Supporting Information

Hydrogen Atom Abstraction and Reduction Study of 21-Thiaporphyrin and 21,23-Dithiaporphyrin

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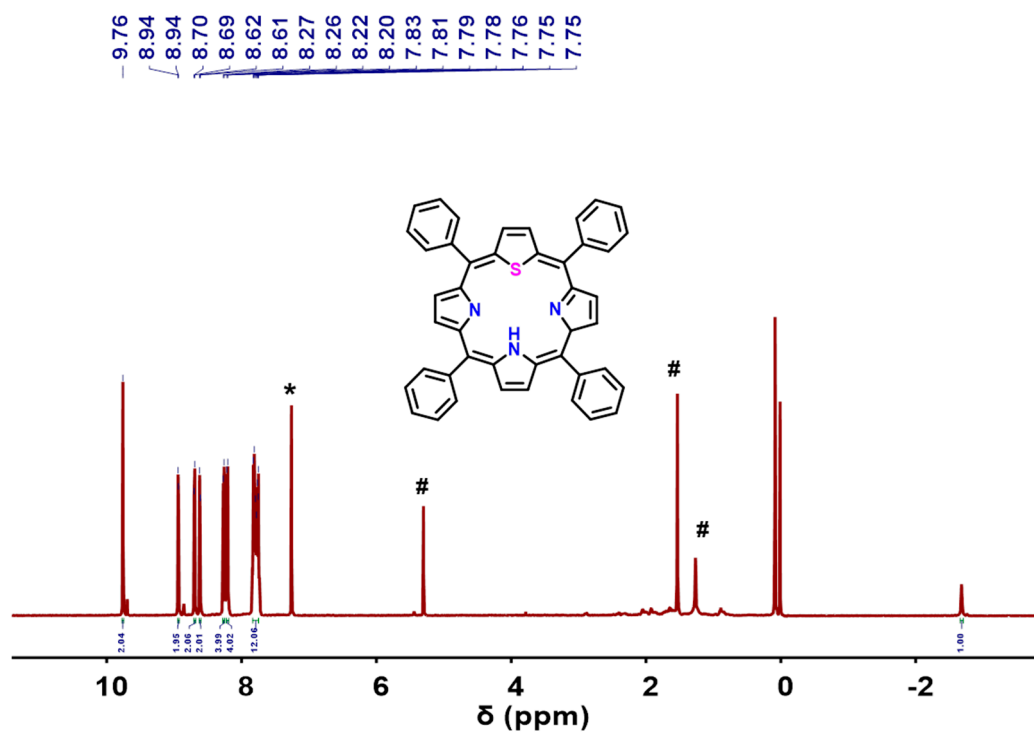
Figure S1: ^{1}H NMR spectrum (500 MHz) of **1** in CDCl$_3$ at 298 K. Solvent signal are marked with an asterisk (*). Other signals are marked with an asterisk (#).
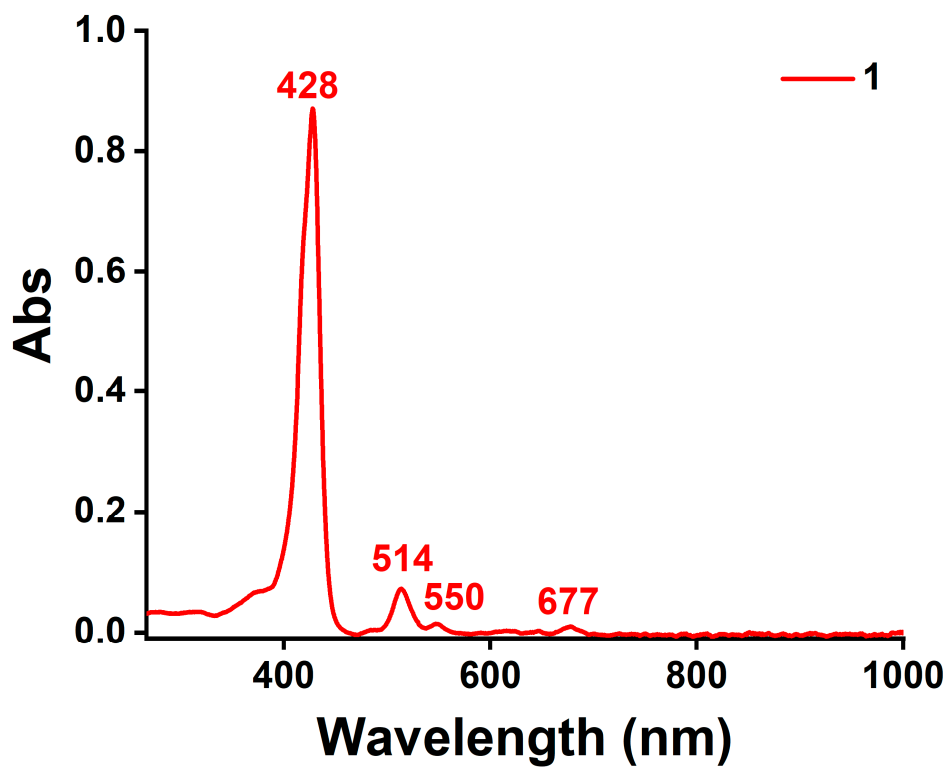

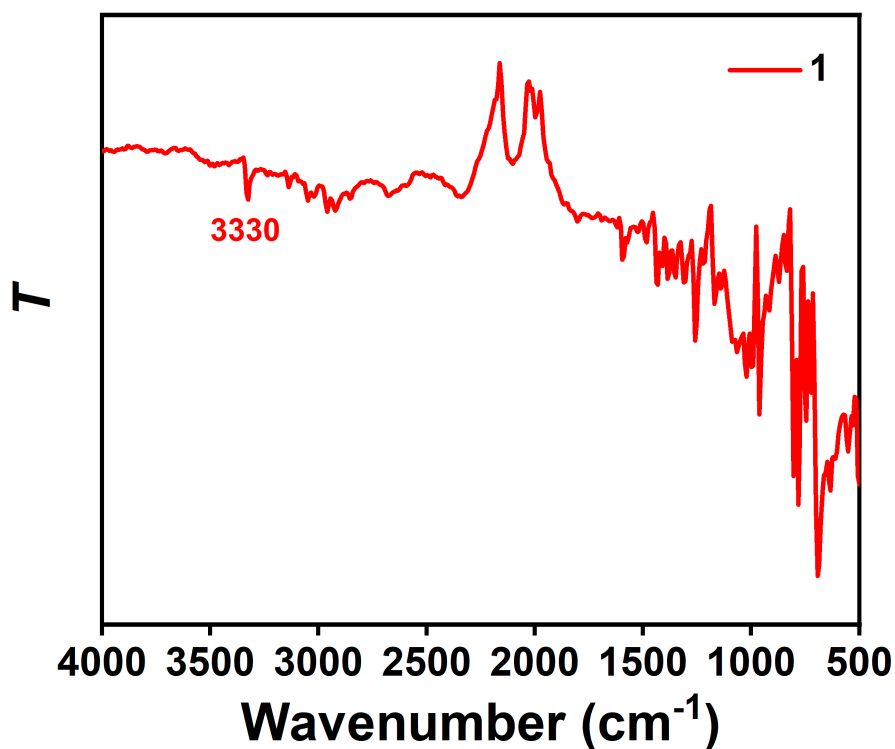**Figure S2:** UV-vis absorption spectra of **1** in DCM solution.

Figure S3: ATR-IR spectrum of **1** in crystalline material.

