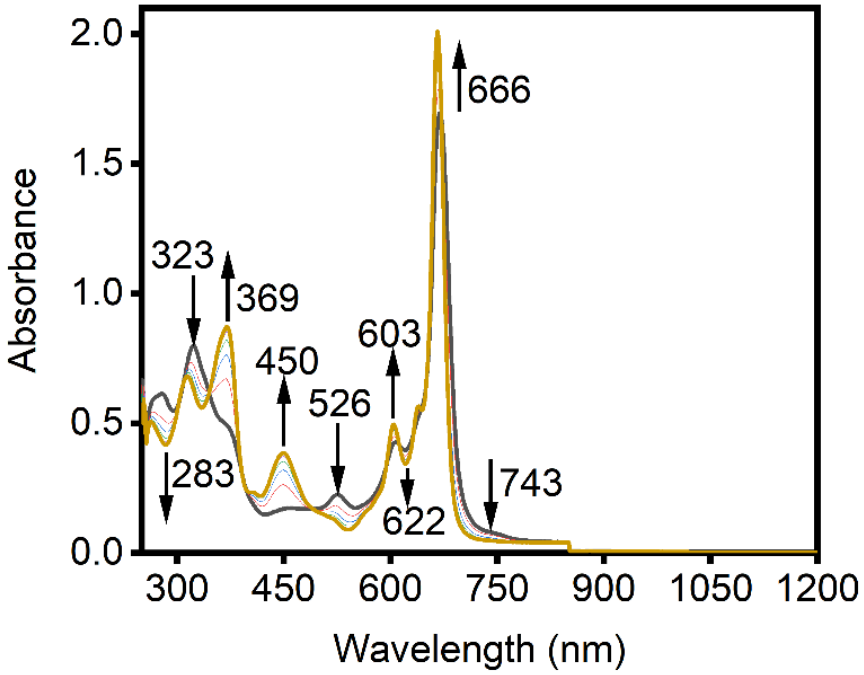


Figure S8.10. Spectroelectrochemical reduction of **8.3** in a DMF/0.3M TBAP system.

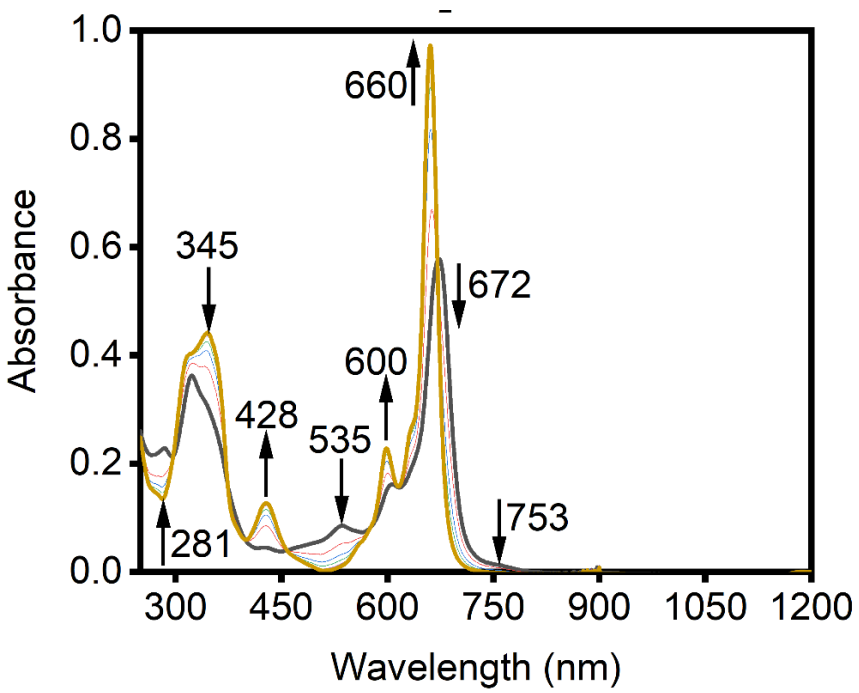


Figure S8.11. Spectroelectrochemical reduction of **8.6** in a DCM/0.3M TBAP system.

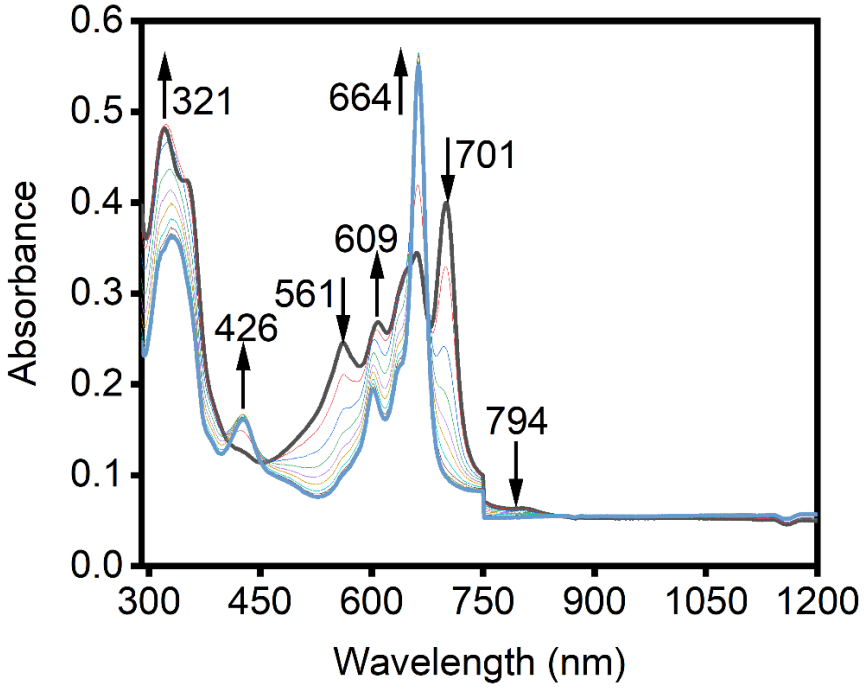


Figure S8.12. Spectroelectrochemical reduction of **8.7** in a DCM/0.3M TFAB system.

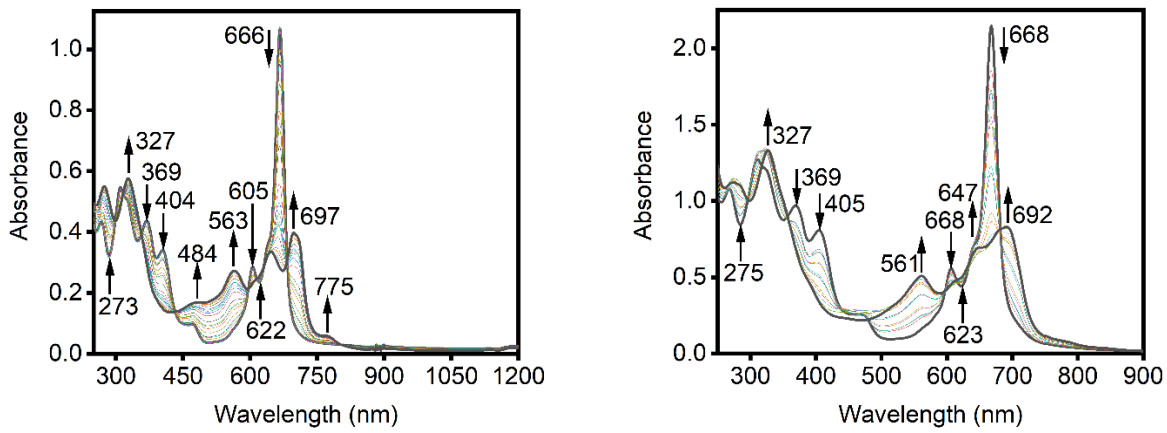


Figure S8.13. Spectroelectrochemical oxidation of **8.9** in a DCM/0.3M TBAP system (left) and chemical oxidation of **8.9** (right).

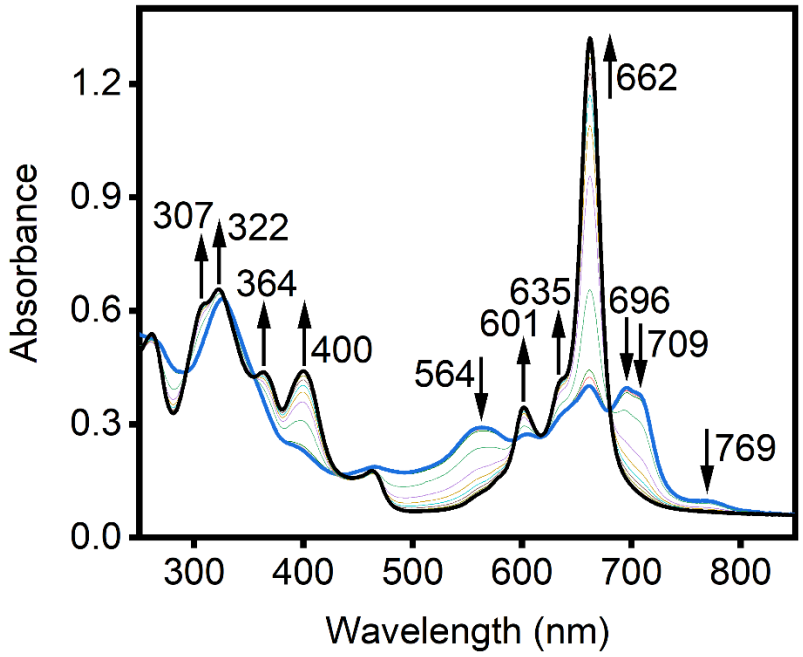


Figure S8.14. Spectroelectrochemical reduction of **8.10** in a DCM/0.3M TBAP system.

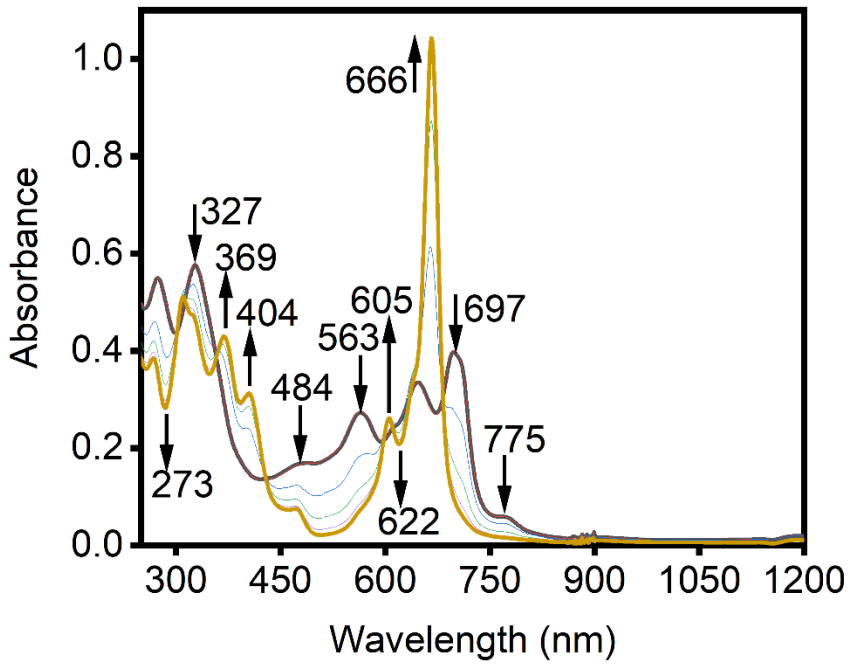


Figure S8.15. Spectroelectrochemical reduction of **8.9** in a DCM/0.3M TBAP system.

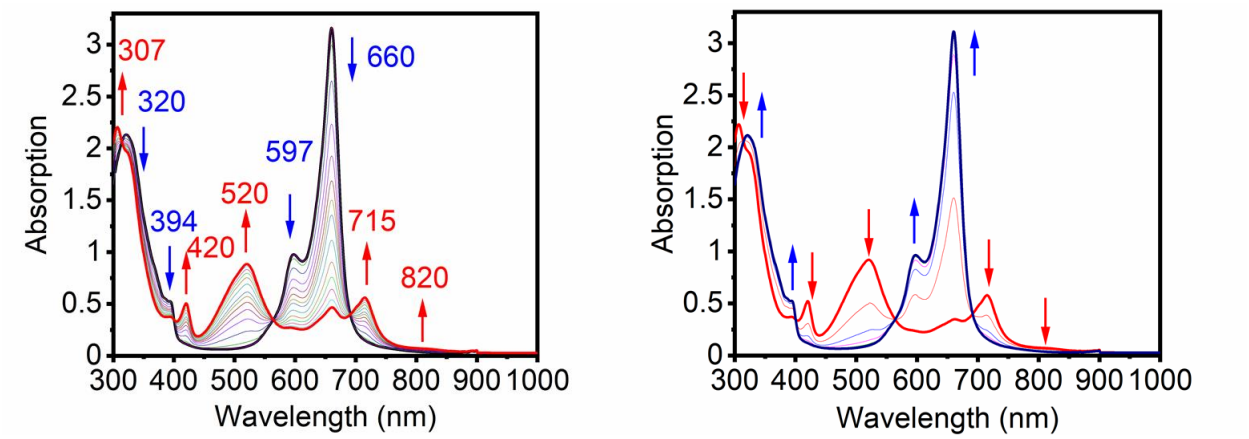


Figure S8.16. Spectroelectrochemical oxidation (left) and reduction (right) of **8.16** in a DCM/0.3M TBAP system.

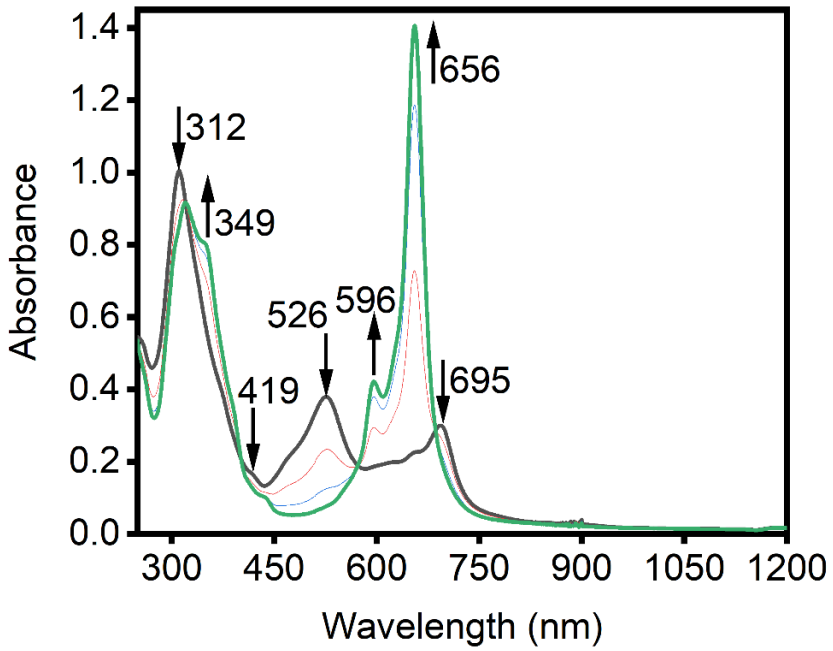


Figure S8.17. Spectroelectrochemical reduction of **8.9** in a DCM/0.3M TBAP system.

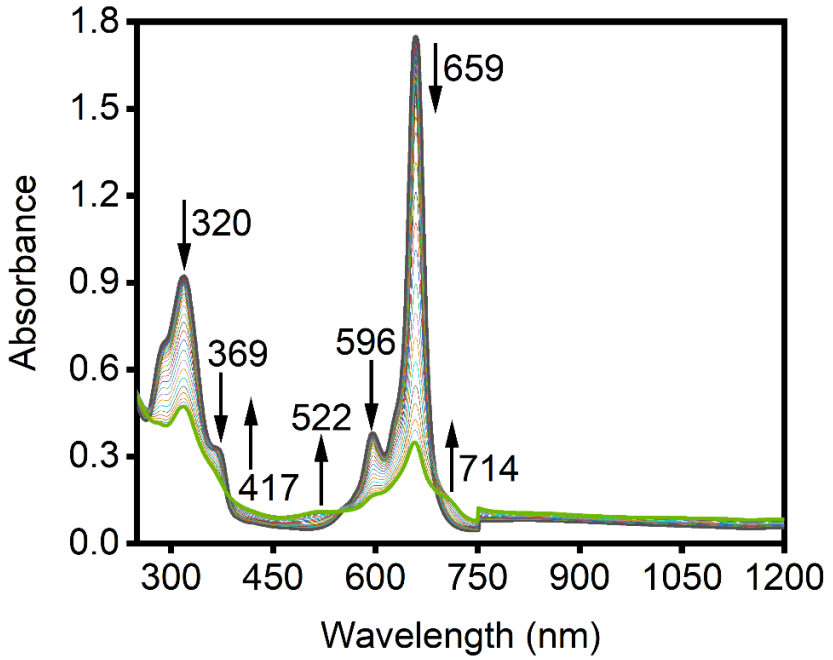


Figure S8.18. Spectroelectrochemical oxidation of **8.13** in a DCM/0.3M TBAP system.

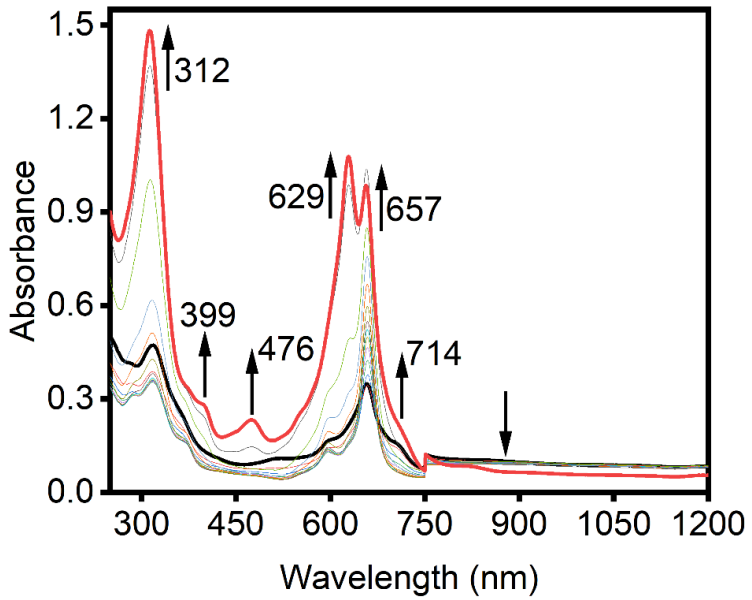


Figure S8.19. Spectroelectrochemical reduction of **8.13** in a DCM/0.3M TBAP system.

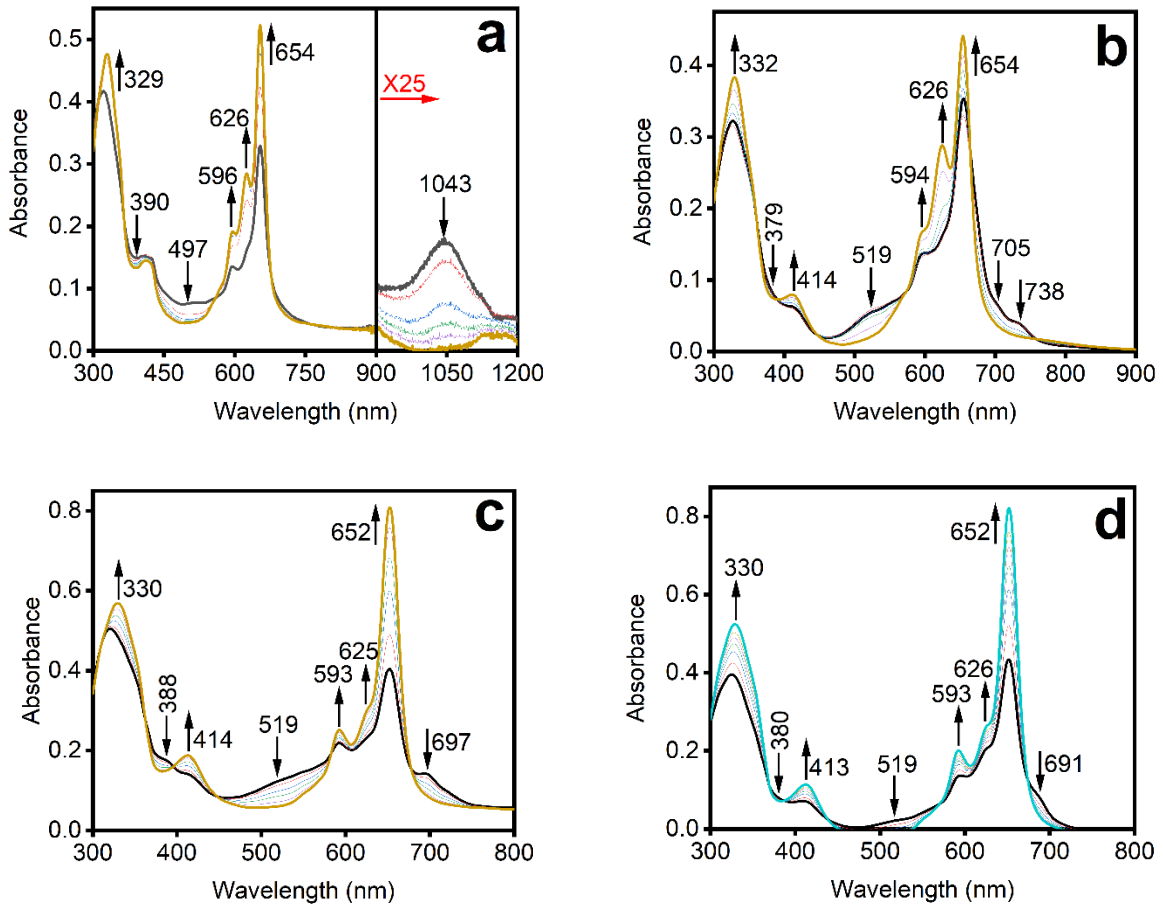


Figure S8.20. Spectroelectrochemical reduction of **8.8** in a Py/0.3M TFAB system (a), Py/0.3M TBAP system (b), DCM/0.3M TBAP (5% Py) system (c), and DMF/0.3M TBAP (5% Py) system (d).

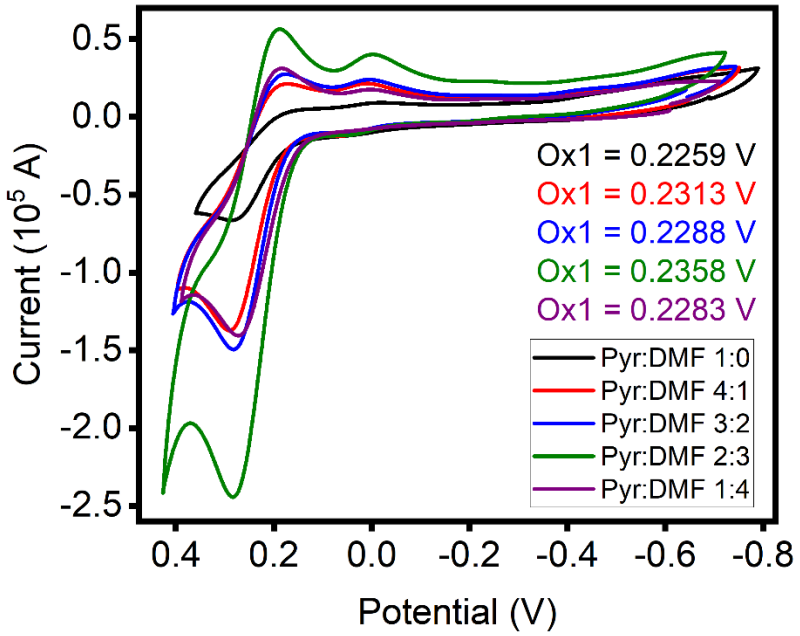


Figure S8.21. CV oxidation of $PcFe^{II}$ in various Py:DMF/0.1M TBAP systems.

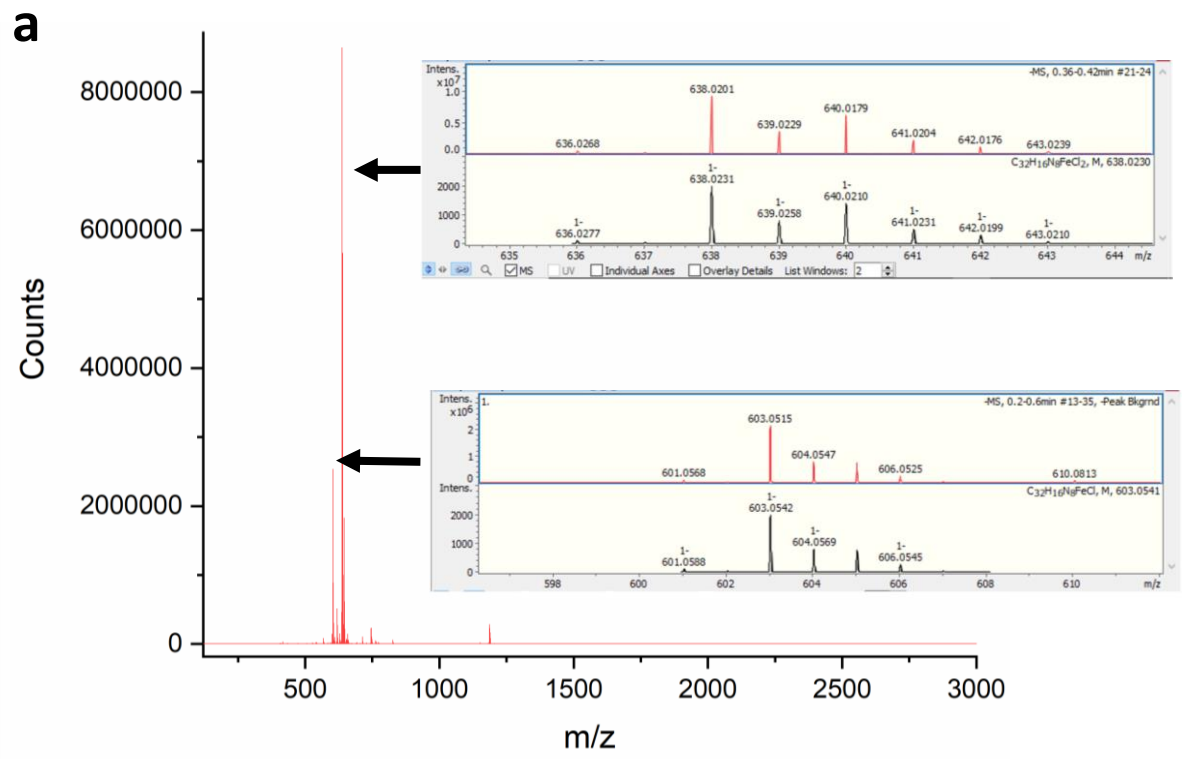


Figure S8.22. ESI HR-MS spectra of **8.14** in DMF/LiCl system. Experimental (red) and theoretical (black) isotope distributions for $[PcFeCl_2]^-$ and $[PcFeCl]^-$ ions are given as inserts.

