Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary Information

Diels-Alder Reaction on Perylenediimides: Synthesis and Theoretical Study of Core-Expanded Diimides

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1. Collection of ^{1}H-NMR, ^{13}C-NMR, IR, UV-vis and fluorescence spectra and HRMS MALDI-TOF data

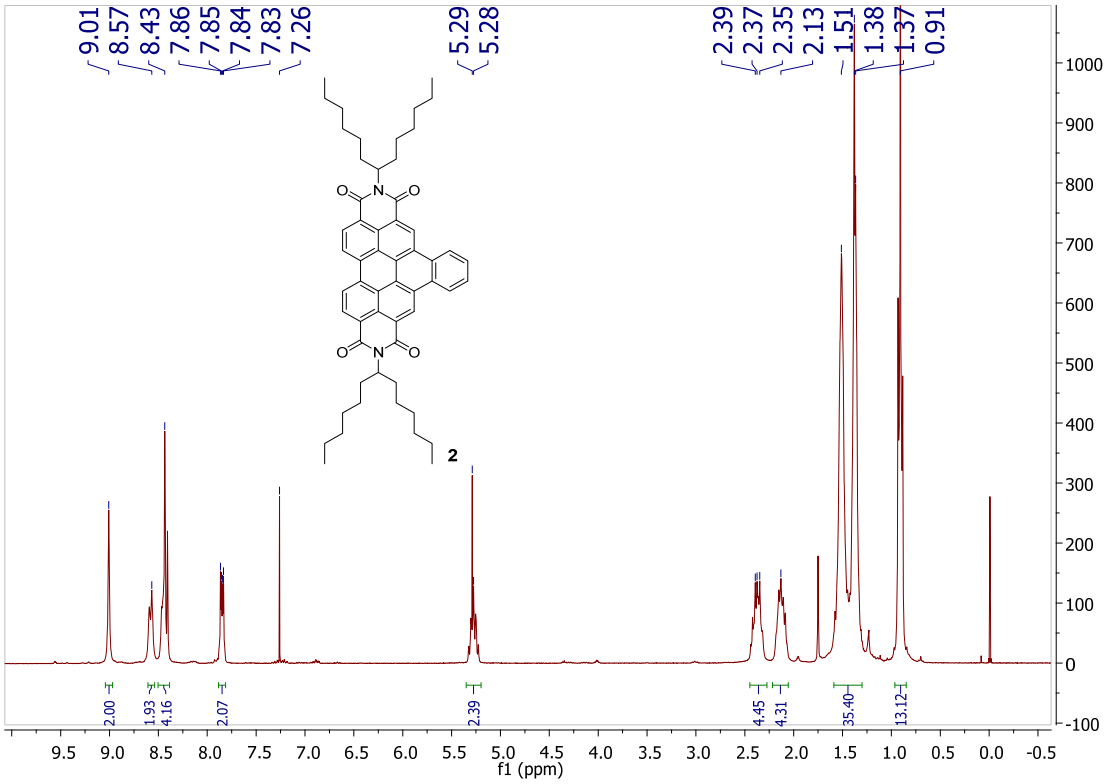

Figure S1. ^{1}H-NMR of **2**

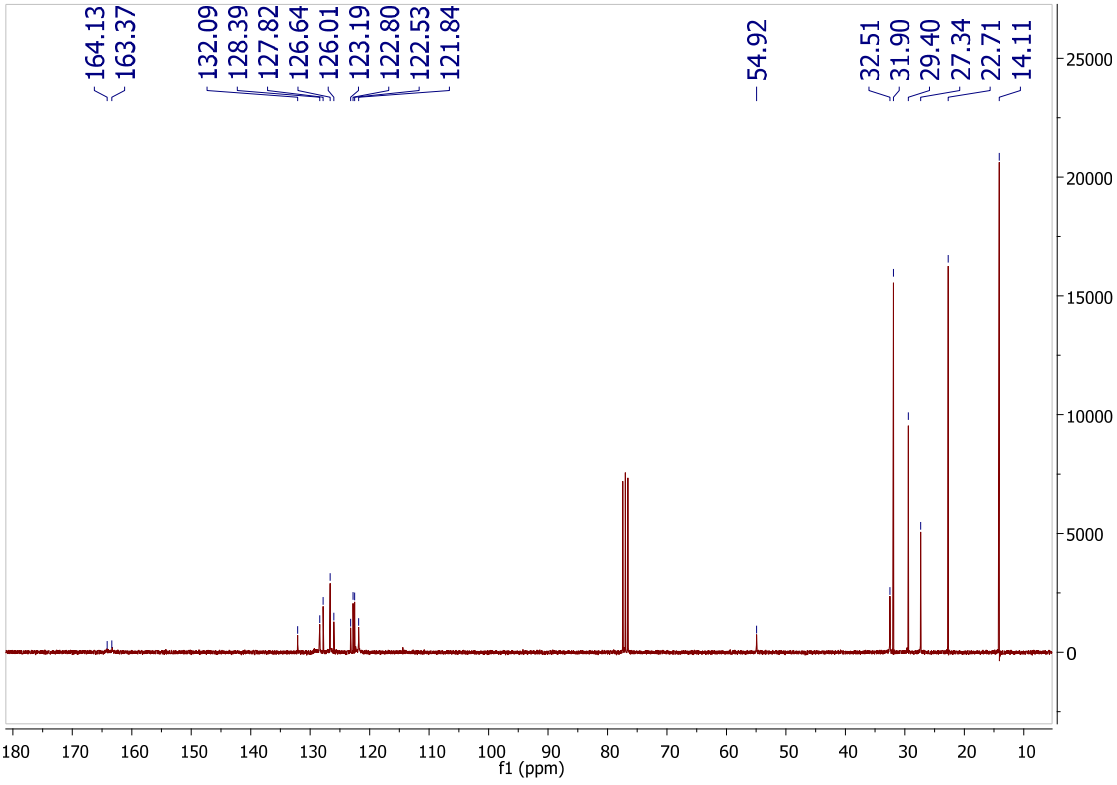

Figure S2. ^{13}C-NMR of **2**.

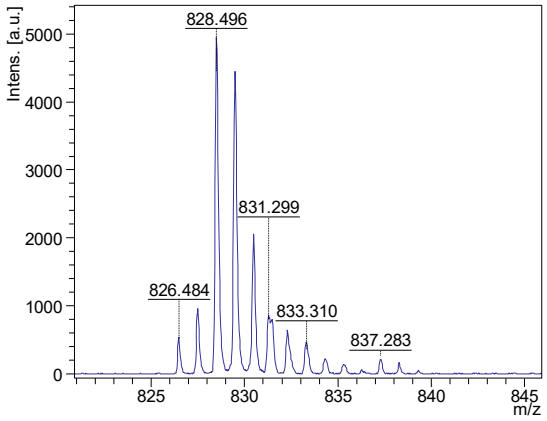

Figure S3. HRMS MALDI-TOF of **2**

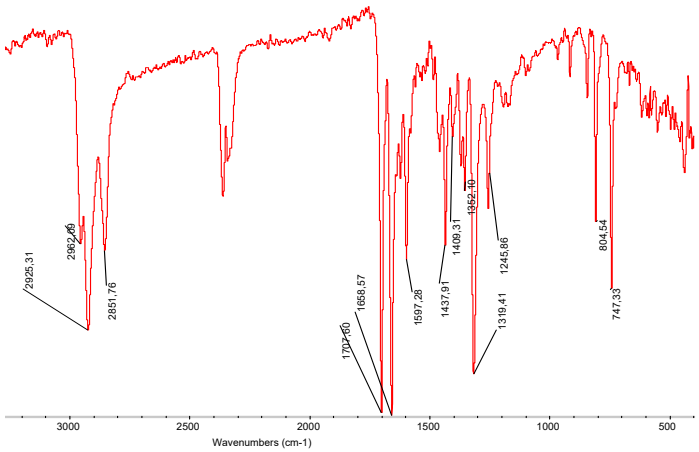

Figure S4. IR of **2**

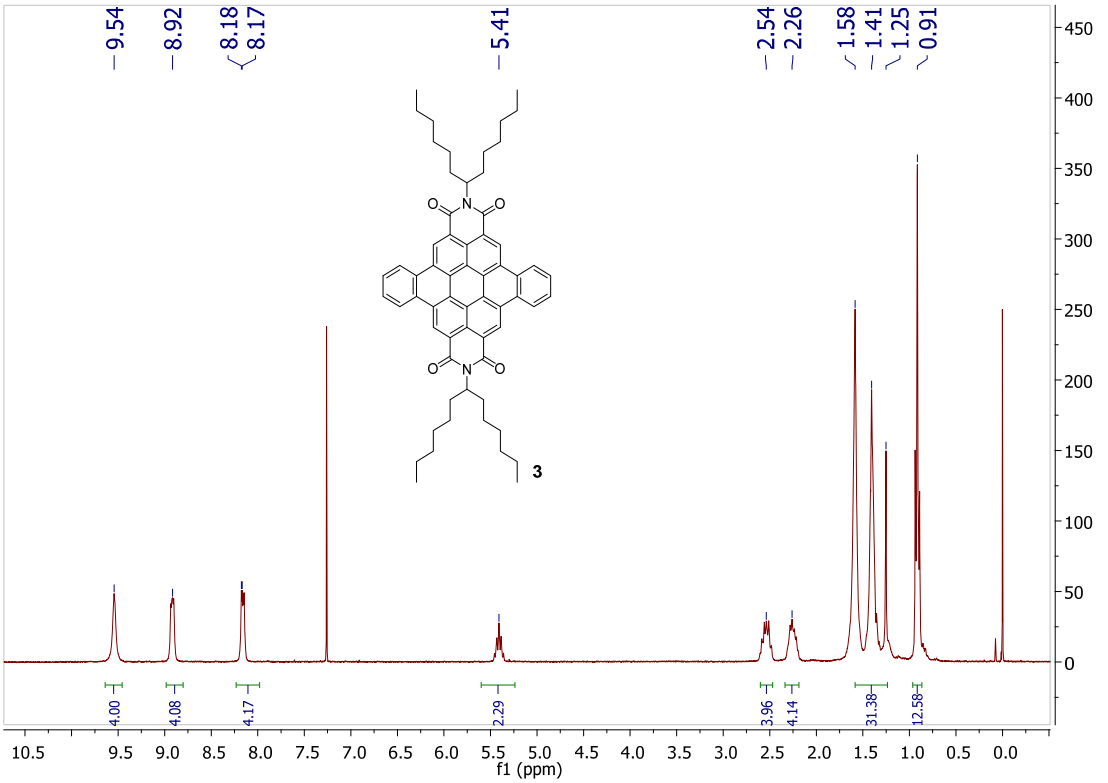

Figure S5. ^{1}H-NMR of **3**.

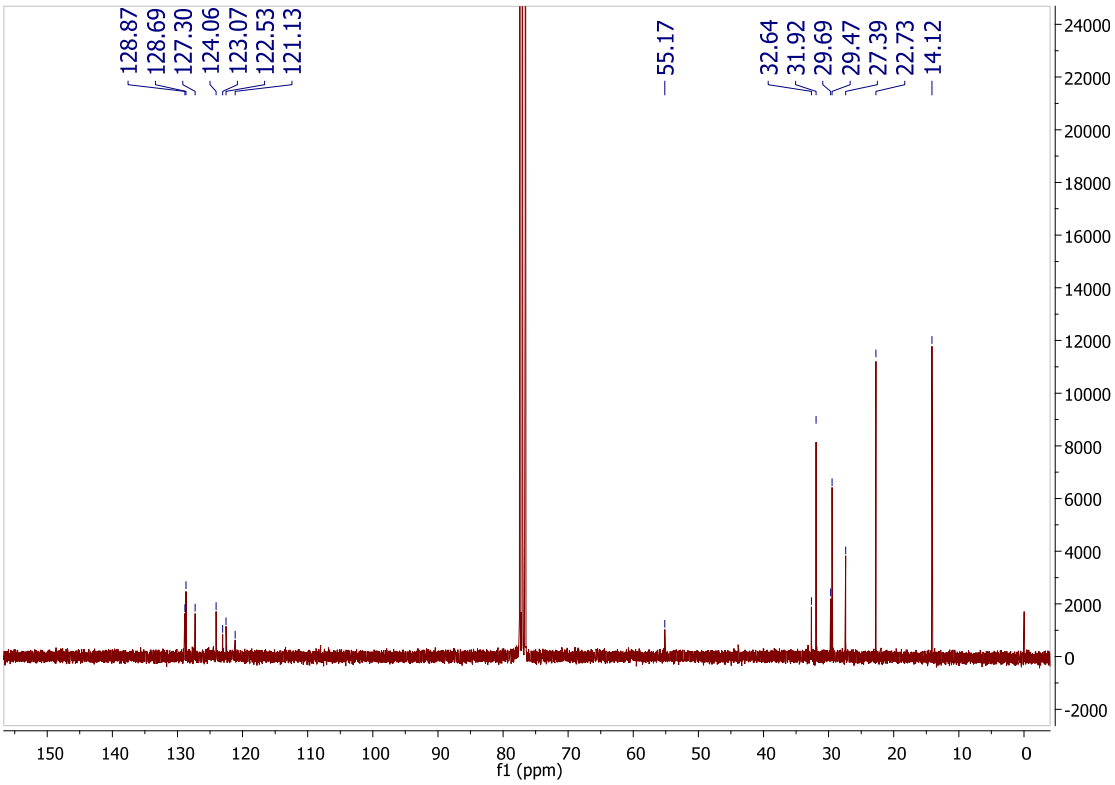

Figure S6. ^{13}C-NMR of **3**.

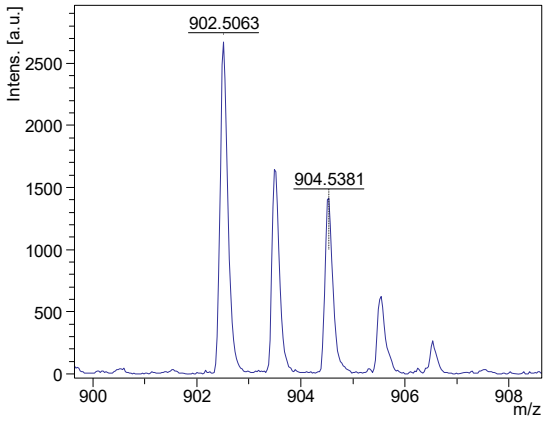

Figure S7. HRMS MALDI-TOF of **3**.

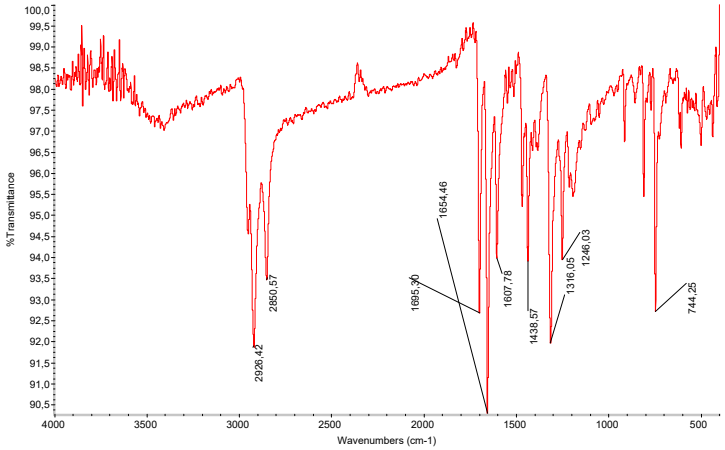

Figure S8. IR of **3**.

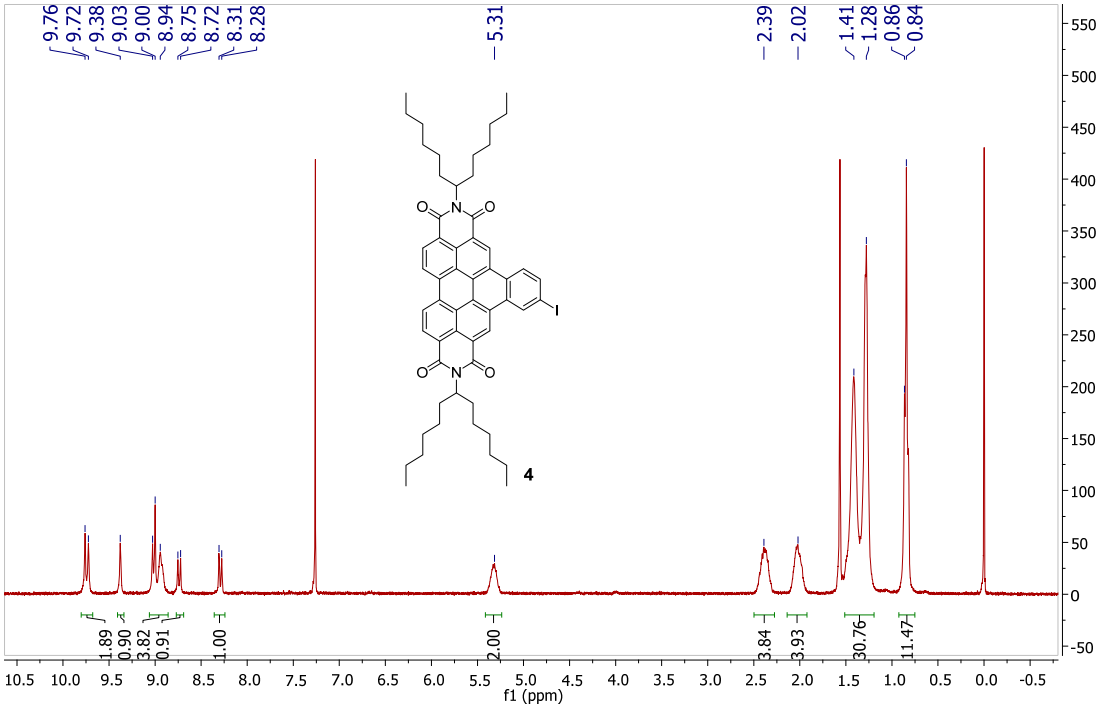

Figure S9. ^{1}H-NMR of **4**.