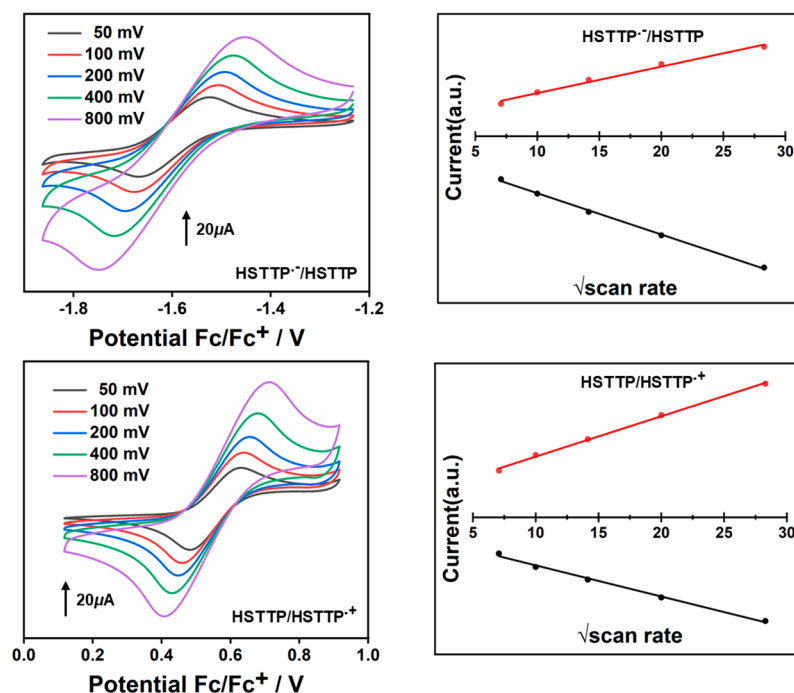**Figure S4:** Left Cyclic voltammograms of **1** in DCM (0.1 M $^{n}Bu_4NPF_6$) at different scan rates. (top) $HSTTP^{-}/HSTTP$ redox couple; (bottom) $HSTTP/HSTTP^{+}$ redox couple. Right: Linear dependence of the current Ifp of the forward peak on the square root of the scan rate. (top) $HSTTP^{-}/HSTTP$ redox couple; (bottom) $HSTTP/HSTTP^{+}$ redox couple
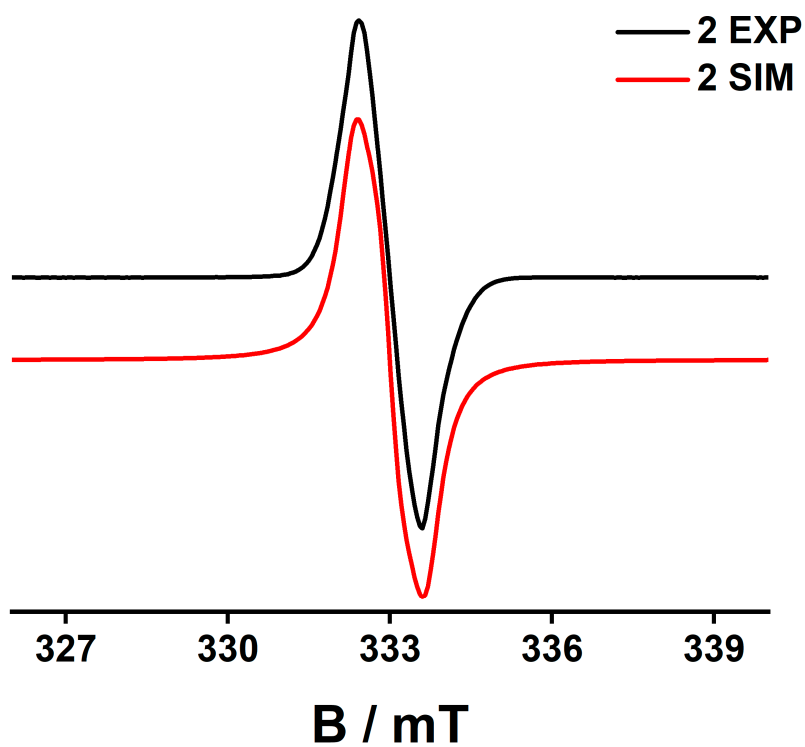
Figure S5: X-band EPR spectrum record at 9.34 GHz, microwave power 1 mW of **2** in THF solution at 293K. The red trace show the simulation with g_{ave} = 2.003.

Figure S6: UV-vis absorption spectra of **2** in THF solution.

Figure S7: ATR-IR spectrum of **2** in crystalline material.

Figure S8: ^{1}H NMR spectrum (500 MHz) of **3** in CDCl$_3$ at 298 K. Solvent signals are marked with an asterisk (*). Other signals are marked with an asterisk (#).

Figure S9: ^{19}F NMR spectrum (471 MHz) of **3** in CDCl$_3$ at 298 K.

Figure S10: ^{1}H NMR spectrum (500 MHz) of **3** in CD$_3$CN at 298 K. Solvent signals are marked with an asterisk (*).
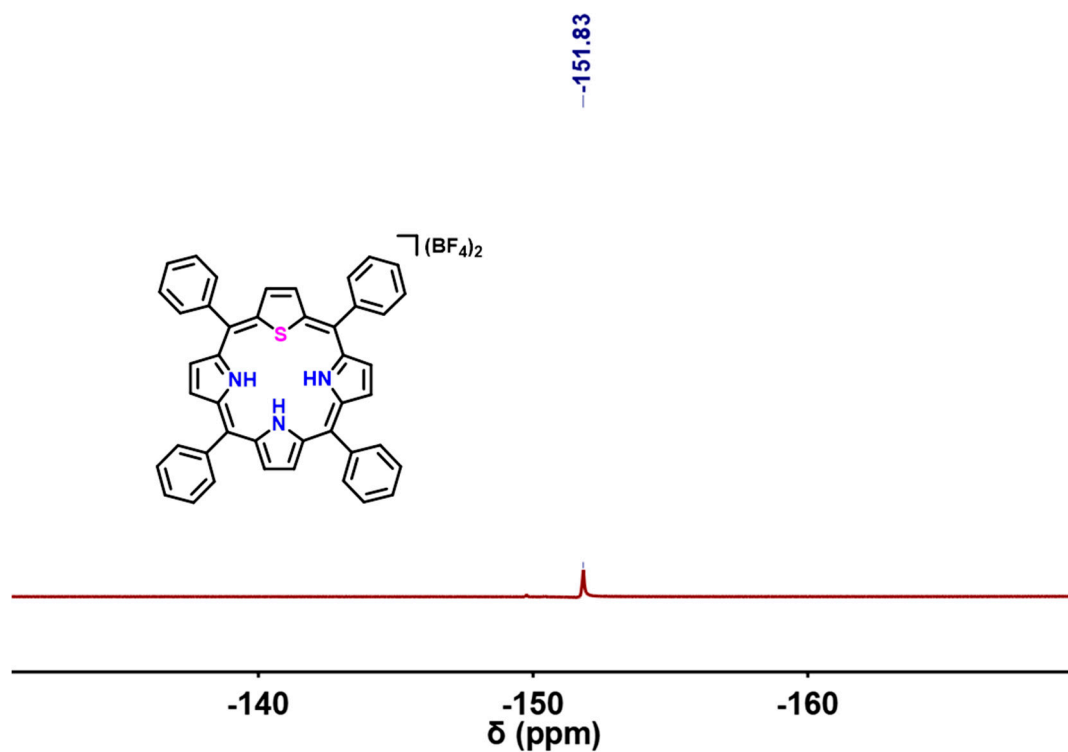
Figure S11: ^{19}F NMR spectrum (471 MHz) of **3** in CD_3CN at 298 K.