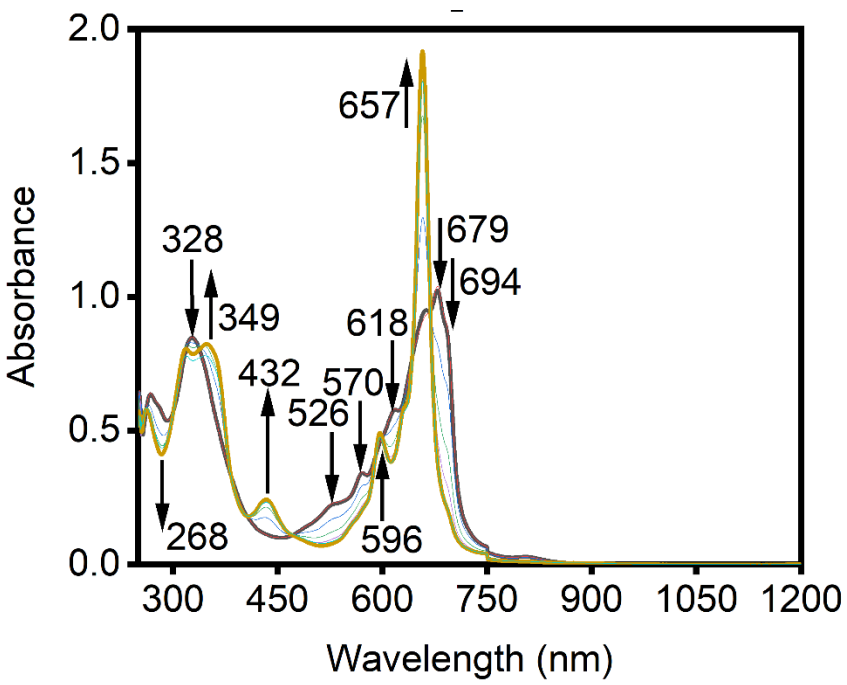


Figure S8.23. Spectroelectrochemical reduction of **8.4** in a DMF/0.3M TBAP system.

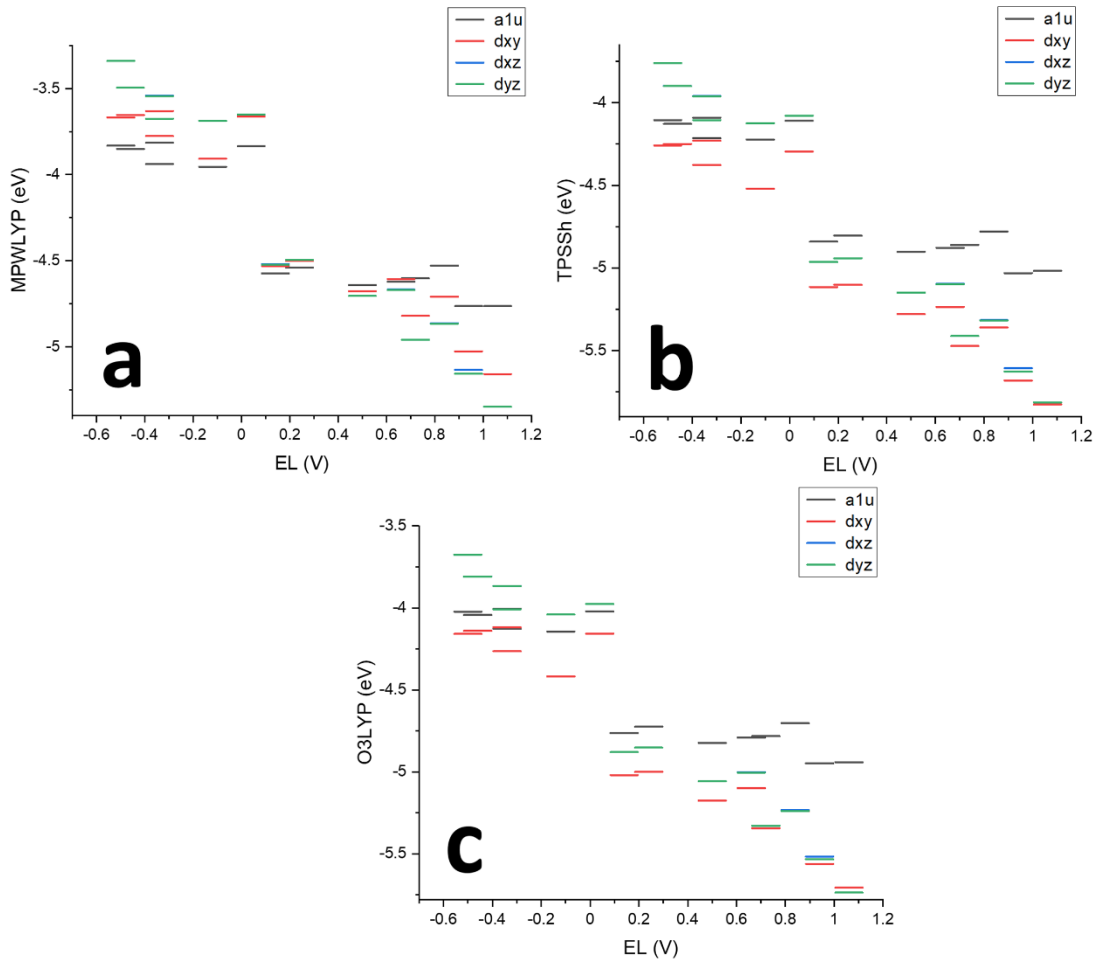


Figure S8.24. DFT-predicted absolute energies of the "a_{1u}" and d_{π} orbitals as a function of E_L parameter using the MPWLYP (a), TPSSh (b), and O3LYP (c) exchange correlation functionals.

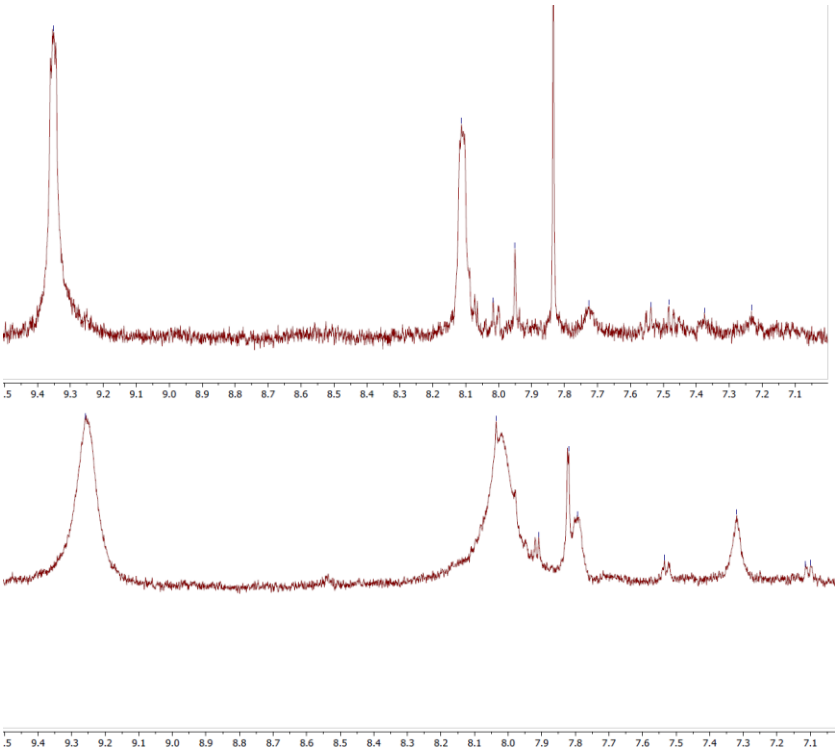


Figure S8.25. ^{1}H NMR spectra (aromatic region) of **8.12** in DMSO-d_6 before (top) and after (bottom) the addition of the KSCN.

<u>Full citation for Gaussian 16</u>:

Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

Table S8.1. Optimized coordinates for **8.18**.

N	0.04308	-1.96109	0.
N	0.04334	0.00022	1.96107
N	0.04305	1.96112	0.
C	0.04343	1.1208	-2.77236
C	0.04803	-0.70654	-4.17482
C	0.04072	-1.12051	-2.77253
C	0.04081	-2.77236	-1.12046
C	0.04666	-4.17478	-0.7067
C	0.04666	-4.17478	0.7067
C	0.04081	-2.77236	1.12046
C	0.04072	-1.12051	2.77253
C	0.04803	-0.70654	4.17482
C	0.0503	0.70689	4.17468
C	0.04343	1.1208	2.77236
C	0.04129	2.77262	1.12084
C	0.04658	4.17482	0.70674
C	0.04658	4.17482	-0.70674
C	0.04129	2.77262	-1.12084
C	0.0503	0.70689	-4.17468
N	0.04334	0.00022	-1.96107
N	0.0415	2.39796	-2.39797
N	0.03901	-2.39783	-2.39776
N	0.03901	-2.39783	2.39776
N	0.0415	2.39796	2.39797
Fe	-0.02263	0.00007	0.
C	0.05373	5.37408	1.43086
C	0.05919	6.5738	0.70624
H	0.0628	7.52801	1.24141
C	0.05919	6.5738	-0.70624
H	0.0628	7.52801	-1.24141
C	0.05373	5.37408	-1.43086
H	0.0533	5.37076	2.52429
H	0.0533	5.37076	-2.52429
C	0.05955	1.43105	-5.37386
C	0.06522	0.70646	-6.57366
H	0.07059	1.2417	-7.52782
C	0.0553	-1.43065	-5.37403
C	0.06309	-0.70596	-6.57375
H	0.06683	-1.2411	-7.52797
C	0.05349	-5.37392	-1.43084
C	0.05885	-6.57374	-0.70619
H	0.06227	-7.52793	-1.2414
C	0.05885	-6.57374	0.70619

H	0.06227	-7.52793	1.2414
C	0.05349	-5.37392	1.43084
H	0.05288	-5.37062	2.52427
H	0.05288	-5.37062	-2.52427
H	0.05311	-2.52408	-5.37076
H	0.06067	2.52448	-5.3705
C	0.0553	-1.43065	5.37403
C	0.06309	-0.70596	6.57375
H	0.06683	-1.2411	7.52797
C	0.06522	0.70646	6.57366
H	0.07059	1.2417	7.52782
C	0.05955	1.43105	5.37386
H	0.06067	2.52448	5.3705
H	0.05311	-2.52408	5.37076
H	2.44297	0.94204	0.
H	2.44418	-0.48366	-0.82388
H	2.44418	-0.48366	0.82388
N	2.06009	-0.00944	0.
C	-1.79249	0.00317	0.
O	-2.95312	0.00479	0.

Table S8.2. Optimized coordinates for **8.12**.

N	-0.00453	1.95316	0.00438
N	0.01323	-0.00665	1.95316
N	0.00453	-1.95316	-0.00438
C	-0.00961	-1.11256	-2.77193
C	0.0256	0.71692	-4.17002
C	0.01207	1.12784	-2.76824
C	-0.0042	2.77485	-1.11347
C	-0.00677	4.17434	-0.6947
C	-0.00362	4.16896	0.71856
C	-0.0001	2.76677	1.12837
C	0.00961	1.11256	2.77193
C	-0.00816	0.69609	4.17223
C	-0.0256	-0.71692	4.17002
C	-0.01207	-1.12784	2.76824
C	0.0042	-2.77485	1.11347
C	0.00677	-4.17434	0.6947
C	0.00362	-4.16896	-0.71856
C	0.0001	-2.76677	-1.12837
C	0.00816	-0.69609	-4.17223

N	-0.01323	0.00665	-1.95316
N	-0.01923	-2.38997	-2.40325
N	0.01209	2.4048	-2.39223
N	0.01923	2.38997	2.40325
N	-0.01209	-2.4048	2.39223
Fe	0.	0.	0.
C	0.00995	-5.3765	1.41489
C	0.01098	-6.57351	0.68619
H	0.01449	-7.52965	1.21796
C	0.0085	-6.56839	-0.72649
H	0.01069	-7.52073	-1.26503
C	0.00437	-5.36628	-1.44674
H	0.01234	-5.37702	2.50837
H	0.00386	-5.3591	-2.54014
C	0.01514	-1.41822	-5.37296
C	0.03873	-0.6919	-6.57134
H	0.04573	-1.22562	-7.52638
C	0.04945	1.44312	-5.36814
C	0.05567	0.72056	-6.56901
H	0.0752	1.25717	-7.52225
C	-0.00995	5.3765	-1.41489
C	-0.01098	6.57351	-0.68619
H	-0.01449	7.52965	-1.21796
C	-0.0085	6.56839	0.72649
H	-0.01069	7.52073	1.26503
C	-0.00437	5.36628	1.44674
H	-0.00386	5.3591	2.54014
H	-0.01234	5.37702	-2.50837
H	0.0642	2.53647	-5.36302
H	0.00477	-2.5116	-5.37145
C	-0.01514	1.41822	5.37296
C	-0.03873	0.6919	6.57134
H	-0.04573	1.22562	7.52638
C	-0.05567	-0.72056	6.56901
H	-0.0752	-1.25717	7.52225
C	-0.04945	-1.44312	5.36814
H	-0.0642	-2.53647	5.36302
H	-0.00477	2.5116	5.37145
C	-3.08777	-1.55797	0.12484
H	-2.76255	-2.06603	1.04079
H	-2.78274	-2.1275	-0.7628
H	-4.17406	-1.39732	0.13987
C	-3.04997	0.74802	-1.42358
H	-4.1375	0.75713	-1.27055

H	-2.77349	0.11522	-2.27599
H	-2.67381	1.76924	-1.55997
C	3.04997	-0.74802	1.42358
H	2.77349	-0.11522	2.27599
H	4.1375	-0.75713	1.27055
H	2.67381	-1.76924	1.55997
C	3.08777	1.55797	-0.12484
H	2.78274	2.1275	0.7628
H	2.76255	2.06603	-1.04079
H	4.17406	1.39732	-0.13987
O	-2.88071	0.88324	1.26477
O	2.88071	-0.88324	-1.26477
S	-2.29734	0.0921	0.10842
S	2.29734	-0.0921	-0.10842

Table S8.3. Optimized coordinates for **8.17**.

N	1.94755	0.19188	0.01354
N	-0.18516	1.95264	-0.00508
N	-1.94757	-0.1799	-0.01338
C	-0.85129	-2.85818	-0.01291
C	1.09979	-4.07991	0.03255
C	1.37731	-2.64487	0.03217
C	2.86229	-0.84579	0.04579
C	4.21889	-0.30163	0.07737
C	4.08494	1.1056	0.06919
C	2.65042	1.38368	0.03418
C	0.85159	2.86843	0.01114
C	0.30743	4.22531	-0.00555
C	-1.09935	4.09011	-0.03669
C	-1.37651	2.65473	-0.03512
C	-2.86317	0.85739	-0.04534
C	-4.2193	0.31256	-0.0754
C	-4.08432	-1.09458	-0.06641
C	-2.6495	-1.37209	-0.03295
C	-0.30701	-4.21485	0.00194
N	0.18581	-1.9428	0.00338
N	-2.15813	-2.60881	-0.03486
N	2.61312	-2.15287	0.0587
N	2.15862	2.61982	0.03475
N	-2.61305	2.16376	-0.06028
Fe	0.00029	0.00612	-0.00038
C	-5.48291	0.91733	-0.10921

C	-6.60858	0.082	-0.13392
H	-7.60927	0.52402	-0.16083
C	-6.4736	-1.32392	-0.12513
H	-7.37185	-1.94863	-0.14527
C	-5.20951	-1.92921	-0.09149
H	-5.58519	2.00618	-0.11666
H	-5.10181	-3.01752	-0.0849
C	-0.91189	-5.4788	-0.007
C	-0.07693	-6.60485	0.01594
H	-0.51905	-7.60584	0.00969
C	1.93399	-5.20534	0.0557
C	1.32864	-6.46985	0.04693
H	1.95302	-7.36836	0.06453
C	5.48214	-0.90725	0.11238
C	6.60833	-0.07263	0.13849
H	7.60872	-0.5153	0.1663
C	6.47427	1.33339	0.12987
H	7.37289	1.95753	0.15095
C	5.2106	1.93949	0.09524
H	5.10357	3.02786	0.08869
H	5.58366	-1.99618	0.11965
H	3.02205	-5.0976	0.0798
H	-2.00051	-5.58123	-0.03073
C	0.91217	5.48938	0.0025
C	0.07706	6.6153	-0.022
H	0.51904	7.61636	-0.01652
C	-1.32852	6.48007	-0.05355
H	-1.95304	7.37847	-0.07232
C	-1.93373	5.21547	-0.06136
H	-3.02177	5.10751	-0.08582
H	2.00076	5.59196	0.02674
P	0.08057	-0.02232	-2.25958
P	-0.08252	0.00562	2.25862
O	-1.3642	-0.28213	-3.00143
O	0.6577	1.37052	-2.91762
O	1.06798	-1.19822	-2.85058
O	-1.09429	1.1508	2.86901
O	-0.63642	-1.40754	2.89251
O	1.3588	0.26823	3.00692
C	-1.54616	-1.04012	-4.22596
H	-1.24548	-0.44537	-5.10216
H	-2.6181	-1.26375	-4.28586
H	-0.97312	-1.97716	-4.18883
C	0.19352	1.96444	-4.15674

H	0.55954	2.99824	-4.15193
H	-0.90472	1.96109	-4.20101
H	0.61014	1.43213	-5.02592
C	1.95126	-1.05018	-3.9913
H	2.68174	-1.86468	-3.91571
H	2.47049	-0.08221	-3.95789
H	1.39009	-1.1471	-4.93379
C	-0.85351	1.91917	4.07482
H	-1.54725	2.76766	4.03578
H	0.18157	2.28803	4.10063
H	-1.06338	1.31532	4.97144
C	-1.5032	-1.51639	4.05082
H	-1.92276	-2.52922	4.01966
H	-2.31458	-0.77707	3.99878
H	-0.92918	-1.38533	4.98112
C	1.76481	-0.33635	4.2624
H	2.84409	-0.16092	4.34605
H	1.56462	-1.417	4.2524
H	1.2494	0.13773	5.11195

Table S8.4. Optimized coordinates for **8.16**.

Fe	0.	0.	0.
N	-1.23076	0.93139	-1.21366
C	-2.13002	0.32912	-2.07219
N	-2.34245	-0.97343	-2.25039
C	-1.67222	-1.90911	-1.58041
N	-0.68669	-1.72839	-0.62936
C	-0.26832	-2.97156	-0.19582
N	0.66423	-3.24846	0.71382
C	1.34631	-2.30075	1.35441
C	2.37159	-2.60282	2.35357
C	2.86643	-1.35832	2.80661
C	3.87302	-1.29082	3.7785
C	4.37349	-2.49774	4.28734
C	3.87904	-3.74079	3.83495
C	2.87155	-3.80844	2.86217
C	-1.01952	-4.0111	-0.89997
C	-1.90558	-3.34051	-1.77412
C	-2.77973	-4.05353	-2.60467
C	-2.74725	-5.45384	-2.54066
C	-1.8623	-6.12362	-1.66745

C	-0.98726	-5.41007	-0.83612
C	-1.32539	0.02887	1.36543
N	-2.14539	0.04659	2.20982
C	-3.15754	0.06937	3.25141
C	-4.52028	-0.22652	2.59301
C	-3.14518	1.47206	3.89187
C	-2.79525	-1.01441	4.28687
H	4.25398	-0.32664	4.12673
H	5.16027	-2.47879	5.04757
H	4.2906	-4.66491	4.25197
H	2.48656	-4.76931	2.50941
H	-3.46404	-3.53216	-3.2799
H	-3.41773	-6.03959	-3.17679
H	-1.86135	-7.21752	-1.6411
H	-0.30061	-5.92558	-0.15885
H	-5.30705	-0.21456	3.36278
H	-4.7633	0.53304	1.83487
H	-4.5181	-1.21637	2.11239
H	-3.90382	1.51483	4.68823
H	-2.16244	1.69312	4.33468
H	-3.37845	2.24682	3.14615
H	-3.54814	-1.01664	5.08988
H	-1.80966	-0.81638	4.73429
H	-2.77776	-2.01187	3.82261
N	1.23076	-0.93139	1.21366
C	2.13002	-0.32912	2.07219
N	2.34245	0.97343	2.25039
C	1.67222	1.90911	1.58041
N	0.68669	1.72839	0.62936
C	0.26832	2.97156	0.19582
N	-0.66423	3.24846	-0.71382
C	-1.34631	2.30075	-1.35441
C	-2.37159	2.60282	-2.35357
C	-2.86643	1.35832	-2.80661
C	-3.87302	1.29082	-3.7785
C	-4.37349	2.49774	-4.28734
C	-3.87904	3.74079	-3.83495
C	-2.87155	3.80844	-2.86217
C	1.01952	4.0111	0.89997
C	1.90558	3.34051	1.77412
C	2.77973	4.05353	2.60467
C	2.74725	5.45384	2.54066
C	1.8623	6.12362	1.66745
C	0.98726	5.41007	0.83612

H	-4.25398	0.32664	-4.12673
H	-5.16027	2.47879	-5.04757
H	-4.2906	4.66491	-4.25197
H	-2.48656	4.76931	-2.50941
H	3.46404	3.53216	3.2799
H	3.41773	6.03959	3.17679
H	1.86135	7.21752	1.6411
H	0.30061	5.92558	0.15885
C	1.32539	-0.02887	-1.36543
N	2.14539	-0.04659	-2.20982
C	3.15754	-0.06937	-3.25141
C	4.52028	0.22652	-2.59301
C	3.14518	-1.47206	-3.89187
C	2.79525	1.01441	-4.28687
H	5.30705	0.21456	-3.36278
H	4.7633	-0.53304	-1.83487
H	4.5181	1.21637	-2.11239
H	3.90382	-1.51483	-4.68823
H	2.16244	-1.69312	-4.33468
H	3.37845	-2.24682	-3.14615
H	3.54814	1.01664	-5.08988
H	1.80966	0.81638	-4.73429
H	2.77776	2.01187	-3.82261

Table S8.5. Optimized coordinates for **8.10**.

N	0.	1.95158	0.00094
N	0.	0.	-1.95093
N	0.	-1.95158	0.00094
C	0.01741	-1.11928	2.77032
C	-0.01254	0.70684	4.17232
C	-0.01741	1.11928	2.77032
C	-0.01542	2.77011	1.12043
C	-0.03373	4.17202	0.70759
C	-0.03936	4.17169	-0.70607
C	-0.02271	2.76975	-1.11871
C	-0.02418	1.11949	-2.76903
C	-0.01771	0.70678	-4.17099
C	0.01771	-0.70678	-4.17099
C	0.02418	-1.11949	-2.76903
C	0.02271	-2.76975	-1.11871
C	0.03936	-4.17169	-0.70607

C	0.03373	-4.17202	0.70759
C	0.01542	-2.77011	1.12043
C	0.01254	-0.70684	4.17232
N	0.	0.	1.9524
N	0.02745	-2.3977	2.39853
N	-0.02745	2.3977	2.39853
N	-0.0397	2.39761	-2.39681
N	0.0397	-2.39761	-2.39681
Fe	0.	0.	0.00134
C	0.05995	-5.37189	-1.42941
C	0.074	-6.57263	-0.70582
H	0.08974	-7.52655	-1.24171
C	0.06861	-6.57293	0.70662
H	0.08033	-7.52707	1.24222
C	0.04908	-5.3725	1.43059
H	0.06498	-5.36854	-2.52309
H	0.04581	-5.36967	2.52428
C	0.02497	-1.42986	5.37291
C	0.01241	-0.70615	6.57352
H	0.02189	-1.24177	7.52767
C	-0.02497	1.42986	5.37291
C	-0.01241	0.70615	6.57352
H	-0.02189	1.24177	7.52767
C	-0.04908	5.3725	1.43059
C	-0.06861	6.57293	0.70662
H	-0.08033	7.52707	1.24222
C	-0.074	6.57263	-0.70582
H	-0.08974	7.52655	-1.24171
C	-0.05995	5.37189	-1.42941
H	-0.06498	5.36854	-2.52309
H	-0.04581	5.36967	2.52428
H	-0.04398	2.52338	5.36987
H	0.04398	-2.52338	5.36987
C	-0.03489	1.42966	-5.37159
C	-0.01732	0.70604	-6.57222
H	-0.03046	1.24159	-7.52636
C	0.01732	-0.70604	-6.57222
H	0.03046	-1.24159	-7.52636
C	0.03489	-1.42966	-5.37159
H	0.06148	-2.52302	-5.36852
H	-0.06148	2.52302	-5.36852
P	2.3404	0.02891	-0.00127
P	-2.3404	-0.02891	-0.00127
C	3.18407	-1.61046	-0.13382

H	2.88961	-2.10935	-1.06854
H	2.89293	-2.25345	0.70948
H	4.27823	-1.48481	-0.12545
C	3.13531	0.76233	1.49683
H	4.23162	0.76138	1.39225
H	2.86247	0.18107	2.38926
H	2.79142	1.79741	1.63706
C	-3.12516	-0.98701	-1.3724
H	-2.84537	-0.55238	-2.34272
H	-4.22229	-0.9706	-1.27794
H	-2.78141	-2.0311	-1.34629
C	-3.13531	-0.76233	1.49683
H	-4.23162	-0.76138	1.39225
H	-2.86247	-0.18107	2.38926
H	-2.79142	-1.79741	1.63706
C	-3.18407	1.61046	-0.13382
H	-2.88961	2.10935	-1.06854
H	-2.89293	2.25345	0.70948
H	-4.27823	1.48481	-0.12545
C	3.12516	0.98701	-1.3724
H	2.84537	0.55238	-2.34272
H	4.22229	0.9706	-1.27794
H	2.78141	2.0311	-1.34629

Table S8.6. Optimized coordinates for **8.8**.

N	1.37734	1.37734	0.
N	-1.37734	1.37734	0.
N	-1.37734	-1.37734	0.
C	1.16675	-2.745	0.08392
C	3.44552	-2.44952	-0.05912
C	2.745	-1.16675	-0.08392
C	2.745	1.16675	-0.08392
C	3.44552	2.44952	-0.05912
C	2.44952	3.44552	0.05912
C	1.16675	2.745	0.08392
C	-1.16675	2.745	0.08392
C	-2.44952	3.44552	0.05912
C	-3.44552	2.44952	-0.05912
C	-2.745	1.16675	-0.08392
C	-2.745	-1.16675	-0.08392
C	-3.44552	-2.44952	-0.05912
C	-2.44952	-3.44552	0.05912

C	-1.16675	-2.745	0.08392
C	2.44952	-3.44552	0.05912
N	1.37734	-1.37734	0.
N	0.	-3.38461	0.14164
N	3.38461	0.	-0.14164
N	0.	3.38461	0.14164
N	-3.38461	0.	-0.14164
Fe	0.	0.	0.
N	0.	0.	-2.03411
C	0.	-1.15935	-2.74006
C	0.	1.15935	-2.74006
C	0.	-1.19942	-4.13503
H	0.	-2.08103	-2.15973
C	0.	1.19942	-4.13503
H	0.	2.08103	-2.15973
C	0.	0.	-4.85472
H	0.	-2.16833	-4.63962
H	0.	2.16833	-4.63962
H	0.	0.	-5.94778
N	0.	0.	2.03411
C	1.15935	0.	2.74006
C	-1.15935	0.	2.74006
C	1.19942	0.	4.13503
H	2.08103	0.	2.15973
C	-1.19942	0.	4.13503
H	-2.08103	0.	2.15973
C	0.	0.	4.85472
H	2.16833	0.	4.63962
H	-2.16833	0.	4.63962
H	0.	0.	5.94778
C	-4.80397	-2.78844	-0.11805
C	-5.14269	-4.14736	-0.05862
H	-6.19479	-4.4446	-0.10348
C	-4.14736	-5.14269	0.05862
H	-4.4446	-6.19479	0.10348
C	-2.78844	-4.80397	0.11805
H	-5.57261	-2.01585	-0.20905
H	-2.01585	-5.57261	0.20905
C	2.78844	-4.80397	0.11805
C	4.14736	-5.14269	0.05862
H	4.4446	-6.19479	0.10348
C	4.80397	-2.78844	-0.11805
C	5.14269	-4.14736	-0.05862
H	6.19479	-4.4446	-0.10348

C	4.80397	2.78844	-0.11805
C	5.14269	4.14736	-0.05862
H	6.19479	4.4446	-0.10348
C	4.14736	5.14269	0.05862
H	4.4446	6.19479	0.10348
C	2.78844	4.80397	0.11805
H	2.01585	5.57261	0.20905
H	5.57261	2.01585	-0.20905
H	5.57261	-2.01585	-0.20905
H	2.01585	-5.57261	0.20905
C	-2.78844	4.80397	0.11805
C	-4.14736	5.14269	0.05862
H	-4.4446	6.19479	0.10348
C	-5.14269	4.14736	-0.05862
H	-6.19479	4.4446	-0.10348
C	-4.80397	2.78844	-0.11805
H	-5.57261	2.01585	-0.20905
H	-2.01585	5.57261	0.20905

Table S8.7. Optimized coordinates for **8.6**.