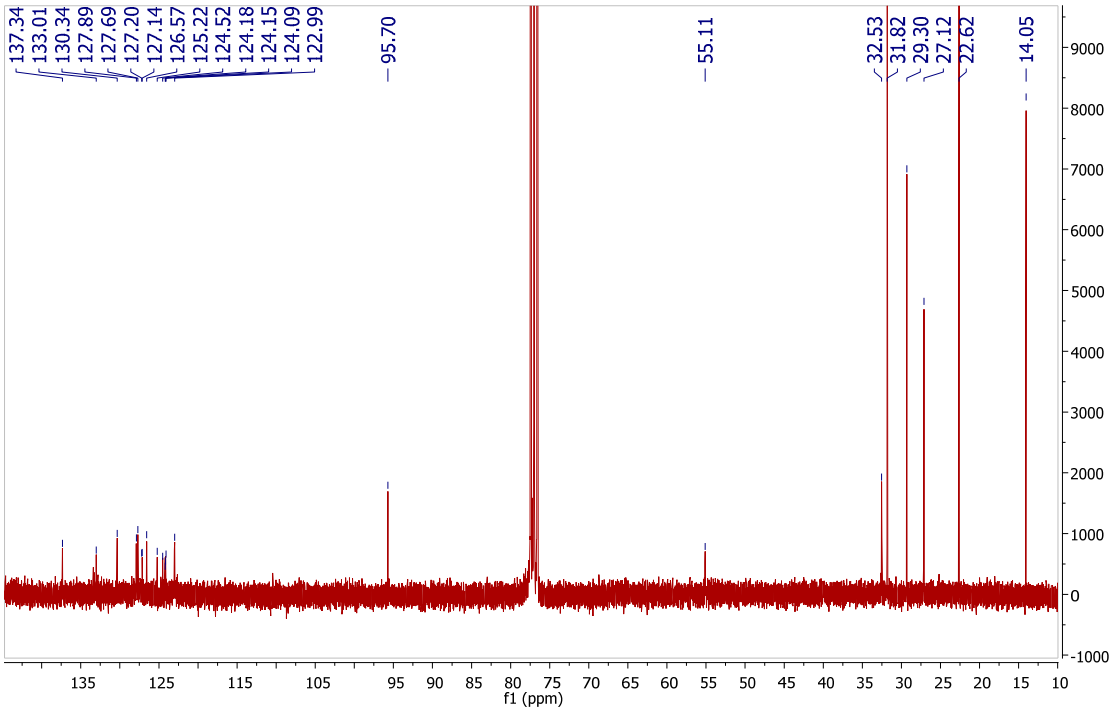

Figure S10. ^{13}C-NMR of **4**.

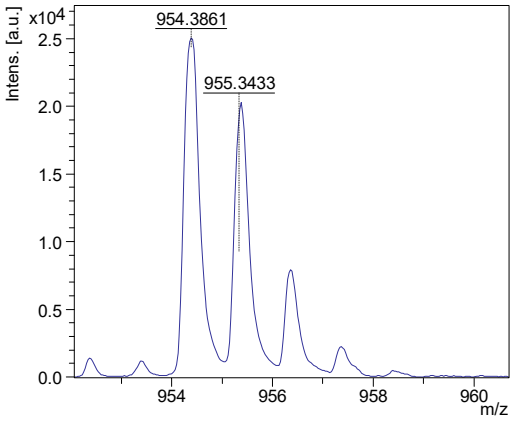

Figure S11. HRMS MALDI-TOF of **4**.

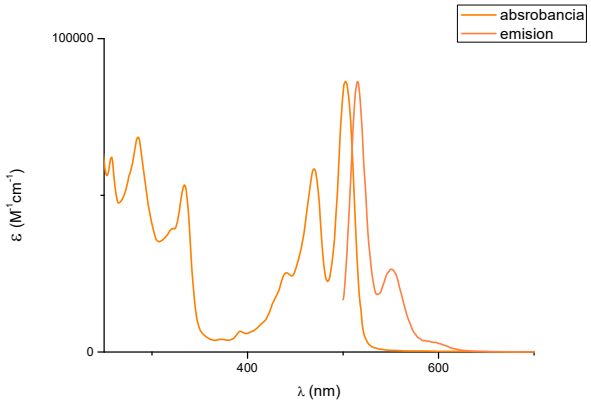

Figure S12. UV-vis and fluorescence of **4**.

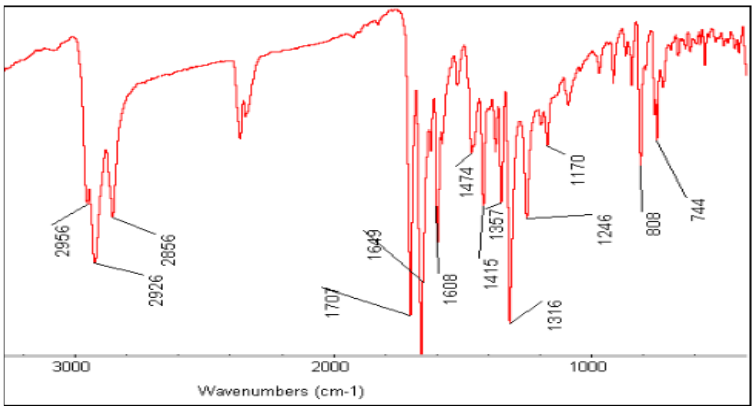

Figure S13. IR of **4**.

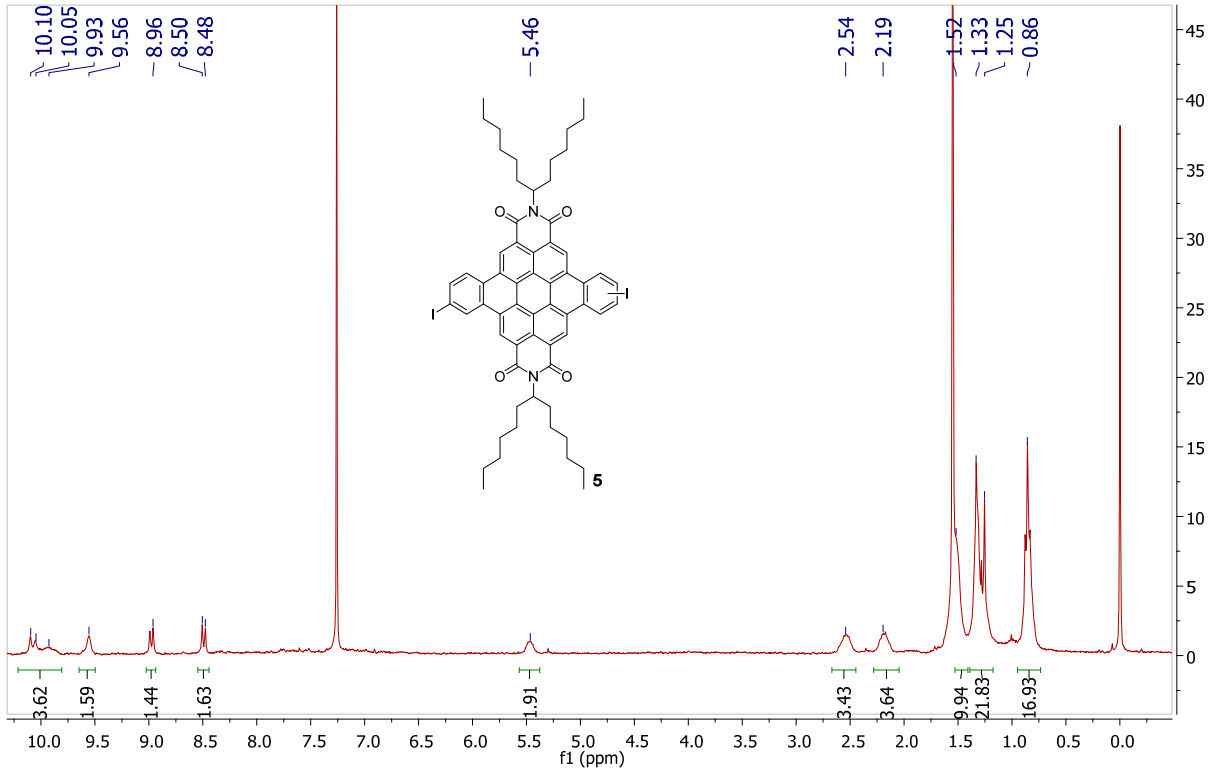

Figure S14. ^{1}H-NMR of **5**.

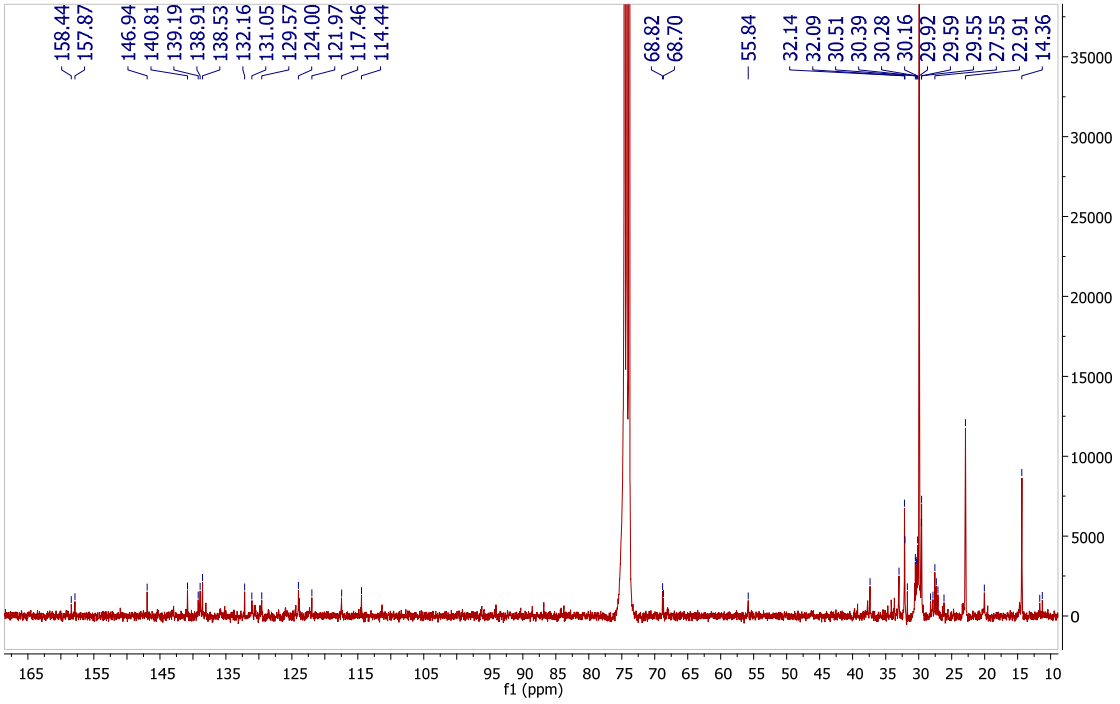

Figure S15. ^{13}C-NMR of **5**.

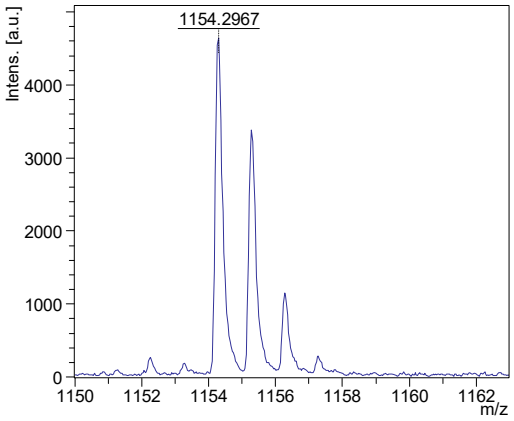

Figure S16. HRMS MALDI-TOF of **5**.

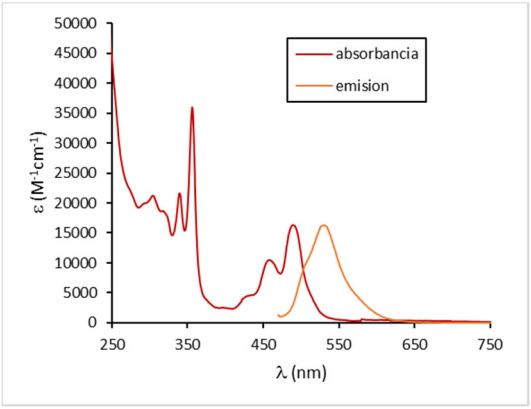

Figure S17. UV-vis and fluorescence of **5**.

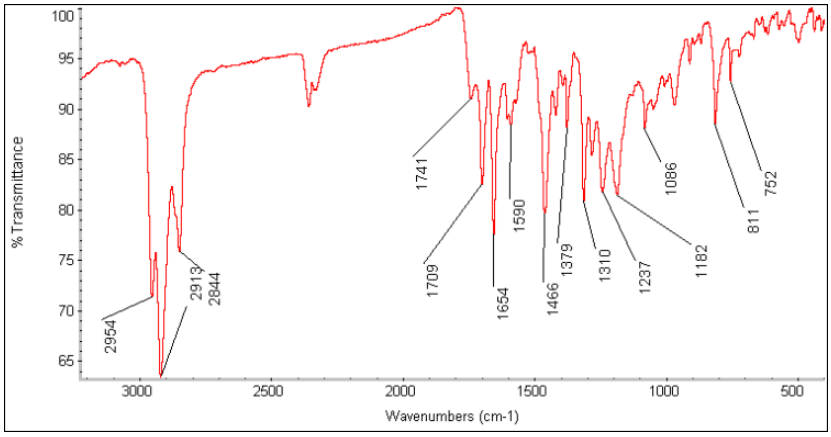

Figure S18. IR of **5**.

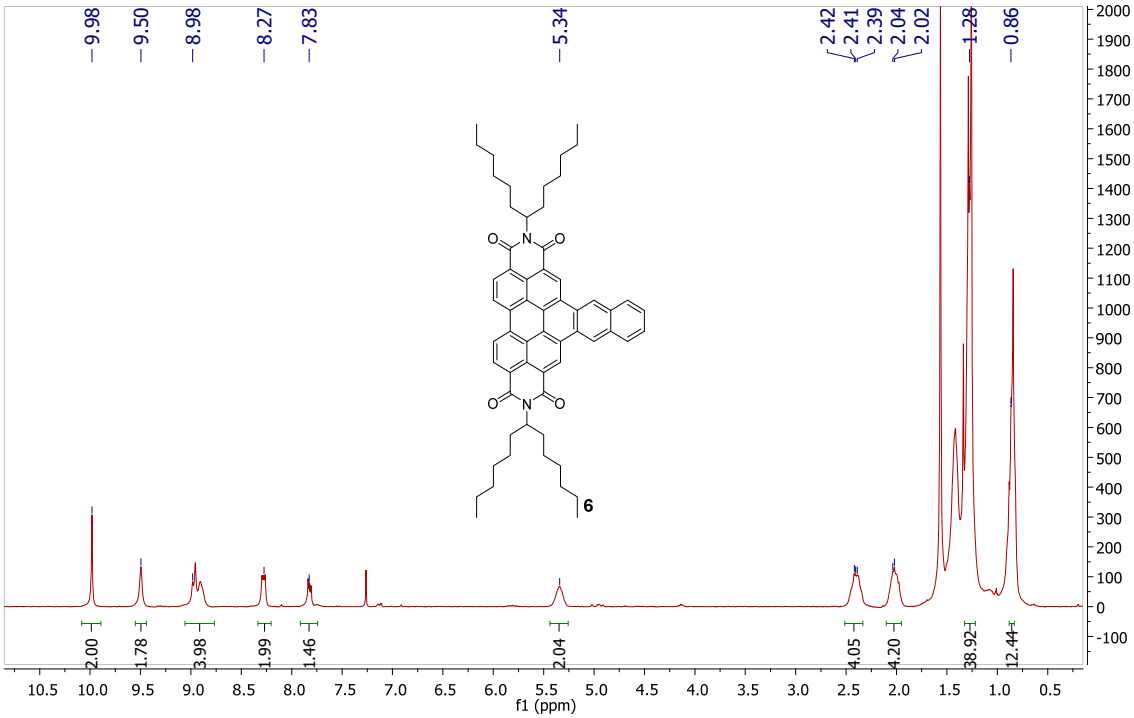

Figure S19. ^{1}H-NMR of **6**.