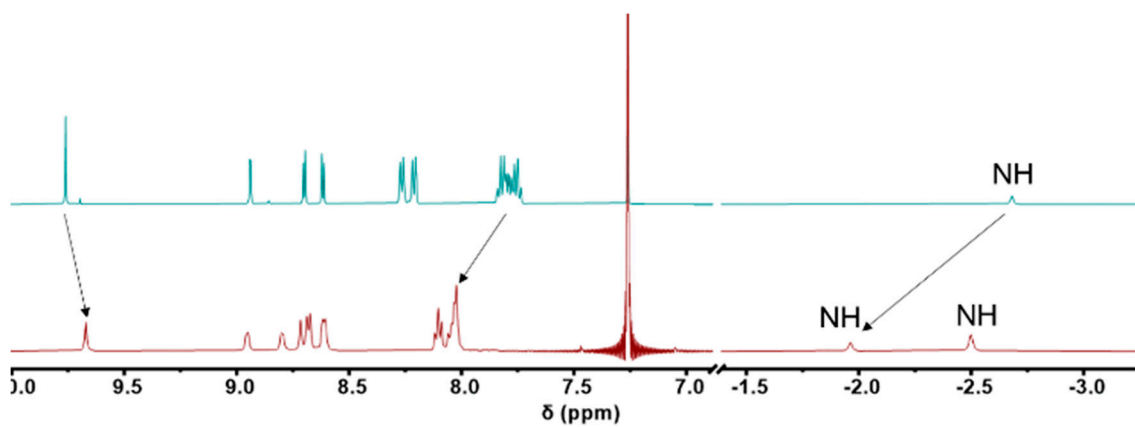
Figure S12: ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of HSTTP **1** (Top) and diacids **3** (Bottom).
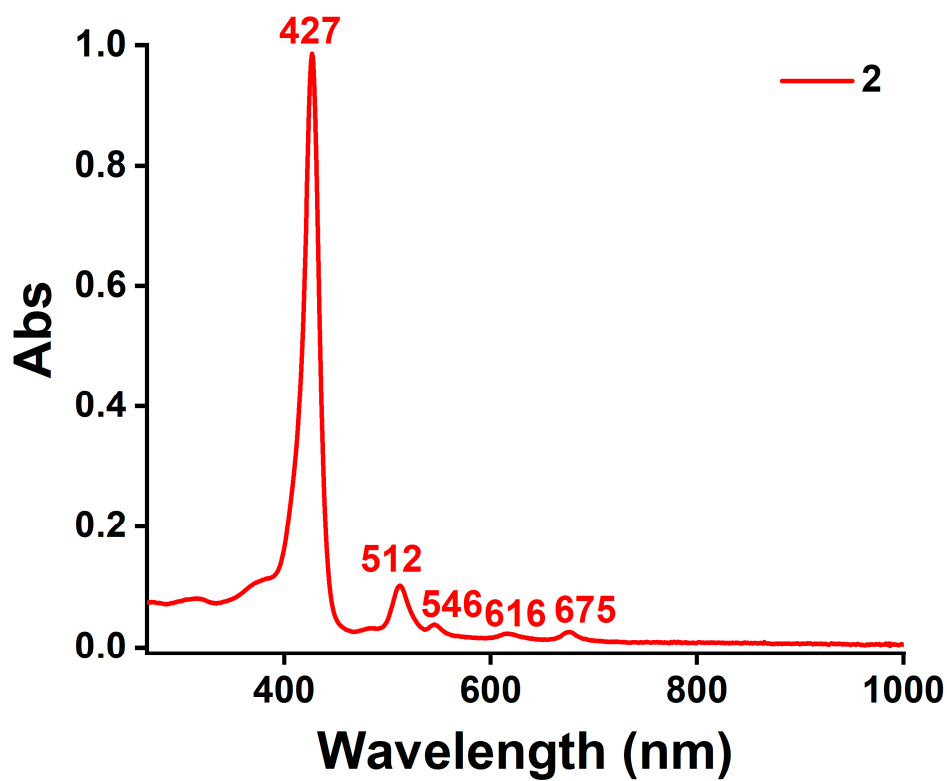
Figure S13: UV-vis absorption spectra of **3** in DCM solution.
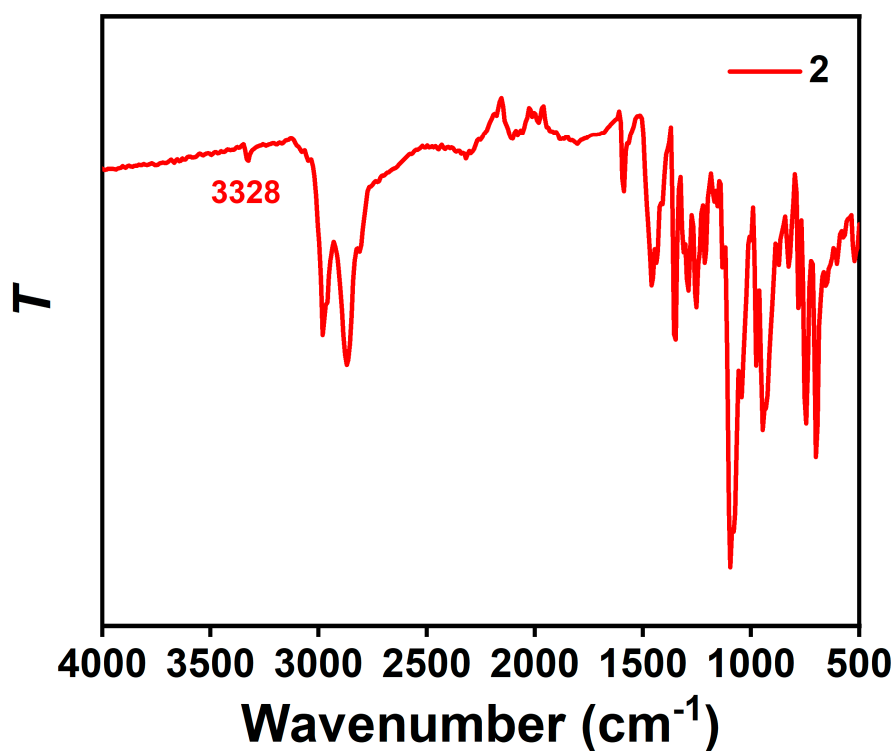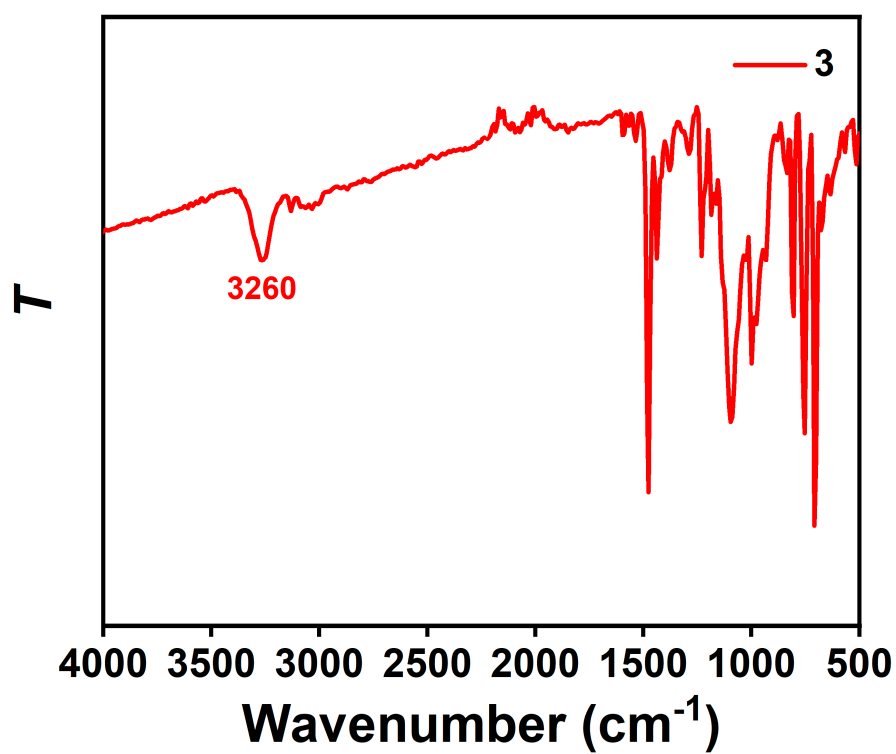

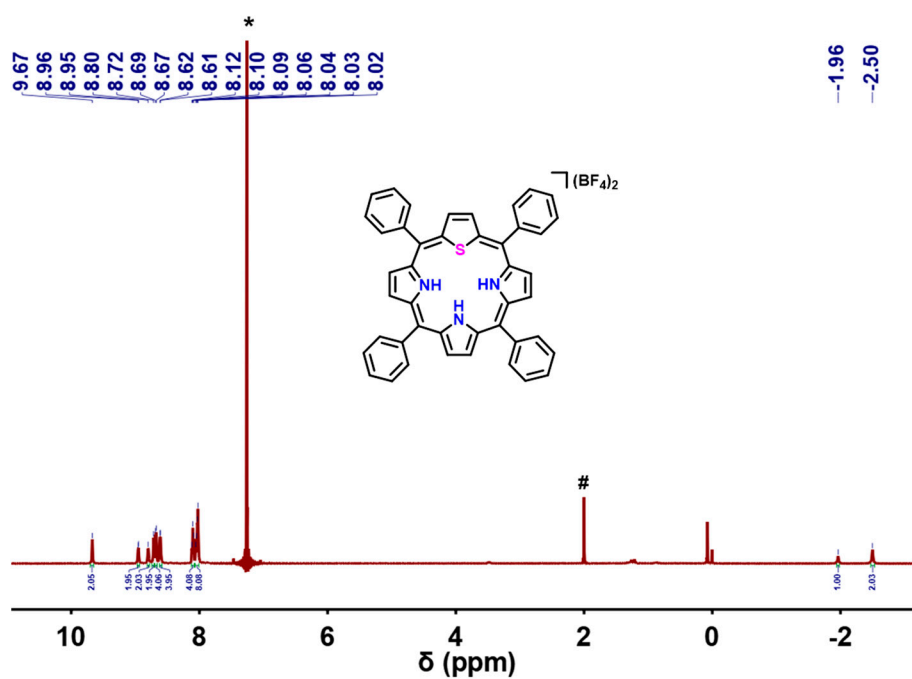**Figure S14**: ATR-IR spectrum of **3** in crystalline material.