C	-2.78056	-1.0764	0.03778
C	4.18169	0.64467	0.01907
C	4.16079	-0.76738	-0.03673
C	2.75186	-1.15794	-0.04265
C	5.39271	1.34936	0.04231
H	5.40591	2.44211	0.08534
C	6.58282	0.60902	0.00963
H	7.54472	1.13056	0.02732
C	6.56193	-0.80221	-0.04563
H	7.50799	-1.35165	-0.07071
C	5.35039	-1.50736	-0.06897
H	5.33105	-2.6001	-0.11164
C	-1.15551	-2.74974	0.0519
C	-0.76477	-4.15848	0.04768
C	0.64741	-4.17903	-0.00891
C	1.079	-2.78241	-0.02904
C	-1.50441	-5.34835	0.08244
H	-2.59712	-5.32931	0.1265
C	-0.79902	-6.5597	0.06026
H	-1.34815	-7.50587	0.08779
C	0.61225	-6.58027	0.00361

H	1.134	-7.54207	-0.01302
C	1.35227	-5.39011	-0.03137
H	2.44498	-5.4031	-0.07532
C	-0.76506	0.76664	2.80308
H	-1.50194	1.49243	2.47521
C	0.78973	-0.76523	2.85763
H	1.51087	-1.47832	2.4711
C	0.48878	-0.46403	4.16637
H	0.87503	-0.84172	5.10785
Fe	0.00208	0.00007	0.00023
N	-1.94561	0.02891	-0.00253
N	-0.02615	-1.94776	0.0094
N	-2.42874	-2.36044	0.07175
N	2.3629	-2.43101	-0.06352
N	0.00242	0.00766	2.01499
N	-0.4949	0.50514	4.10905
H	-0.94429	0.95139	4.90464
C	2.7849	1.07641	0.03629
C	-4.17697	-0.64466	0.01903
C	-4.15609	0.76757	-0.04025
C	-2.74749	1.15821	-0.04767
C	-5.38832	-1.34918	0.04472
H	-5.40157	-2.4418	0.0912
C	-6.5783	-0.60899	0.01033
H	-7.54022	-1.13044	0.0296
C	-6.55745	0.80227	-0.0489
H	-7.50356	1.35157	-0.07518
C	-5.34607	1.50734	-0.07441
H	-5.32685	2.59995	-0.12054
C	1.16055	2.74943	0.03816
C	0.77019	4.15829	0.02889
C	-0.6419	4.17955	-0.02923
C	-1.07384	2.78293	-0.04476
C	1.51033	5.34795	0.06023
H	2.60298	5.32843	0.10472
C	0.80552	6.55954	0.03351
H	1.35521	7.5055	0.05708
C	-0.60569	6.58076	-0.02405
H	-1.1269	7.54278	-0.04443
C	-1.34625	5.39082	-0.05577
H	-2.43893	5.40425	-0.10109
N	1.95016	-0.02874	-0.00066
N	0.03139	1.94791	-0.00585
N	2.43365	2.36027	0.0655

N	-2.35789	2.43148	-0.07369
C	-0.75793	-0.77122	-2.80343
H	-1.49141	-1.50071	-2.47622
C	0.78839	0.76926	-2.85673
H	1.5058	1.48584	-2.4696
C	0.49059	0.46599	-4.16576
H	0.87559	0.84568	-5.10694
N	0.00464	-0.00783	-2.01477
N	-0.48793	-0.5084	-4.10917
H	-0.93386	-0.95743	-4.90516

Table S8.8. Optimized coordinates for **8.15**.

N	1.9473	-0.0047	0.00001
N	-0.00001	-0.00271	-1.94725
N	-1.9473	0.0047	-0.00001
C	-1.1194	0.0093	2.76818
C	0.70682	0.00255	4.16981
C	1.11941	-0.00119	2.76819
C	2.76824	-0.00796	1.11942
C	4.16985	-0.01425	0.70684
C	4.16985	-0.01635	-0.70681
C	2.76823	-0.01124	-1.1194
C	1.1194	-0.0093	-2.76818
C	0.7068	-0.01021	-4.1698
C	-0.70682	-0.00255	-4.16981
C	-1.11941	0.00119	-2.76819
C	-2.76824	0.00796	-1.11942
C	-4.16985	0.01425	-0.70684
C	-4.16985	0.01635	0.70681
C	-2.76823	0.01124	1.1194
C	-0.7068	0.01021	4.1698
N	0.00001	0.00271	1.94725
N	-2.39766	0.01293	2.39762
N	2.39767	-0.00586	2.39765
N	2.39766	-0.01293	-2.39762
N	-2.39767	0.00586	-2.39765
Fe	0.	0.	0.
C	-5.37069	0.01911	-1.42991
C	-6.57123	0.02591	-0.70642
H	-7.52539	0.02976	-1.24214
C	-6.57123	0.02805	0.70636

H	-7.52538	0.03353	1.24208
C	-5.37068	0.02341	1.42986
H	-5.36756	0.01768	-2.52364
H	-5.36754	0.02527	2.52359
C	-1.42985	0.01597	5.37064
C	-0.70637	0.01437	6.57121
H	-1.24208	0.0189	7.52537
C	1.42987	0.00105	5.37066
C	0.70639	0.00691	6.57122
H	1.24211	0.00579	7.52539
C	5.37069	-0.01911	1.42991
C	6.57123	-0.02591	0.70642
H	7.52539	-0.02976	1.24214
C	6.57123	-0.02805	-0.70636
H	7.52538	-0.03353	-1.24208
C	5.37068	-0.02341	-1.42986
H	5.36754	-0.02527	-2.52359
H	5.36756	-0.01768	2.52364
H	2.52359	-0.00464	5.36753
H	-2.52357	0.0217	5.36749
C	1.42985	-0.01597	-5.37064
C	0.70637	-0.01437	-6.57121
H	1.24208	-0.0189	-7.52537
C	-0.70639	-0.00691	-6.57122
H	-1.24211	-0.00579	-7.52539
C	-1.42987	-0.00105	-5.37066
H	-2.52359	0.00464	-5.36753
H	2.52357	-0.0217	-5.36749
H	-0.93708	2.42216	-0.00261
H	0.48951	2.42043	0.82063
H	0.48862	2.41831	-0.8274
H	0.93708	-2.42216	0.00261
H	-0.48862	-2.41831	0.8274
H	-0.48951	-2.42043	-0.82063
N	-0.01354	-2.03741	0.00264
N	0.01354	2.03741	-0.00264

Table S8.9. Optimized coordinates for **8.5**.

N	-1.95299	0.	0.00268
N	0.	-1.95299	-0.00268
N	1.95299	0.	0.00268

C	1.11747	2.76646	-0.00741
C	-0.70729	4.17027	-0.02114
C	-1.11747	2.76646	-0.00741
C	-2.76646	1.11747	0.00741
C	-4.17027	0.70729	0.02114
C	-4.17027	-0.70729	0.02114
C	-2.76646	-1.11747	0.00741
C	-1.11747	-2.76646	-0.00741
C	-0.70729	-4.17027	-0.02114
C	0.70729	-4.17027	-0.02114
C	1.11747	-2.76646	-0.00741
C	2.76646	-1.11747	0.00741
C	4.17027	-0.70729	0.02114
C	4.17027	0.70729	0.02114
C	2.76646	1.11747	0.00741
C	0.70729	4.17027	-0.02114
N	0.	1.95299	-0.00268
N	2.39719	2.39719	0.
N	-2.39719	2.39719	0.
N	-2.39719	-2.39719	0.
N	2.39719	-2.39719	0.
Fe	0.	0.	0.
C	5.3715	-1.4286	0.03614
C	6.57378	-0.70624	0.05168
H	7.52789	-1.24306	0.0642
C	6.57378	0.70624	0.05168
H	7.52789	1.24306	0.0642
C	5.3715	1.4286	0.03614
H	5.36794	-2.52282	0.037
H	5.36794	2.52282	0.037
C	1.4286	5.3715	-0.03614
C	0.70624	6.57378	-0.05168
H	1.24306	7.52789	-0.0642
C	-1.4286	5.3715	-0.03614
C	-0.70624	6.57378	-0.05168
H	-1.24306	7.52789	-0.0642
C	-5.3715	1.4286	0.03614
C	-6.57378	0.70624	0.05168
H	-7.52789	1.24306	0.0642
C	-6.57378	-0.70624	0.05168
H	-7.52789	-1.24306	0.0642
C	-5.3715	-1.4286	0.03614
H	-5.36794	-2.52282	0.037
H	-5.36794	2.52282	0.037

H	-2.52282	5.36794	-0.037
H	2.52282	5.36794	-0.037
C	-1.4286	-5.3715	-0.03614
C	-0.70624	-6.57378	-0.05168
H	-1.24306	-7.52789	-0.0642
C	0.70624	-6.57378	-0.05168
H	1.24306	-7.52789	-0.0642
C	1.4286	-5.3715	-0.03614
H	2.52282	-5.36794	-0.037
H	-2.52282	-5.36794	-0.037
N	0.	0.	3.15392
N	0.	0.	-3.15392
C	0.	0.	1.97365
C	0.	0.	-1.97365

Table S8.10. Optimized coordinates for **8.4**.

N	-1.95277	0.	0.00244
N	0.	-1.95277	-0.00244
N	1.95277	0.	0.00244
C	1.11747	2.76579	-0.00704
C	-0.70696	4.16973	-0.01998
C	-1.11747	2.76579	-0.00704
C	-2.76579	1.11747	0.00704
C	-4.16973	0.70696	0.01998
C	-4.16973	-0.70696	0.01998
C	-2.76579	-1.11747	0.00704
C	-1.11747	-2.76579	-0.00704
C	-0.70696	-4.16973	-0.01998
C	0.70696	-4.16973	-0.01998
C	1.11747	-2.76579	-0.00704
C	2.76579	-1.11747	0.00704
C	4.16973	-0.70696	0.01998
C	4.16973	0.70696	0.01998
C	2.76579	1.11747	0.00704
C	0.70696	4.16973	-0.01998
N	0.	1.95277	-0.00244
N	2.39659	2.39659	0.
N	-2.39659	2.39659	0.
N	-2.39659	-2.39659	0.
N	2.39659	-2.39659	0.

Fe	0.	0.	0.
C	5.37042	-1.42909	0.03411
C	6.5719	-0.70633	0.04874
H	7.5261	-1.2427	0.06055
C	6.5719	0.70633	0.04874
H	7.5261	1.2427	0.06055
C	5.37042	1.42909	0.03411
H	5.3668	-2.52313	0.03481
H	5.3668	2.52313	0.03481
C	1.42909	5.37042	-0.03411
C	0.70633	6.5719	-0.04874
H	1.2427	7.5261	-0.06055
C	-1.42909	5.37042	-0.03411
C	-0.70633	6.5719	-0.04874
H	-1.2427	7.5261	-0.06055
C	-5.37042	1.42909	0.03411
C	-6.5719	0.70633	0.04874
H	-7.5261	1.2427	0.06055
C	-6.5719	-0.70633	0.04874
H	-7.5261	-1.2427	0.06055
C	-5.37042	-1.42909	0.03411
H	-5.3668	-2.52313	0.03481
H	-5.3668	2.52313	0.03481
H	-2.52313	5.3668	-0.03481
H	2.52313	5.3668	-0.03481
C	-1.42909	-5.37042	-0.03411
C	-0.70633	-6.5719	-0.04874
H	-1.2427	-7.5261	-0.06055
C	0.70633	-6.5719	-0.04874
H	1.2427	-7.5261	-0.06055
C	1.42909	-5.37042	-0.03411
H	2.52313	-5.3668	-0.03481
H	-2.52313	-5.3668	-0.03481
C	0.	0.	3.1285
C	0.	0.	-3.1285
N	0.	0.	1.94505
N	0.	0.	-1.94505
S	0.	0.	4.78268
S	0.	0.	-4.78268

Table S8.11. Optimized coordinates for **8.3.2** with C_2 symmetry.

C	-0.03305	-2.76075	-1.1161
C	-0.03455	4.1654	0.70589
C	0.01849	4.16408	-0.70724
C	0.03305	2.76075	-1.1161
C	-0.06547	5.3672	1.42633
H	-0.10761	5.36417	2.51979
C	-0.04058	6.56903	0.70398
H	-0.06356	7.5236	1.23964
C	0.0139	6.56802	-0.70786
H	0.03287	7.52197	-1.24483
C	0.0437	5.3655	-1.42877
H	0.08505	5.36127	-2.52222
C	-0.03504	-1.11552	-2.75851
C	-0.02599	-0.70634	-4.16262
C	0.02599	0.70634	-4.16262
C	0.03504	1.11552	-2.75851
C	-0.05421	-1.42743	-5.36376
H	-0.09555	-2.52092	-5.36004
C	-0.02716	-0.70579	-6.56631
H	-0.04812	-1.24227	-7.52052
C	0.02716	0.70579	-6.56631
H	0.04812	1.24227	-7.52052
C	0.05421	1.42743	-5.36376
H	0.09555	2.52092	-5.36004
C	-2.85925	-0.73775	0.74158
H	-2.5185	-1.47514	1.46765
C	-4.03171	0.5006	-0.4723
H	-4.88628	0.988	-0.94725
Fe	0.	0.	-0.00272
N	0.	-1.94408	-0.00025
N	0.	0.	-1.94213
N	-0.06335	-2.39479	-2.39493
N	0.06335	2.39479	-2.39493
N	-2.00723	0.00469	0.0018
C	-0.03977	2.76209	1.11573
C	-0.01849	-4.16408	-0.70724
C	0.03455	-4.1654	0.70589
C	0.03977	-2.76209	1.11573
C	-0.0437	-5.3655	-1.42877
H	-0.08505	-5.36127	-2.52222
C	-0.0139	-6.56802	-0.70786
H	-0.03287	-7.52197	-1.24483
C	0.04058	-6.56903	0.70398

H	0.06356	-7.5236	1.23964
C	0.06547	-5.3672	1.42633
H	0.10761	-5.36417	2.51979
C	-0.03793	1.11642	2.76437
C	-0.02721	0.70683	4.16689
C	0.02721	-0.70683	4.16689
C	0.03793	-1.11642	2.76437
C	-0.05553	1.4277	5.36899
H	-0.09819	2.52112	5.36547
C	-0.02762	0.70606	6.57078
H	-0.04887	1.24226	7.52508
C	0.02762	-0.70606	6.57078
H	0.04887	-1.24226	7.52508
C	0.05553	-1.4277	5.36899
H	0.09819	-2.52112	5.36547
N	0.	1.94408	-0.00025
N	0.	0.	1.94604
N	-0.0652	2.39622	2.39595
N	0.0652	-2.39622	2.39595
C	2.85925	0.73775	0.74158
H	2.5185	1.47514	1.46765
C	4.03171	-0.5006	-0.4723
H	4.88628	-0.988	-0.94725
N	2.00723	-0.00469	0.0018
N	2.76935	-0.82005	-0.79748
N	-2.76935	0.82005	-0.79748
N	4.15801	0.46537	0.48241
N	-4.15801	-0.46537	0.48241

Table S8.12. Optimized coordinates for **8.3.2** with D_{2h} symmetry.

C	2.74357	-1.16475	-0.03815
C	-3.44592	2.44682	-0.02708
C	-2.44682	3.44592	0.02708
C	-1.16475	2.74357	0.03815
C	-4.80561	2.78655	-0.05411
H	-5.57716	2.01213	-0.09627
C	-5.14492	4.14683	-0.02718
H	-6.19883	4.44212	-0.04815
C	-4.14683	5.14492	0.02718
H	-4.44212	6.19883	0.04815

C	-2.78655	4.80561	0.05411
H	-2.01213	5.57716	0.09627
C	2.74357	1.16475	-0.03815
C	3.44592	2.44682	-0.02708
C	2.44682	3.44592	0.02708
C	1.16475	2.74357	0.03815
C	4.80561	2.78655	-0.05411
H	5.57716	2.01213	-0.09627
C	5.14492	4.14683	-0.02718
H	6.19883	4.44212	-0.04815
C	4.14683	5.14492	0.02718
H	4.44212	6.19883	0.04815
C	2.78655	4.80561	0.05411
H	2.01213	5.57716	0.09627
C	1.06064	0.	2.88056
H	2.09794	0.	2.54685
Fe	0.	0.	0.
N	1.37549	-1.37549	0.
N	1.37549	1.37549	0.
N	3.38804	0.	-0.06505
N	0.	3.38804	0.06505
N	0.	0.	2.0195
C	-2.74357	1.16475	-0.03815
C	3.44592	-2.44682	-0.02708
C	2.44682	-3.44592	0.02708
C	1.16475	-2.74357	0.03815
C	4.80561	-2.78655	-0.05411
H	5.57716	-2.01213	-0.09627
C	5.14492	-4.14683	-0.02718
H	6.19883	-4.44212	-0.04815
C	4.14683	-5.14492	0.02718
H	4.44212	-6.19883	0.04815
C	2.78655	-4.80561	0.05411
H	2.01213	-5.57716	0.09627
C	-2.74357	-1.16475	-0.03815
C	-3.44592	-2.44682	-0.02708
C	-2.44682	-3.44592	0.02708
C	-1.16475	-2.74357	0.03815
C	-4.80561	-2.78655	-0.05411
H	-5.57716	-2.01213	-0.09627
C	-5.14492	-4.14683	-0.02718
H	-6.19883	-4.44212	-0.04815
C	-4.14683	-5.14492	0.02718
H	-4.44212	-6.19883	0.04815

C	-2.78655	-4.80561	0.05411
H	-2.01213	-5.57716	0.09627
N	-1.37549	1.37549	0.
N	-1.37549	-1.37549	0.
N	-3.38804	0.	-0.06505
N	0.	-3.38804	0.06505
C	0.	1.06064	-2.88056
H	0.	2.09794	-2.54685
N	0.	0.	-2.0195
N	0.	0.69686	-4.16565
N	0.69686	0.	4.16565
C	0.	-1.06064	-2.88056
C	-1.06064	0.	2.88056
N	-0.69686	0.	4.16565
N	0.	-0.69686	-4.16565
H	0.	-2.09794	-2.54685
H	-2.09794	0.	2.54685

Table S8.13. Optimized coordinates for **8.2**.

C	2.87042	0.79363	0.04124
C	-4.21967	-0.22842	0.02286
C	-4.05885	1.17509	-0.04402
C	-2.61813	1.42233	-0.0527
C	-5.49589	-0.80756	0.05376
H	-5.61773	-1.89363	0.10627
C	-6.60806	0.04566	0.01673
H	-7.61714	-0.37858	0.04044
C	-6.4475	1.44756	-0.05057
H	-7.33443	2.08887	-0.07961
C	-5.17119	2.02729	-0.08142
H	-5.04396	3.11264	-0.13463
C	1.42165	2.61679	0.05598
C	1.17455	4.05763	0.0488
C	-0.22884	4.21859	-0.01838
C	-0.79499	2.87115	-0.03901
C	2.02687	5.16965	0.08778
H	3.11219	5.0422	0.14066
C	1.44723	6.44607	0.05832
H	2.08866	7.33286	0.08842
C	0.04543	6.60688	-0.00936

H	-0.37866	7.61604	-0.03233
C	-0.80794	5.49483	-0.04819
H	-1.89395	5.61677	-0.10152
C	0.69414	-0.82531	2.86123
H	1.35587	-1.6063	2.48473
C	-0.7081	0.83058	2.87276
H	-1.36569	1.60866	2.48828
C	-0.40067	0.46421	4.17739
H	-0.76774	0.89528	5.11221
Fe	-0.00087	-0.0003	-0.00008
N	1.93047	-0.2216	-0.00272
N	0.22009	1.93107	0.00531
N	2.65126	2.10638	0.08292
N	-2.10785	2.6522	-0.07961
N	-0.00098	-0.00247	2.02515
N	0.49293	-0.5914	4.1724
C	-2.87221	-0.79447	0.04113
C	4.21799	0.22761	0.02098
C	4.05717	-1.1758	-0.04578
C	2.61631	-1.42306	-0.05357
C	5.49409	0.80688	0.05031
H	5.61589	1.89296	0.10222
C	6.60622	-0.04635	0.01183
H	7.61531	0.37792	0.03389
C	6.44564	-1.44821	-0.05494
H	7.33255	-2.0895	-0.08458
C	5.16932	-2.02803	-0.08431
H	5.042	-3.11339	-0.13681
C	-1.42351	-2.61774	0.04999
C	-1.17639	-4.0585	0.04102
C	0.22704	-4.2194	-0.02532
C	0.79322	-2.87184	-0.04345
C	-2.02869	-5.17067	0.07797
H	-3.11406	-5.04338	0.13064
C	-1.44894	-6.44701	0.04729
H	-2.09034	-7.33388	0.07585
C	-0.04706	-6.60768	-0.019
H	0.37717	-7.61678	-0.04178
C	0.80627	-5.49551	-0.05562
H	1.89238	-5.61724	-0.10661
N	-1.93218	0.22078	-0.00295
N	-0.22208	-1.93179	-0.00003
N	-2.65327	-2.10736	0.07912
N	2.10601	-2.65287	-0.08263

C	0.822	0.69679	-2.86159
H	1.60983	1.35058	-2.48542
C	-0.84444	-0.69304	-2.87221
H	-1.62524	-1.34717	-2.48709
C	-0.48208	-0.3814	-4.17695
H	-0.92021	-0.74046	-5.11159
N	-0.00241	0.00403	-2.02515
N	0.58022	0.50419	-4.17258

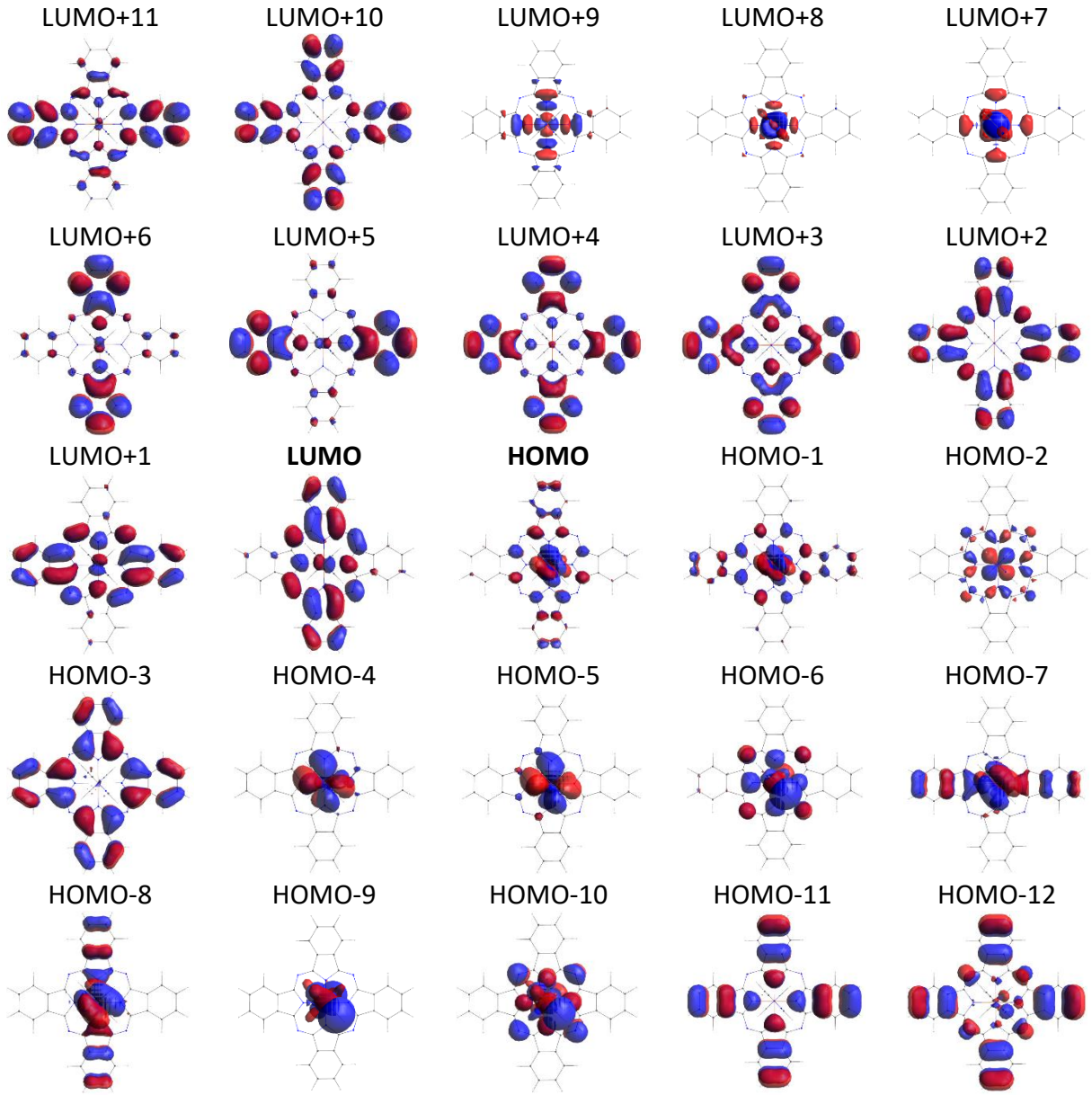
Table S8.14. Optimized coordinates for **8.1**.