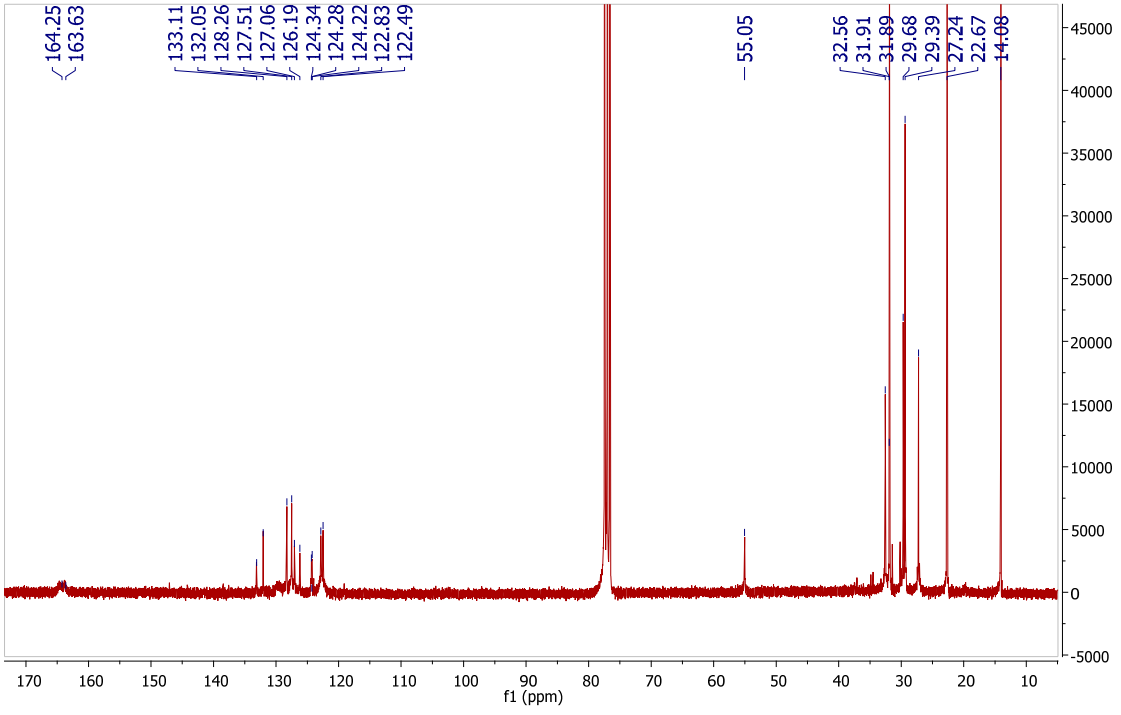

Figure S20. ^{13}C-NMR of **6**.

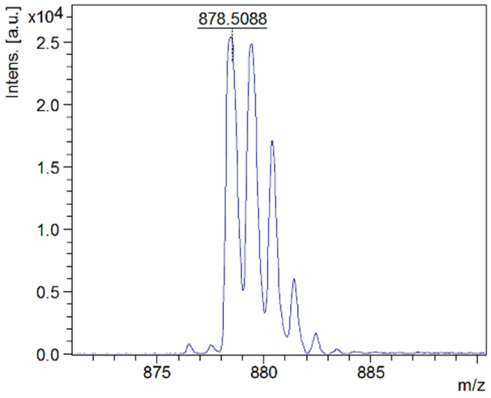

Figure S21. HRMS MALDI-TOF of **6**.

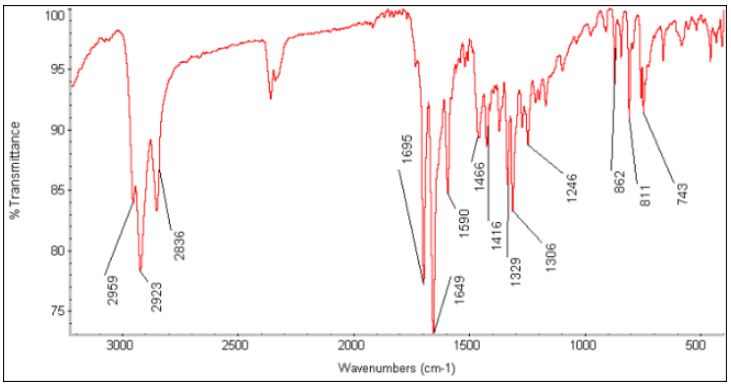

Figure S22. IR of **6**.

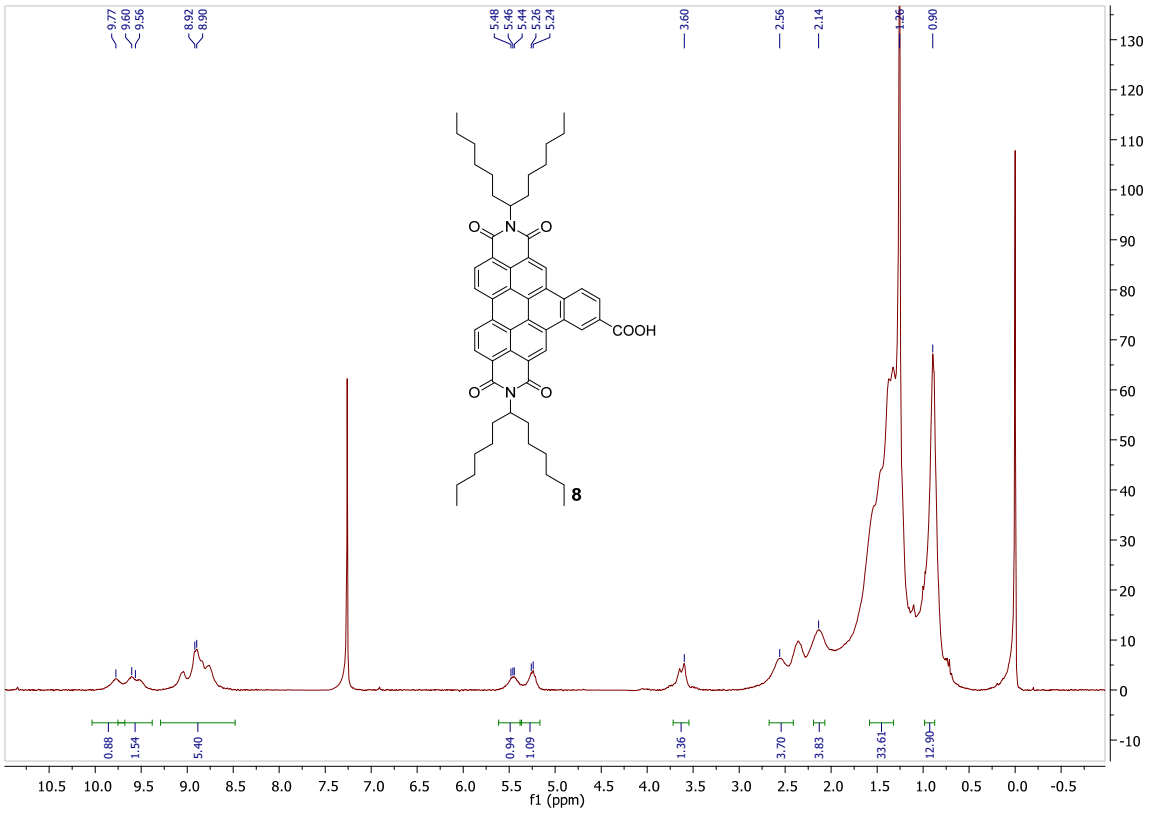

Figure S23. ^{1}H-NMR of **8**.

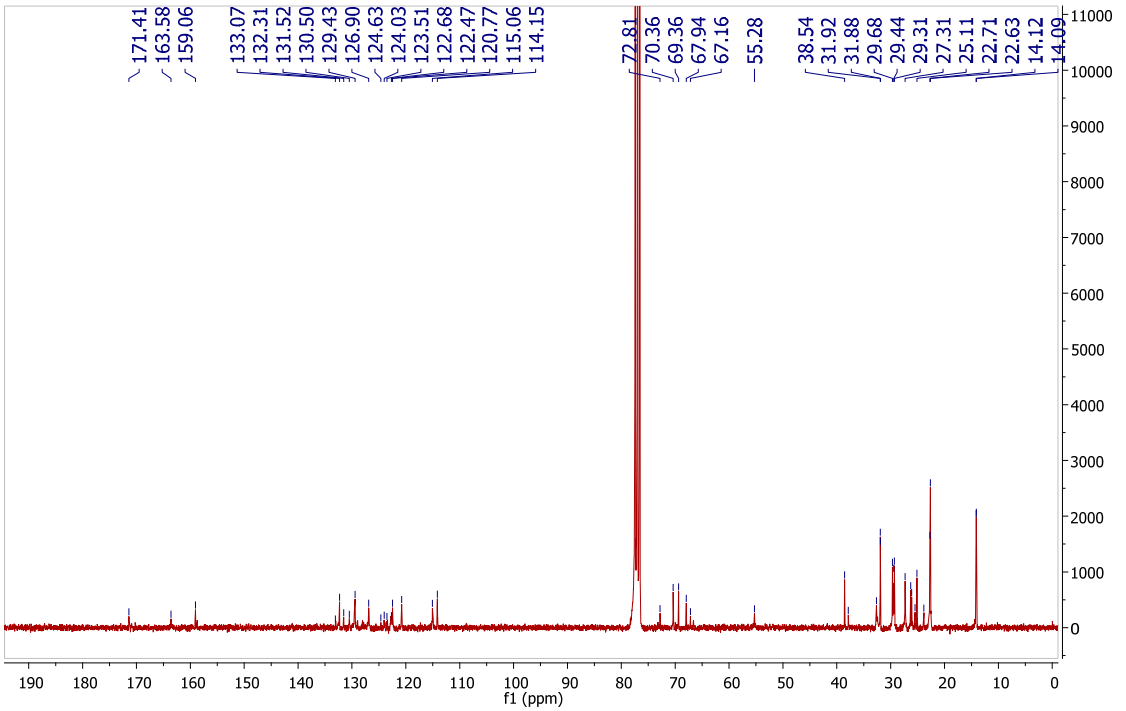

Figure S24. ^{13}C-NMR of **8**.

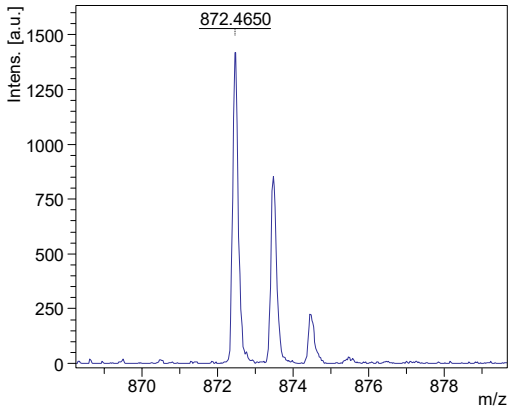

Figure S25. HRMS MALDI-TOF of **8**.

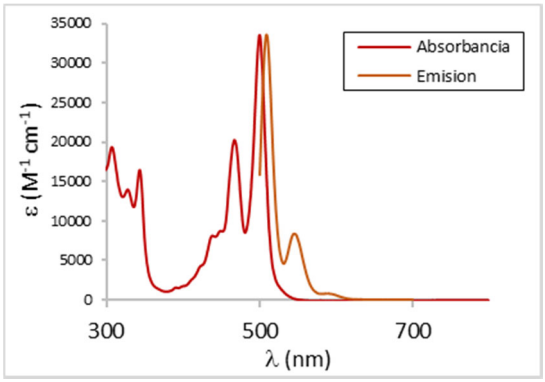

Figure S26. UV-vis and fluorescence of **8**.

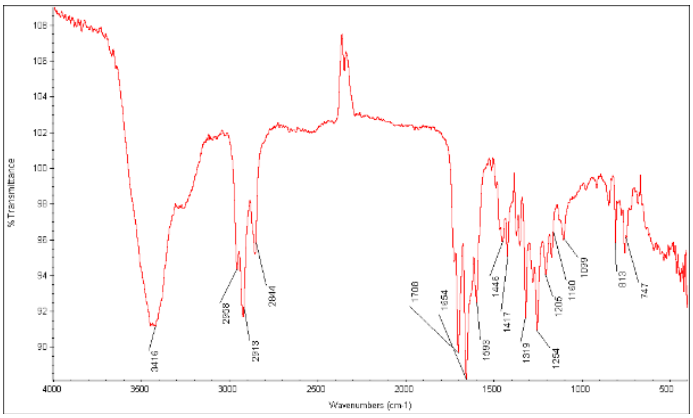

Figure S27. IR of **8**.

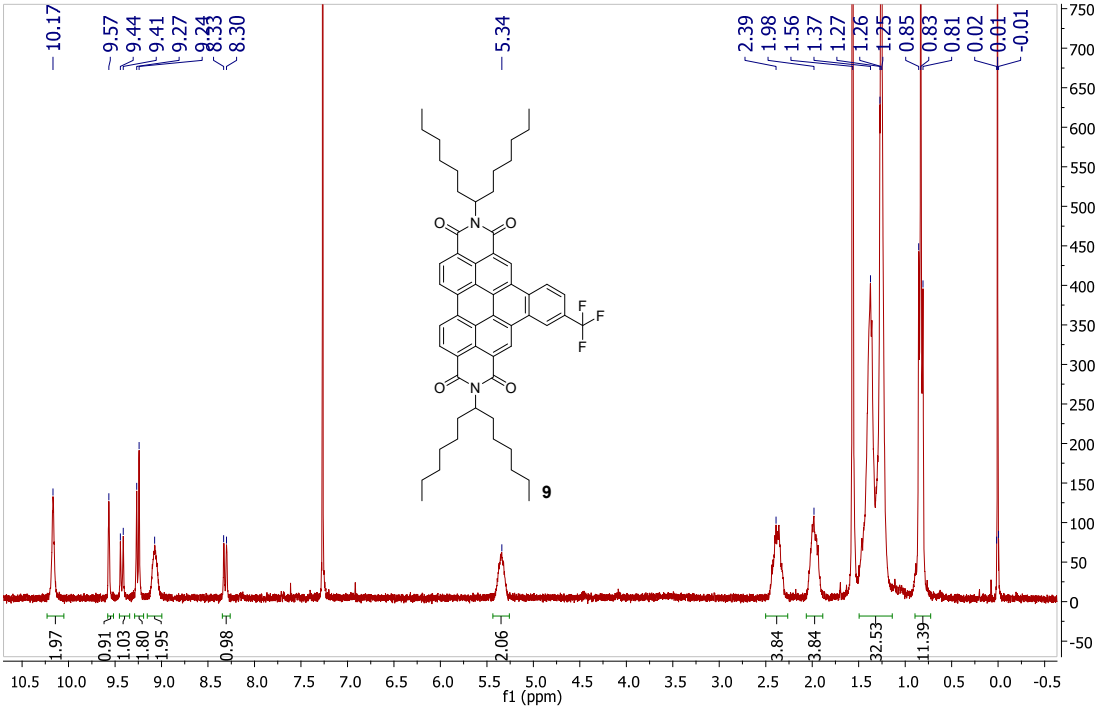

Figure S28. ^{1}H-NMR N of **9**.

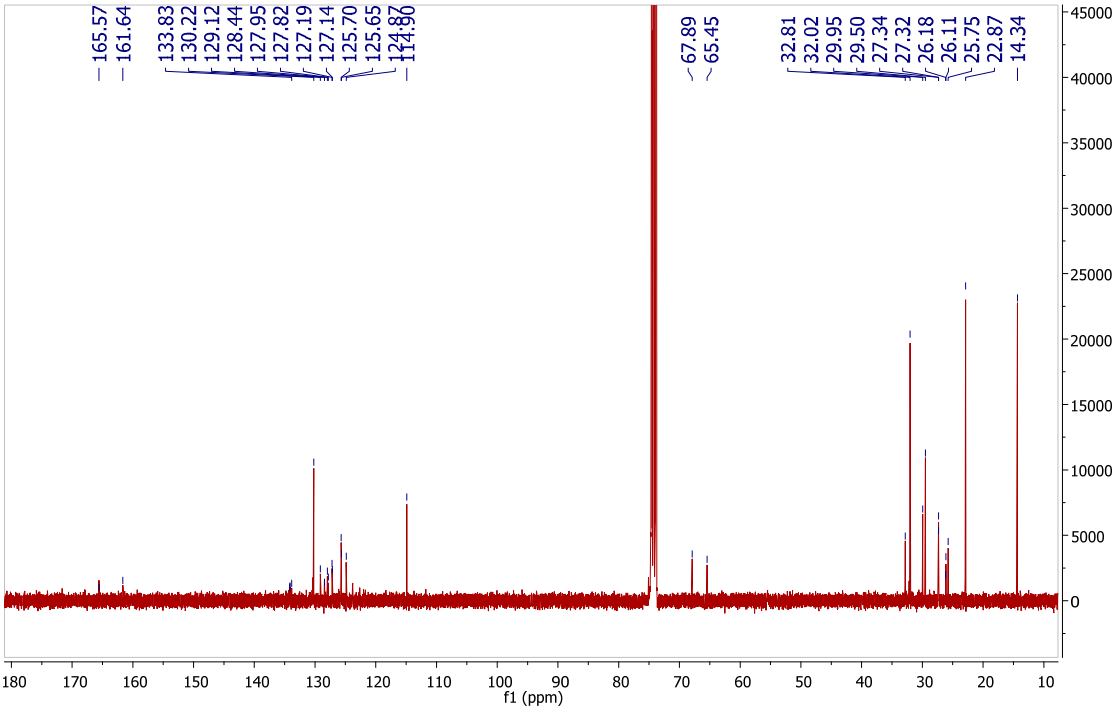

Figure S29. ^{13}C-NMR of **9**.