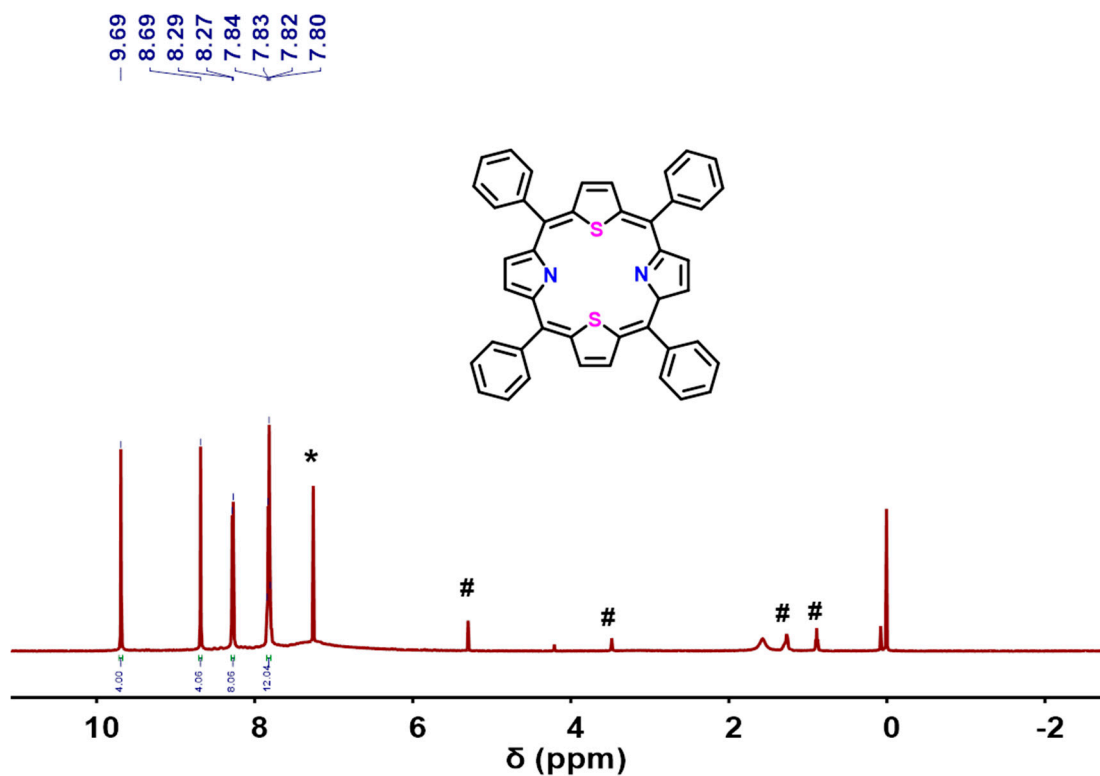
Figure S15: ^{1}H NMR spectrum (500 MHz) of **4** in CDCl$_3$ at 298 K. Solvent signals are marked with an asterisk (*). Other signals are marked with an asterisk (#).
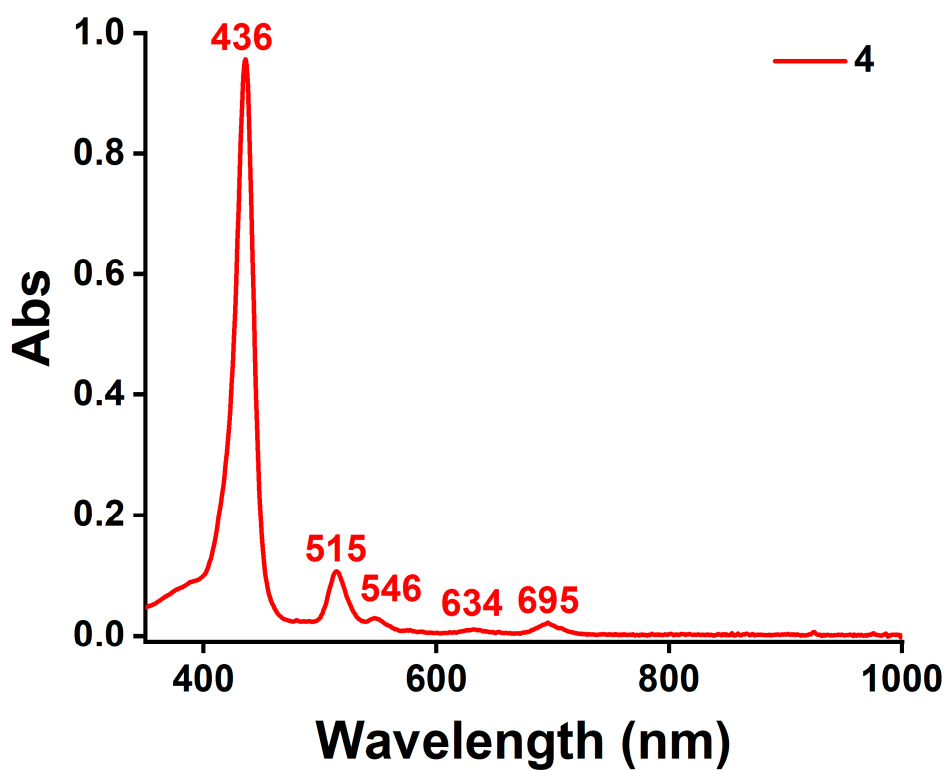
Figure S16: UV-vis absorption spectra of **4** in CHCl$_3$ solution.