N	-1.94913	0.	0.00347
N	0.	-1.94913	-0.00347
N	1.94913	0.	0.00347
C	1.11661	2.76369	-0.00993
C	-0.70721	4.16758	-0.02814
C	-1.11661	2.76369	-0.00993
C	-2.76369	1.11661	0.00993
C	-4.16758	0.70721	0.02814
C	-4.16758	-0.70721	0.02814
C	-2.76369	-1.11661	0.00993
C	-1.11661	-2.76369	-0.00993
C	-0.70721	-4.16758	-0.02814
C	0.70721	-4.16758	-0.02814
C	1.11661	-2.76369	-0.00993
C	2.76369	-1.11661	0.00993
C	4.16758	-0.70721	0.02814
C	4.16758	0.70721	0.02814
C	2.76369	1.11661	0.00993
C	0.70721	4.16758	-0.02814
N	0.	1.94913	-0.00347
N	2.39652	2.39652	0.
N	-2.39652	2.39652	0.
N	-2.39652	-2.39652	0.
N	2.39652	-2.39652	0.
Fe	0.	0.	0.
C	5.36899	-1.42864	0.04774
C	6.57094	-0.70643	0.06801
H	7.52506	-1.24313	0.08433
C	6.57094	0.70643	0.06801
H	7.52506	1.24313	0.08433

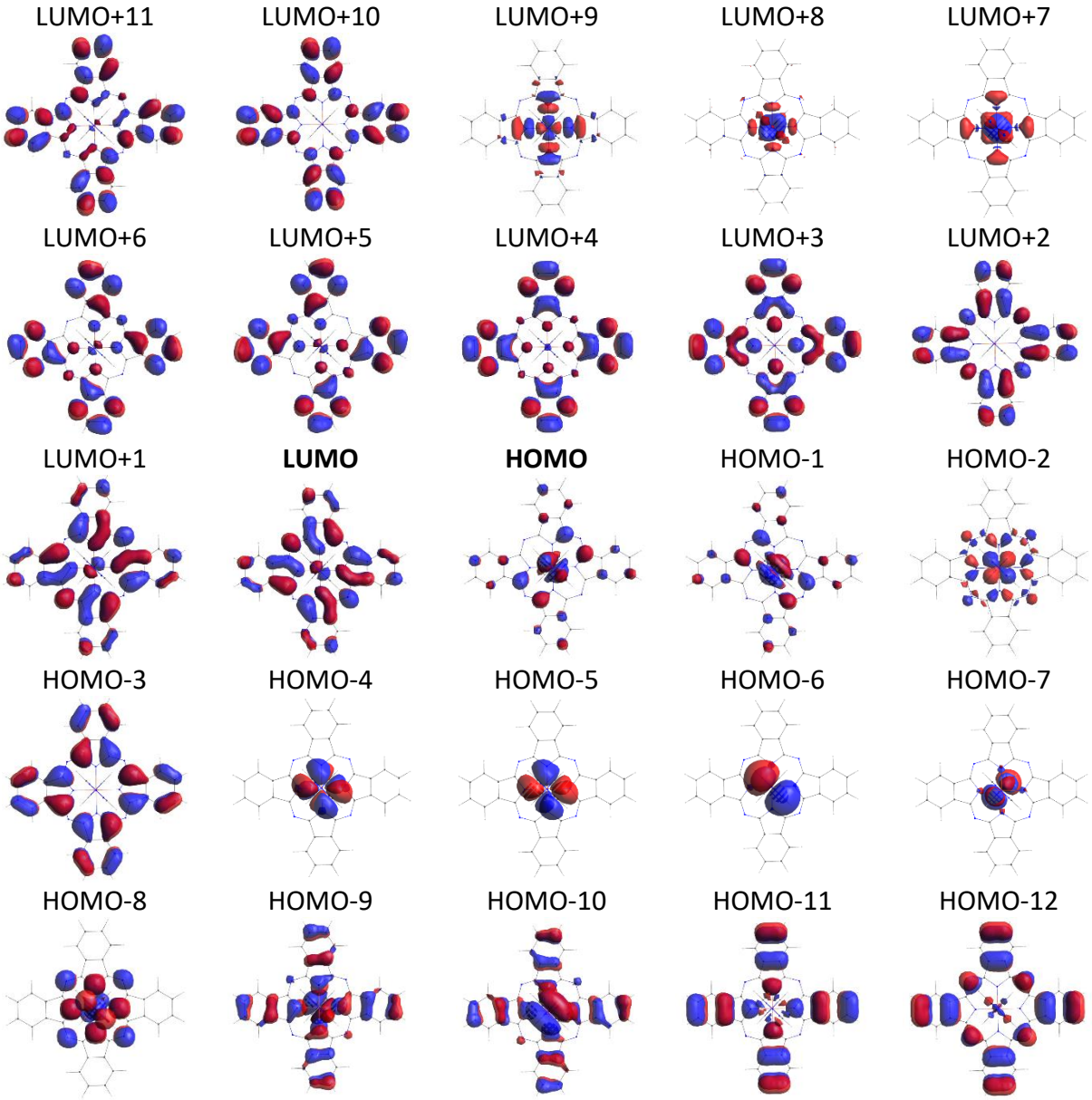
C	5.36899	1.42864	0.04774
H	5.36554	-2.52289	0.04876
H	5.36554	2.52289	0.04876
C	1.42864	5.36899	-0.04774
C	0.70643	6.57094	-0.06801
H	1.24313	7.52506	-0.08433
C	-1.42864	5.36899	-0.04774
C	-0.70643	6.57094	-0.06801
H	-1.24313	7.52506	-0.08433
C	-5.36899	1.42864	0.04774
C	-6.57094	0.70643	0.06801
H	-7.52506	1.24313	0.08433
C	-6.57094	-0.70643	0.06801
H	-7.52506	-1.24313	0.08433
C	-5.36899	-1.42864	0.04774
H	-5.36554	-2.52289	0.04876
H	-5.36554	2.52289	0.04876
H	-2.52289	5.36554	-0.04876
H	2.52289	5.36554	-0.04876
C	-1.42864	-5.36899	-0.04774
C	-0.70643	-6.57094	-0.06801
H	-1.24313	-7.52506	-0.08433
C	0.70643	-6.57094	-0.06801
H	1.24313	-7.52506	-0.08433
C	1.42864	-5.36899	-0.04774
H	2.52289	-5.36554	-0.04876
H	-2.52289	-5.36554	-0.04876
C	0.	0.	3.16657
C	0.	0.	-3.16657
N	0.	0.	1.97313
N	0.	0.	-1.97313
O	0.	0.	4.38724
O	0.	0.	-4.38724

Chapter 9 Supporting Information:

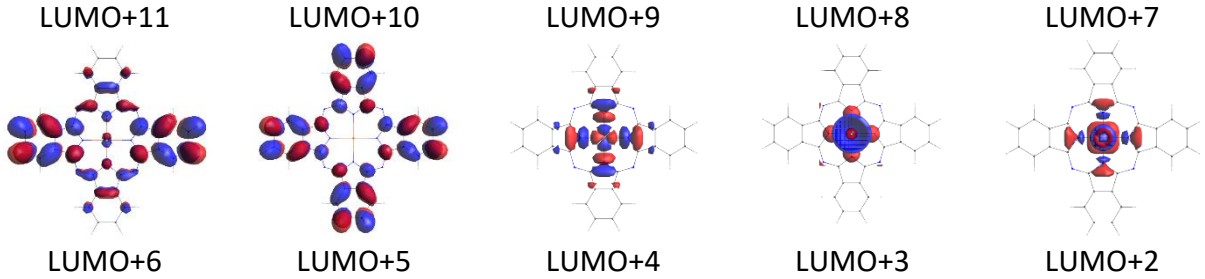
8.2

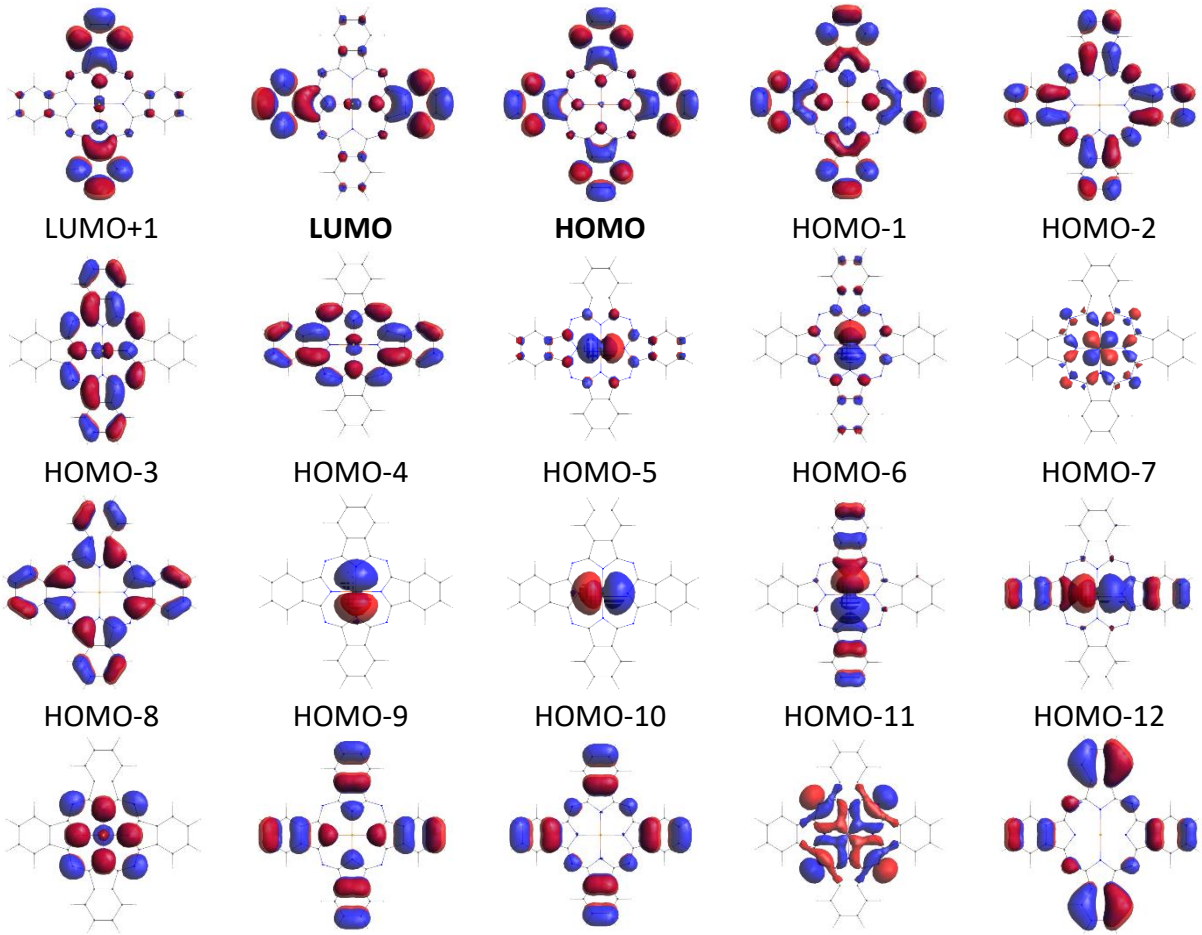


8.3

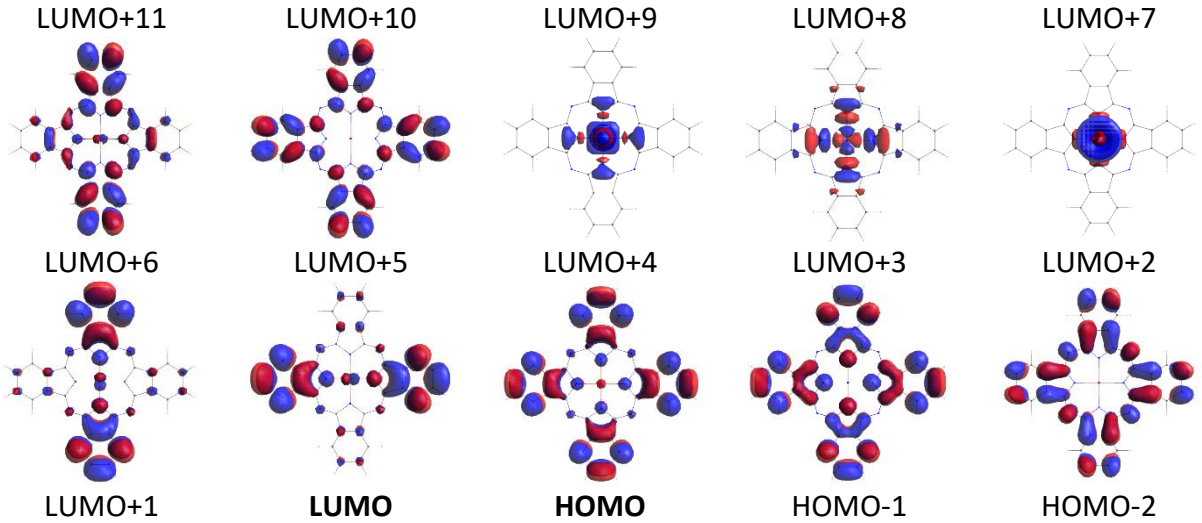

LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2
LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-8
HOMO-9
HOMO-10
HOMO-11
HOMO-12

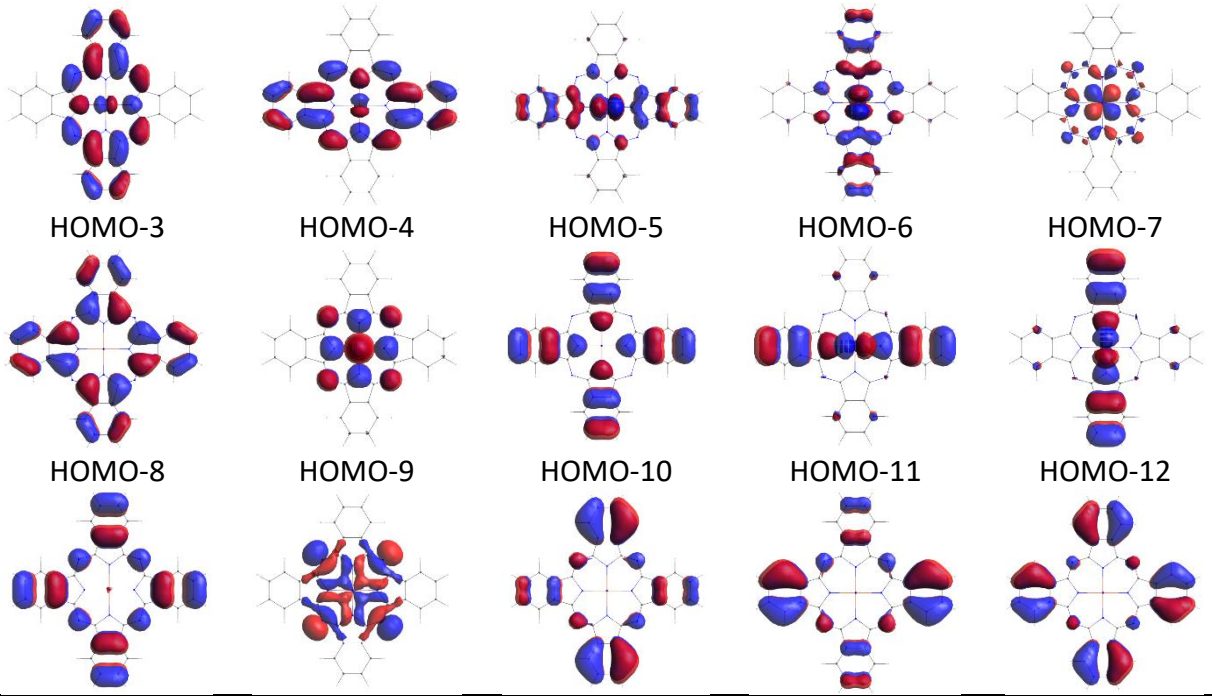
8.4


LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2

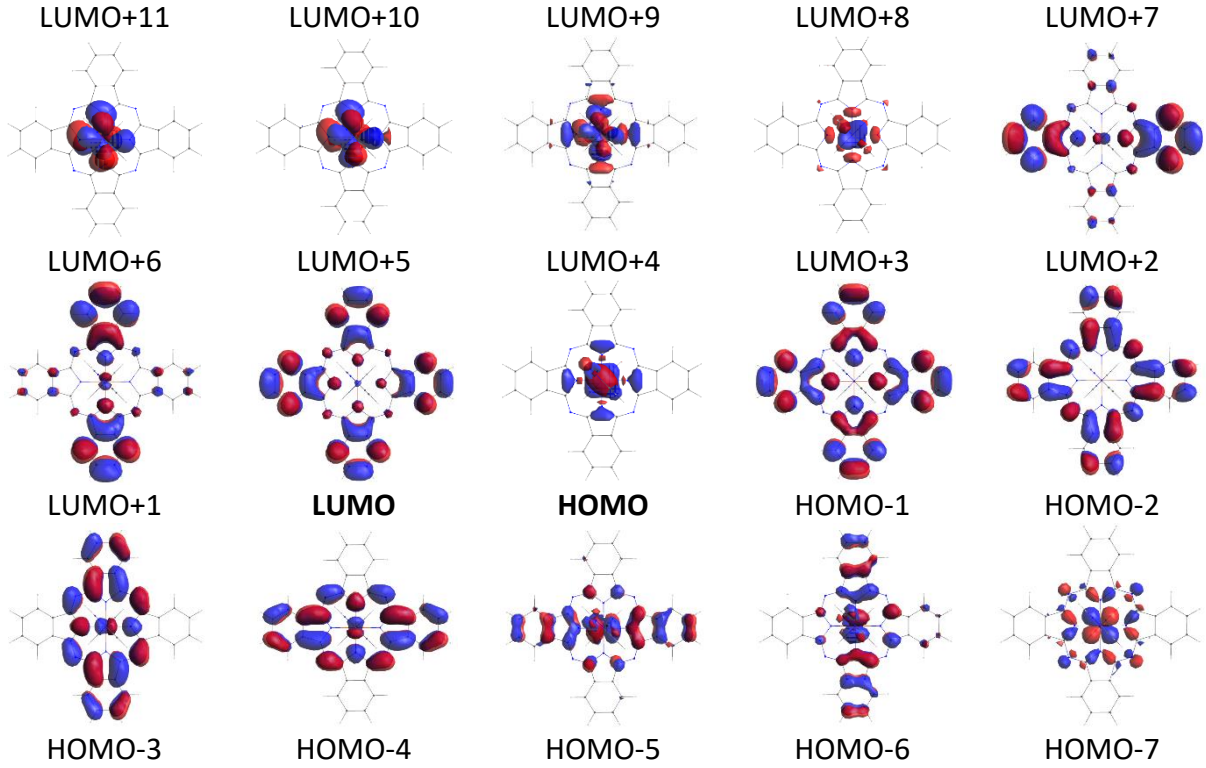

LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-8
HOMO-9
HOMO-10
HOMO-11
HOMO-12

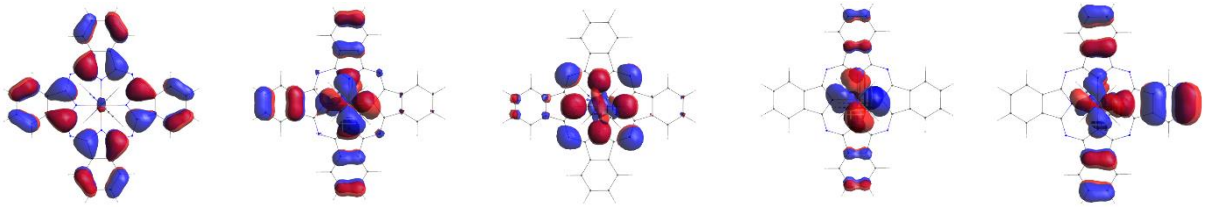
8.5


LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2
LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2

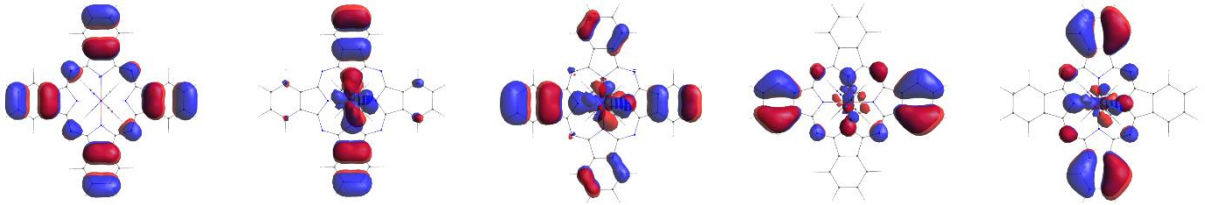

HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-8
HOMO-9
HOMO-10
HOMO-11
HOMO-12

8.6


LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2
LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7