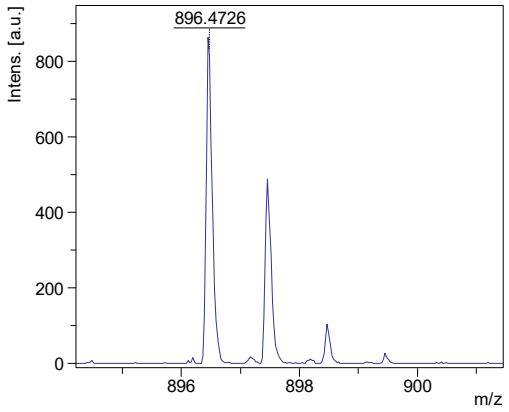

Figure S30. HRMS MALDI-TOF of **9**.

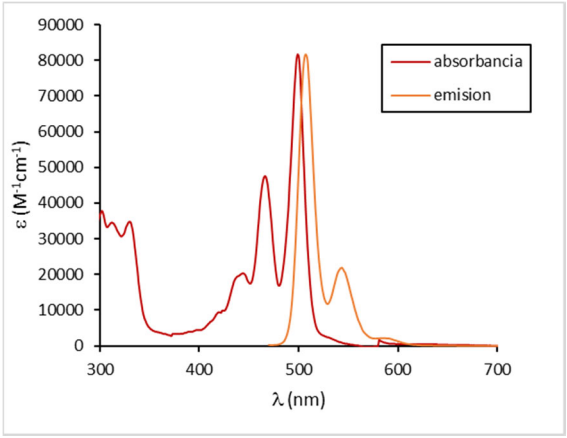

Figure S31. UV-vis and fluorescence of **9**.

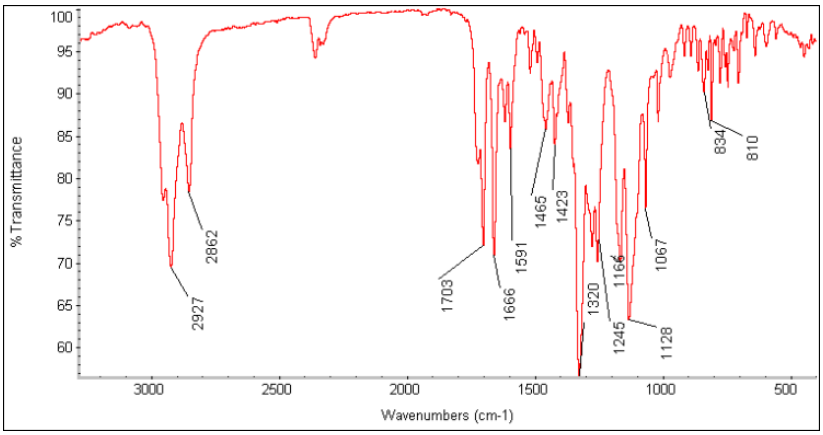

Figure S32. IR of **9**.

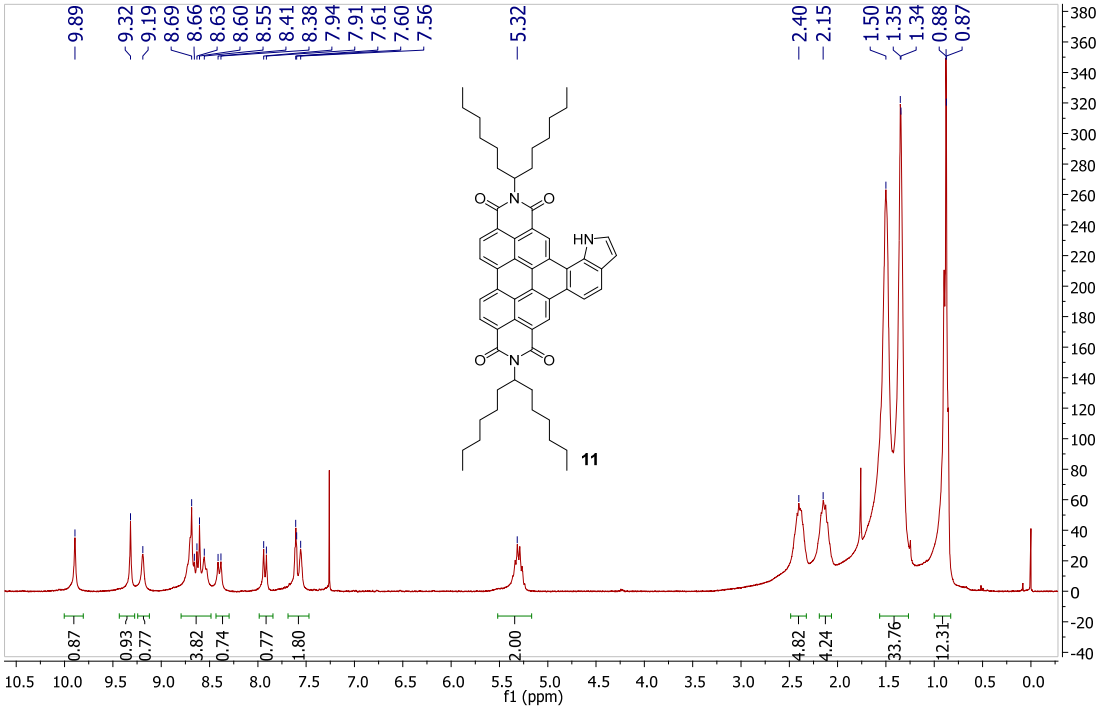

Figure S33. ^{1}H-NMR of **11**.

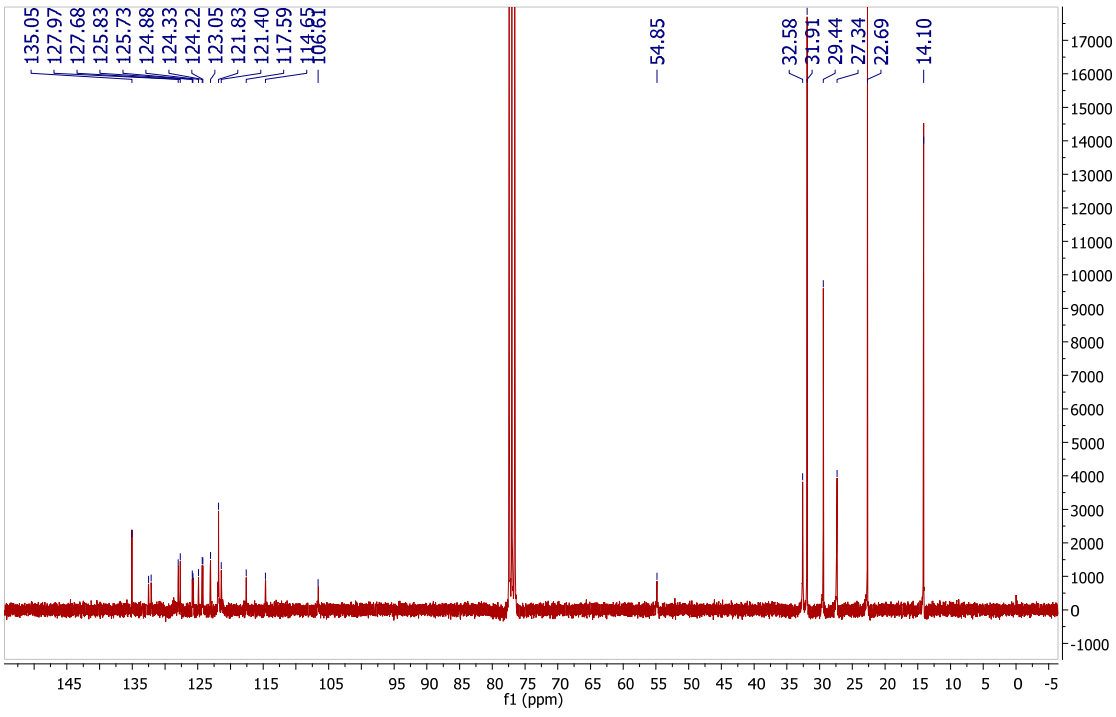

Figure S34. ^{13}C-NMR of **11**.

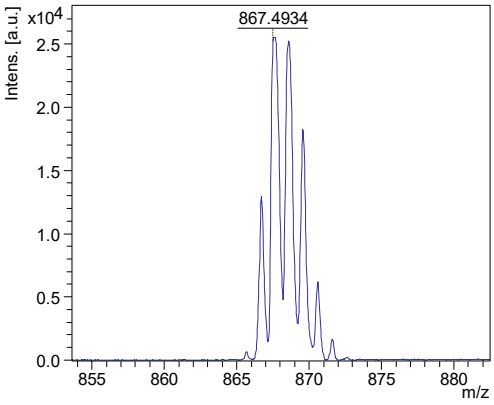

Figure S35. HRMS MALDI-TOF of **11**.

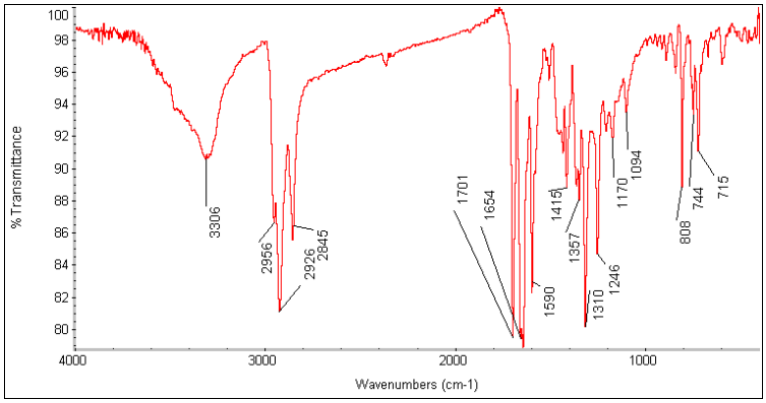

Figure S36. IR of **11**.

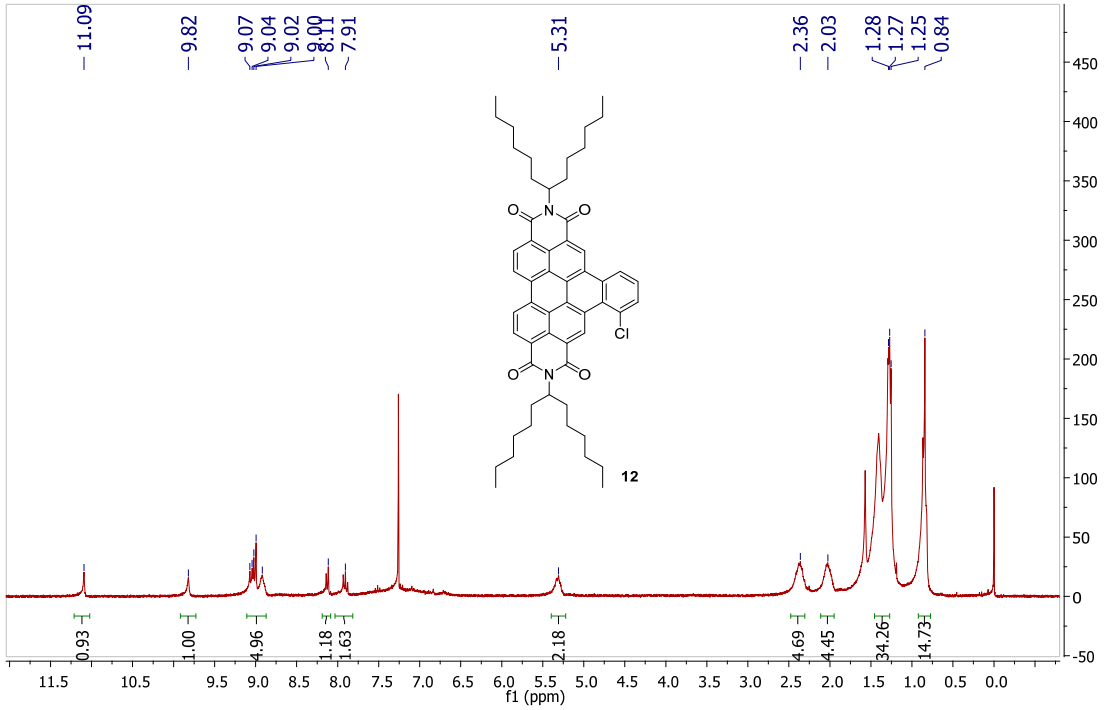

Figure S37. ^{1}H-NMR of **12**.

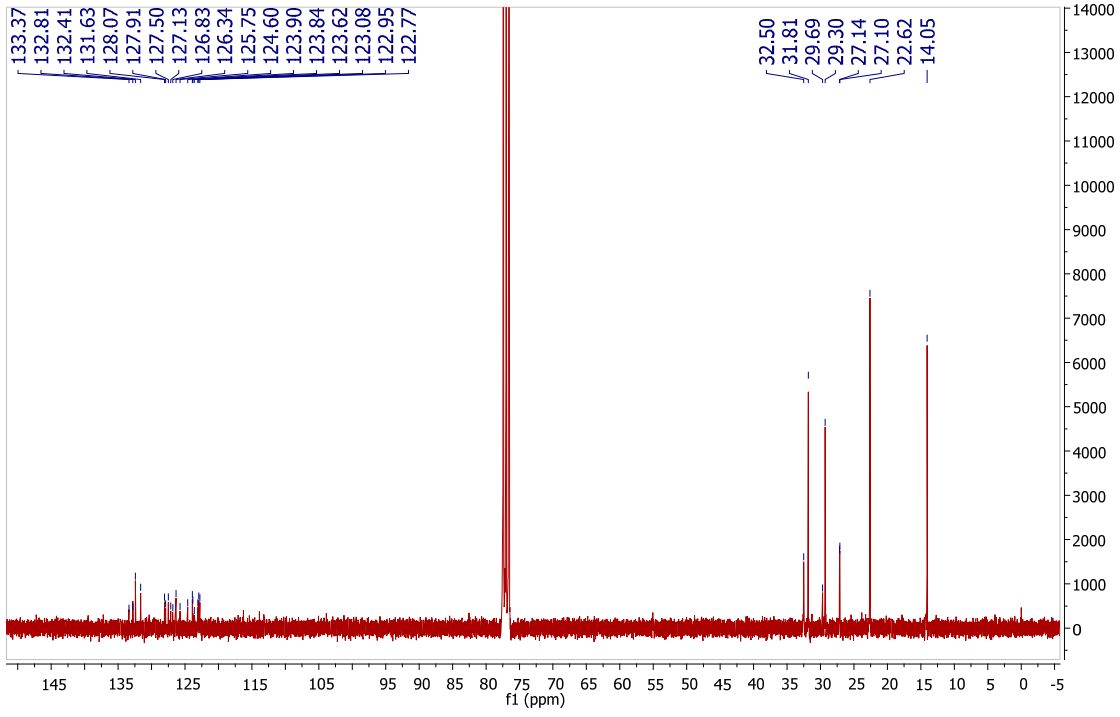

Figure S38. ^{13}C-NMR of **12**.