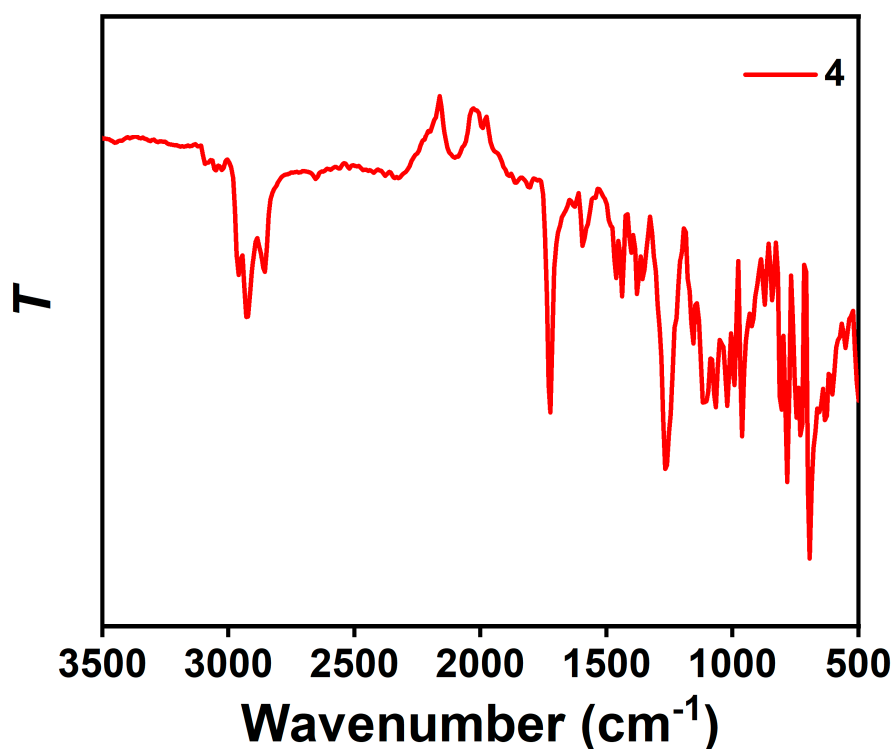
Figure S17: ATR-IR spectrum of **4** in crystalline material.
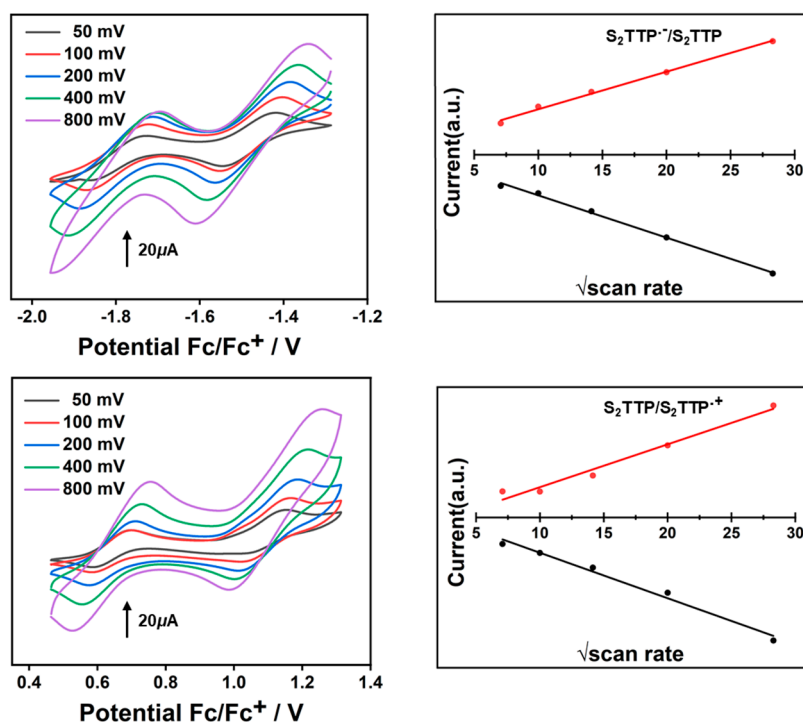
Figure S18: Left Cyclic voltammograms of **4** in DCM (0.1 M ^{n}Bu$_4$NPF$_6$) at different scan rates. (top) S$_2$TTP$^-$/S$_2$TTP redox couple; (bottom) S$_2$TTP/S$_2$TTP$^+$ redox couple. Right: Linear dependence of the current Ifp of the forward peak on the square root of the scan rate. (top) S$_2$TTP$^-$/S$_2$TTP redox couple; (bottom) S$_2$TTP/S$_2$TTP$^+$ redox couple
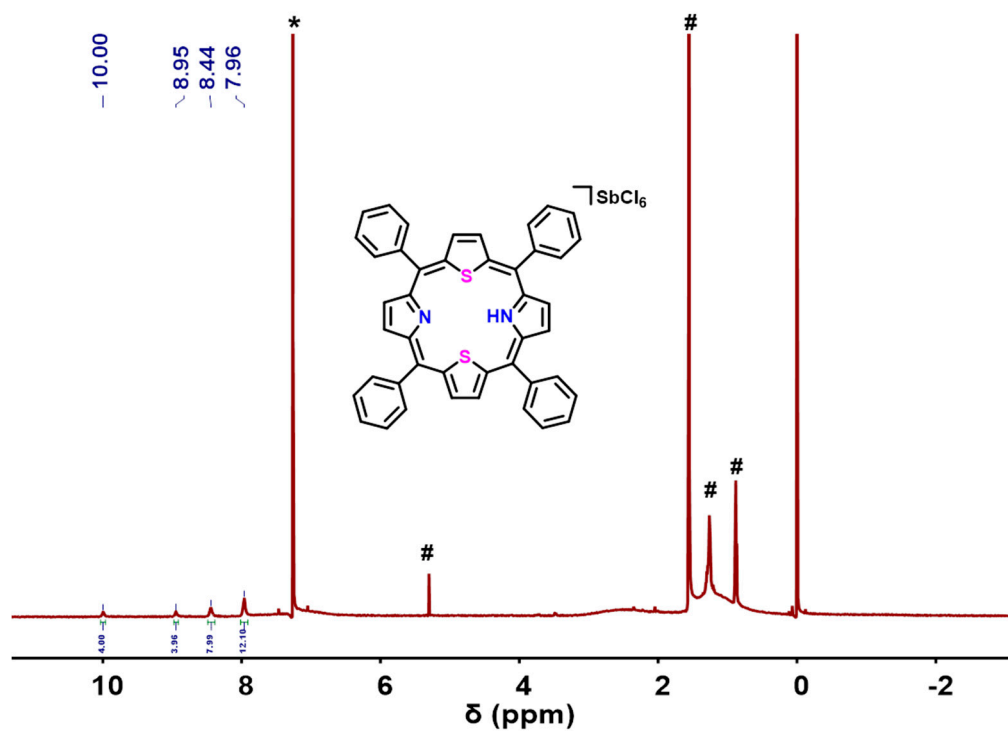
Figure S19: ^{1}H NMR spectrum (500 MHz) of **5** in CDCl$_3$ at 298 K. Solvent signals are marked with an asterisk (*). Other signals are marked with an asterisk (#).