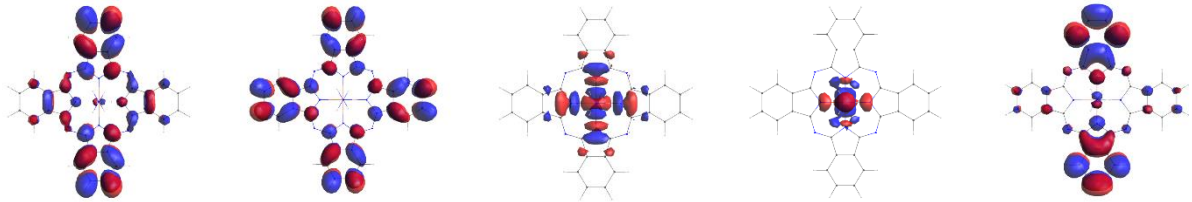


HOMO-8 HOMO-9 HOMO-10 HOMO-11 HOMO-12

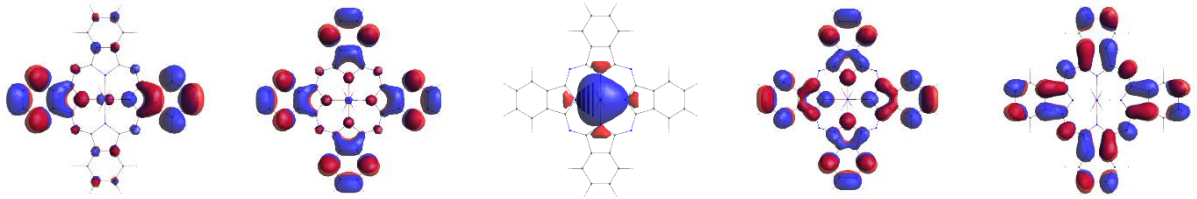


8.15

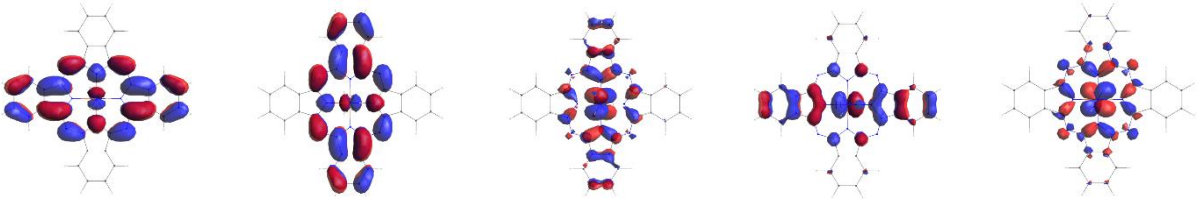
LUMO+11 LUMO+10 LUMO+9 LUMO+8 LUMO+7



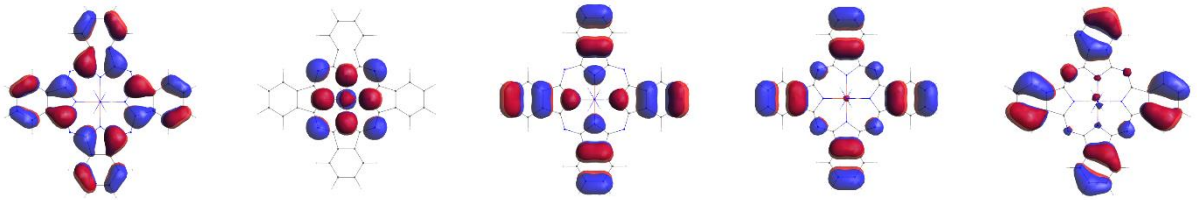
LUMO+6 LUMO+5 LUMO+4 LUMO+3 LUMO+2



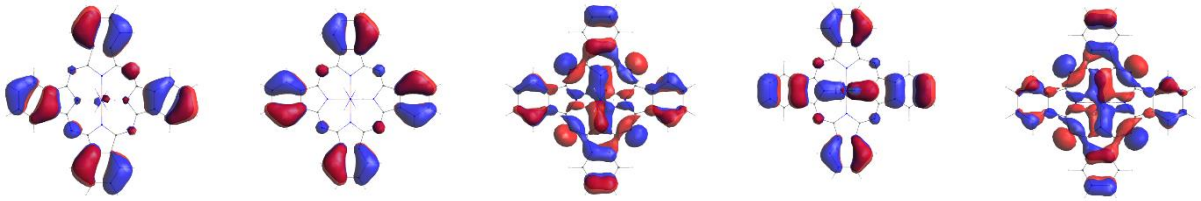
LUMO+1 **LUMO** **HOMO** HOMO-1 HOMO-2



HOMO-3 HOMO-4 HOMO-5 HOMO-6 HOMO-7

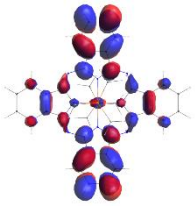


HOMO-8 HOMO-9 HOMO-10 HOMO-11 HOMO-12

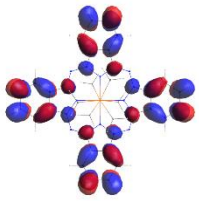


8.10

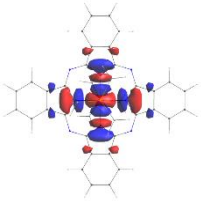
LUMO+11



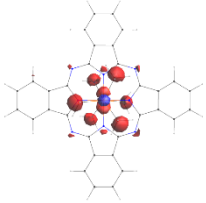
LUMO+10



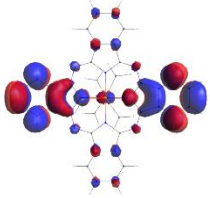
LUMO+9



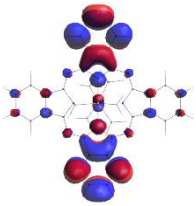
LUMO+8



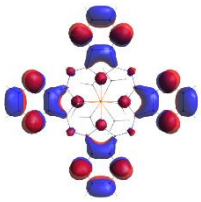
LUMO+7



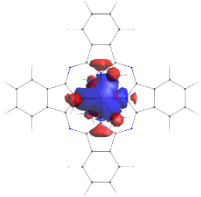
LUMO+6



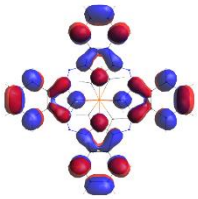
LUMO+5



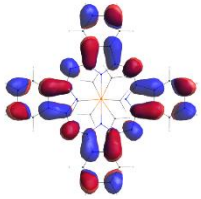
LUMO+4



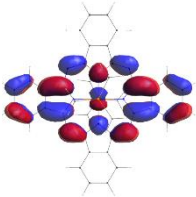
LUMO+3



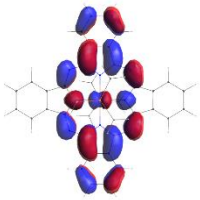
LUMO+2



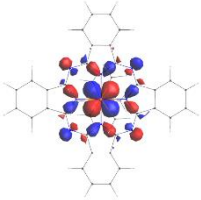
LUMO+1



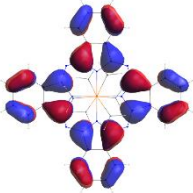
LUMO



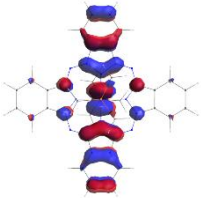
HOMO



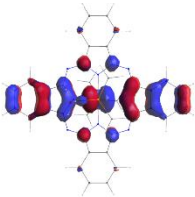
HOMO-1



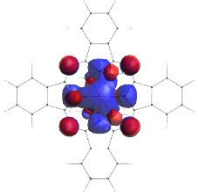
HOMO-2



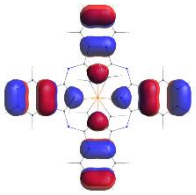
HOMO-3



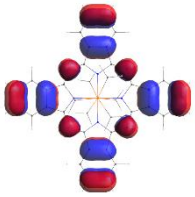
HOMO-4



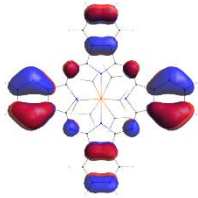
HOMO-5



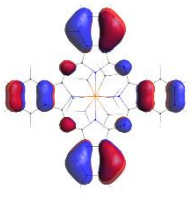
HOMO-6



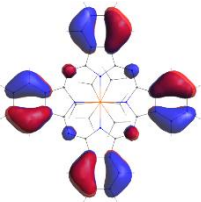
HOMO-7



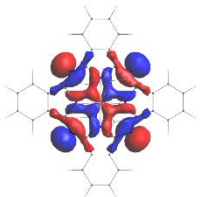
HOMO-8



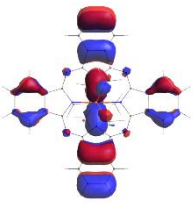
HOMO-9



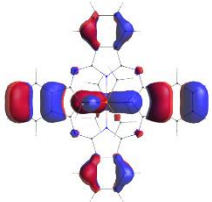
HOMO-10



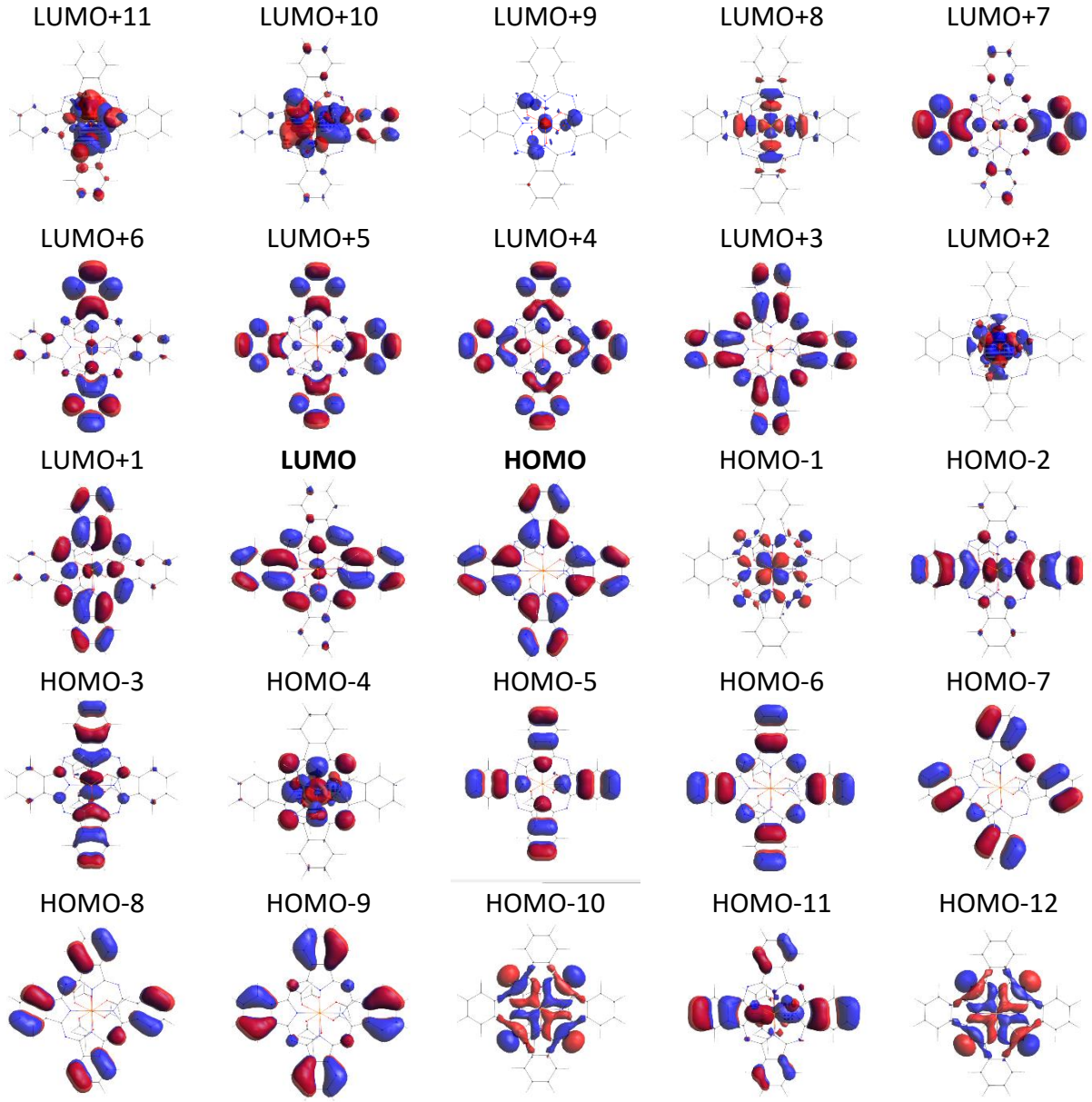
HOMO-11



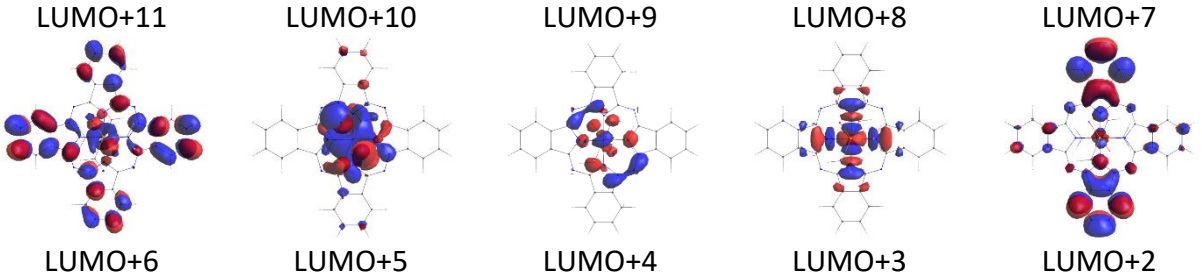
HOMO-12



8.17


LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2
LUMO+1
LUMO
HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-8
HOMO-9
HOMO-10
HOMO-11
HOMO-12

8.12


LUMO+11
LUMO+10
LUMO+9
LUMO+8
LUMO+7
LUMO+6
LUMO+5
LUMO+4
LUMO+3
LUMO+2

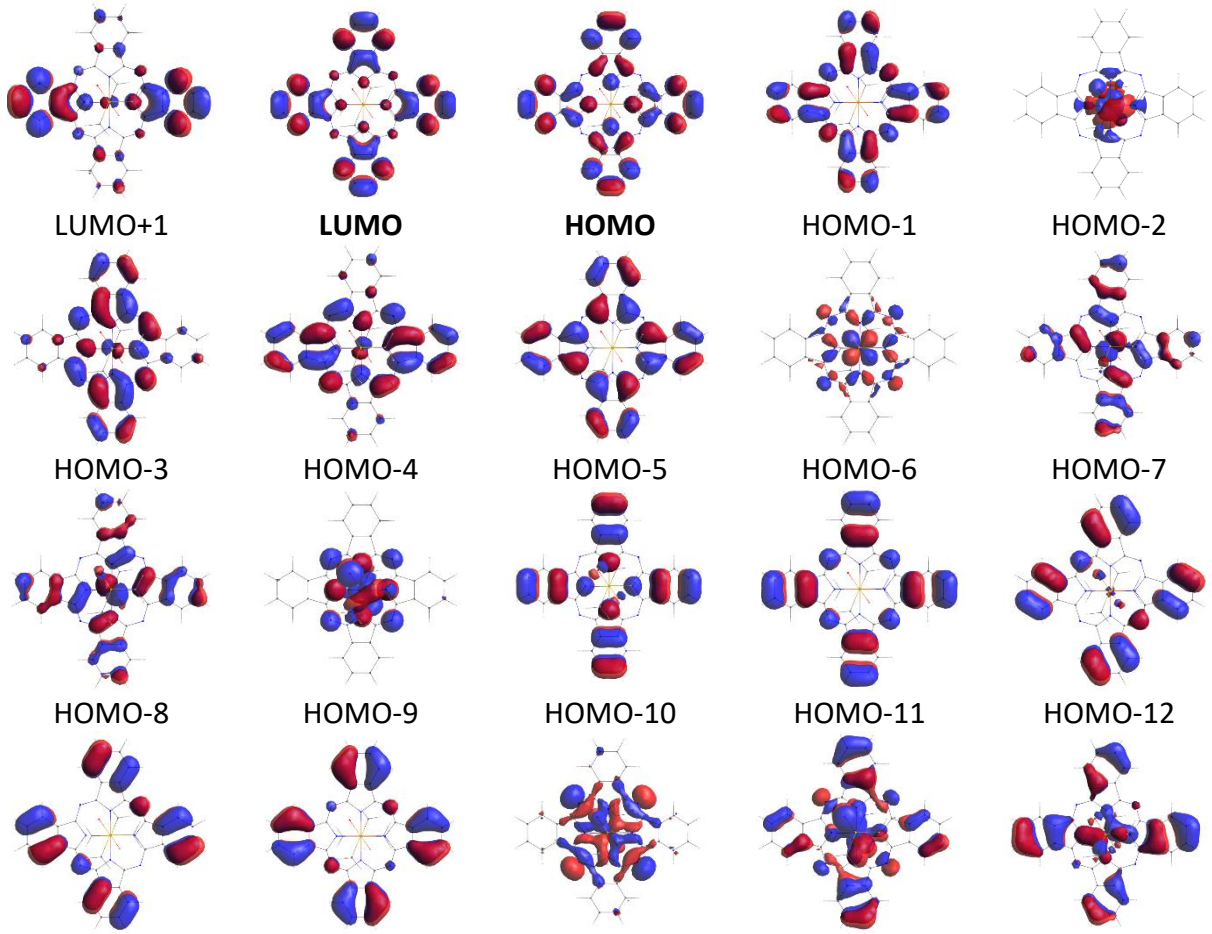


Figure S9.1. Additional DFT-predicted (MPWLYP) MOs for the example compounds not shown in the main text.

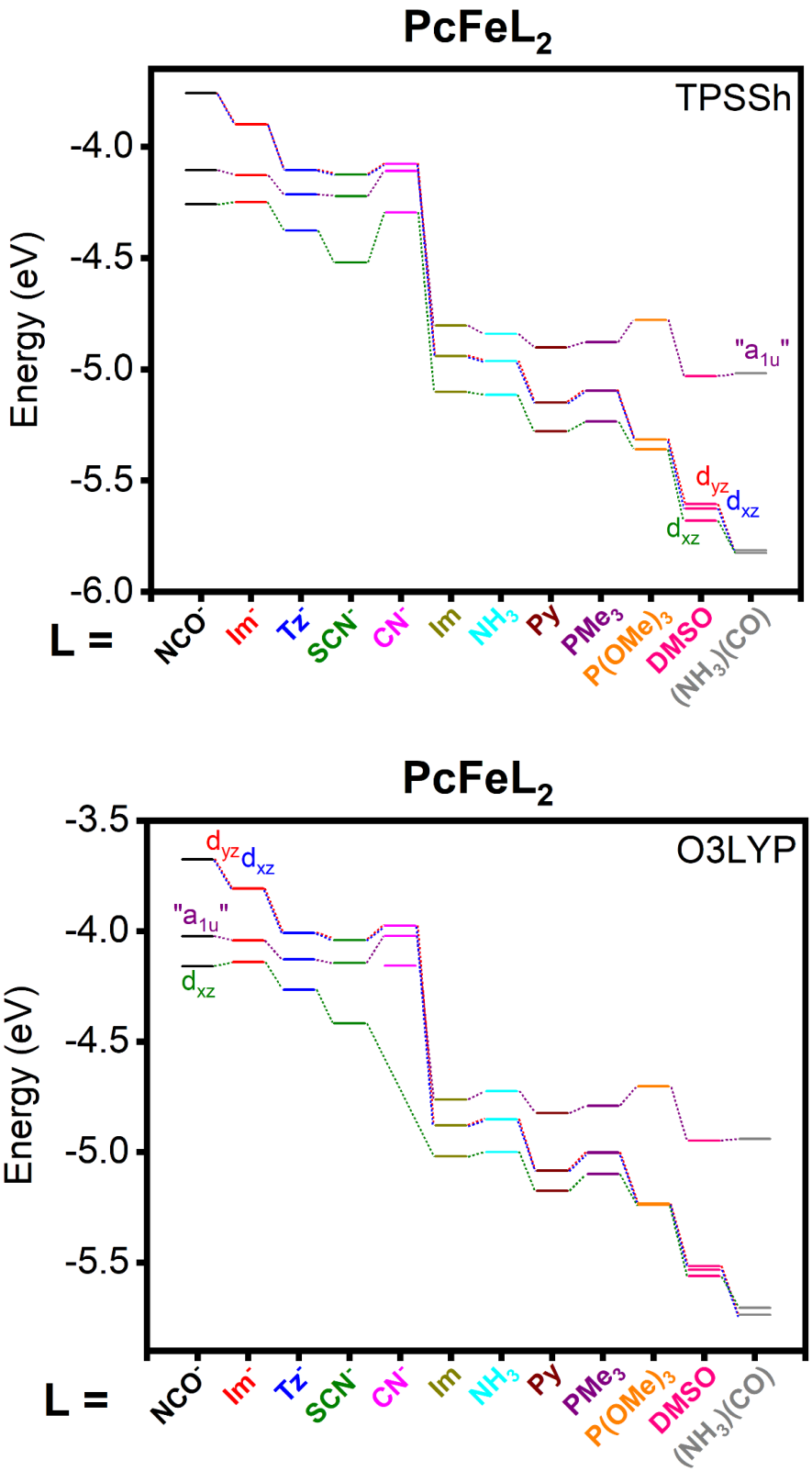
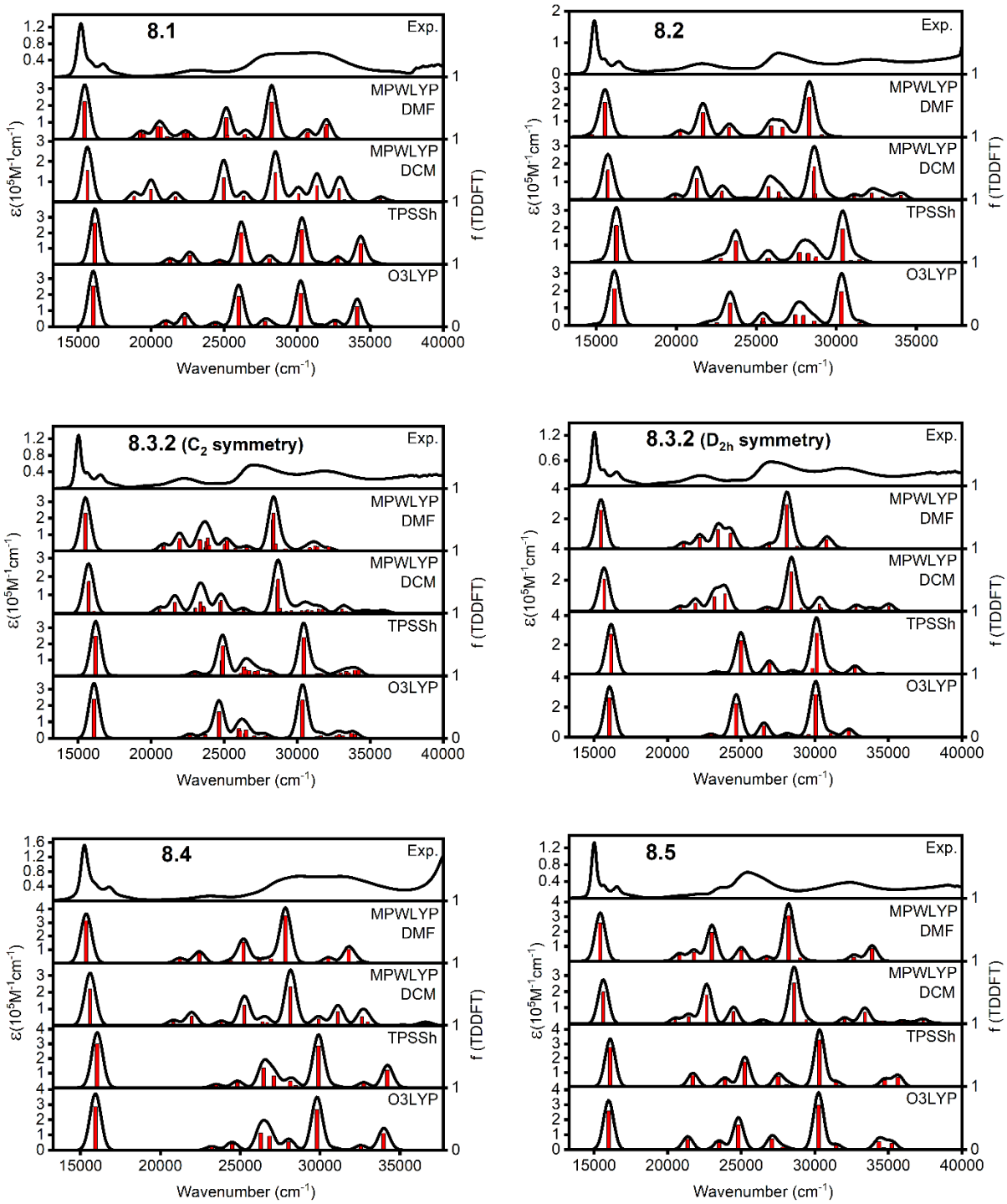
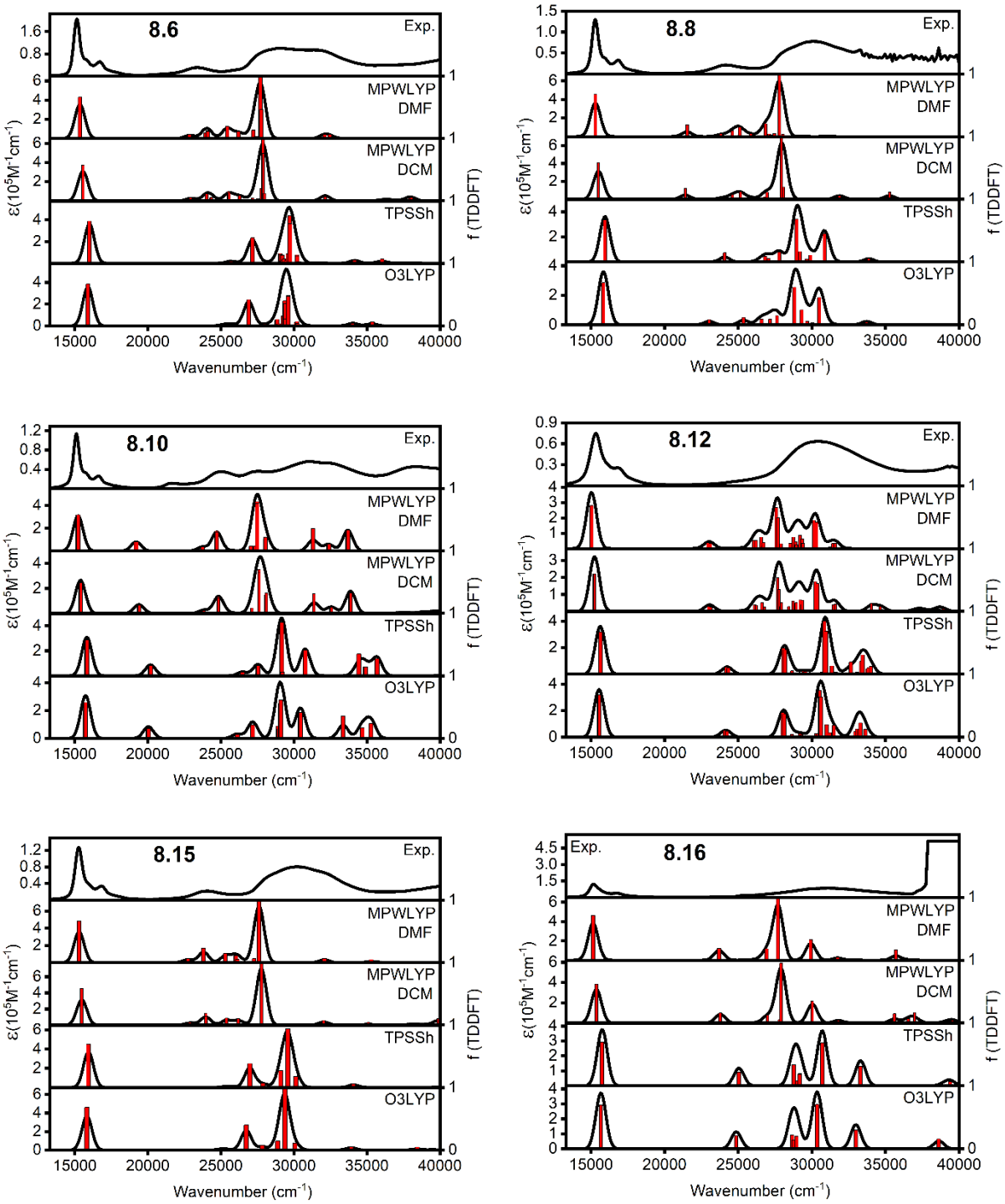


Figure S9.2. DFT-predicted energy-level diagrams of select frontier orbitals for all compounds using the TPSSh (upper) and O3LYP (lower) exchange correlation functionals.


8.1
8.2
8.3.2 (C2 symmetry)
8.3.2 (D2h symmetry)
8.4
8.5
Exp.
MPWLYP DMF
MPWLYP DCM
TPSSh
O3LYP
ε(10^5M^-1cm^-1)
f (TDDFT)
Wavenumber (cm^-1)


8.6
8.8
8.10
8.12
8.15
8.16
Exp.
MPWLYP DMF
MPWLYP DCM
TPSSh
O3LYP
ε(10^5M^-1cm^-1)
f (TDDFT)
Wavenumber (cm^-1)

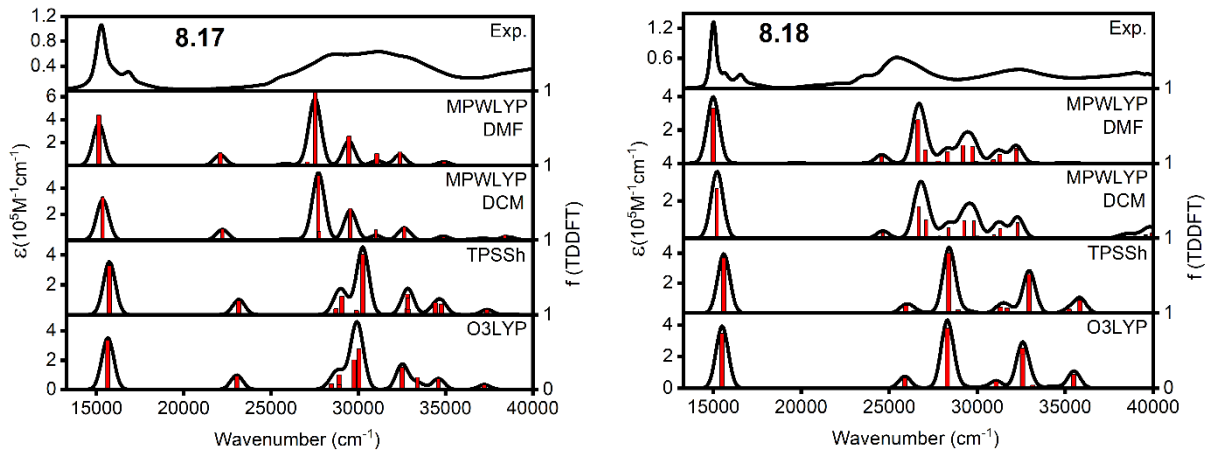


Figure S9.3. TDDFT-predicted UV-vis spectra for all compounds using the MPWLYP (DMF and DCM), TPSSh, and O3LYP exchange correlation functionals.

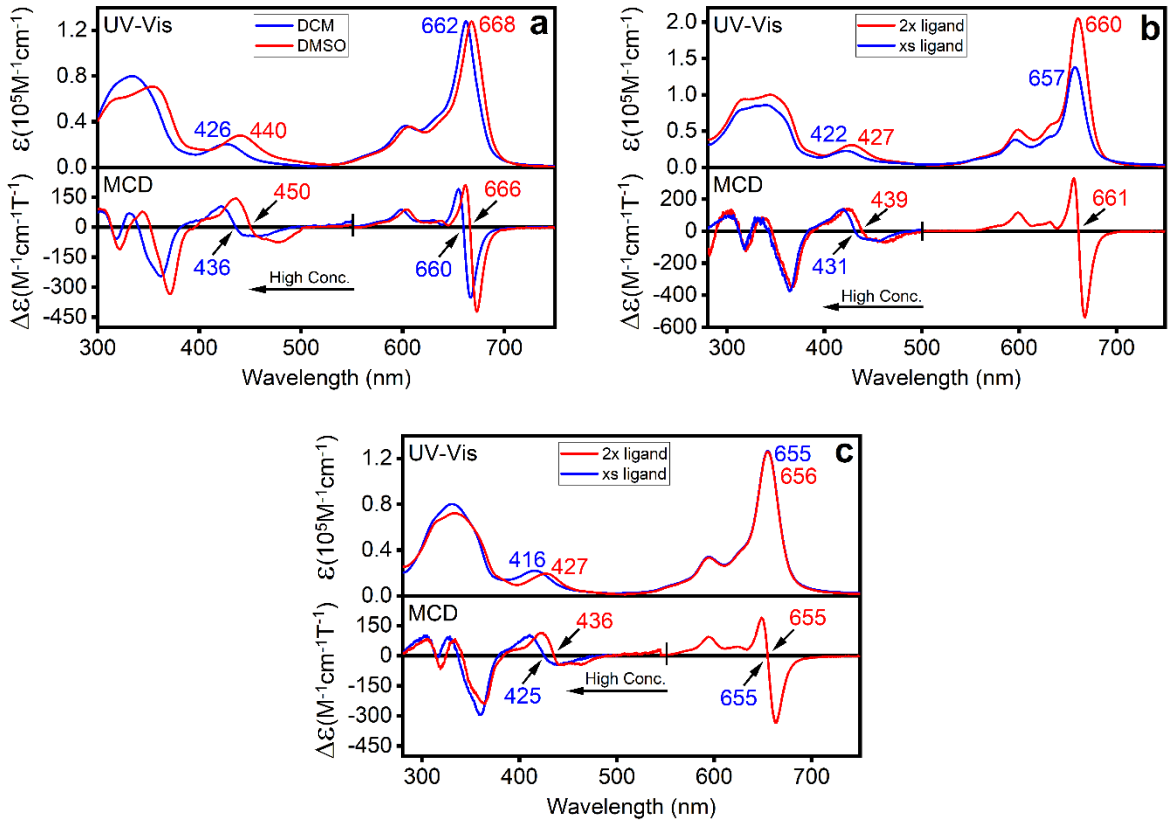


Figure S9.4. Experimental UV-vis (upper) and MCD (lower) spectra demonstrating solvatochromic effects for (a) **8.15** in DCM vs. DMSO, (b) **8.6** with low and high ligand concentration, and (c) **8.7** with low and high ligand concentration.