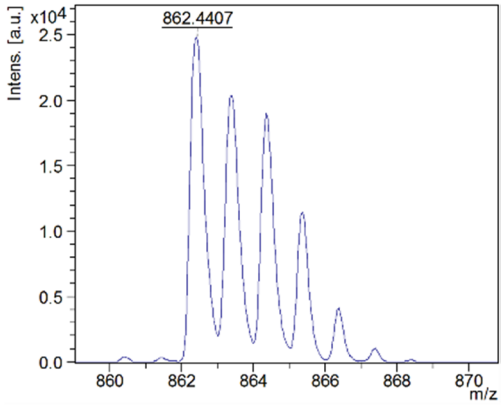

Figure S39. HRMS MALDI-TOF of **12.**

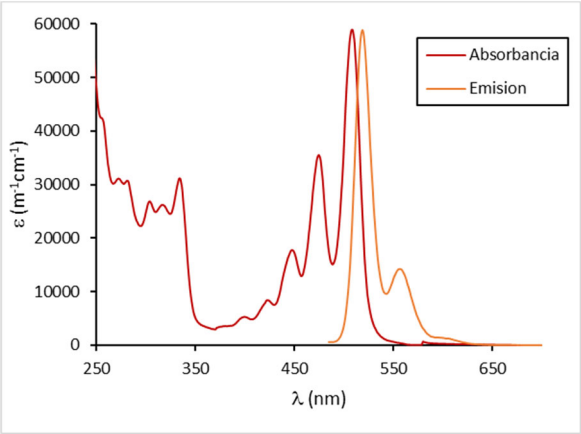

Figure S40. UV-vis and fluorescence of **12**.

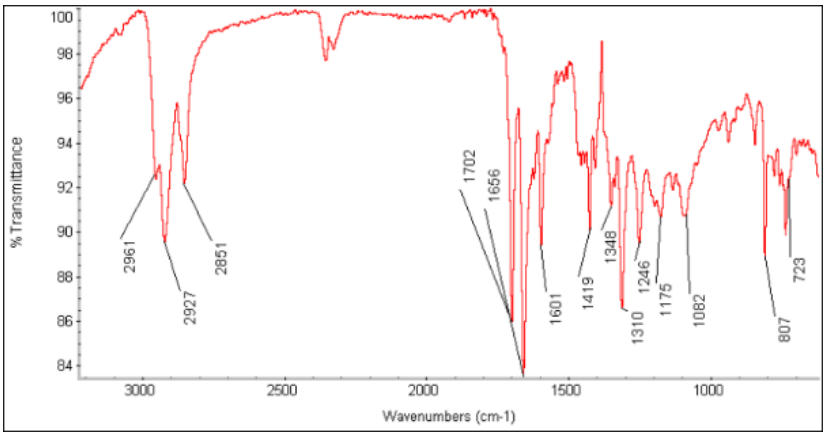

Figure S41. IR of **12**.

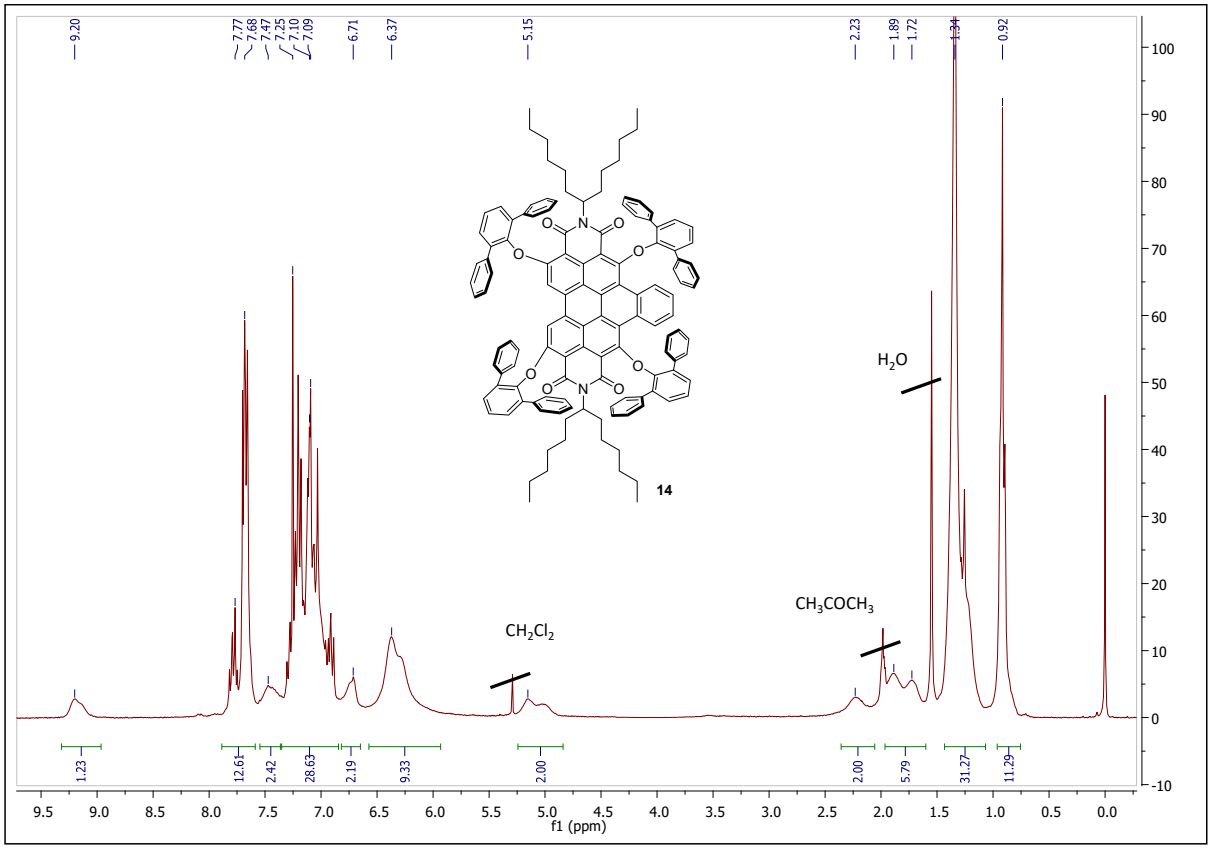

Figure S42. ^{1}H-NMR of **14**.

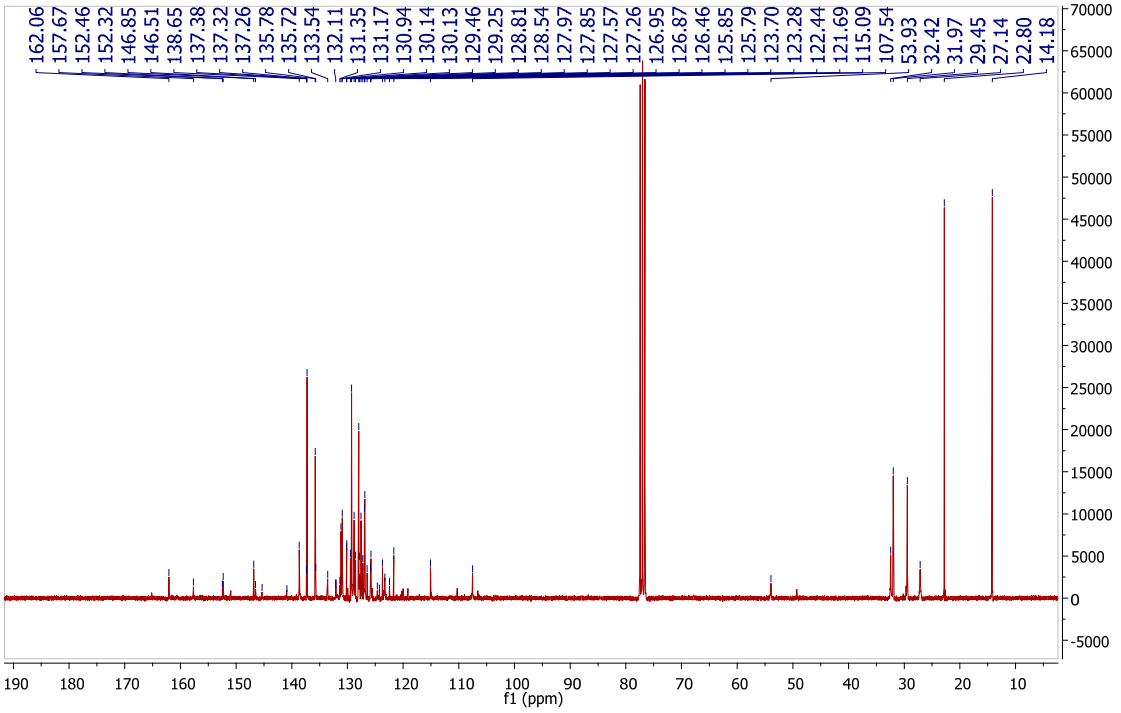

Figure S43. ^{13}C-NMR of **14**.

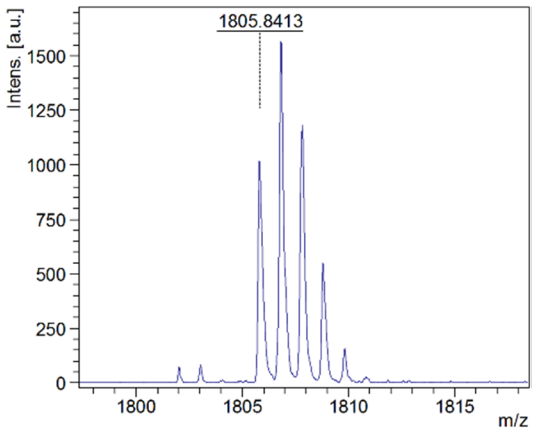

Figure S44. HRMS MALDI-TOF of **14.**

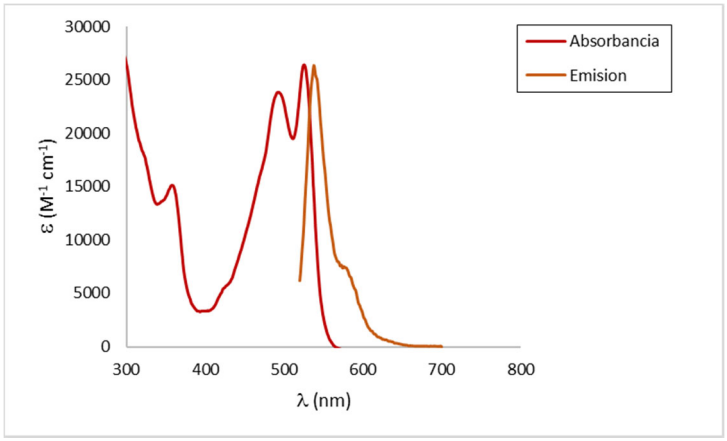

Figure S45. UV-vis and fluorescence of **14**.

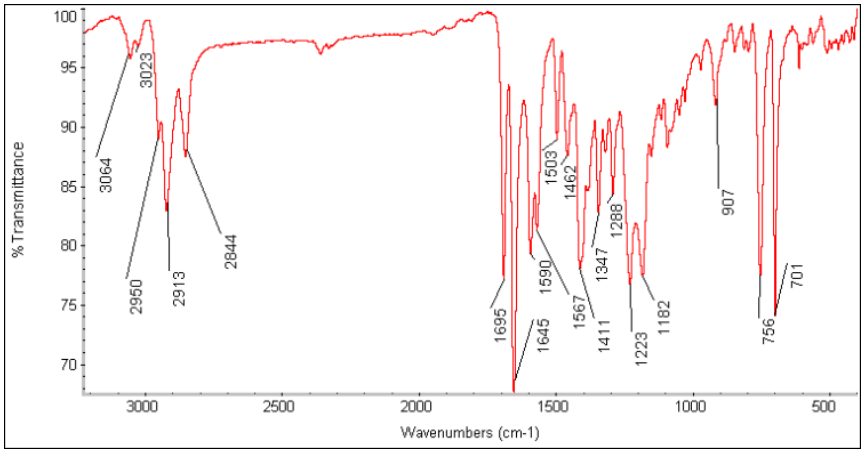

Figure S46. IR of **14**.

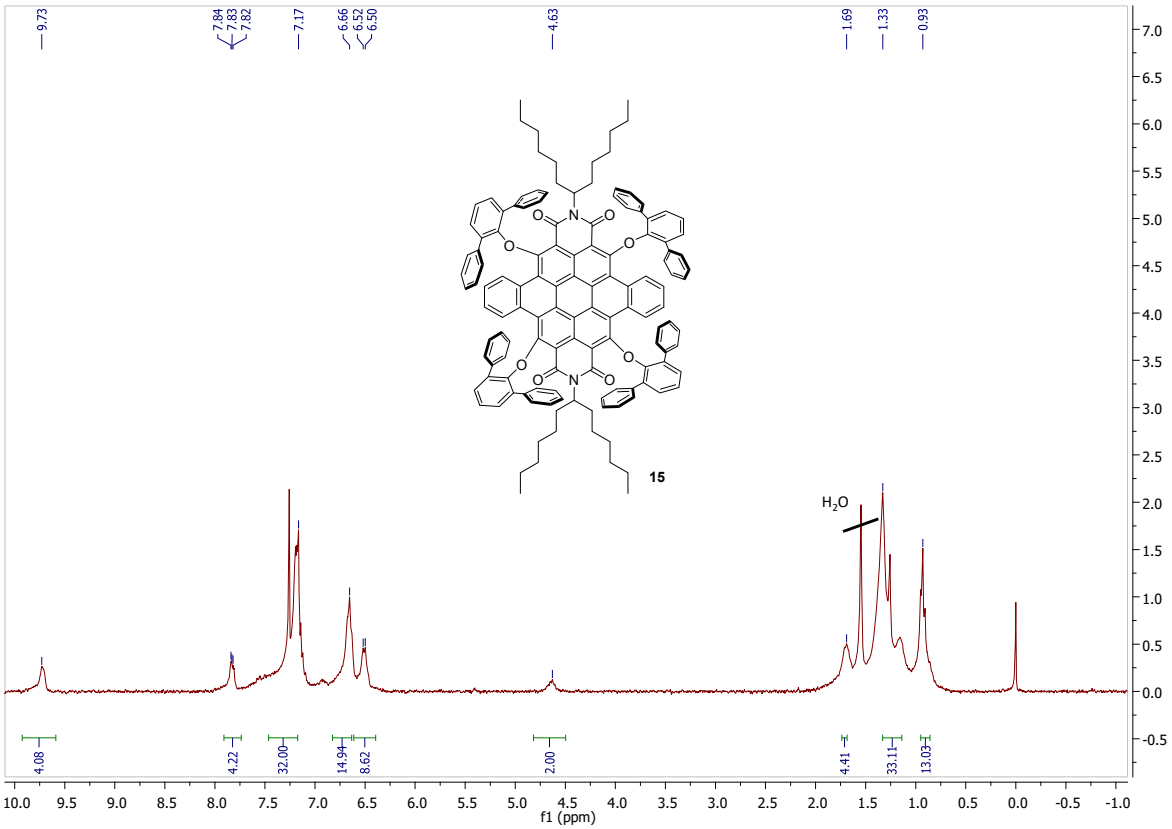

Figure S47. ^{1}H-NMR of **15**.

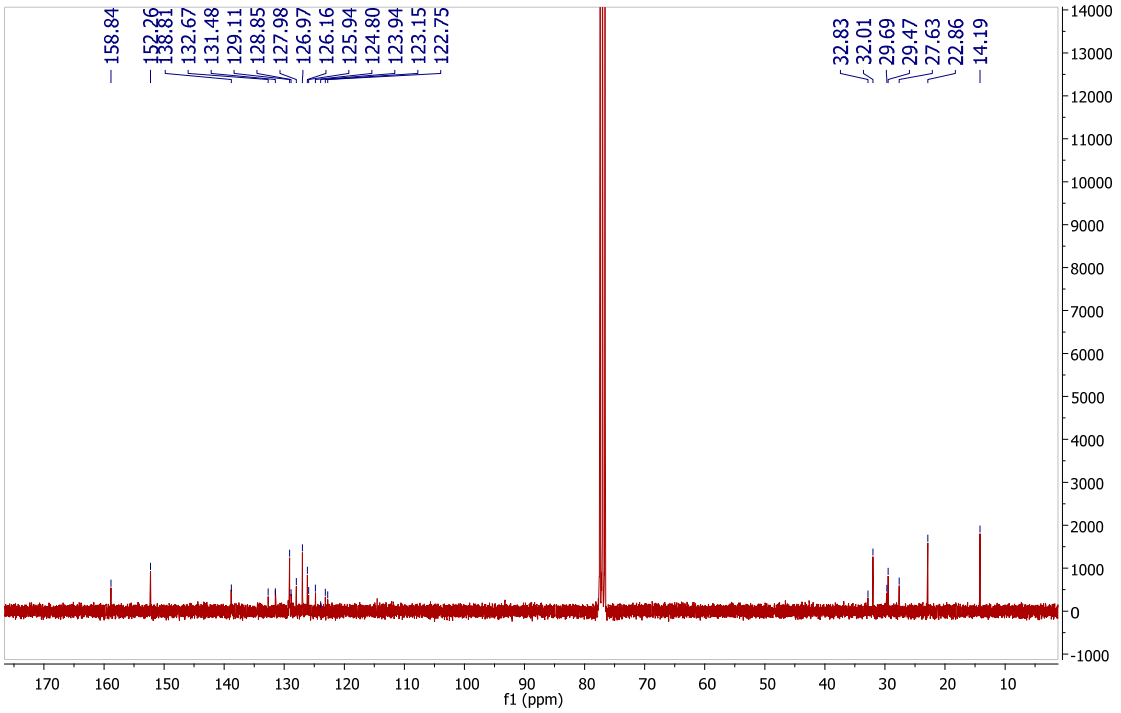

Figure S48. ^{13}C-NMR of **15**.