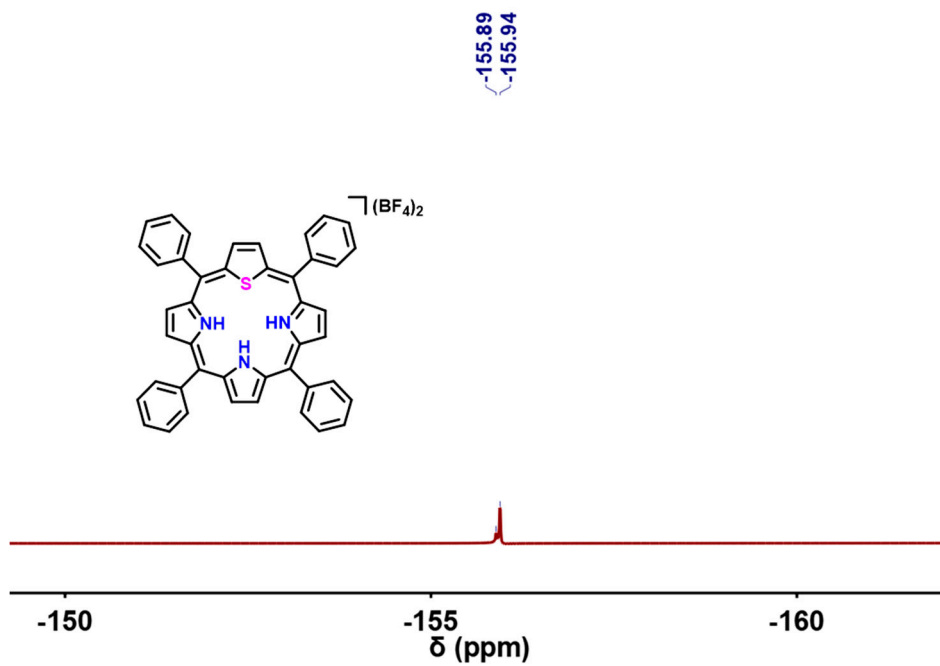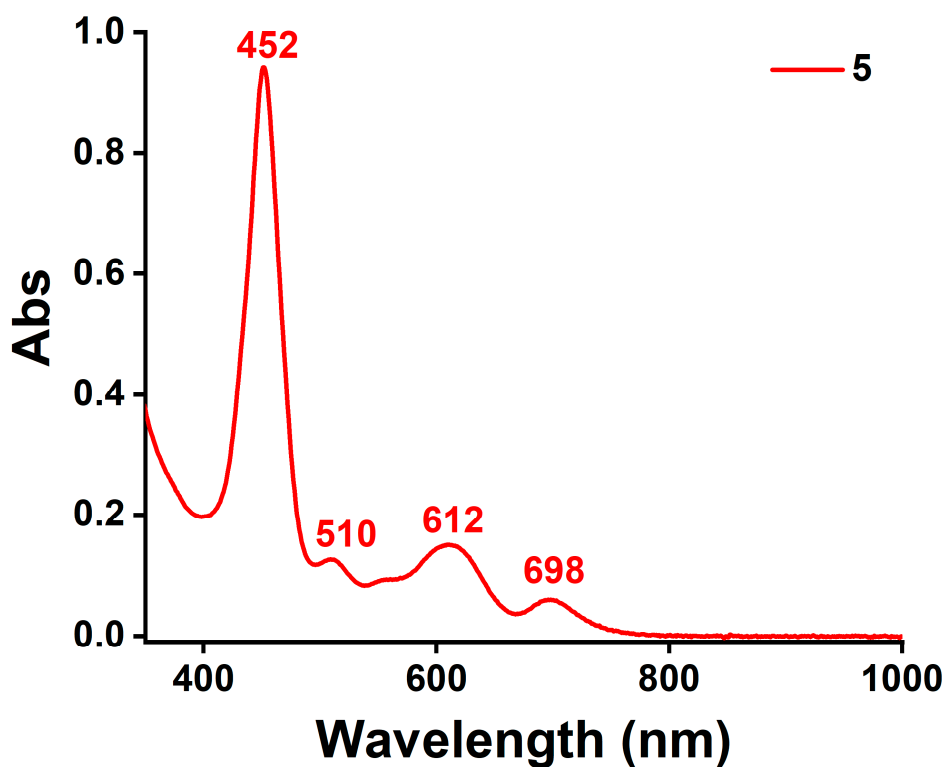

Figure S20: UV-vis absorption spectra of **5** in CHCl$_3$ solution.
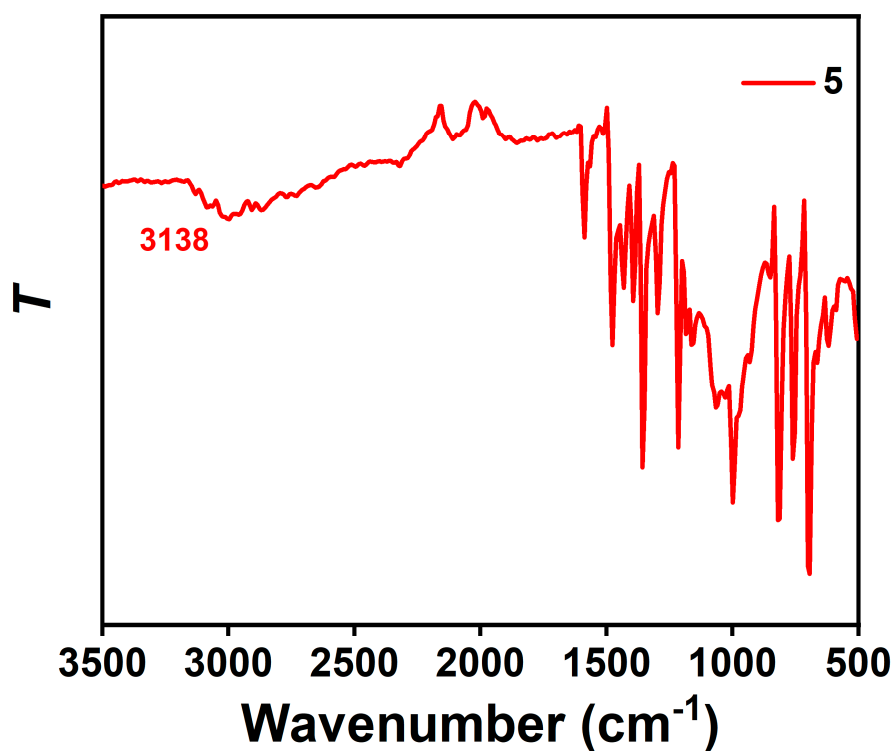
Figure S21: ATR-IR spectrum of **5** in crystalline material.
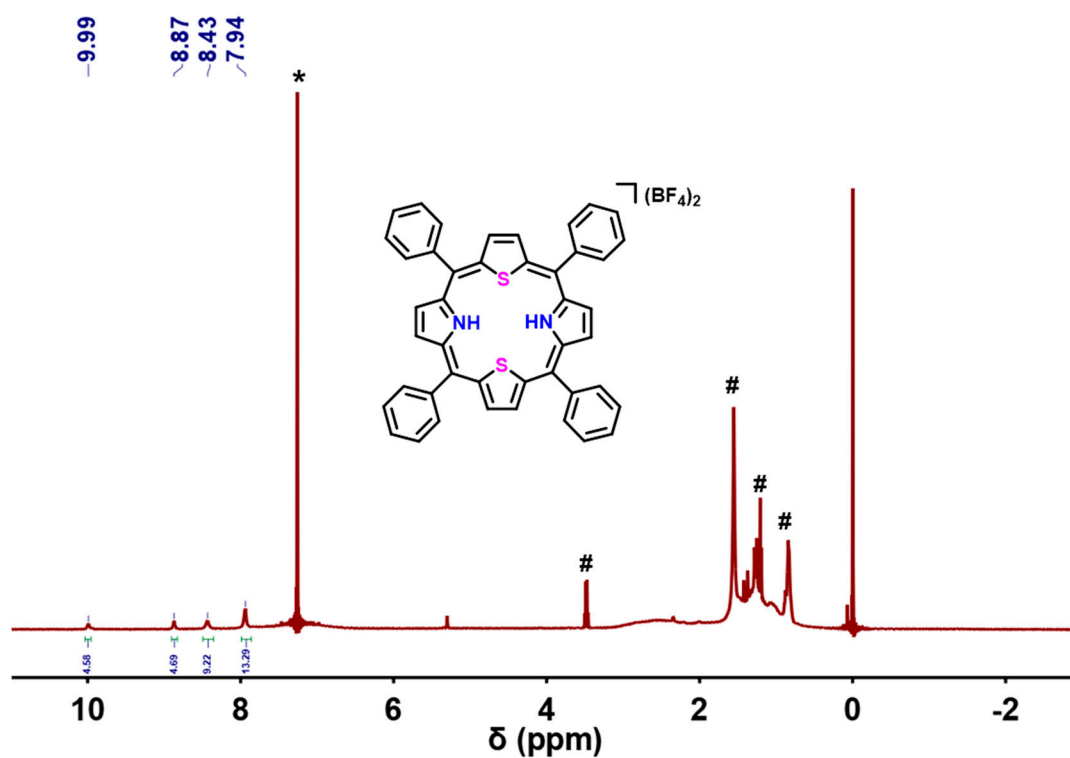
Figure S22: ^{1}H NMR spectrum (500 MHz) of **6** in CDCl₃ at 298 K. Solvent signals are marked with an asterisk (*). Other signals are marked with an asterisk (#).