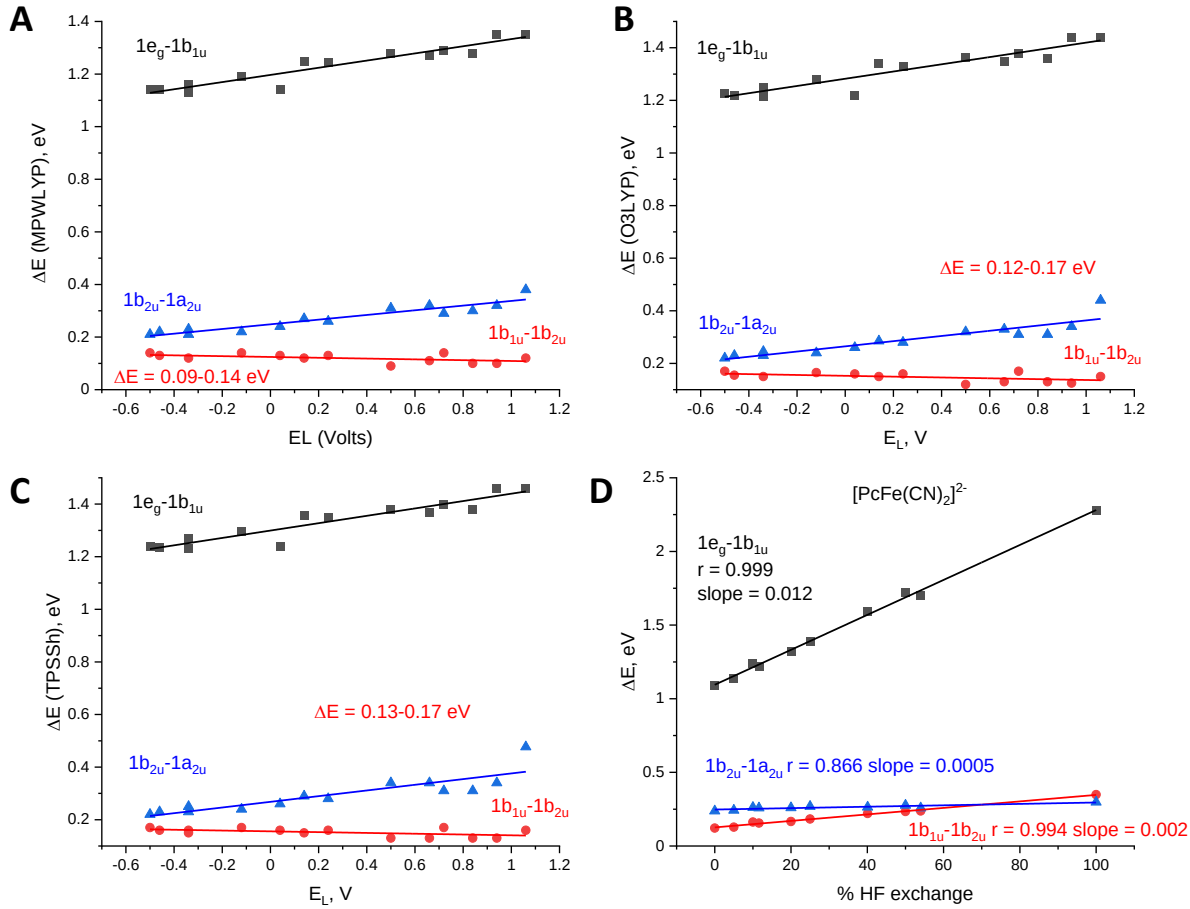


Figure S9.5. Energy difference between $1e_g$ and $1b_{1u}$, $1b_{1u}$ and $1b_{2u}$, and $1b_{2u}$-$1a_{2u}$ MOs across E_L series for MPWLYP (**A**), O3LYP (**B**), and TPSSh (**C**) calculations. Same dependency for $[PcFe(CN)_2]^{2-}$ complex as a function of Hartree-Fock percentage present in the exchange-correlation functional.

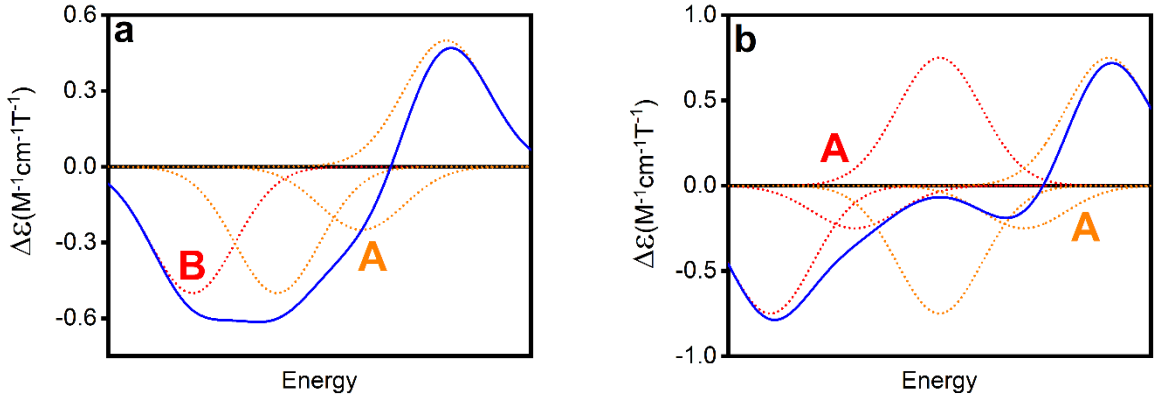


Figure S9.6. Examples of overlapping MCD (a) *B*- and *A*-terms, and (b) two *A*-terms.

Table S9.1. DFT-predicted compositions (MPWLYP functional) of the frontier MOs in iron(II) phthalocyanine complexes.

8.1

MO	Energy/eV	C,H	N	Fe	L_2
179	0.782	96.63	2.92	0.38	0.07
178	0.691	99.96	0.04	0	0
177	0.333	33.31	23.11	43.57	0
176	-0.054	5.61	1.48	91.86	1.05
175	-0.296	5.83	7.83	63.63	22.71
174	-0.495	92.75	5.99	1.21	0.04
173	-0.495	92.75	5.99	1.21	0.04
172	-0.534	90.72	4.66	1.88	2.74
171	-0.739	84.88	15.11	0.01	0
170	-0.878	80.52	19.48	0	0
169	-2.018	56.83	33.06	9.95	0.16
168	**-2.018**	**56.83**	**33.06**	**9.95**	**0.16**
167	**-3.339**	**16.76**	**0.31**	**56.18**	**26.75**
166	-3.339	16.76	0.31	56.18	26.75
165	-3.667	21.49	5.23	73.28	0
164	-3.831	99.66	0.21	0.13	0
163	-4.639	4.11	8.51	2.84	84.54
162	-4.639	4.11	8.51	2.84	84.54
161	-4.715	27.89	13.4	6.48	52.23
160	-4.715	27.89	13.4	6.48	52.23
159	-5.033	2.87	86.4	0.02	10.71
158	-5.388	72.93	27.06	0	0
157	-5.578	83.62	14.02	0.59	1.77
156	-5.588	51.58	45.49	2.94	0
155	-5.703	89.52	10.3	0.14	0.03

8.2

MO	Energy/eV	C,H	N	Fe	L_2
193	0.764	95.13	2.83	0.44	1.6
192	0.68	99.93	0.05	0.01	0.02
191	0.369	33.26	23.62	42.86	0.26
190	0.106	6.53	1.11	89.76	2.6
189	-0.135	6.17	4.2	79.34	10.29
188	-0.507	92.06	6.14	1.41	0.39
187	-0.507	92.1	6.15	1.41	0.34
186	-0.549	91.11	4.88	1.42	2.59
185	-0.768	84.37	15.53	0	0.1

184	-0.894	79.8	19.69	0.25	0.26
183	-2.029	55.24	32.34	11.02	1.4
182	**-2.03**	**55.24**	**32.35**	**11.03**	**1.38**
181	**-3.494**	**21.69**	**0.94**	**58.84**	**18.53**
180	-3.494	21.89	1.06	59.28	17.76
179	-3.653	20.14	5.31	74.35	0.21
178	-3.85	93.07	0.28	0.48	6.16
177	-3.899	6.17	1.33	5.54	86.96
176	-3.949	15.23	2.03	4.3	78.45
175	-4.692	4.1	30.74	1.07	64.09
174	-4.869	17.9	11.47	1.35	69.27
173	-4.872	18.1	11.33	1.47	69.1
172	-5.056	5.04	1.78	8.68	84.5
171	-5.238	2.69	46.26	0.84	50.2
170	-5.429	72.77	26.15	0.02	1.06
169	-5.593	74.12	20	1.22	4.66

8.3.2 (C_2 Symmetry)

MO	Energy/eV	C,H	N	Fe	L_2
193	0.79	95.15	2.92	0.49	1.44
192	0.7	99.69	0.19	0.04	0.09
191	0.396	33.52	23.39	42.83	0.26
190	0.105	6.67	1.12	89.23	2.97
189	-0.094	6.42	3.91	79.16	10.51
188	-0.477	92.3	5.92	1.38	0.4
187	-0.485	92.34	6.06	1.37	0.23
186	-0.534	91.56	5.04	1.29	2.11
185	-0.741	84.66	15.22	0	0.12
184	-0.861	80.36	19.39	0.13	0.12
183	-1.992	56.13	32.56	10.38	0.93
182	**-1.992**	**56.14**	**32.51**	**10.37**	**0.98**
181	**-3.541**	**24.03**	**0.96**	**63.59**	**11.41**
180	-3.544	24.24	0.98	63.63	11.14
179	-3.629	20.88	5.35	73.53	0.24
178	-3.815	99.29	0.26	0.35	0.09
177	-4.755	11.46	6.98	1.25	80.32
176	-4.796	12.77	7.43	1.28	78.52
175	-4.863	4.14	58.45	0.56	36.84
174	-5.131	8.01	2.14	19.06	70.79
173	-5.16	7.93	14	2.14	75.93
172	-5.257	28.55	16.64	1.59	53.22
171	-5.319	18.68	11.2	2.88	67.24

170	-5.46	57.73	19.7	0.45	22.12
169	-5.553	72.05	18.83	0.83	8.29

8.3.2 (D_{2h} Symmetry)

MO	Energy/eV	C,H	N	Fe	L_2
193	0.697	96.33	2.87	0.45	0.35
192	0.624	99.9	0.04	0	0.06
191	0.236	32.67	23.28	43.64	0.4
190	0.062	6.73	1.02	90.21	2.04
189	-0.285	6.9	6.06	72.63	14.4
188	-0.562	92.49	6.21	1.27	0.04
187	-0.568	91.94	6.19	1.33	0.54
186	-0.604	91.11	4.98	1.42	2.49
185	-0.835	83.97	15.93	0	0.11
184	-0.959	79.69	20.11	0.01	0.19
183	-2.121	55.82	33.21	10.76	0.2
182	**-2.128**	**55.66**	**31.91**	**10.03**	**2.4**
181	**-3.604**	**22.34**	**0.43**	**63.52**	**13.71**
180	-3.745	25.81	1.29	65.14	7.76
179	-3.779	19.7	5.38	74.79	0.13
178	-3.938	99.59	0.21	0	0.2
177	-4.76	2.36	2.01	0	95.63
176	-4.808	5.25	0.73	0.09	93.93
175	-4.813	5.37	1.74	0.73	92.16
174	-4.816	2.99	1.61	0.97	94.43
173	-4.987	3.61	58.97	0.52	36.9
172	-5.168	32.74	18.92	0.05	48.29
171	-5.401	9.36	12.61	0.66	77.38
170	-5.509	71.83	25.11	0	3.06
169	-5.627	67.82	24.91	0.27	7

8.4

MO	Energy/eV	C,H	N	Fe	L_2
187	0.685	96.47	2.67	0.48	0.38
186	0.607	99.96	0.04	0	0
185	0.082	31.65	23.66	44.69	0
184	-0.18	4.62	1.14	92.17	2.07
183	-0.487	6.31	10.4	49.78	33.51
182	-0.581	92.67	6.08	1.19	0.06
181	-0.581	92.67	6.08	1.19	0.06
180	-0.615	89.6	4.71	2.32	3.38

179	-0.838	84.25	15.74	0	0
178	-0.976	79.91	20.09	0	0
177	-2.169	58.36	33.28	8.22	0.15
176	**-2.169**	**58.36**	**33.28**	**8.22**	**0.15**
175	**-3.687**	**15.6**	**0.33**	**53.66**	**30.42**
174	-3.687	15.6	0.33	53.66	30.42
173	-3.908	21.18	5.74	73.08	0
172	-3.954	98.9	0.26	0.84	0
171	-4.677	3.59	4.13	2.18	90.1
170	-4.677	3.59	4.13	2.18	90.1
169	-4.788	18.85	8.38	7.49	65.27
168	-4.788	18.85	8.38	7.49	65.27
167	-5.229	2.68	86.22	0	11.1
166	-5.501	73.21	26.78	0	0
165	-5.671	83.88	13.53	0.75	1.83
164	-5.72	50.66	45.96	3.39	0
163	-5.785	90.28	9.34	0.24	0.15

8.5

MO	Energy/eV	C,H	N	Fe	L_2
171	0.776	96.49	2.82	0.48	0.22
170	0.692	99.96	0.04	0	0
169	0.51	12.03	5.54	71.36	11.07
168	0.301	32.73	22.79	44.48	0
167	-0.119	5.26	2.06	90.6	2.08
166	-0.494	92.58	5.98	1.42	0.03
165	-0.494	92.58	5.98	1.42	0.03
164	-0.507	92.64	5.37	0.37	1.62
163	-0.75	84.64	15.36	0	0
162	-0.878	80.4	19.6	0	0
161	-2.018	56.08	33.05	10.55	0.31
160	**-2.018**	**56.08**	**33.05**	**10.55**	**0.31**
159	**-3.651**	**26.59**	**1.11**	**65.25**	**7.05**
158	-3.651	26.59	1.11	65.25	7.05
157	-3.662	20.77	5.17	74.06	0
156	-3.834	99.73	0.21	0.06	0
155	-4.57	4.89	60.46	2.22	32.43
154	-5.405	73	27	0	0
153	-5.412	45.87	24.85	2.97	26.32
152	-5.412	45.87	24.85	2.97	26.32
151	-5.553	74.59	23.12	0.08	2.21
150	-5.584	51.45	45.67	2.88	0

149	-5.699	89.12	10.68	0.16	0.04
148	-5.699	89.12	10.68	0.16	0.04
147	-5.736	94.79	5.21	0	0

8.15

MO	Energy/eV	C,H	N	Fe	L_2
167	0.148	96.56	2.44	0.65	0.35
166	0.088	99.95	0.04	0.01	0
165	-0.509	31.24	23	45.49	0.27
164	-0.739	9.96	6.44	74.15	9.44
163	-1.116	92.12	6.55	1.27	0.06
162	-1.116	92.07	6.56	1.31	0.06
161	-1.162	86.42	4.7	5.59	3.29
160	-1.43	82.16	17.44	0.11	0.3
159	-1.432	4.29	2.86	64.87	27.99
158	-1.552	78.13	21.81	0.01	0.04
157	-2.805	57.39	32.95	9.09	0.57
156	**-2.805**	**57.31**	**32.97**	**9.11**	**0.6**
155	**-4.52**	**22.29**	**3.88**	**71.91**	**1.91**
154	-4.524	26.33	2.13	68.17	3.37
153	-4.531	23.69	4.63	70.38	1.3
152	-4.575	99.79	0.21	0	0
151	-5.954	2.83	80.13	0.14	16.9
150	-6.091	73.13	26.41	0.16	0.3
149	-6.216	83.47	14.32	0.63	1.58
148	-6.307	91.27	7.56	0.99	0.19
147	-6.307	91.23	7.54	1.03	0.2
146	-6.335	94.91	5.01	0.03	0.04
145	-6.351	49.42	46.57	3.95	0.05
144	-6.362	61.47	24.8	12.05	1.69
143	-6.363	60.54	26.7	11.26	1.5

8.6

MO	Energy/eV	C,H	N	Fe	L_2
193	-0.381	6.68	1.3	5.16	86.86
192	-0.383	16.35	14.83	14.86	53.97
191	-0.536	21.58	12.52	30.74	35.17
190	-0.582	4.06	0.85	90.66	4.42
189	-1.084	91.46	6.51	1.35	0.67
188	-1.085	91.35	6.59	1.42	0.64
187	-1.123	89.79	5.19	1.73	3.3

186	-1.186	6.21	7.98	55.6	30.21
185	-1.386	82.27	16.98	0.01	0.74
184	-1.518	77.82	21.52	0.23	0.43
183	-2.763	57.23	32.67	8.57	1.54
182	**-2.763**	**57.23**	**32.69**	**8.57**	**1.51**
181	**-4.496**	**26.26**	**1.89**	**64.91**	**6.94**
180	-4.496	23.7	2.73	67.88	5.7
179	-4.501	20.15	5.33	72.92	1.6
178	-4.54	97.78	0.29	1.72	0.2
177	-5.88	3.71	79.48	0.19	16.62
176	-5.907	32.69	15.81	0.06	51.45
175	-6.039	12.71	6.83	0.81	79.65
174	-6.135	52.56	17.72	1.93	27.8
173	-6.187	81.63	15.15	0.6	2.62
172	-6.269	68.34	9.59	5.48	16.58
171	-6.278	80.22	7.38	2.37	10.03
170	-6.289	67.16	17.96	4.02	10.86
169	-6.298	54.13	19.58	6.01	20.29

8.8

MO	Energy/eV	C,H	N	Fe	L_2
199	-1.153	90.83	6.79	1.33	1.05
198	-1.153	90.83	6.79	1.33	1.05
197	-1.189	86.26	5.07	1.68	6.99
196	-1.205	15.55	4.36	0	80.09
195	-1.358	5.79	3.8	1.93	88.49
194	-1.445	5.75	8.28	49.95	36.01
193	-1.515	68.02	13.13	0	18.85
192	-1.604	76.26	22	0.56	1.18
191	-1.897	3.2	1.56	4.74	90.51
190	-1.897	3.2	1.56	4.74	90.51
189	-2.881	57.88	32.5	7.58	2.05
188	**-2.881**	**57.88**	**32.5**	**7.58**	**2.05**
187	**-4.642**	**99.7**	**0.27**	**0.01**	**0.03**
186	-4.678	18.15	6.94	74.51	0.4
185	-4.705	25.23	2.61	65.51	6.64
184	-4.705	25.23	2.61	65.51	6.64
183	-6.028	5.58	76.95	0.21	17.26
182	-6.113	70.42	26.31	0	3.26
181	-6.257	80.68	14.72	0.71	3.89
180	-6.335	84.23	9.15	3.92	2.7
179	-6.335	84.23	9.15	3.92	2.7

178	-6.369	93.54	5.13	0.32	1
177	-6.374	61.85	24.06	8.77	5.33
176	-6.374	61.85	24.06	8.77	5.33
175	-6.43	48.56	46.15	4.36	0.93

8.10

MO	Energy/eV	C,H	N	Fe	L_2
199	0.095	88.36	1.89	1.24	8.5
198	0.057	99.04	0.08	0.15	0.73
197	-0.627	28.03	25.2	44.4	2.37
196	-0.705	3.73	0.8	89.81	5.66
195	-1.145	91.04	6.73	1.79	0.44
194	-1.149	90.76	6.65	1.44	1.15
193	-1.159	77.18	4.83	7.51	10.49
192	-1.376	1.74	4.09	40.17	53.99
191	-1.479	79.25	17.44	0.17	3.13
190	-1.585	77.61	22.06	0.1	0.23
189	-2.848	56.34	32.25	9.51	1.9
188	**-2.854**	**53.78**	**30.39**	**10.99**	**4.84**
187	**-4.607**	**17.43**	**6.38**	**75.99**	**0.21**
186	-4.622	99.05	0.23	0.11	0.61
185	-4.668	28.82	3.74	63.72	3.73
184	-4.671	29.12	3.56	63.31	4.01
183	-5.29	4.11	33.02	3.05	59.81
182	-6.132	72.12	26.32	0.12	1.44
181	-6.236	70.64	23.08	2.81	3.47
180	-6.329	90.59	8.71	0.17	0.52
179	-6.33	90.53	8.58	0.48	0.41
178	-6.354	94.56	5.08	0.03	0.32
177	-6.387	48.17	47.53	3.85	0.46
176	-6.462	60.62	19.84	14.15	5.39
175	-6.463	60.42	19.64	14.11	5.82

8.16

MO	Energy/eV	C,H	N	Fe	L_2
203	-0.495	9.73	9.02	10.14	71.12
202	-0.495	9.74	9.01	10.15	71.09
201	-0.754	5.79	2.76	80.22	11.22
200	-0.889	28.4	24.38	47.17	0.05
199	-1.041	4.02	6.17	71.76	18.05
198	-1.141	90.79	5.55	1.1	2.57

197	-1.146	91.45	6.22	1.52	0.8
196	-1.147	91.47	6.22	1.52	0.78
195	-1.435	82.58	17.34	0	0.09
194	-1.578	78.12	21.74	0	0.14
193	-2.87	59.84	33.16	6.65	0.35
192	**-2.871**	**59.84**	**33.17**	**6.65**	**0.34**
191	**-4.603**	**99.77**	**0.21**	**0**	**0.02**
190	-4.82	18.87	7.31	73.81	0.01
189	-4.96	27.62	6.03	59.3	7.05
188	-4.96	27.62	6.03	59.3	7.04
187	-5.776	5.06	70.97	1.52	22.45
186	-6.119	73.92	26.03	0	0.05
185	-6.234	79.44	19.16	0.38	1.02
184	-6.333	90.63	8.6	0.51	0.25
183	-6.333	90.63	8.59	0.51	0.26
182	-6.359	94.95	5.04	0	0.01
181	-6.385	48.95	46.38	4.66	0.01
180	-6.458	54.57	18.29	16.59	10.56
179	-6.458	54.56	18.27	16.59	10.58

8.17

MO	Energy/eV	C,H	N	Fe	L_2
223	0.038	29.26	4.21	32.47	34.06
222	0.013	31.61	4.17	32.02	32.2
221	-0.732	26.56	22.59	49.67	1.18
220	-0.738	2.9	0.53	88.19	8.38
219	-1.106	91.49	6.26	1.49	0.76
218	-1.108	91.23	6.29	1.72	0.76
217	-1.116	87.73	5.41	1.43	5.43
216	-1.412	81.6	17.18	0.03	1.19
215	-1.515	78.56	21.14	0.08	0.22
214	-1.566	5.03	5.89	27.21	61.87
213	-2.79	59.61	32.53	7.33	0.54
212	**-2.791**	**59.47**	**32.48**	**7.56**	**0.49**
211	**-4.529**	**99.59**	**0.23**	**0.01**	**0.17**
210	-4.709	17.74	7.61	74.53	0.12
209	-4.864	29.97	6.89	59.77	3.38
208	-4.867	29.77	6.87	59.95	3.41
207	-5.535	4.31	53.17	1.43	41.09
206	-6.072	72.15	26.7	0.02	1.12
205	-6.179	76.74	20.65	0.51	2.11
204	-6.286	89.98	9.14	0.49	0.38

203	-6.287	90.12	9.17	0.35	0.36
202	-6.315	94.57	5.23	0.01	0.19
201	-6.331	48.85	46.4	4.66	0.08
200	-6.489	55.36	15.43	20.34	8.87
199	-6.497	55.89	15.24	20.48	8.39

8.12

MO	Energy/eV	C,H	N	Fe	L_2
199	-0.053	74.2	2.24	3.3	20.25
198	-0.14	27.58	6.22	14.09	52.11
197	-0.739	3.51	0.84	87.21	8.44
196	-1.029	26.64	26.67	45.23	1.46
195	-1.264	88.93	6.74	2.76	1.56
194	-1.27	90.41	6.93	1.93	0.73
193	-1.296	81.33	5.25	5.41	8.01
192	-1.616	78.25	18.17	0.44	3.14
191	-1.716	76.97	22.76	0.08	0.18
190	-2.328	2.29	4.35	39.83	53.53
189	-3.059	59.47	31.82	6.95	1.76
188	**-3.066**	**59.55**	**31.86**	**7.04**	**1.55**
187	**-4.776**	**99.09**	**0.28**	**0.01**	**0.61**
186	-5.027	16.97	8.54	74.21	0.29
185	-5.135	28.39	7.68	59.62	4.32
184	-5.157	28.34	7.14	59.91	4.61
183	-5.984	5.14	33.86	3.51	57.5
182	-6.252	70.21	26.33	0.27	3.18
181	-6.36	78.3	17.8	1.92	1.98
180	-6.428	86.78	8.85	2.45	1.92
179	-6.442	90.52	8.7	0.31	0.47
178	-6.458	94.07	5.61	0.06	0.26
177	-6.581	45.91	45.2	6.2	2.68
176	-6.627	36.88	14.76	22.74	25.63
175	-6.686	12.19	35.68	9.07	43.07

8.18

MO	Energy/eV	C,H	N	Fe	L_2
169	-0.859	6.38	2.37	80.55	10.7
168	-0.879	12.75	11.07	13.97	62.21
167	-0.879	12.81	11.11	13.55	62.53
166	-1.205	75.99	7.51	12.54	3.96
165	-1.21	29.36	24.81	45.71	0.12

164	-1.264	90.07	6.41	2.11	1.41
163	-1.264	90.03	6.41	2.14	1.42
162	-1.588	79.21	18.72	1.8	0.27
161	-1.594	19.21	10.48	49.25	21.07
160	-1.714	77.35	22.62	0	0.03
159	-3.064	62.01	32.87	4.89	0.24
158	**-3.064**	**62**	**32.85**	**4.89**	**0.26**
157	**-4.764**	**99.79**	**0.21**	**0**	**0**
156	-5.159	18.55	9.26	72.18	0.02
155	-5.349	31.35	10.14	52.46	6.06
154	-5.349	31.44	10.13	52.4	6.03
153	-6.132	5.4	73.49	1.84	19.27
152	-6.258	73.94	25.78	0.09	0.19
151	-6.357	79.74	18.77	0.68	0.8
150	-6.443	90.56	8.99	0.37	0.09
149	-6.443	90.55	8.99	0.38	0.09
148	-6.463	94.96	5.01	0.02	0.02
147	-6.578	47.54	46.19	6.27	0.01
146	-6.719	54.57	13.38	26.4	5.66
145	-6.72	54.56	13.47	26.34	5.63

Table S9.2. Major TDDFT-predicted excited state contributions for compounds not included in main text using the MPWLYP exchange correlation functional (the MLCT signals are emboldened).