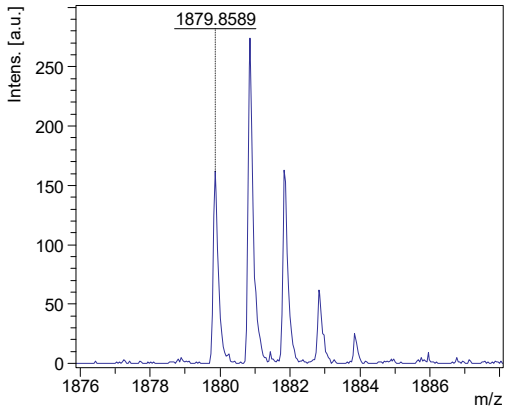

Figure S49. HRMS MALDI-TOF of **15**.

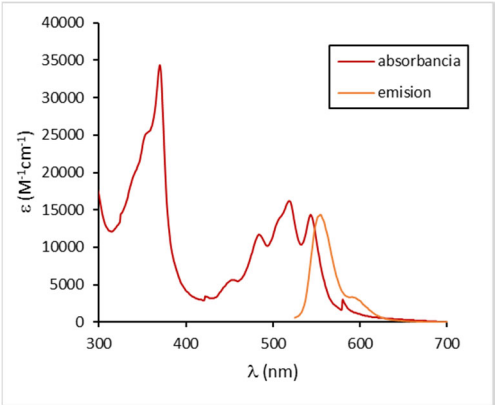

Figure S50. UV-vis and fluorescence of **15**.

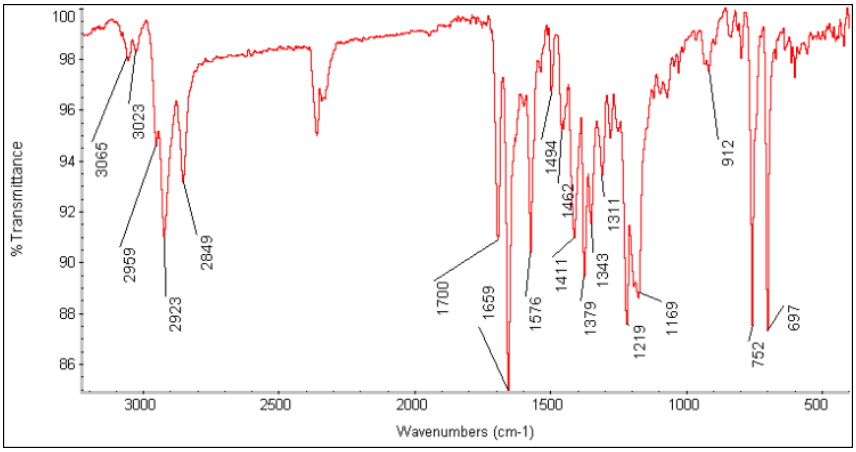

Figure S51. IR of **15**.

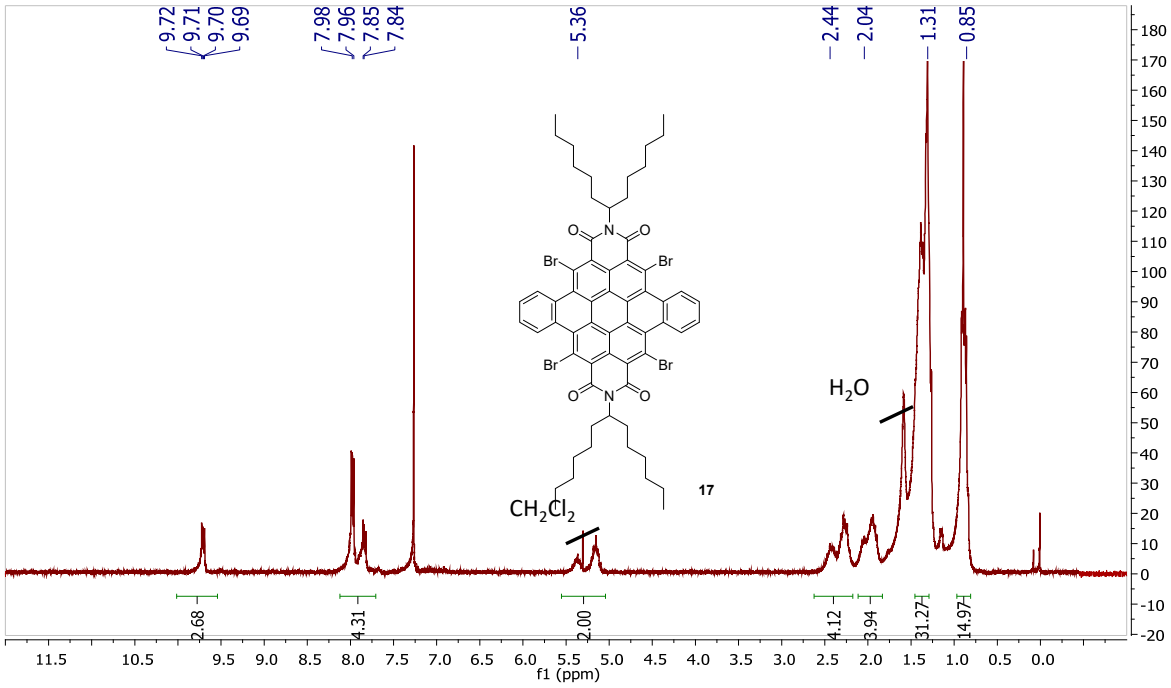

Figure S52. ^{1}H-NMR of **17**

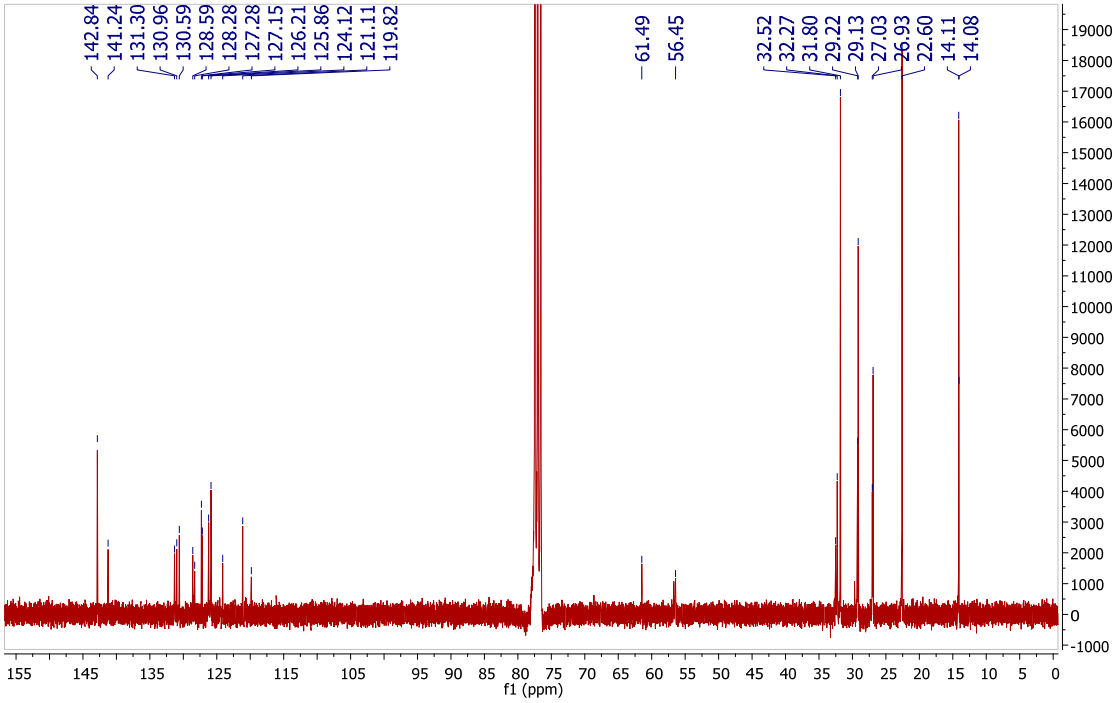

Figure S53. ^{13}C-NMR of **17**.

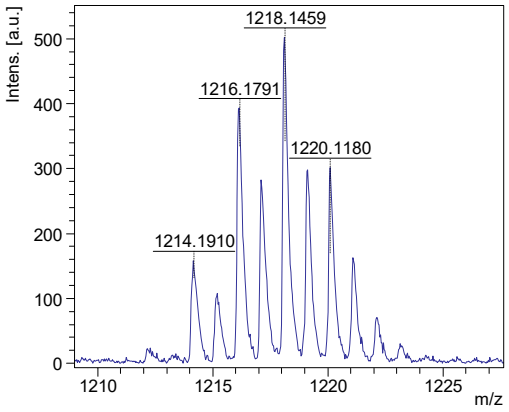

Figure S54. HRMS MALDI-TOF of **17**.

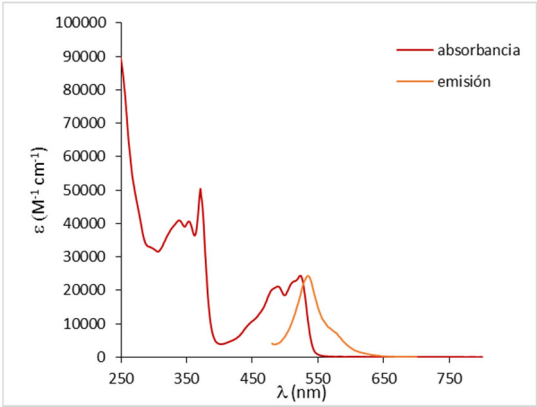

Figure S55. UV-vis and fluorescence of **17**.

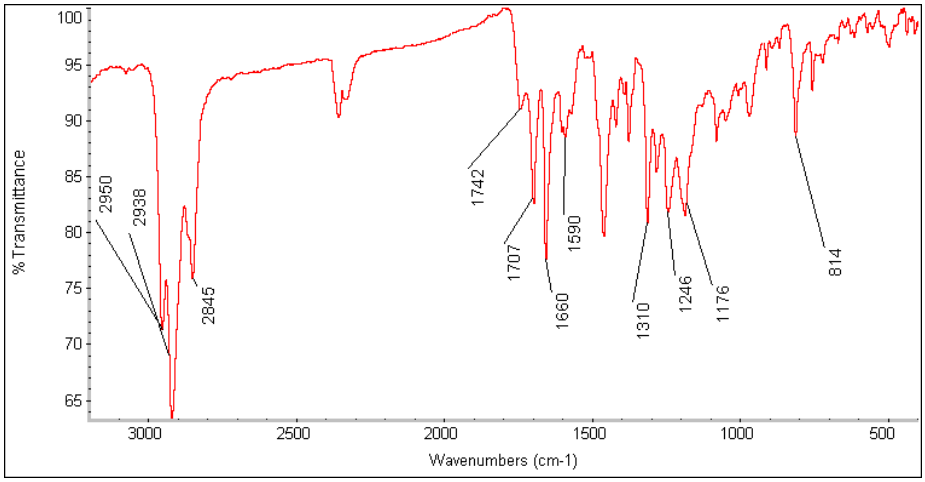

Figure S56. IR of **17**.

2. Theoretical calculations

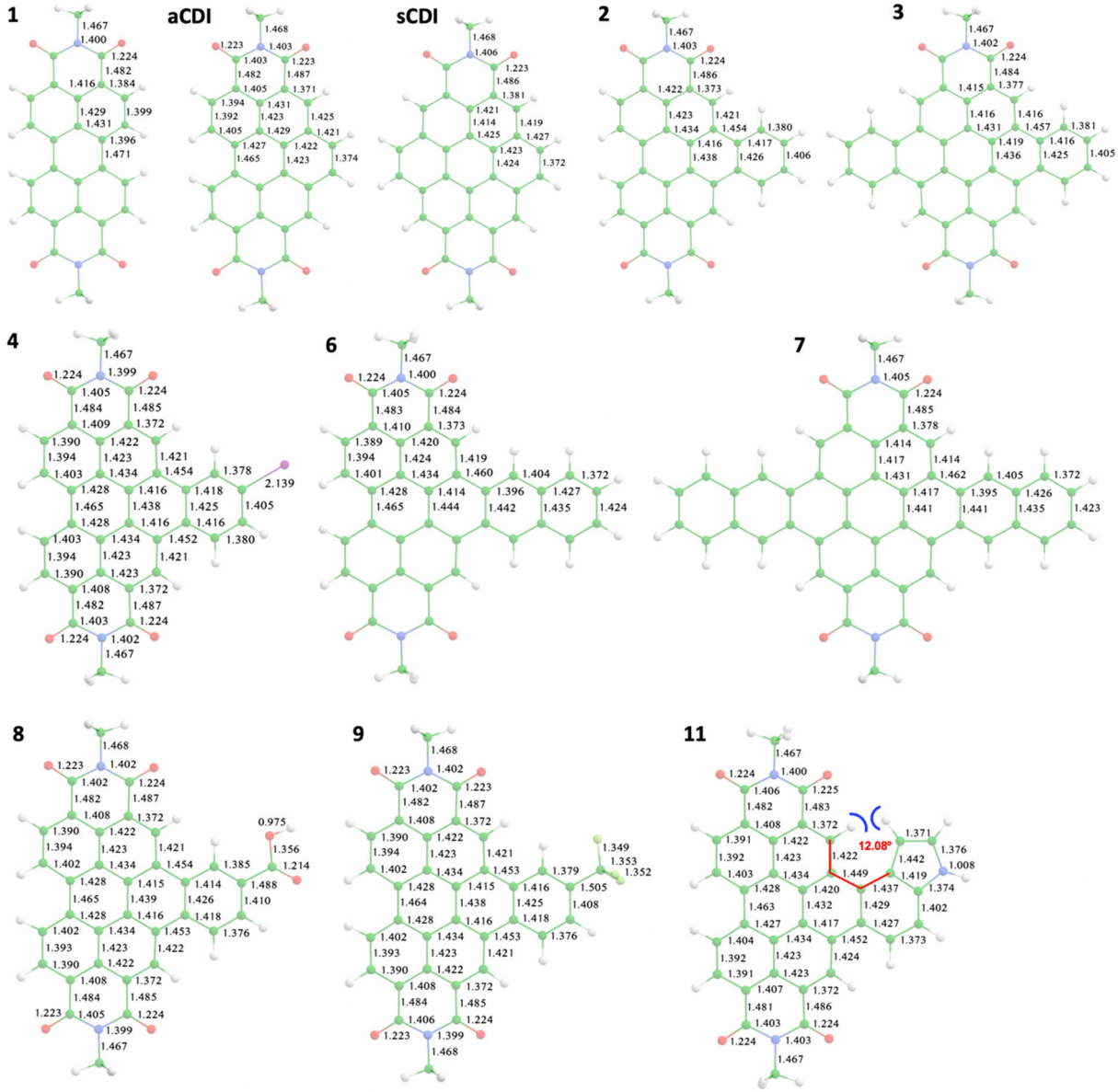

Figure S57. Minimum-energy fully optimized structures calculated at the B3LYP/6-31G* level of theory for the series of PDIs (**1**, **aCDI**, **sCDI**, **2**-**4**, **6**-**9**, and **11**) with symmetric and asymmetric core expansion. C–H bond lengths are not displayed.