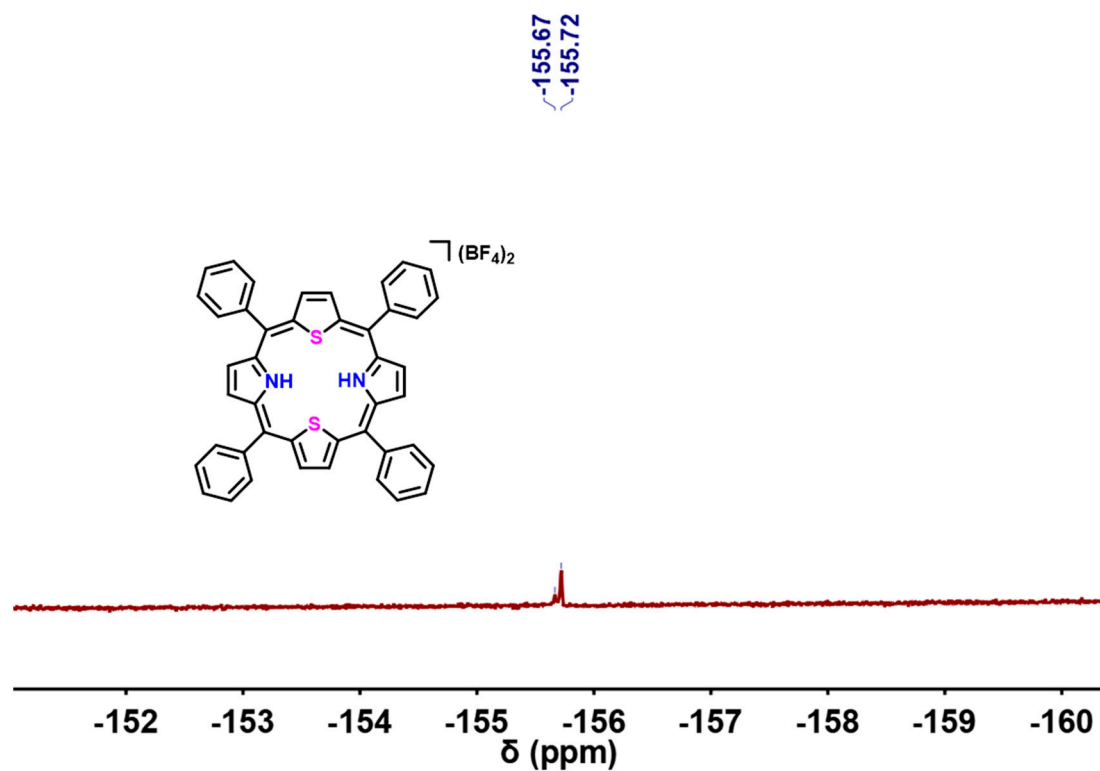
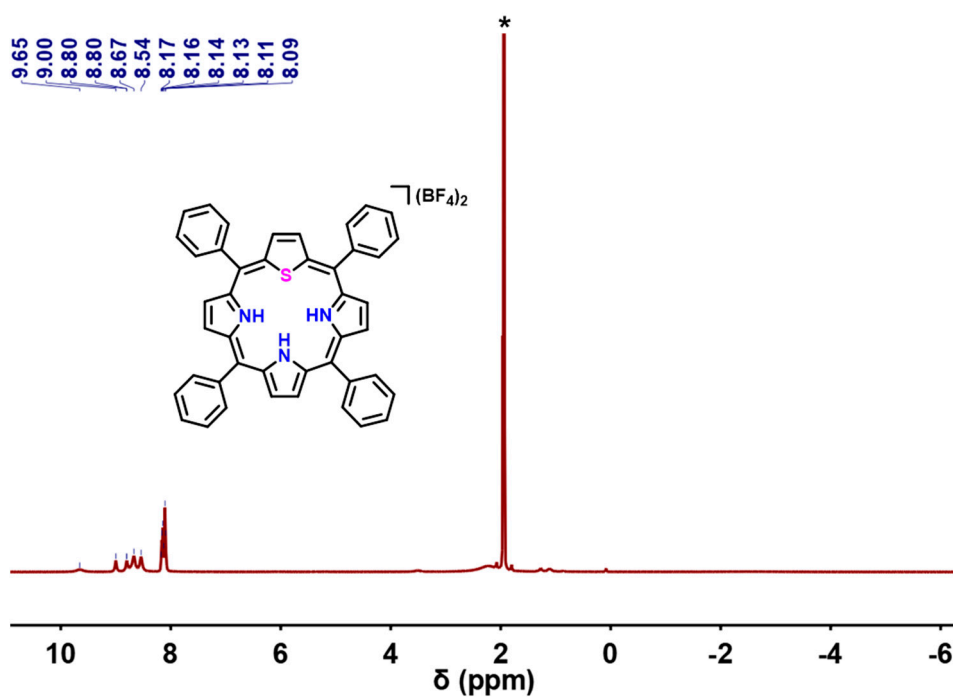**Figure S23**: ^{19}F NMR spectrum (471 MHz) of **6** in CDCl$_3$ at 298 K.
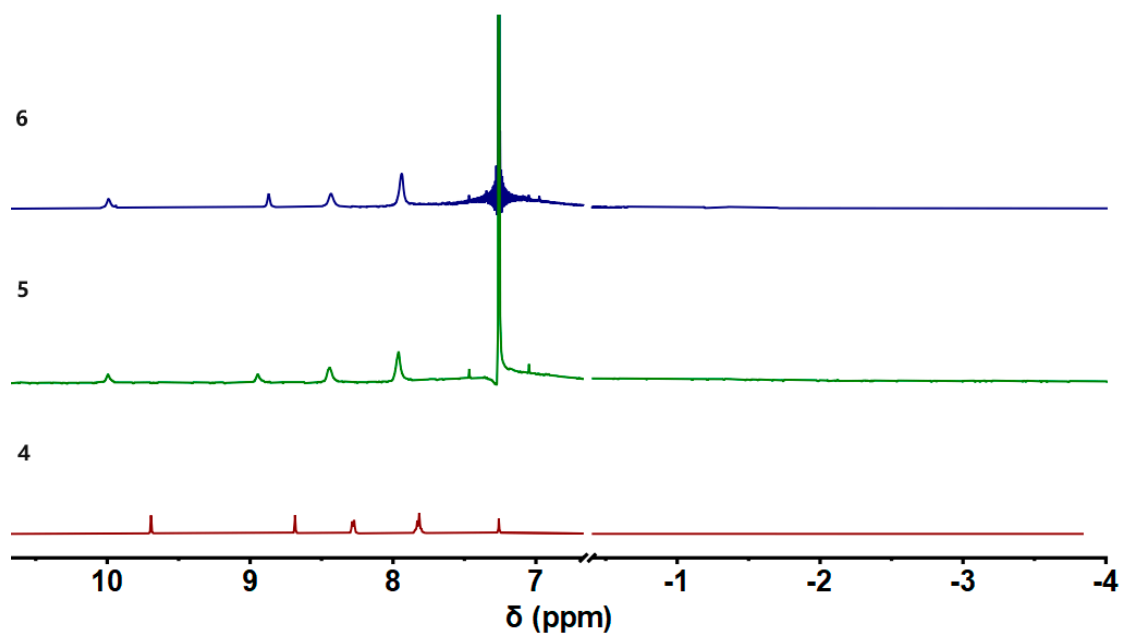
Figure S24: ^{1}H NMR spectrum (500 MHz, CDCl$_3$, 298 K) of S$_2$TTP **4**, monoacid **5** and diacids **6**.