8.2

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
10,11	636	15720	0.4659	H-3→L/L+1 (80%), H-5→L/L+1 (11%)
12	622	16083	0.0195	H-1→L (28%), H→L+1 (28%), H-5→L (22%), H-4→L+1 (14%), H-1→L+5 (3%), H→L+6 (3%)
13,14	**502**	**19937**	**0.0602**	**H/H-1→L+2 (92%), H-6→L/L+1 (4%), H/H-1→L+3 (3%)**
18,19	**470**	**21291**	**0.3391**	**H/H-1→L+3 (39%), H/H-1→L+3 (20%), H-6→L/L+1 (15%), H-6→L/L+1 (11%), H/H-1→L+2 (3%), H-10→L/L+1 (2%)**
27,28	438	22849	0.1285	H/H-1→L+4 (93%), H-1→L+6 (4%)
32	431	23206	0.0280	H-4→L+2 (97%)
35	425	23518	0.0143	H-5→L+2 (82%), H-3→L+2 (11%), H-1→L+5 (3%), H→L+6 (3%)

39	413	24234	0.0239	H-4→L+3 (89%), H-1→L+5 (5%), H→L+6 (4%)
40	411	24358	0.0129	H-3→L+3 (76%), H-5→L+3 (22%)
45,46	388	25765	0.2108	H-10→L/L+1 (68%), H-11→L/L+1 (16%), H-3→L+5/6 (5%), H-12→L/L+1 (3%)
48	384	26070	0.0117	H-4→L+4 (94%), H-3→L+5 (4%)
49,50	379	26355	0.0386	H-3/4→L+5/6 (53%), H-3/4→L+5/6 (34%), H-5→L+4/6 (5%), H-2→L+7 (3%), H-10→L (2%)
51	379	26397	0.1260	H-3→L+5 (81%), H-10→L+1 (7%), H-4→L+4 (4%), H-5→L+5 (3%)
53	377	26531	0.0459	H-5→L+4 (88%), H-3→L+6 (5%), H-3→L+4 (3%)
54,55	373	26829	0.0341	H-5→L+5/6 (53%), H-11→L/L+1 (31%), H-10→L/L+1 (5%), H-3→L+6 (2%), H-2→L+7 (2%), H-12→L+1 (2%)
63	350	28542	0.0169	H-3→L+7 (91%), H-12→L+1 (3%)
64,65	350	28605	0.4931	H-12→L/L+1 (57%), H-13→L/L+1 (16%), H-3/4→L+7 (7%), H-10→L/L+1 (5%), H-16→L/L+1 (4%), H-11→L/L+1 (3%)
67	348	28699	0.0967	H-4→L+7 (73%), H-12→L (7%), H→L+8 (5%), H-13→L (4%), H-14→L+1 (2%), H-15→L (2%)
69	344	29084	0.0130	H-5→L+7 (78%), H-1→L+9 (8%), H-1→L+8 (5%), H-3→L+7 (3%)
73,75	340	29411	0.0119	H-15/16→L+1 (20%), H-14→L (22%), H-16→L (18%), H-20→L+1 (7%), H-17→L+1 (5%), H-19→L (5%), H-20→L (4%), H-18→L (3%), H-19→L+1 (2%), H-15→L+1 (2%)
74,76	340	29423	0.0260	H-16→L/L+1 (56%), H-15→L+1 (10%), H-16→L/L+1 (8%), H-18→L (4%) H-19→L (3%), H-19→L+1 (2%), H-17→L+1 (2%), H-20→L+1 (2%)

8.3.2

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
6,7	638	15675	0.5159	H-3→L/L+1 (95%), H-8→L/L+1 (2%)
17,18	**480**	**20845**	**0.0623**	**H/H-1→L+2 (94%), H/H-1→L+3 (4%)**
20,21	**457**	**21887**	**0.1317**	**H/H-1→L+3 (77%), H-8→L/L+1 (10%), H/H-1→L+7 (9%)**

22,23	457	21897	0.0171	H/H-1→L+7 (75%), H/H-1→L+3 (10%), H/H-1→L+9, H/H-1→L+8
25,26	431	23176	0.2367	H-8→L/L+1 (74%), H/H-1→L+4 (9%), H/H-1→L+3 (6%), H-12→L/L+1 (3%), H-3→L/L+1 (2%)
30,31	418	23915	0.2827	H/H-1→L+4 (90%), H-8→L/L+1 (5%)
46,47	374	26766	0.0434	H-3→L+5/6 (59%), H-11→L/L+1 (35%), H-12→L/L+1 (4%)
53,54	352	28400	0.6317	H-12→L/L+1 (71%), H-13→L/L+1 (9%), H-16→L/L+1 (7%), H-19→L/L+1 (4%), H-11→L/L+1 (4%), H-8→L/L+1 (2%)
58,59	344	29074	0.0534	H-16→L/L+1 (90%), H-12→L/L+1 (4%)
73,74	330	30305	0.1159	H-19→L/L+1 (67%), H-20→L/L+1 (18%), H-6/7→L+2 (6%), H-12→L/L+1 (2%)
77,78	329	30436	0.0555	H-20→L/L+1 (56%), H/H-1→L+9 (20%), H-19→L/L+1 (15%), H-6/7→L+2 (2%), H/H-1→L+8 (2%)

8.4

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
7,8	641	15602	0.5878	H-3→L/L+1 (95%), H-8→L/L+1 (2%)
18,19	**480**	**20820**	**0.0610**	**H/H-1→L+2 (97%)**
21,22	**455**	**21967**	**0.1493**	**H/H-1→L+3 (95%)**
23	448	22313	0.0001	H-2→L+2 (99%)
26,27	420	23823	0.0520	H/H-1→L+4 (98%)
34,35	396	25268	0.3302	H-8→L/L+1 (67%), H-9→L/L+1 (21%), H-10→L/L+1 (5%)
40,41	379	26394	0.0618	H-9→L/L+1 (68%), H-8→L/L+1 (15%), H-10→L/L+1 (9%), H-3→L+5/6 (5%)
44,45	375	26694	0.0508	H-3→L+5/6 (90%), H-9→L/L+1 (6%)
50,51	355	28149	0.6206	H-10→L/L+1 (76%), H-14→L/L+1 (8%), H-8→L/L+1 (7%), H-9→L/L+1 (3%)
61,62	346	28896	0.0158	H-14→L/L+1 (89%), H-10→L/L+1 (5%)
71,72	334	29905	0.1021	H-6/7→L+2
77,78	321	31120	0.2258	H-6/7→L+3

8.5

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
6,7	640	15625	0.5103	H-3→L/L+1 (93%), H-4→L/L+1 (5%)

9,10	488	20511	0.0663	H-4→L/L+1 (82%), H/H-1→L+2 (12%), H-3→L/L+1 (2%), H/H-1→L+3 (2%)
12,13	**466**	**21438**	**0.1150**	**H/H-1→L+2 (81%), H/H-1→L+3 (10%), H-4→L/L+1 (7%)**
15,16	**442**	**22646**	**0.4594**	**H/H-1→L+3 (85%), H/H-1→L+2 (6%), H-4→L/L+1 (4%), H-3→L/L+1 (2%)**
24,25	409	24477	0.1958	H/H-1→L+4 (97%)
32,33	380	26325	0.0371	H-3→L+5/6 (82%), H-5→L/L+1 (17%)
37,38	375	26692	0.0167	H-5→L/L+1 (78%), H-3→L+5/6 (16%), H-8→L/L+1 (4%)
43,44	350	28589	0.6539	H-8→L/L+1 (87%), H-12→L/L+1 (4%), H-5→L/L+1 (3%)
54,55	340	29417	0.0637	H-12→L/L+1 (93%), H-8→L/L+1 (3%)
67,68	312	32035	0.0743	H-4→L+5/6 (98%)
73,74	299	33402	0.1839	H-18→L/L+1 (64%), H-17→L/L+1 (25%), H/H-1→L+10 (3%), H-3→L+11/12 (2%)

8.6

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
6,7	643	15553	0.5768	H-3→L/L+1 (95%), H→L (2%)
11	440	22703	0.0003	H-2→L+2 (74%), H-1→L+2 (24%)
12,13	**436**	**22941**	**0.0501**	**H/H-1→L+2 (80%), H-1/2→L+2 (14%), H→L+2 (2%), H→L+3 (2%)**
15,16	**416**	**24036**	**0.1177**	**H/H-1→L+3 (70%), H-1/2→L+3 (11%) H-5→L/L+1 (8%), H-4→L/L+1 (7%), H→L+3 (2%)**
17,18	411	24343	0.0566	H-5→L/L+1 (86%), H/H-1→L+3 (8%), H-2→L+3 (2%), H-4→L+1 (2%)
25,26	391	25550	0.1408	H-4→L/L+1 (57%), H-7→L/L+1 (12%), H-8→L/L+1 (11%), H-3→L+4 (6%), H/H-1→L+5 (3%), H-5→L+1 (2%)
27	391	25574	0.0211	H-3→L+4 (85%), H-4→L+1 (8%)
31	381	26242	0.0603	H→L+5 (72%), H→L+7 (7%), H-1→L+6 (6%), H-2→L+6 (4%), H-1→L+5 (2%), H-8→L (2%)
32	381	26278	0.0854	H-1→L+5 (59%), H-2→L+5 (23%), H-8→L+1 (7%), H-4→L+1 (2%)
33	380	26332	0.0231	H→L+7 (32%), H-7→L (26%), H-8→L (11%), H-1→L+6 (10%), H→L+5 (9%), H-4→L (4%), H-2→L+6 (3%)

39,40	368	27174	0.0448	H-14→L/L+1 (80%), H-8→L/L+1 (8%), H-14→L+1/L (3%)
42,43	366	27325	0.0174	H-3→L+6/7 (79%), H-13→L/L+1 (6%) H-11→L/L+1 (5%)
44	365	27416	0.0156	H-10→L (33%), H-9→L+1 (20%), H-11→L+1 (20%), H-12→L (14%), H-3→L+7 (5%), H-13→L+1 (5%)
45,46	363	27527	0.0349	H-9→L/L+1 (27%), H-12→L/L+1 (23%), H-10→L/L+1 (17%), H-11→L/L+1 (14%), H-3→L+5 (9%), H-8→L/L+1 (3%)
47	360	27757	0.1954	H-12→L (28%), H-11→L+1 (25%), H-8→L (9%), H-2→L+4 (9%), H-9→L+1 (7%), H-1→L+6 (3%), H→L+7 (3%), H-4→L (2%), H-1→L+4 (2%), H-7→L (2%)
49	358	27908	0.7603	H-8→L (30%), H-13→L+1 (24%), H-12→L (18%), H-4→L (8%), H-14→L (4%), H-9→L+1 (3%), H→L+5 (2%), H-7→L (2%), H-11→L+1 (2%)
50	357	27977	0.1205	H-10→L (38%), H-9→L+1 (27%), H-11→L+1 (14%), H-13→L+1 (4%), H→L+7 (3%)
71,72	311	32126	0.0731	H-17→L/L+1 (63%), H→L+11 (16%), H-1→L+10 (12%), H-2→L+10 (2%)
73	311	32150	0.0494	H-17→L+1 (58%), H→L+11 (22%), H-1→L+10 (10%)

8.15

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
6,7	646	15476	0.5875	H-3→L/L+1 (97%)
12,13	**437**	**22892**	**0.0501**	**H-1/2→L+2 (76%), H→L+2 (20%), H-1→L+4 (3%)**
16,17	**417**	**23963**	**0.1640**	**H-1/2→L+4 (63%), H→L+4 (16%), H-3→L+3 (13%), H-4→L/L+1 (4%)**
18	417	23977	0.0505	H-3→L+3 (74%), H-2→L+4 (12%), H→L+4 (12%)
22,23	394	25382	0.1118	H-5→L/L+1 (48%), H-4→L/L+1 (38%), H/H-1→L+5 (4%), H-6→L/L+1 (4%)
29,30	382	26200	0.1077	H-1/2→L+5 (56%), H→L+5 (15%), H-6→L/L+1 (15%), H-4→L/L+1 (7%),

				H-5→L (2%)
39,40	366	27350	0.0117	H-3→L+6/7 (83%), H-9→L/L+1(14%)
42,43	360	27773	1.3015	H-6→L/L+1 (49%), H-9→L/L+1 (18%), H-4→L/L+1 (17%), H/H-1→L+5 (4%), H-5→L/L+1 (3%), H-1→L+4 (2%), H-2→L+5 (2%)
63,64	312	32048	0.0738	H-15→L/L+1 (93%)
68	285	35091	0.0423	H-4→L+3 (99%)

8.17

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
4,5	651	15359	0.5751	H→L/L+1 (93%), H-4→L/L+1 (3%)
6	647	15459	0.0154	H-3→L+1 (49%), H-2→L (44%), H-1→L+2 (4%), H→L+1 (2%)
11,12	450	22216	0.1519	H-4→L/L+1 (88%), H-4→L/L+1 (4%), H-6→L/L+1 (2%), H→L/L+1 (2%)
15	410	24414	0.0002	H-1→L+3 (100%)
22,23	**385**	**25965**	**0.0172**	**H-2/3→L+3 (86%), H-6→L/L+1 (8%), H-5→L/L+1 (6%)**
24,25	**374**	**26731**	**0.0020**	**H-2/3→L+4 (66%), H-6→L/L+1 (21%), H-9→L/L+1 (4%), H→L+6/7 (3%), H-5→L/L+1 (3%)**
27,28	370	27056	0.0177	H→L+6/7 (86%), H-9→L/L+1 (8%), H-2→L+4 (2%)
33	361	27708	0.0714	H-1→L+7 (73%), H-1→L+5 (8%), H-6→L+1 (4%), H-7→L+1 (3%), H-8→L+1 (3%), H-3→L+9 (2%)
34,35	361	27722	0.7879	H-6→L/L+1 (35%), H-2/3→L+4 (21%), H-9→L/L+1 (8%), H-7/8→L+1 (6%), H-1→L+7 (5%), H-6→L/L+1 (5%), H-2/3→L+3 (4%), H-2/3→L+5 (2%)
36,37	360	27756	0.0797	H-8→L (28%), H-7→L (24%), H-7→L+1 (18%), H-8→L+1 (14%), H-2/3→L+4 (2%), H-2→L+7 (2%), H-12→L (2%), H-6→L (2%), H-9→L (2%)
38	360	27779	0.1150	H-8→L+1 (24%), H-7→L+1 (23%), H-7→L (14%), H-8→L (11%), H-3→L+6 (6%), H-6→L+1 (5%), H-2→L+7 (4%), H-9→L (3%),

				H-2→L+4 (3%)
51,52	338	29542	0.4231	H-2/3→L+5 (87%), H-9→L/L+1 (4%), H-3→L+7 (3%)
53	338	29595	0.0102	H→L+8 (97%)
59	322	31018	0.1382	H-4→L+2 (98%)
67,68	306	32634	0.1724	H-16→L/L+1 (73%), H-15→L/L+1 (13%), H-16→L/L+1 (5%), H-4→L+4 (2%)
74	287	34845	0.0110	H-4→L+5 (46%), H-18→L+1 (39%), H-4→L+6 (6%), H-18→L (4%), H-4→L+7 (3%)
75,76	287	34874	0.0501	H-4→L+6/7 (89%), H-4→L+5 (8%)

8.12

Excited State	*Wavelength (nm)*	*Energy (cm^{-1})*	*Oscillator Strength, f*	*% Contributions*
4,5	656	15239	0.5973	H→L/L+1 (89%), H→L+1/L (9%)
13,14	434	23065	0.0741	H-4→L/L+1 (88%), H-4→L+1/L (3%), H-6→L/L+1 (2%), H-12→L+1 (2%)
20	394	25354	0.0003	H-1→L+3 (100%)
22,24	**382**	**26173**	**0.1021**	**H-6→L+1 (33%), H-6→L (31%), H-2→L+3/4 (14%), H-3→L+3/4 (11%), H-9→L/L+1 (4%), H-12→L+1 (2%)**
25	376	26612	0.1412	H-2→L+3 (66%), H-9→L (14%), H-3→L+4 (9%), H-6→L (5%)
26	375	26685	0.0213	H-9→L+1 (48%), H-9→L (35%), H-6→L+1 (6%), H-2→L+4 (3%), H→L+7 (2%)
28	373	26778	0.0718	H-3→L+3 (69%), H-2→L+4 (14%), H-6→L+1 (7%), H-9→L+1 (4%), H-12→L+1 (2%)
35,36	**361**	**27733**	**0.4438**	**H-3→L+3/4 (41%), H-2→L+3/4 (38%), H-6→L/L+1 (4%), H→L+7 (4%), H-12→L/L+1 (3%), H-9→L+1 (2%), H→L+6 (2%)**
39	358	27899	0.0785	H→L+6 (86%), H-9→L+1 (5%), H-3→L+4 (2%)
40	358	27933	0.1367	H→L+7 (82%), H-3→L+4 (7%), H-9→L (5%)
41	352	28430	0.0768	H-14→L (48%), H-12→L (26%), H-14→L+1 (13%), H-12→L+1 (6%)
44	348	28729	0.1664	H-12→L+1 (37%), H-14→L+1 (19%), H-4→L+2 (17%), H-12→L (12%),

				H-14→L (2%), H-17→L (2%)
47	346	28900	0.0201	H-1→L+5 (86%), H-4→L+2 (11%)
50	346	28940	0.1360	H-4→L+2 (61%), H-14→L+1 (12%), H-1→L+5 (11%), H-12→L+1 (4%), H-14→L (3%), H-12→L+2 (2%)
51,52	342	29263	0.1468	H-15→L (30%), H-14→L (20%) H-12→L (17%), H-15→L+1 (16%), H-17→L+1 (4%), H-12→L+1 (3%), H-6→L (2%)
53	341	29358	0.1793	H-14→L+1 (50%), H-12→L+1 (21%), H-17→L (8%), H-15→L (8%), H-14→L (4%), H-6→L+1 (2%)
57,59	330	30316	0.4567	H-2/3→L+5
58	330	30278	0.0103	H-5→L+2
64	322	31092	0.0146	H-18→L (31%), H-17→L+1 (31%), H-18→L+1 (28%), H-17→L (6%)
66	321	31196	0.0179	H-18→L (42%), H-18→L+1 (37%), H-17→L (5%), H-17→L+1 (5%)
70	318	31463	0.1055	H-17→L (61%), H-18→L (15%), H-18→L+1 (5%), H-17→L+1 (5%), H-12→L+1 (4%)
72	316	31598	0.1176	H-17→L+1 (44%), H-18→L+1 (27%), H-18→L (11%), H→L+9 (4%) H-17→L (3%), H-12→L (3%)

Table S9.2. Optimized coordinates for **8.1** using the MPWLYP exchange correlation functional.

N	-1.94913	0.	0.00347
N	0.	-1.94913	-0.00347
N	1.94913	0.	0.00347
C	1.11661	2.76369	-0.00993
C	-0.70721	4.16758	-0.02814
C	-1.11661	2.76369	-0.00993
C	-2.76369	1.11661	0.00993
C	-4.16758	0.70721	0.02814
C	-4.16758	-0.70721	0.02814
C	-2.76369	-1.11661	0.00993
C	-1.11661	-2.76369	-0.00993
C	-0.70721	-4.16758	-0.02814
C	0.70721	-4.16758	-0.02814
C	1.11661	-2.76369	-0.00993

C	2.76369	-1.11661	0.00993
C	4.16758	-0.70721	0.02814
C	4.16758	0.70721	0.02814
C	2.76369	1.11661	0.00993
C	0.70721	4.16758	-0.02814
N	0.	1.94913	-0.00347
N	2.39652	2.39652	0.
N	-2.39652	2.39652	0.
N	-2.39652	-2.39652	0.
N	2.39652	-2.39652	0.
Fe	0.	0.	0.
C	5.36899	-1.42864	0.04774
C	6.57094	-0.70643	0.06801
H	7.52506	-1.24313	0.08433
C	6.57094	0.70643	0.06801
H	7.52506	1.24313	0.08433
C	5.36899	1.42864	0.04774
H	5.36554	-2.52289	0.04876
H	5.36554	2.52289	0.04876
C	1.42864	5.36899	-0.04774
C	0.70643	6.57094	-0.06801
H	1.24313	7.52506	-0.08433
C	-1.42864	5.36899	-0.04774
C	-0.70643	6.57094	-0.06801
H	-1.24313	7.52506	-0.08433
C	-5.36899	1.42864	0.04774
C	-6.57094	0.70643	0.06801
H	-7.52506	1.24313	0.08433
C	-6.57094	-0.70643	0.06801
H	-7.52506	-1.24313	0.08433
C	-5.36899	-1.42864	0.04774
H	-5.36554	-2.52289	0.04876
H	-5.36554	2.52289	0.04876
H	-2.52289	5.36554	-0.04876
H	2.52289	5.36554	-0.04876
C	-1.42864	-5.36899	-0.04774
C	-0.70643	-6.57094	-0.06801
H	-1.24313	-7.52506	-0.08433
C	0.70643	-6.57094	-0.06801
H	1.24313	-7.52506	-0.08433
C	1.42864	-5.36899	-0.04774

H	2.52289	-5.36554	-0.04876
H	-2.52289	-5.36554	-0.04876
C	0.	0.	3.16657
C	0.	0.	-3.16657
N	0.	0.	1.97313
N	0.	0.	-1.97313
O	0.	0.	4.38724
O	0.	0.	-4.38724

Table S9.3. Optimized coordinates for **8.2** using the MPWLYP exchange correlation functional.

C	2.87042	0.79363	0.04124
C	-4.21967	-0.22842	0.02286
C	-4.05885	1.17509	-0.04402
C	-2.61813	1.42233	-0.0527
C	-5.49589	-0.80756	0.05376
H	-5.61773	-1.89363	0.10627
C	-6.60806	0.04566	0.01673
H	-7.61714	-0.37858	0.04044
C	-6.4475	1.44756	-0.05057
H	-7.33443	2.08887	-0.07961
C	-5.17119	2.02729	-0.08142
H	-5.04396	3.11264	-0.13463
C	1.42165	2.61679	0.05598
C	1.17455	4.05763	0.0488
C	-0.22884	4.21859	-0.01838
C	-0.79499	2.87115	-0.03901
C	2.02687	5.16965	0.08778
H	3.11219	5.0422	0.14066
C	1.44723	6.44607	0.05832
H	2.08866	7.33286	0.08842
C	0.04543	6.60688	-0.00936
H	-0.37866	7.61604	-0.03233
C	-0.80794	5.49483	-0.04819
H	-1.89395	5.61677	-0.10152
C	0.69414	-0.82531	2.86123
H	1.35587	-1.6063	2.48473
C	-0.7081	0.83058	2.87276
H	-1.36569	1.60866	2.48828
C	-0.40067	0.46421	4.17739
H	-0.76774	0.89528	5.11221

Fe	-0.00087	-0.0003	-0.00008
N	1.93047	-0.2216	-0.00272
N	0.22009	1.93107	0.00531
N	2.65126	2.10638	0.08292
N	-2.10785	2.6522	-0.07961
N	-0.00098	-0.00247	2.02515
N	0.49293	-0.5914	4.1724
C	-2.87221	-0.79447	0.04113
C	4.21799	0.22761	0.02098
C	4.05717	-1.1758	-0.04578
C	2.61631	-1.42306	-0.05357
C	5.49409	0.80688	0.05031
H	5.61589	1.89296	0.10222
C	6.60622	-0.04635	0.01183
H	7.61531	0.37792	0.03389
C	6.44564	-1.44821	-0.05494
H	7.33255	-2.0895	-0.08458
C	5.16932	-2.02803	-0.08431
H	5.042	-3.11339	-0.13681
C	-1.42351	-2.61774	0.04999
C	-1.17639	-4.0585	0.04102
C	0.22704	-4.2194	-0.02532
C	0.79322	-2.87184	-0.04345
C	-2.02869	-5.17067	0.07797
H	-3.11406	-5.04338	0.13064
C	-1.44894	-6.44701	0.04729
H	-2.09034	-7.33388	0.07585
C	-0.04706	-6.60768	-0.019
H	0.37717	-7.61678	-0.04178
C	0.80627	-5.49551	-0.05562
H	1.89238	-5.61724	-0.10661
N	-1.93218	0.22078	-0.00295
N	-0.22208	-1.93179	-0.00003
N	-2.65327	-2.10736	0.07912
N	2.10601	-2.65287	-0.08263
C	0.822	0.69679	-2.86159
H	1.60983	1.35058	-2.48542
C	-0.84444	-0.69304	-2.87221
H	-1.62524	-1.34717	-2.48709
C	-0.48208	-0.3814	-4.17695
H	-0.92021	-0.74046	-5.11159

N	-0.00241	0.00403	-2.02515
N	0.58022	0.50419	-4.17258

Table S9.4. Optimized coordinates for **8.3.2** using the MPWLYP exchange correlation functional.

C	2.74357	-1.16475	-0.03815
C	-3.44592	2.44682	-0.02708
C	-2.44682	3.44592	0.02708
C	-1.16475	2.74357	0.03815
C	-4.80561	2.78655	-0.05411
H	-5.57716	2.01213	-0.09627
C	-5.14492	4.14683	-0.02718
H	-6.19883	4.44212	-0.04815
C	-4.14683	5.14492	0.02718
H	-4.44212	6.19883	0.04815
C	-2.78655	4.80561	0.05411
H	-2.01213	5.57716	0.09627
C	2.74357	1.16475	-0.03815
C	3.44592	2.44682	-0.02708
C	2.44682	3.44592	0.02708
C	1.16475	2.74357	0.03815
C	4.80561	2.78655	-0.05411
H	5.57716	2.01213	-0.09627
C	5.14492	4.14683	-0.02718
H	6.19883	4.44212	-0.04815
C	4.14683	5.14492	0.02718
H	4.44212	6.19883	0.04815
C	2.78655	4.80561	0.05411
H	2.01213	5.57716	0.09627
C	1.06064	0.	2.88056
H	2.09794	0.	2.54685
Fe	0.	0.	0.
N	1.37549	-1.37549	0.
N	1.37549	1.37549	0.
N	3.38804	0.	-0.06505
N	0.	3.38804	0.06505
N	0.	0.	2.0195
C	-2.74357	1.16475	-0.03815
C	3.44592	-2.44682	-0.02708
C	2.44682	-3.44592	0.02708
C	1.16475	-2.74357	0.03815

C	4.80561	-2.78655	-0.05411
H	5.57716	-2.01213	-0.09627
C	5.14492	-4.14683	-0.02718
H	6.19883	-4.44212	-0.04815
C	4.14683	-5.14492	0.02718
H	4.44212	-6.19883	0.04815
C	2.78655	-4.80561	0.05411
H	2.01213	-5.57716	0.09627
C	-2.74357	-1.16475	-0.03815
C	-3.44592	-2.44682	-0.02708
C	-2.44682	-3.44592	0.02708
C	-1.16475	-2.74357	0.03815
C	-4.80561	-2.78655	-0.05411
H	-5.57716	-2.01213	-0.09627
C	-5.14492	-4.14683	-0.02718
H	-6.19883	-4.44212	-0.04815
C	-4.14683	-5.14492	0.02718
H	-4.44212	-6.19883	0.04815
C	-2.78655	-4.80561	0.05411
H	-2.01213	-5.57716	0.09627
N	-1.37549	1.37549	0.
N	-1.37549	-1.37549	0.
N	-3.38804	0.	-0.06505
N	0.	-3.38804	0.06505
C	0.	1.06064	-2.88056
H	0.	2.09794	-2.54685
N	0.	0.	-2.0195
N	0.	0.69686	-4.16565
N	0.69686	0.	4.16565
C	0.	-1.06064	-2.88056
C	-1.06064	0.	2.88056
N	-0.69686	0.	4.16565
N	0.	-0.69686	-4.16565
H	0.	-2.09794	-2.54685
H	-2.09794	0.	2.54685

Table S9.5. Optimized coordinates for **8.4** using the MPWLYP exchange correlation functional.

N	-1.95277	0.	0.00244

N	0.	-1.95277	-0.00244
N	1.95277	0.	0.00244
C	1.11747	2.76579	-0.00704
C	-0.70696	4.16973	-0.01998
C	-1.11747	2.76579	-0.00704
C	-2.76579	1.11747	0.00704
C	-4.16973	0.70696	0.01998
C	-4.16973	-0.70696	0.01998
C	-2.76579	-1.11747	0.00704
C	-1.11747	-2.76579	-0.00704
C	-0.70696	-4.16973	-0.01998
C	0.70696	-4.16973	-0.01998
C	1.11747	-2.76579	-0.00704
C	2.76579	-1.11747	0.00704
C	4.16973	-0.70696	0.01998
C	4.16973	0.70696	0.01998
C	2.76579	1.11747	0.00704
C	0.70696	4.16973	-0.01998
N	0.	1.95277	-0.00244
N	2.39659	2.39659	0.
N	-2.39659	2.39659	0.
N	-2.39659	-2.39659	0.
N	2.39659	-2.39659	0.
Fe	0.	0.	0.
C	5.37042	-1.42909	0.03411
C	6.5719	-0.70633	0.04874
H	7.5261	-1.2427	0.06055
C	6.5719	0.70633	0.04874
H	7.5261	1.2427	0.06055
C	5.37042	1.42909	0.03411
H	5.3668	-2.52313	0.03481
H	5.3668	2.52313	0.03481
C	1.42909	5.37042	-0.03411
C	0.70633	6.5719	-0.04874
H	1.2427	7.5261	-0.06055
C	-1.42909	5.37042	-0.03411
C	-0.70633	6.5719	-0.04874
H	-1.2427	7.5261	-0.06055
C	-5.37042	1.42909	0.03411
C	-6.5719	0.70633	0.04874
H	-7.5261	1.2427	0.06055

C	-6.5719	-0.70633	0.04874
H	-7.5261	-1.2427	0.06055
C	-5.37042	-1.42909	0.03411
H	-5.3668	-2.52313	0.03481
H	-5.3668	2.52313	0.03481
H	-2.52313	5.3668	-0.03481
H	2.52313	5.3668	-0.03481
C	-1.42909	-5.37042	-0.03411
C	-0.70633	-6.5719	-0.04874
H	-1.2427	-7.5261	-0.06055
C	0.70633	-6.5719	-0.04874
H	1.2427	-7.5261	-0.06055
C	1.42909	-5.37042	-0.03411
H	2.52313	-5.3668	-0.03481
H	-2.52313	-5.3668	-0.03481
C	0.	0.	3.1285
C	0.	0.	-3.1285
N	0.	0.	1.94505
N	0.	0.	-1.94505
S	0.	0.	4.78268
S	0.	0.	-4.78268

Table S9.6. Optimized coordinates for **8.5** using the MPWLYP exchange correlation functional.