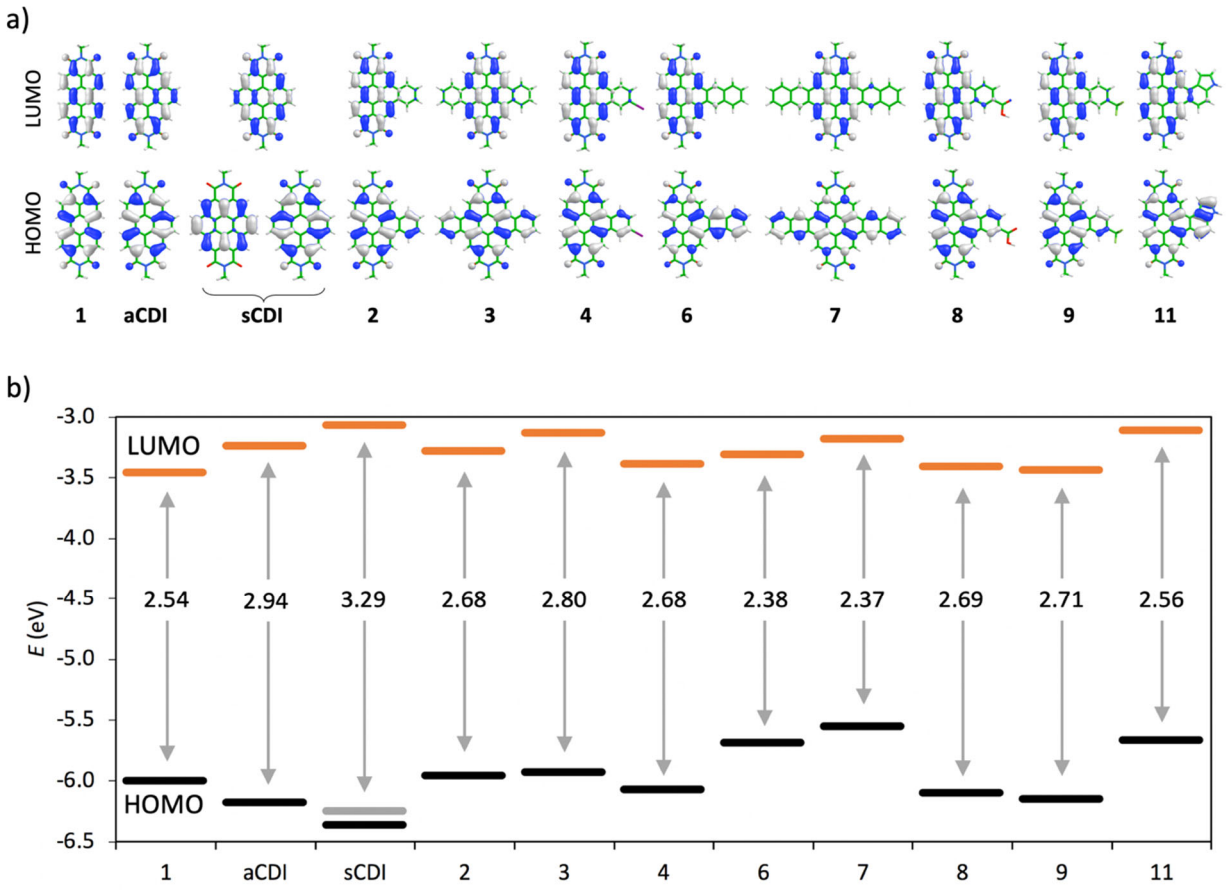

Figure S58. a) Topology of the frontier molecular orbitals. The HOMO (left) and HOMO-1 (right) of **sCDI** are displayed. b) Energy diagram of the highest-occupied (HOMO) and lowest-unoccupied (LUMO) molecular orbitals of the series of PDIs (**1**, aCDI, sCDI, **2**-**4**, **6**-**9**, and **11**) with symmetric and asymmetric core expansion. The HOMO (in grey) and HOMO-1 (in black) of **sCDI** are indicated.

Ionization potential and electron affinity and reorganization energies were calculated for the set of molecules according to the following expressions:

$$\mathrm{IP} = E_C^{+1} - E_N^0 \quad \text{(S1)}$$

$$\mathrm{EA} = E_N^0 - E_C^{-1} \quad \text{(S2)}$$

$$\lambda^+ = (E_N^{+1} - E_C^{+1}) + (E_C^0 - E_N^0) \quad \text{(S3)}$$

$$\lambda^- = (E_N^{-1} - E_C^{-1}) + (E_C^0 - E_N^0) \quad \text{(S4)}$$

where E_Y^X is the energy of the neutral (X = 0), cation (X = +1) or anion (X = −1) species at the minimum-energy geometry of the neutral (Y = N) or the corresponding charged species (Y = C). Table S1 summarizes the values for all these magnitudes.

Table S1. Ionization potential (IP), electron affinity (EA), and reorganization energy for holes (λ^+) and electrons (λ^-), in eV units.

Compound	IP	EA	λ^+	λ^-
1	7.21	2.34	0.156	0.262
aCDI	7.37	2.11	0.151	0.246
sCDI	7.44	1.95	0.176	0.233
2	7.10	2.20	0.129	0.234
3	7.00	2.10	0.109	0.213
4	7.16	2.33	0.119	0.232
6	6.77	2.27	0.108	0.231
7	6.52	2.23	0.082	0.189
8	7.21	2.35	0.141	0.239
9	7.27	2.37	0.143	0.241
11	6.77	2.05	0.128	0.234

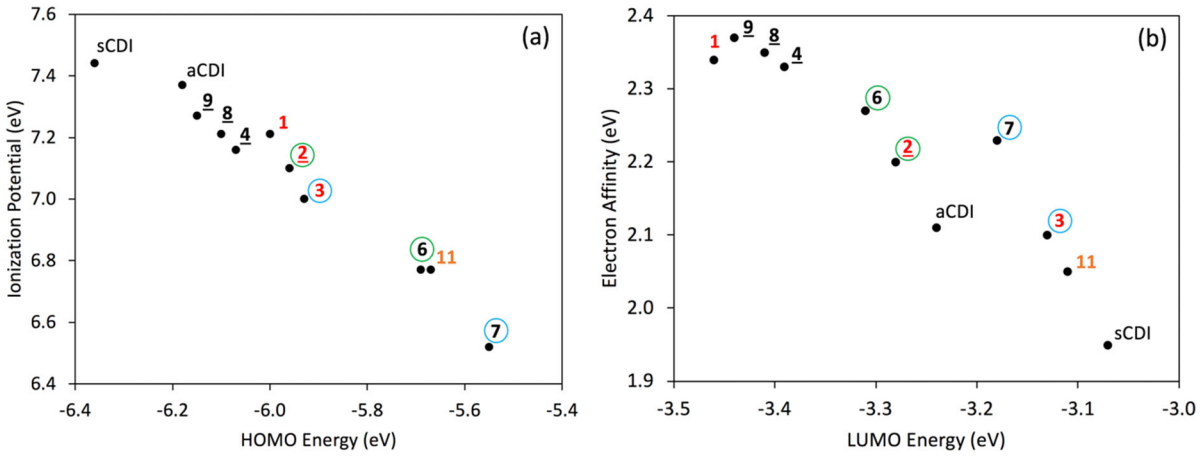

Figure S59. Correlation between the ionization potential and the HOMO energy (a), and between the electron affinity and the LUMO energy (b). Key comparisons are highlighted.

XYZ Coordinates

46
Compound 1
C -2.8614 0.0012 -0.0001
C -3.5738 -1.2223 -0.0002
C -5.0559 -1.2382 -0.0002
N -5.7055 0.0025 0.0000
C -5.0588 1.2482 0.0003
C -3.5750 1.2243 0.0001
C -1.4320 0.0011 -0.0001
C -2.8810 -2.4202 -0.0004
O -5.7063 -2.2751 -0.0001
O -5.6926 2.2952 0.0006
C -7.1723 -0.0297 0.0003
H -7.5298 -0.5600 0.8862
H -7.5253 0.9989 0.0003
H -7.5302 -0.5601 -0.8853
C -1.4820 -2.4294 -0.0004
C -0.7353 1.2512 -0.0001
C -2.8809 2.4219 0.0002
C -1.4820 2.4311 0.0001
C -0.7353 -1.2493 -0.0002
H -3.4438 -3.3477 -0.0006
H -3.4430 3.3496 0.0004
H -0.9833 3.3929 0.0002
H -0.9830 -3.3911 -0.0006
C 0.7353 -1.2493 -0.0001
C 0.7353 1.2512 -0.0003
C 1.4320 0.0011 -0.0002
C 1.4820 -2.4294 0.0002
C 2.8613 0.0012 -0.0002
C 1.4820 2.4311 -0.0005
C 2.8809 2.4219 -0.0005
C 2.8810 -2.4202 0.0002
C 3.5750 1.2243 -0.0003
C 3.5738 -1.2223 -0.0000
H 0.9830 -3.3911 0.0004
H 3.4438 -3.3477 0.0004
H 3.4430 3.3497 -0.0006
H 0.9832 3.3929 -0.0006
C 5.0559 -1.2382 -0.0001
C 5.0588 1.2482 -0.0002
N 5.7055 0.0025 -0.0001
O 5.7063 -2.2751 0.0008
O 5.6925 2.2952 0.0001
C 7.1723 -0.0297 0.0003
H 7.5303 -0.5594 -0.8857
H 7.5253 0.9989 0.0012
H 7.5297 -0.5608 0.8858

48
Compound aCDI
C -2.8464 -0.2259 0.0000
C -3.5692 -1.4313 0.0000
C -5.0527 -1.4341 0.0000
N -5.6844 -0.1783 0.0001
C -5.0241 1.0564 0.0000
C -3.5392 1.0258 0.0000

```
C     -1.4233  -0.2478   0.0000
C     -2.8853  -2.6460  -0.0000
O     -5.7018  -2.4710  -0.0000
O     -5.6650   2.0987   0.0000
C     -7.1511  -0.1302   0.0001
H     -7.5030   0.4041   0.8857
H     -7.5030   0.4040  -0.8857
H     -7.5153  -1.1548   0.0001
C     -1.4938  -2.6755  -0.0000
C     -0.7127   0.9926   0.0000
C     -2.8449   2.2080   0.0000
C     -1.4203   2.2257   0.0000
C     -0.7312  -1.4960  -0.0000
H     -3.4622  -3.5645  -0.0000
H     -3.4021   3.1401   0.0000
C     -0.6900   3.4445   0.0000
C      0.7342  -1.4947  -0.0000
C      0.7104   0.9938   0.0000
C      1.4237  -0.2448  -0.0000
C      1.4987  -2.6730  -0.0000
C      2.8467  -0.2201  -0.0000
C      1.4161   2.2279   0.0000
C      2.8407   2.2129   0.0000
C      2.8902  -2.6410  -0.0000
C      3.5385   1.0325  -0.0000
C      3.5705  -1.4246  -0.0000
H      3.4696  -3.5581  -0.0001
H      3.3953   3.1464   0.0000
C      0.6839   3.4456   0.0000
C      5.0524  -1.4167  -0.0000
C      5.0250   1.0739  -0.0000
N      5.6846  -0.1647  -0.0000
O      5.7198  -2.4421  -0.0001
O      5.6472   2.1272  -0.0000
C      7.1521  -0.1791  -0.0000
H      7.5163  -0.7049  -0.8858
H      7.4926   0.8536   0.0001
H      7.5163  -0.7051   0.8856
H      1.2320   4.3837   0.0000
H     -1.2396   4.3817   0.0000
H      1.0086  -3.6398  -0.0000
H     -1.0023  -3.6415  -0.0000

50
Compound sCDI
C     -2.8322   0.0030  -0.0000
C     -3.5316   1.2399   0.0000
C     -5.0178   1.2580   0.0001
N     -5.6603   0.0072  -0.0002
C     -5.0174  -1.2398   0.0000
C     -3.5328  -1.2328  -0.0000
C     -1.4183   0.0016  -0.0000
C     -2.8423   2.4365   0.0000
O     -5.6576   2.3002   0.0004
O     -5.6760  -2.2704   0.0004
C     -7.1279  -0.0242  -0.0002
H     -7.4859  -0.5544  -0.8859
H     -7.4859  -0.5544   0.8855
H     -7.4807   1.0044  -0.0001
```

```
C     -1.4241   2.4686  -0.0000
C     -0.7132  -1.2364  -0.0001
C     -2.8472  -2.4312  -0.0001
C     -1.4290  -2.4661  -0.0001
C     -0.7104   1.2378  -0.0000
H     -3.4107   3.3616   0.0001
H     -3.4182  -3.3548  -0.0001
C     -0.6893  -3.6870  -0.0002
C     -0.6824   3.6882  -0.0000
C      0.7132   1.2364  -0.0000
C      0.7104  -1.2378  -0.0001
C      1.4183  -0.0016  -0.0000
C      1.4290   2.4662  -0.0000
C      2.8322  -0.0030  -0.0000
C      1.4241  -2.4686  -0.0001
C      2.8423  -2.4365  -0.0000
C      2.8472   2.4312  -0.0001
C      3.5316  -1.2399   0.0000
C      3.5328   1.2328  -0.0001
C      0.6894   3.6870  -0.0000
H      3.4182   3.3548  -0.0001
H      3.4107  -3.3616   0.0000
C      0.6824  -3.6882  -0.0001
C      5.0174   1.2398  -0.0001
C      5.0178  -1.2580   0.0002
N      5.6603  -0.0072  -0.0000
O      5.6760   2.2703  -0.0001
O      5.6575  -2.3002   0.0004
C      7.1279   0.0242   0.0001
H      7.4858   0.5544   0.8858
H      7.4806  -1.0044   0.0001
H      7.4859   0.5544  -0.8855
H      1.2366   4.6258   0.0000
H     -1.2279   4.6280  -0.0000
H      1.2280  -4.6280  -0.0001
H     -1.2366  -4.6259  -0.0002

54
Compound 2
C      2.8478  -0.7835   0.0000
C      3.5440   0.4564   0.0000
C      5.0296   0.4962   0.0001
N      5.6867  -0.7432   0.0001
C      5.0496  -1.9923   0.0001
C      3.5680  -1.9938   0.0001
C      1.4245  -0.7875  -0.0000
C      2.8512   1.6413  -0.0000
O      5.6543   1.5488   0.0001
O      5.7129  -3.0206   0.0001
C      7.1539  -0.7620   0.0001
H      7.5164  -1.2890   0.8859
H      7.5164  -1.2892  -0.8855
H      7.4975   0.2697  -0.0001
C      1.4310   1.6836  -0.0001
C      0.7348  -2.0379   0.0000
C      2.8828  -3.2029   0.0001
C      1.4895  -3.2195   0.0001
C      0.7182   0.4603  -0.0000
H      3.4423   2.5481  -0.0000
```

```
H      3.4532  -4.1256   0.0001
C      0.7096   2.9457  -0.0002
C     -0.7197   0.4586  -0.0000
C     -0.7297  -2.0396   0.0000
C     -1.4227  -0.7912   0.0000
C     -1.4351   1.6805  -0.0000
C     -2.8460  -0.7908   0.0000
C     -1.4819  -3.2228  -0.0000
C     -2.8752  -3.2094   0.0000
C     -2.8554   1.6349   0.0000
C     -3.5646  -2.0024   0.0000
C     -3.5438   0.4478   0.0001
C     -0.7164   2.9441  -0.0001
H     -3.4494   2.5398   0.0001
H     -3.4426  -4.1338   0.0000
C     -5.0279   0.4762   0.0001
C     -5.0478  -2.0124   0.0001
N     -5.6850  -0.7597   0.0000
O     -5.6717   1.5174   0.0002
O     -5.6922  -3.0524   0.0001
C     -7.1516  -0.7171   0.0000
H     -7.5056  -0.1840  -0.8855
H     -7.5117  -1.7432  -0.0003
H     -7.5057  -0.1846   0.8860
C     -1.3953   4.1874  -0.0001
C      1.3855   4.1906  -0.0004
C     -0.7091   5.3845  -0.0002
C      0.6966   5.3861  -0.0004
H     -1.2574   6.3220  -0.0002
H      1.2427   6.3249  -0.0005
H     -2.4781   4.2132  -0.0000
H      2.4682   4.2191  -0.0005
H      0.9921  -4.1824   0.0001
H     -0.9826  -4.1846  -0.0000

62
Compound 3
C      2.8329   0.0073   0.0000
C      3.5338   1.2364   0.0001
C      5.0190   1.2621   0.0002
N      5.6666   0.0155   0.0002
C      5.0222  -1.2292   0.0001
C      3.5386  -1.2188   0.0001
C      1.4170   0.0037  -0.0000
C      2.8454   2.4298   0.0000
O      5.6544   2.3079   0.0004
O      5.6793  -2.2617   0.0001
C      7.1337  -0.0135   0.0003
H      7.4926  -0.5430   0.8861
H      7.4927  -0.5432  -0.8853
H      7.4845   1.0157   0.0002
C      1.4304   2.4748  -0.0001
C      0.7211  -1.2462  -0.0000
C      2.8575  -2.4160   0.0000
C      1.4426  -2.4680   0.0000
C      0.7145   1.2498  -0.0001
H      3.4404   3.3338   0.0002
H      3.4578  -3.3167   0.0000
C      0.7218  -3.7338  -0.0000
```

```
C      0.7035   3.7372  -0.0003
C     -0.7211   1.2462   0.0000
C     -0.7145  -1.2498  -0.0001
C     -1.4170  -0.0037   0.0000
C     -1.4426   2.4680   0.0001
C     -2.8329  -0.0073   0.0001
C     -1.4304  -2.4748  -0.0002
C     -2.8454  -2.4298  -0.0001
C     -2.8575   2.4160   0.0002
C     -3.5338  -1.2364   0.0000
C     -3.5386   1.2188   0.0002
C     -0.7218   3.7338   0.0000
H     -3.4578   3.3167   0.0003
H     -3.4404  -3.3338  -0.0002
C     -0.7035  -3.7372  -0.0003
C     -5.0222   1.2292   0.0003
C     -5.0190  -1.2621   0.0001
N     -5.6666  -0.0155   0.0001
O     -5.6793   2.2617   0.0006
O     -5.6544  -2.3079   0.0001
C     -7.1337   0.0135   0.0001
H     -7.4926   0.5434  -0.8854
H     -7.4845  -1.0158  -0.0004
H     -7.4927   0.5426   0.8861
C     -1.3774  -4.9821  -0.0005
C      1.4017  -4.9753   0.0001
C     -1.4017   4.9753   0.0001
C      1.3774   4.9821  -0.0008
C     -0.6872  -6.1778  -0.0005
C      0.7175  -6.1744  -0.0001
C     -0.7174   6.1744  -0.0002
C      0.6872   6.1778  -0.0007
H     -1.2326  -7.1171  -0.0007
H      1.2674  -7.1111  -0.0001
H     -1.2674   7.1111  -0.0001
H      1.2326   7.1172  -0.0011
H     -2.4846   4.9987   0.0004
H      2.4602   5.0109  -0.0012
H     -2.4602  -5.0109  -0.0007
H      2.4846  -4.9987   0.0005

54
Compound 4
C     -3.6988  -0.5462   0.0002
C     -3.4111  -1.9393   0.0002
C     -4.5067  -2.9445   0.0002
N     -5.8152  -2.4406   0.0001
C     -6.1538  -1.0795   0.0003
C     -5.0365  -0.1062   0.0003
C     -2.6274   0.3910   0.0002
C     -2.1114  -2.3796   0.0001
O     -4.2861  -4.1486  -0.0003
O     -7.3289  -0.7383  -0.0002
C     -6.9354  -3.3886  -0.0003
H     -7.5547  -3.2285   0.8854
H     -7.5546  -3.2279  -0.8861
H     -6.5187  -4.3932  -0.0006
C     -1.0120  -1.4785   0.0001
C     -2.9277   1.7872   0.0003
```

```
C     -5.3133   1.2560   0.0003
C     -4.2731   2.1835   0.0003
C     -1.2758  -0.0874   0.0002
H     -1.9633  -3.4517   0.0001
H     -6.3494   1.5772   0.0003
C      0.3597  -1.9557   0.0000
C     -0.1910   0.8571   0.0002
C     -1.8235   2.7493   0.0003
C     -0.4811   2.2618   0.0002
C      1.1513   0.4057   0.0001
C      0.5932   3.1955   0.0002
C     -2.0322   4.1362   0.0003
C     -0.9715   5.0402   0.0002
C      2.1937   1.3721   0.0001
C      0.3408   4.5814   0.0002
C      1.9330   2.7192   0.0001
C      1.4350  -1.0207   0.0000
H      3.2365   1.0814   0.0000
H     -1.1489   6.1102   0.0003
C      3.0717   3.6726   0.0002
C      1.4536   5.5627   0.0002
N      2.7564   5.0360   0.0000
O      4.2403   3.3085  -0.0003
O      1.2564   6.7703  -0.0001
C      3.8915   5.9662  -0.0003
H      4.5081   5.7956  -0.8861
H      3.4906   6.9771  -0.0006
H      4.5081   5.7962   0.8856
C      2.7663  -1.5080  -0.0001
C      0.6696  -3.3374  -0.0001
C      3.0213  -2.8625  -0.0002
C      1.9711  -3.7955  -0.0002
H      2.1742  -4.8604  -0.0002
H      3.5970  -0.8160  -0.0001
H     -0.1247  -4.0737  -0.0001
H     -4.5299   3.2361   0.0003
H     -3.0399   4.5341   0.0003
I      5.0417  -3.5662  -0.0003

60
Compound 6
C      2.8482  -1.4745   0.0000
C      3.5461  -0.2376  -0.0002
C      5.0299  -0.2087  -0.0003
N      5.6875  -1.4442  -0.0001
C      5.0504  -2.6970   0.0001
C      3.5675  -2.6867   0.0001
C      1.4244  -1.4734   0.0001
C      2.8562   0.9495  -0.0003
O      5.6733   0.8328  -0.0006
O      5.6950  -3.7370   0.0003
C      7.1540  -1.4014  -0.0002
H      7.5144  -2.4274  -0.0002
H      7.5080  -0.8685  -0.8860
H      7.5081  -0.8684   0.8855
C      1.4376   0.9954  -0.0001
C      0.7325  -2.7229   0.0002
C      2.8784  -3.8928   0.0002
C      1.4844  -3.9055   0.0003
```

```
C      0.7219  -0.2236   0.0000
H      3.4497   1.8547  -0.0005
H      3.4454  -4.8174   0.0003
C      0.7208   2.2671  -0.0000
C     -0.7219  -0.2236   0.0000
C     -0.7325  -2.7229   0.0002
C     -1.4244  -1.4734   0.0001
C     -1.4377   0.9954  -0.0001
C     -2.8482  -1.4745  -0.0000
C     -1.4844  -3.9055   0.0003
C     -2.8784  -3.8928   0.0002
C     -2.8562   0.9495  -0.0003
C     -3.5675  -2.6867   0.0001
C     -3.5461  -0.2376  -0.0002
C     -0.7208   2.2671  -0.0000
H     -3.4497   1.8547  -0.0005
H     -3.4455  -4.8174   0.0003
C     -5.0299  -0.2087  -0.0004
C     -5.0504  -2.6970   0.0001
N     -5.6875  -1.4442  -0.0002
O     -5.6733   0.8329  -0.0006
O     -5.6950  -3.7371   0.0003
C     -7.1541  -1.4013  -0.0002
H     -7.5144  -2.4274  -0.0001
H     -7.5080  -0.8683   0.8855
H     -7.5080  -0.8685  -0.8860
C     -1.3917   3.4910   0.0001
C      1.3917   3.4910   0.0000
C     -0.7176   4.7223   0.0002
C      0.7176   4.7223   0.0001
C     -1.4078   5.9707   0.0003
C      1.4079   5.9707   0.0002
C     -0.7119   7.1531   0.0003
C      0.7119   7.1531   0.0003
H     -2.4752   3.5209   0.0002
H      2.4752   3.5209   0.0000
H      2.4951   5.9671   0.0001
H     -2.4950   5.9671   0.0003
H     -1.2455   8.0994   0.0004
H      1.2455   8.0994   0.0003
H     -0.9854  -4.8672   0.0003
H      0.9853  -4.8672   0.0003

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Compound 7
C     -0.0009   2.8357  -0.0000
C     -1.2270   3.5403   0.0000
C     -1.2500   5.0252   0.0002
N     -0.0022   5.6702   0.0001
C      1.2406   5.0223  -0.0001
C      1.2255   3.5391  -0.0001
C     -0.0008   1.4183  -0.0000
C     -2.4215   2.8539   0.0000
O     -2.2946   5.6629   0.0005
O      2.2752   5.6764  -0.0001
C      0.0301   7.1371   0.0003
H      0.5600   7.4948   0.8863
H      0.5607   7.4951  -0.8852
H     -0.9984   7.4903  -0.0001
```