N	-1.95299	0.	0.00268
N	0.	-1.95299	-0.00268
N	1.95299	0.	0.00268
C	1.11747	2.76646	-0.00741
C	-0.70729	4.17027	-0.02114
C	-1.11747	2.76646	-0.00741
C	-2.76646	1.11747	0.00741
C	-4.17027	0.70729	0.02114
C	-4.17027	-0.70729	0.02114
C	-2.76646	-1.11747	0.00741
C	-1.11747	-2.76646	-0.00741
C	-0.70729	-4.17027	-0.02114
C	0.70729	-4.17027	-0.02114
C	1.11747	-2.76646	-0.00741
C	2.76646	-1.11747	0.00741

C	4.17027	-0.70729	0.02114
C	4.17027	0.70729	0.02114
C	2.76646	1.11747	0.00741
C	0.70729	4.17027	-0.02114
N	0.	1.95299	-0.00268
N	2.39719	2.39719	0.
N	-2.39719	2.39719	0.
N	-2.39719	-2.39719	0.
N	2.39719	-2.39719	0.
Fe	0.	0.	0.
C	5.3715	-1.4286	0.03614
C	6.57378	-0.70624	0.05168
H	7.52789	-1.24306	0.0642
C	6.57378	0.70624	0.05168
H	7.52789	1.24306	0.0642
C	5.3715	1.4286	0.03614
H	5.36794	-2.52282	0.037
H	5.36794	2.52282	0.037
C	1.4286	5.3715	-0.03614
C	0.70624	6.57378	-0.05168
H	1.24306	7.52789	-0.0642
C	-1.4286	5.3715	-0.03614
C	-0.70624	6.57378	-0.05168
H	-1.24306	7.52789	-0.0642
C	-5.3715	1.4286	0.03614
C	-6.57378	0.70624	0.05168
H	-7.52789	1.24306	0.0642
C	-6.57378	-0.70624	0.05168
H	-7.52789	-1.24306	0.0642
C	-5.3715	-1.4286	0.03614
H	-5.36794	-2.52282	0.037
H	-5.36794	2.52282	0.037
H	-2.52282	5.36794	-0.037
H	2.52282	5.36794	-0.037
C	-1.4286	-5.3715	-0.03614
C	-0.70624	-6.57378	-0.05168
H	-1.24306	-7.52789	-0.0642
C	0.70624	-6.57378	-0.05168
H	1.24306	-7.52789	-0.0642
C	1.4286	-5.3715	-0.03614
H	2.52282	-5.36794	-0.037

H	-2.52282	-5.36794	-0.037
N	0.	0.	3.15392
N	0.	0.	-3.15392
C	0.	0.	1.97365
C	0.	0.	-1.97365

Table S9.7. Optimized coordinates for **8.6** using the MPWLYP exchange correlation functional.

C	-2.78056	-1.0764	0.03778
C	4.18169	0.64467	0.01907
C	4.16079	-0.76738	-0.03673
C	2.75186	-1.15794	-0.04265
C	5.39271	1.34936	0.04231
H	5.40591	2.44211	0.08534
C	6.58282	0.60902	0.00963
H	7.54472	1.13056	0.02732
C	6.56193	-0.80221	-0.04563
H	7.50799	-1.35165	-0.07071
C	5.35039	-1.50736	-0.06897
H	5.33105	-2.6001	-0.11164
C	-1.15551	-2.74974	0.0519
C	-0.76477	-4.15848	0.04768
C	0.64741	-4.17903	-0.00891
C	1.079	-2.78241	-0.02904
C	-1.50441	-5.34835	0.08244
H	-2.59712	-5.32931	0.1265
C	-0.79902	-6.5597	0.06026
H	-1.34815	-7.50587	0.08779
C	0.61225	-6.58027	0.00361
H	1.134	-7.54207	-0.01302
C	1.35227	-5.39011	-0.03137
H	2.44498	-5.4031	-0.07532
C	-0.76506	0.76664	2.80308
H	-1.50194	1.49243	2.47521
C	0.78973	-0.76523	2.85763
H	1.51087	-1.47832	2.4711
C	0.48878	-0.46403	4.16637
H	0.87503	-0.84172	5.10785
Fe	0.00208	0.00007	0.00023

N	-1.94561	0.02891	-0.00253
N	-0.02615	-1.94776	0.0094
N	-2.42874	-2.36044	0.07175
N	2.3629	-2.43101	-0.06352
N	0.00242	0.00766	2.01499
N	-0.4949	0.50514	4.10905
H	-0.94429	0.95139	4.90464
C	2.7849	1.07641	0.03629
C	-4.17697	-0.64466	0.01903
C	-4.15609	0.76757	-0.04025
C	-2.74749	1.15821	-0.04767
C	-5.38832	-1.34918	0.04472
H	-5.40157	-2.4418	0.0912
C	-6.5783	-0.60899	0.01033
H	-7.54022	-1.13044	0.0296
C	-6.55745	0.80227	-0.0489
H	-7.50356	1.35157	-0.07518
C	-5.34607	1.50734	-0.07441
H	-5.32685	2.59995	-0.12054
C	1.16055	2.74943	0.03816
C	0.77019	4.15829	0.02889
C	-0.6419	4.17955	-0.02923
C	-1.07384	2.78293	-0.04476
C	1.51033	5.34795	0.06023
H	2.60298	5.32843	0.10472
C	0.80552	6.55954	0.03351
H	1.35521	7.5055	0.05708
C	-0.60569	6.58076	-0.02405
H	-1.1269	7.54278	-0.04443
C	-1.34625	5.39082	-0.05577
H	-2.43893	5.40425	-0.10109
N	1.95016	-0.02874	-0.00066
N	0.03139	1.94791	-0.00585
N	2.43365	2.36027	0.0655
N	-2.35789	2.43148	-0.07369
C	-0.75793	-0.77122	-2.80343
H	-1.49141	-1.50071	-2.47622
C	0.78839	0.76926	-2.85673
H	1.5058	1.48584	-2.4696
C	0.49059	0.46599	-4.16576
H	0.87559	0.84568	-5.10694

N	0.00464	-0.00783	-2.01477
N	-0.48793	-0.5084	-4.10917
H	-0.93386	-0.95743	-4.90516

Table S9.8. Optimized coordinates for **8.15** using the MPWLYP exchange correlation functional.

N	1.9473	-0.0047	0.00001
N	-0.00001	-0.00271	-1.94725
N	-1.9473	0.0047	-0.00001
C	-1.1194	0.0093	2.76818
C	0.70682	0.00255	4.16981
C	1.11941	-0.00119	2.76819
C	2.76824	-0.00796	1.11942
C	4.16985	-0.01425	0.70684
C	4.16985	-0.01635	-0.70681
C	2.76823	-0.01124	-1.1194
C	1.1194	-0.0093	-2.76818
C	0.7068	-0.01021	-4.1698
C	-0.70682	-0.00255	-4.16981
C	-1.11941	0.00119	-2.76819
C	-2.76824	0.00796	-1.11942
C	-4.16985	0.01425	-0.70684
C	-4.16985	0.01635	0.70681
C	-2.76823	0.01124	1.1194
C	-0.7068	0.01021	4.1698
N	0.00001	0.00271	1.94725
N	-2.39766	0.01293	2.39762
N	2.39767	-0.00586	2.39765
N	2.39766	-0.01293	-2.39762
N	-2.39767	0.00586	-2.39765
Fe	0.	0.	0.
C	-5.37069	0.01911	-1.42991
C	-6.57123	0.02591	-0.70642
H	-7.52539	0.02976	-1.24214
C	-6.57123	0.02805	0.70636
H	-7.52538	0.03353	1.24208
C	-5.37068	0.02341	1.42986
H	-5.36756	0.01768	-2.52364
H	-5.36754	0.02527	2.52359

C	-1.42985	0.01597	5.37064
C	-0.70637	0.01437	6.57121
H	-1.24208	0.0189	7.52537
C	1.42987	0.00105	5.37066
C	0.70639	0.00691	6.57122
H	1.24211	0.00579	7.52539
C	5.37069	-0.01911	1.42991
C	6.57123	-0.02591	0.70642
H	7.52539	-0.02976	1.24214
C	6.57123	-0.02805	-0.70636
H	7.52538	-0.03353	-1.24208
C	5.37068	-0.02341	-1.42986
H	5.36754	-0.02527	-2.52359
H	5.36756	-0.01768	2.52364
H	2.52359	-0.00464	5.36753
H	-2.52357	0.0217	5.36749
C	1.42985	-0.01597	-5.37064
C	0.70637	-0.01437	-6.57121
H	1.24208	-0.0189	-7.52537
C	-0.70639	-0.00691	-6.57122
H	-1.24211	-0.00579	-7.52539
C	-1.42987	-0.00105	-5.37066
H	-2.52359	0.00464	-5.36753
H	2.52357	-0.0217	-5.36749
H	-0.93708	2.42216	-0.00261
H	0.48951	2.42043	0.82063
H	0.48862	2.41831	-0.8274
H	0.93708	-2.42216	0.00261
H	-0.48862	-2.41831	0.8274
H	-0.48951	-2.42043	-0.82063
N	-0.01354	-2.03741	0.00264
N	0.01354	2.03741	-0.00264

Table S9.9. Optimized coordinates for **8.8** using the MPWLYP exchange correlation functional.

N	1.37734	1.37734	0.
N	-1.37734	1.37734	0.
N	-1.37734	-1.37734	0.
C	1.16675	-2.745	0.08392

C	3.44552	-2.44952	-0.05912
C	2.745	-1.16675	-0.08392
C	2.745	1.16675	-0.08392
C	3.44552	2.44952	-0.05912
C	2.44952	3.44552	0.05912
C	1.16675	2.745	0.08392
C	-1.16675	2.745	0.08392
C	-2.44952	3.44552	0.05912
C	-3.44552	2.44952	-0.05912
C	-2.745	1.16675	-0.08392
C	-2.745	-1.16675	-0.08392
C	-3.44552	-2.44952	-0.05912
C	-2.44952	-3.44552	0.05912
C	-1.16675	-2.745	0.08392
C	2.44952	-3.44552	0.05912
N	1.37734	-1.37734	0.
N	0.	-3.38461	0.14164
N	3.38461	0.	-0.14164
N	0.	3.38461	0.14164
N	-3.38461	0.	-0.14164
Fe	0.	0.	0.
N	0.	0.	-2.03411
C	0.	-1.15935	-2.74006
C	0.	1.15935	-2.74006
C	0.	-1.19942	-4.13503
H	0.	-2.08103	-2.15973
C	0.	1.19942	-4.13503
H	0.	2.08103	-2.15973
C	0.	0.	-4.85472
H	0.	-2.16833	-4.63962
H	0.	2.16833	-4.63962
H	0.	0.	-5.94778
N	0.	0.	2.03411
C	1.15935	0.	2.74006
C	-1.15935	0.	2.74006
C	1.19942	0.	4.13503
H	2.08103	0.	2.15973
C	-1.19942	0.	4.13503
H	-2.08103	0.	2.15973
C	0.	0.	4.85472
H	2.16833	0.	4.63962

H	-2.16833	0.	4.63962
H	0.	0.	5.94778
C	-4.80397	-2.78844	-0.11805
C	-5.14269	-4.14736	-0.05862
H	-6.19479	-4.4446	-0.10348
C	-4.14736	-5.14269	0.05862
H	-4.4446	-6.19479	0.10348
C	-2.78844	-4.80397	0.11805
H	-5.57261	-2.01585	-0.20905
H	-2.01585	-5.57261	0.20905
C	2.78844	-4.80397	0.11805
C	4.14736	-5.14269	0.05862
H	4.4446	-6.19479	0.10348
C	4.80397	-2.78844	-0.11805
C	5.14269	-4.14736	-0.05862
H	6.19479	-4.4446	-0.10348
C	4.80397	2.78844	-0.11805
C	5.14269	4.14736	-0.05862
H	6.19479	4.4446	-0.10348
C	4.14736	5.14269	0.05862
H	4.4446	6.19479	0.10348
C	2.78844	4.80397	0.11805
H	2.01585	5.57261	0.20905
H	5.57261	2.01585	-0.20905
H	5.57261	-2.01585	-0.20905
H	2.01585	-5.57261	0.20905
C	-2.78844	4.80397	0.11805
C	-4.14736	5.14269	0.05862
H	-4.4446	6.19479	0.10348
C	-5.14269	4.14736	-0.05862
H	-6.19479	4.4446	-0.10348
C	-4.80397	2.78844	-0.11805
H	-5.57261	2.01585	-0.20905
H	-2.01585	5.57261	0.20905

Table S9.10. Optimized coordinates for **8.10** using the MPWLYP exchange correlation functional.

N	0.	1.95158	0.00094

N	0.	0.	-1.95093
N	0.	-1.95158	0.00094
C	0.01741	-1.11928	2.77032
C	-0.01254	0.70684	4.17232
C	-0.01741	1.11928	2.77032
C	-0.01542	2.77011	1.12043
C	-0.03373	4.17202	0.70759
C	-0.03936	4.17169	-0.70607
C	-0.02271	2.76975	-1.11871
C	-0.02418	1.11949	-2.76903
C	-0.01771	0.70678	-4.17099
C	0.01771	-0.70678	-4.17099
C	0.02418	-1.11949	-2.76903
C	0.02271	-2.76975	-1.11871
C	0.03936	-4.17169	-0.70607
C	0.03373	-4.17202	0.70759
C	0.01542	-2.77011	1.12043
C	0.01254	-0.70684	4.17232
N	0.	0.	1.9524
N	0.02745	-2.3977	2.39853
N	-0.02745	2.3977	2.39853
N	-0.0397	2.39761	-2.39681
N	0.0397	-2.39761	-2.39681
Fe	0.	0.	0.00134
C	0.05995	-5.37189	-1.42941
C	0.074	-6.57263	-0.70582
H	0.08974	-7.52655	-1.24171
C	0.06861	-6.57293	0.70662
H	0.08033	-7.52707	1.24222
C	0.04908	-5.3725	1.43059
H	0.06498	-5.36854	-2.52309
H	0.04581	-5.36967	2.52428
C	0.02497	-1.42986	5.37291
C	0.01241	-0.70615	6.57352
H	0.02189	-1.24177	7.52767
C	-0.02497	1.42986	5.37291
C	-0.01241	0.70615	6.57352
H	-0.02189	1.24177	7.52767
C	-0.04908	5.3725	1.43059
C	-0.06861	6.57293	0.70662
H	-0.08033	7.52707	1.24222

C	-0.074	6.57263	-0.70582
H	-0.08974	7.52655	-1.24171
C	-0.05995	5.37189	-1.42941
H	-0.06498	5.36854	-2.52309
H	-0.04581	5.36967	2.52428
H	-0.04398	2.52338	5.36987
H	0.04398	-2.52338	5.36987
C	-0.03489	1.42966	-5.37159
C	-0.01732	0.70604	-6.57222
H	-0.03046	1.24159	-7.52636
C	0.01732	-0.70604	-6.57222
H	0.03046	-1.24159	-7.52636
C	0.03489	-1.42966	-5.37159
H	0.06148	-2.52302	-5.36852
H	-0.06148	2.52302	-5.36852
P	2.3404	0.02891	-0.00127
P	-2.3404	-0.02891	-0.00127
C	3.18407	-1.61046	-0.13382
H	2.88961	-2.10935	-1.06854
H	2.89293	-2.25345	0.70948
H	4.27823	-1.48481	-0.12545
C	3.13531	0.76233	1.49683
H	4.23162	0.76138	1.39225
H	2.86247	0.18107	2.38926
H	2.79142	1.79741	1.63706
C	-3.12516	-0.98701	-1.3724
H	-2.84537	-0.55238	-2.34272
H	-4.22229	-0.9706	-1.27794
H	-2.78141	-2.0311	-1.34629
C	-3.13531	-0.76233	1.49683
H	-4.23162	-0.76138	1.39225
H	-2.86247	-0.18107	2.38926
H	-2.79142	-1.79741	1.63706
C	-3.18407	1.61046	-0.13382
H	-2.88961	2.10935	-1.06854
H	-2.89293	2.25345	0.70948
H	-4.27823	1.48481	-0.12545
C	3.12516	0.98701	-1.3724
H	2.84537	0.55238	-2.34272
H	4.22229	0.9706	-1.27794
H	2.78141	2.0311	-1.34629

Table S9.11. Optimized coordinates for **8.17** using the MPWLYP exchange correlation functional.

N	1.94755	0.19188	0.01354
N	-0.18516	1.95264	-0.00508
N	-1.94757	-0.1799	-0.01338
C	-0.85129	-2.85818	-0.01291
C	1.09979	-4.07991	0.03255
C	1.37731	-2.64487	0.03217
C	2.86229	-0.84579	0.04579
C	4.21889	-0.30163	0.07737
C	4.08494	1.1056	0.06919
C	2.65042	1.38368	0.03418
C	0.85159	2.86843	0.01114
C	0.30743	4.22531	-0.00555
C	-1.09935	4.09011	-0.03669
C	-1.37651	2.65473	-0.03512
C	-2.86317	0.85739	-0.04534
C	-4.2193	0.31256	-0.0754
C	-4.08432	-1.09458	-0.06641
C	-2.6495	-1.37209	-0.03295
C	-0.30701	-4.21485	0.00194
N	0.18581	-1.9428	0.00338
N	-2.15813	-2.60881	-0.03486
N	2.61312	-2.15287	0.0587
N	2.15862	2.61982	0.03475
N	-2.61305	2.16376	-0.06028
Fe	0.00029	0.00612	-0.00038
C	-5.48291	0.91733	-0.10921
C	-6.60858	0.082	-0.13392
H	-7.60927	0.52402	-0.16083
C	-6.4736	-1.32392	-0.12513
H	-7.37185	-1.94863	-0.14527
C	-5.20951	-1.92921	-0.09149
H	-5.58519	2.00618	-0.11666
H	-5.10181	-3.01752	-0.0849
C	-0.91189	-5.4788	-0.007
C	-0.07693	-6.60485	0.01594
H	-0.51905	-7.60584	0.00969
C	1.93399	-5.20534	0.0557
C	1.32864	-6.46985	0.04693

H	1.95302	-7.36836	0.06453
C	5.48214	-0.90725	0.11238
C	6.60833	-0.07263	0.13849
H	7.60872	-0.5153	0.1663
C	6.47427	1.33339	0.12987
H	7.37289	1.95753	0.15095
C	5.2106	1.93949	0.09524
H	5.10357	3.02786	0.08869
H	5.58366	-1.99618	0.11965
H	3.02205	-5.0976	0.0798
H	-2.00051	-5.58123	-0.03073
C	0.91217	5.48938	0.0025
C	0.07706	6.6153	-0.022
H	0.51904	7.61636	-0.01652
C	-1.32852	6.48007	-0.05355
H	-1.95304	7.37847	-0.07232
C	-1.93373	5.21547	-0.06136
H	-3.02177	5.10751	-0.08582
H	2.00076	5.59196	0.02674
P	0.08057	-0.02232	-2.25958
P	-0.08252	0.00562	2.25862
O	-1.3642	-0.28213	-3.00143
O	0.6577	1.37052	-2.91762
O	1.06798	-1.19822	-2.85058
O	-1.09429	1.1508	2.86901
O	-0.63642	-1.40754	2.89251
O	1.3588	0.26823	3.00692
C	-1.54616	-1.04012	-4.22596
H	-1.24548	-0.44537	-5.10216
H	-2.6181	-1.26375	-4.28586
H	-0.97312	-1.97716	-4.18883
C	0.19352	1.96444	-4.15674
H	0.55954	2.99824	-4.15193
H	-0.90472	1.96109	-4.20101
H	0.61014	1.43213	-5.02592
C	1.95126	-1.05018	-3.9913
H	2.68174	-1.86468	-3.91571
H	2.47049	-0.08221	-3.95789
H	1.39009	-1.1471	-4.93379
C	-0.85351	1.91917	4.07482
H	-1.54725	2.76766	4.03578

H	0.18157	2.28803	4.10063
H	-1.06338	1.31532	4.97144
C	-1.5032	-1.51639	4.05082
H	-1.92276	-2.52922	4.01966
H	-2.31458	-0.77707	3.99878
H	-0.92918	-1.38533	4.98112
C	1.76481	-0.33635	4.2624
H	2.84409	-0.16092	4.34605
H	1.56462	-1.417	4.2524
H	1.2494	0.13773	5.11195

Table S9.12. Optimized coordinates for **8.12** using the MPWLYP exchange correlation functional.

N	-0.00453	1.95316	0.00438
N	0.01323	-0.00665	1.95316
N	0.00453	-1.95316	-0.00438
C	-0.00961	-1.11256	-2.77193
C	0.0256	0.71692	-4.17002
C	0.01207	1.12784	-2.76824
C	-0.0042	2.77485	-1.11347
C	-0.00677	4.17434	-0.6947
C	-0.00362	4.16896	0.71856
C	-0.0001	2.76677	1.12837
C	0.00961	1.11256	2.77193
C	-0.00816	0.69609	4.17223
C	-0.0256	-0.71692	4.17002
C	-0.01207	-1.12784	2.76824
C	0.0042	-2.77485	1.11347
C	0.00677	-4.17434	0.6947
C	0.00362	-4.16896	-0.71856
C	0.0001	-2.76677	-1.12837
C	0.00816	-0.69609	-4.17223
N	-0.01323	0.00665	-1.95316
N	-0.01923	-2.38997	-2.40325
N	0.01209	2.4048	-2.39223
N	0.01923	2.38997	2.40325
N	-0.01209	-2.4048	2.39223
Fe	0.	0.	0.
C	0.00995	-5.3765	1.41489

C	0.01098	-6.57351	0.68619
H	0.01449	-7.52965	1.21796
C	0.0085	-6.56839	-0.72649
H	0.01069	-7.52073	-1.26503
C	0.00437	-5.36628	-1.44674
H	0.01234	-5.37702	2.50837
H	0.00386	-5.3591	-2.54014
C	0.01514	-1.41822	-5.37296
C	0.03873	-0.6919	-6.57134
H	0.04573	-1.22562	-7.52638
C	0.04945	1.44312	-5.36814
C	0.05567	0.72056	-6.56901
H	0.0752	1.25717	-7.52225
C	-0.00995	5.3765	-1.41489
C	-0.01098	6.57351	-0.68619
H	-0.01449	7.52965	-1.21796
C	-0.0085	6.56839	0.72649
H	-0.01069	7.52073	1.26503
C	-0.00437	5.36628	1.44674
H	-0.00386	5.3591	2.54014
H	-0.01234	5.37702	-2.50837
H	0.0642	2.53647	-5.36302
H	0.00477	-2.5116	-5.37145
C	-0.01514	1.41822	5.37296
C	-0.03873	0.6919	6.57134
H	-0.04573	1.22562	7.52638
C	-0.05567	-0.72056	6.56901
H	-0.0752	-1.25717	7.52225
C	-0.04945	-1.44312	5.36814
H	-0.0642	-2.53647	5.36302
H	-0.00477	2.5116	5.37145
C	-3.08777	-1.55797	0.12484
H	-2.76255	-2.06603	1.04079
H	-2.78274	-2.1275	-0.7628
H	-4.17406	-1.39732	0.13987
C	-3.04997	0.74802	-1.42358
H	-4.1375	0.75713	-1.27055
H	-2.77349	0.11522	-2.27599
H	-2.67381	1.76924	-1.55997
C	3.04997	-0.74802	1.42358
H	2.77349	-0.11522	2.27599

H	4.1375	-0.75713	1.27055
H	2.67381	-1.76924	1.55997
C	3.08777	1.55797	-0.12484
H	2.78274	2.1275	0.7628
H	2.76255	2.06603	-1.04079
H	4.17406	1.39732	-0.13987
O	-2.88071	0.88324	1.26477
O	2.88071	-0.88324	-1.26477
S	-2.29734	0.0921	0.10842
S	2.29734	-0.0921	-0.10842

Table S9.13. Optimized coordinates for **8.18** using the MPWLYP exchange correlation functional.

N	0.04308	-1.96109	0.
N	0.04334	0.00022	1.96107
N	0.04305	1.96112	0.
C	0.04343	1.1208	-2.77236
C	0.04803	-0.70654	-4.17482
C	0.04072	-1.12051	-2.77253
C	0.04081	-2.77236	-1.12046
C	0.04666	-4.17478	-0.7067
C	0.04666	-4.17478	0.7067
C	0.04081	-2.77236	1.12046
C	0.04072	-1.12051	2.77253
C	0.04803	-0.70654	4.17482
C	0.0503	0.70689	4.17468
C	0.04343	1.1208	2.77236
C	0.04129	2.77262	1.12084
C	0.04658	4.17482	0.70674
C	0.04658	4.17482	-0.70674
C	0.04129	2.77262	-1.12084
C	0.0503	0.70689	-4.17468
N	0.04334	0.00022	-1.96107
N	0.0415	2.39796	-2.39797
N	0.03901	-2.39783	-2.39776
N	0.03901	-2.39783	2.39776
N	0.0415	2.39796	2.39797
Fe	-0.02263	0.00007	0.

C	0.05373	5.37408	1.43086
C	0.05919	6.5738	0.70624
H	0.0628	7.52801	1.24141
C	0.05919	6.5738	-0.70624
H	0.0628	7.52801	-1.24141
C	0.05373	5.37408	-1.43086
H	0.0533	5.37076	2.52429
H	0.0533	5.37076	-2.52429
C	0.05955	1.43105	-5.37386
C	0.06522	0.70646	-6.57366
H	0.07059	1.2417	-7.52782
C	0.0553	-1.43065	-5.37403
C	0.06309	-0.70596	-6.57375
H	0.06683	-1.2411	-7.52797
C	0.05349	-5.37392	-1.43084
C	0.05885	-6.57374	-0.70619
H	0.06227	-7.52793	-1.2414
C	0.05885	-6.57374	0.70619
H	0.06227	-7.52793	1.2414
C	0.05349	-5.37392	1.43084
H	0.05288	-5.37062	2.52427
H	0.05288	-5.37062	-2.52427
H	0.05311	-2.52408	-5.37076
H	0.06067	2.52448	-5.3705
C	0.0553	-1.43065	5.37403
C	0.06309	-0.70596	6.57375
H	0.06683	-1.2411	7.52797
C	0.06522	0.70646	6.57366
H	0.07059	1.2417	7.52782
C	0.05955	1.43105	5.37386
H	0.06067	2.52448	5.3705
H	0.05311	-2.52408	5.37076
H	2.44297	0.94204	0.
H	2.44418	-0.48366	-0.82388
H	2.44418	-0.48366	0.82388
N	2.06009	-0.00944	0.
C	-1.79249	0.00317	0.
O	-2.95312	0.00479	0.