C	-2.4699	1.4403	-0.0000
C	1.2486	0.7205	-0.0000
C	2.4204	2.8541	-0.0001
C	2.4689	1.4403	-0.0001
C	-1.2498	0.7204	-0.0000
H	-3.3244	3.4507	0.0001
H	3.3230	3.4515	-0.0001
C	3.7414	0.7206	-0.0001
C	-3.7425	0.7206	-0.0000
C	-1.2498	-0.7204	-0.0000
C	1.2486	-0.7205	0.0000
C	-0.0008	-1.4183	0.0000
C	-2.4699	-1.4403	-0.0001
C	-0.0009	-2.8358	0.0000
C	2.4689	-1.4403	0.0001
C	2.4205	-2.8540	0.0001
C	-2.4215	-2.8539	-0.0001
C	1.2255	-3.5391	0.0001
C	-1.2270	-3.5403	-0.0000
C	-3.7425	-0.7207	-0.0001
H	-3.3244	-3.4507	-0.0002
H	3.3230	-3.4515	0.0002
C	3.7414	-0.7206	0.0000
C	-1.2500	-5.0252	-0.0000
C	1.2406	-5.0223	0.0002
N	-0.0022	-5.6702	0.0001
O	-2.2946	-5.6629	-0.0001
O	2.2751	-5.6765	0.0003
C	0.0304	-7.1371	0.0001
H	0.5609	-7.4948	-0.8855
H	0.5608	-7.4948	0.8859
H	-0.9980	-7.4904	0.0001
C	4.9645	-1.3911	0.0001
C	4.9645	1.3912	-0.0002
C	-4.9656	-1.3911	-0.0001
C	-4.9656	1.3911	-0.0000
C	6.1968	-0.7173	0.0000
C	6.1968	0.7173	-0.0002
C	-6.1979	-0.7173	-0.0001
C	-6.1979	0.7173	-0.0001
C	7.4447	-1.4075	0.0001
C	7.4447	1.4076	-0.0003
C	-7.4458	-1.4076	-0.0001
C	-7.4459	1.4075	-0.0001
C	8.6276	-0.7116	-0.0000
C	8.6276	0.7117	-0.0002
C	-8.6287	-0.7116	-0.0002
C	-8.6288	0.7116	-0.0001
H	4.9937	-2.4748	0.0002
H	7.4411	-2.4948	0.0002
H	9.5738	-1.2455	0.0000
H	9.5738	1.2455	-0.0003
H	7.4411	2.4948	-0.0005
H	4.9937	2.4748	-0.0004
H	-4.9949	-2.4748	-0.0001
H	-4.9949	2.4748	0.0000
H	-7.4423	2.4947	-0.0000
H	-7.4423	-2.4948	-0.0002
H	-9.5749	-1.2455	-0.0002

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H     -9.5750   1.2455  -0.0001

57
Compound 8
C      2.4298  -1.8018   0.0001
C      3.3323  -0.7026   0.0000
C      4.8030  -0.9239   0.0000
N      5.2330  -2.2586   0.0001
C      4.3871  -3.3767   0.0002
C      2.9277  -3.1190   0.0002
C      1.0278  -1.5572   0.0001
C      2.8586   0.5852  -0.0001
O      5.6009   0.0037  -0.0002
O      4.8595  -4.5053   0.0002
C      6.6745  -2.5338  -0.0000
H      6.9392  -3.1159   0.8859
H      6.9390  -3.1163  -0.8857
H      7.1938  -1.5783  -0.0003
C      1.4669   0.8738  -0.0001
C      0.1303  -2.6678   0.0003
C      2.0421  -4.1898   0.0004
C      0.6671  -3.9631   0.0004
C      0.5511  -0.2052   0.0000
H      3.5989   1.3749  -0.0002
H      2.4427  -5.1978   0.0004
C      0.9741   2.2419  -0.0002
C     -0.8655   0.0449   0.0000
C     -1.3119  -2.4132   0.0003
C     -1.7759  -1.0629   0.0002
C     -1.3580   1.3725  -0.0001
C     -3.1774  -0.8132   0.0002
C     -2.2597  -3.4465   0.0004
C     -3.6290  -3.1889   0.0004
C     -2.7648   1.5769  -0.0000
C     -4.0967  -1.8800   0.0003
C     -3.6490   0.5283   0.0001
C     -0.4304   2.4904  -0.0002
H     -3.1907   2.5719  -0.0001
H     -4.3497  -3.9995   0.0005
C     -5.1063   0.8148   0.0001
C     -5.5592  -1.6314   0.0003
N     -5.9686  -0.2871   0.0002
O     -5.5574   1.9524   0.0000
O     -6.3740  -2.5438   0.0004
C     -7.4056   0.0103   0.0001
H     -7.6611   0.5968  -0.8856
H     -7.9393  -0.9372  -0.0001
H     -7.6613   0.5963   0.8861
C     -0.8812   3.8351  -0.0003
C      1.8580   3.3453  -0.0004
C     -0.0000   4.8918  -0.0005
C      1.3888   4.6482  -0.0005
H     -0.3518   5.9177  -0.0005
H     -1.9422   4.0509  -0.0003
H      2.9282   3.1911  -0.0004
H      0.0095  -4.8242   0.0005
H     -1.9368  -4.4807   0.0004
C      2.3053   5.8200  -0.0007
O      1.9413   6.9785  -0.0008
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O      3.6160   5.4707  -0.0006
H      4.1161   6.3077  -0.0006

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Compound 9
C     -2.0921  -2.2828  -0.0018
C     -3.1195  -1.2993  -0.0064
C     -4.5534  -1.6947  -0.0069
N     -4.8209  -3.0711  -0.0022
C     -3.8475  -4.0801   0.0024
C     -2.4293  -3.6500   0.0025
C     -0.7293  -1.8732  -0.0014
C     -2.8029   0.0357  -0.0103
O     -5.4560  -0.8689  -0.0106
O     -4.1811  -5.2571   0.0062
C     -6.2190  -3.5176  -0.0020
H     -6.4102  -4.1310  -0.8857
H     -6.4120  -4.1244   0.8858
H     -6.8498  -2.6319  -0.0060
C     -1.4555   0.4880  -0.0099
C      0.2943  -2.8688   0.0033
C     -1.4224  -4.6075   0.0071
C     -0.0842  -4.2189   0.0075
C     -0.4171  -0.4739  -0.0055
H     -3.6322   0.7313  -0.0136
H     -1.7003  -5.6561   0.0105
C     -1.1297   1.9043  -0.0126
C      0.9594  -0.0571  -0.0050
C      1.6958  -2.4445   0.0038
C      1.9955  -1.0483  -0.0004
C      1.2894   1.3197  -0.0089
C      3.3568  -0.6334   0.0001
C      2.7601  -3.3571   0.0083
C      4.0890  -2.9381   0.0087
C      2.6614   1.6905  -0.0082
C      4.3971  -1.5827   0.0047
C      3.6644   0.7549  -0.0039
C      0.2337   2.3176  -0.0126
H      2.9673   2.7288  -0.0109
H      4.9013  -3.6570   0.0123
C      5.0767   1.2141  -0.0034
C      5.8194  -1.1602   0.0052
N      6.0646   0.2238   0.0010
O      5.3874   2.3979  -0.0069
O      6.7380  -1.9678   0.0092
C      7.4554   0.6922   0.0014
H      7.6368   1.3081   0.8855
H      8.0999  -0.1836   0.0051
H      7.6392   1.3024  -0.8861
C      0.5199   3.7064  -0.0171
C     -2.1404   2.8962  -0.0148
C     -0.4811   4.6511  -0.0199
C     -1.8277   4.2389  -0.0181
H     -0.2364   5.7084  -0.0279
H      1.5469   4.0491  -0.0203
H     -3.1845   2.6141  -0.0172
H      0.6711  -4.9957   0.0111
H      2.5630  -4.4225   0.0116
C     -2.9067   5.2881   0.0121
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F     -2.7034   6.2257  -0.9412
F     -4.1367   4.7701  -0.1813
F     -2.9237   5.9380   1.1985

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Compound 11
C     -2.4920  -1.5674  -0.0050
C     -3.0438  -2.8615  -0.0505
C     -4.5095  -3.0697   0.0264
N     -5.3013  -1.9169   0.1731
C     -4.8113  -0.6068   0.2322
C     -3.3424  -0.4356   0.1240
C     -1.0828  -1.3744  -0.0519
C     -2.2014  -3.9638  -0.1531
O     -5.0148  -4.1831  -0.0265
O     -5.5846   0.3354   0.3553
C     -6.7569  -2.0715   0.2664
H     -7.1127  -1.6556   1.2121
H     -7.2397  -1.5288  -0.5500
H     -6.9814  -3.1339   0.2057
C     -0.8206  -3.7899  -0.1960
C     -0.5516  -0.0428  -0.0098
C     -2.8166   0.8311   0.1531
C     -1.4217   1.0786   0.0281
C     -0.2311  -2.5176  -0.1374
H     -2.6415  -4.9545  -0.1901
H     -3.5072   1.6420   0.3197
C     -0.8881   2.4256  -0.0055
C      1.2189  -2.3209  -0.1477
C      0.8679   0.1467   0.0117
C      1.7349  -0.9934  -0.0510
C      2.1259  -3.3889  -0.2293
C      3.1440  -0.8014  -0.0148
C      1.4029   1.4542   0.1223
C      2.8186   1.5956   0.1735
C      3.5032  -3.1868  -0.2054
C      3.6644   0.5176   0.1042
C      4.0196  -1.9002  -0.0926
H      4.1931  -4.0216  -0.2680
H      3.2868   2.5676   0.2531
C      0.5226   2.6087   0.1358
C      5.4864  -1.7007  -0.0564
C      5.1303   0.7549   0.1489
N      5.9485  -0.3818   0.0645
O      6.2844  -2.6263  -0.1259
O      5.6093   1.8770   0.2530
C      7.4043  -0.2057   0.1018
H      7.8475  -0.5922  -0.8192
H      7.6062   0.8576   0.2074
H      7.8221  -0.7632   0.9434
C      1.0621   3.9237   0.2648
C     -1.7022   3.5986  -0.1694
C      0.2768   5.0480   0.2041
C     -1.0928   4.8732  -0.0410
H      0.7096   6.0387   0.3127
H      2.1239   4.0552   0.4240
H     -0.1982  -4.6740  -0.2676
H      1.7613  -4.4061  -0.3100
C     -3.0813   3.8592  -0.5011
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C	-3.2506	5.2195	-0.5368
N	-2.0543	5.8331	-0.2443
H	-3.8639	3.1572	-0.7388
H	-4.1346	5.8012	-0.7553
H	-1.8916	6.8282	-0.2350