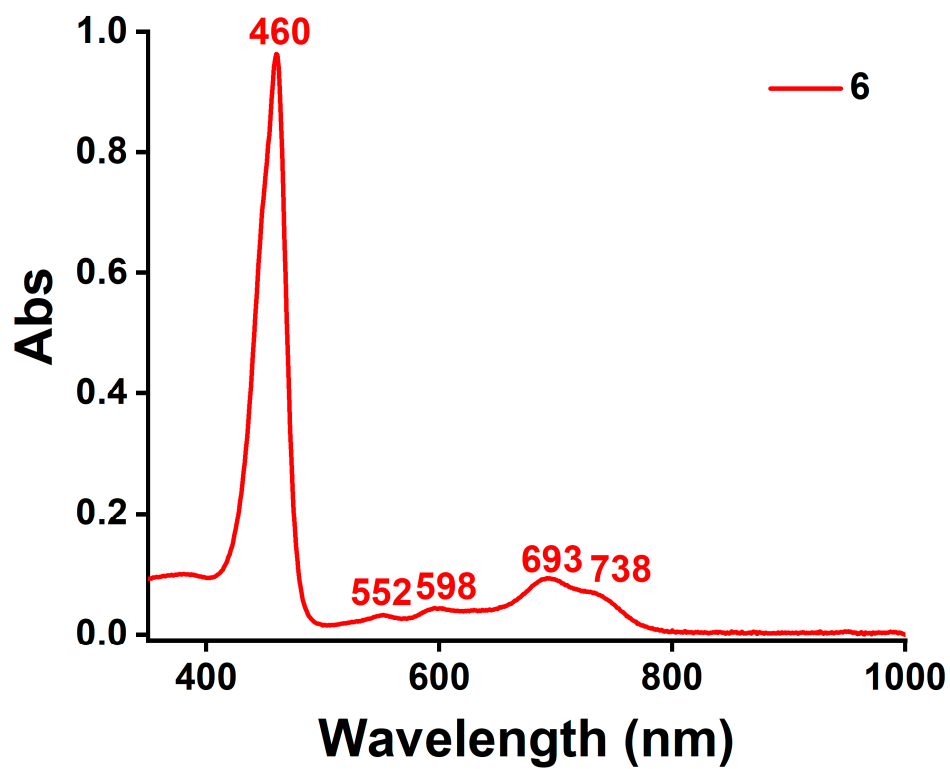
Figure S25: UV-vis absorption spectra of **6** in CHCl$_3$ solution.

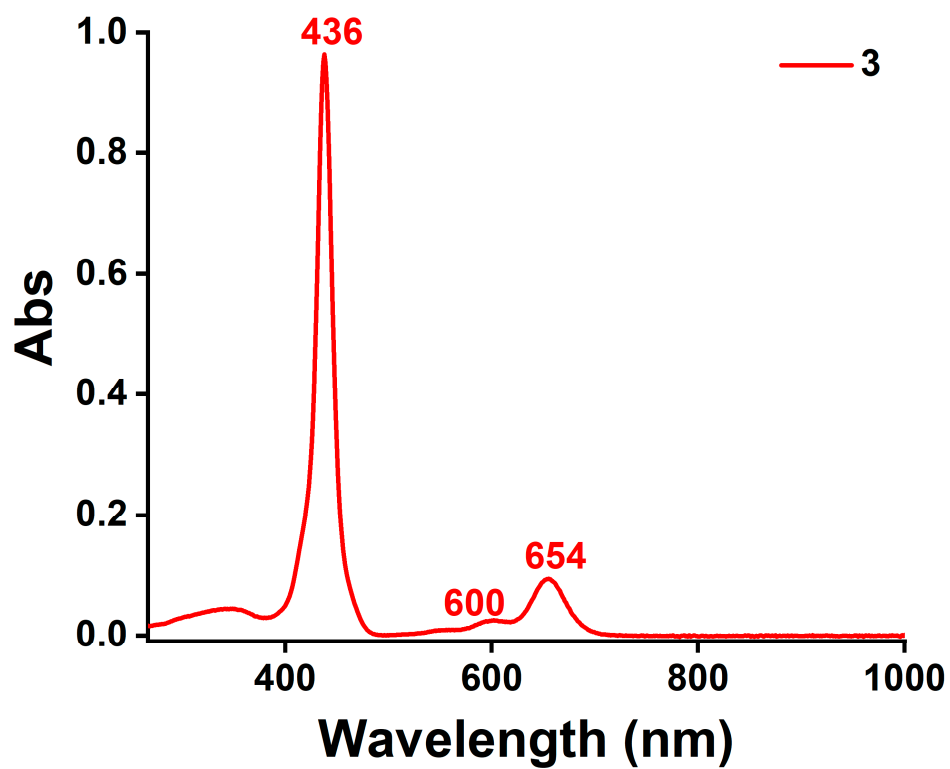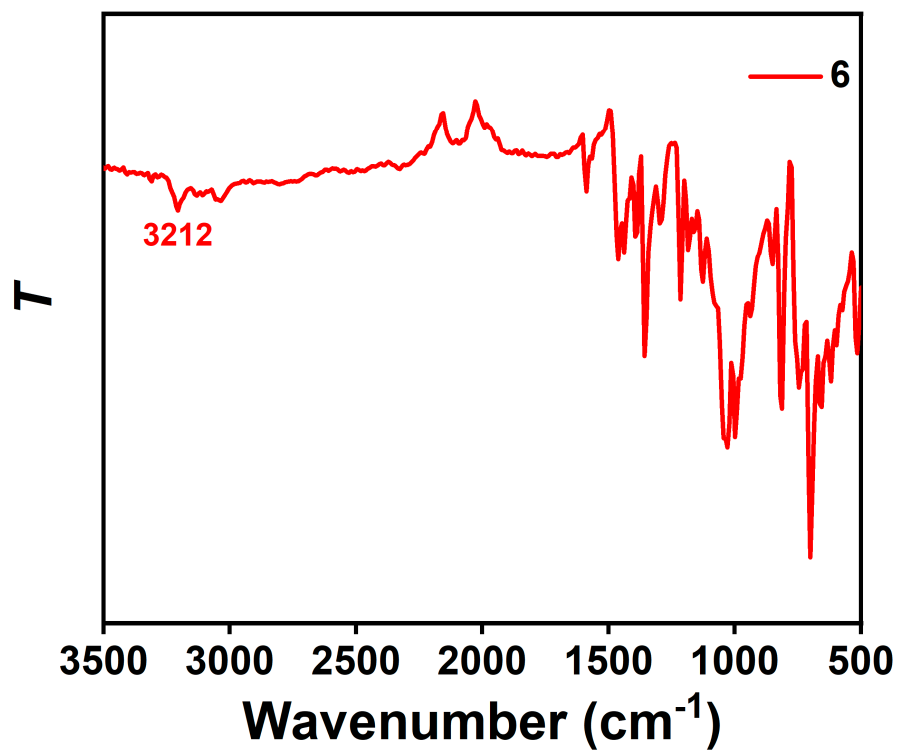**Figure S26**: ATR-IR spectrum of **6** in crystalline material.
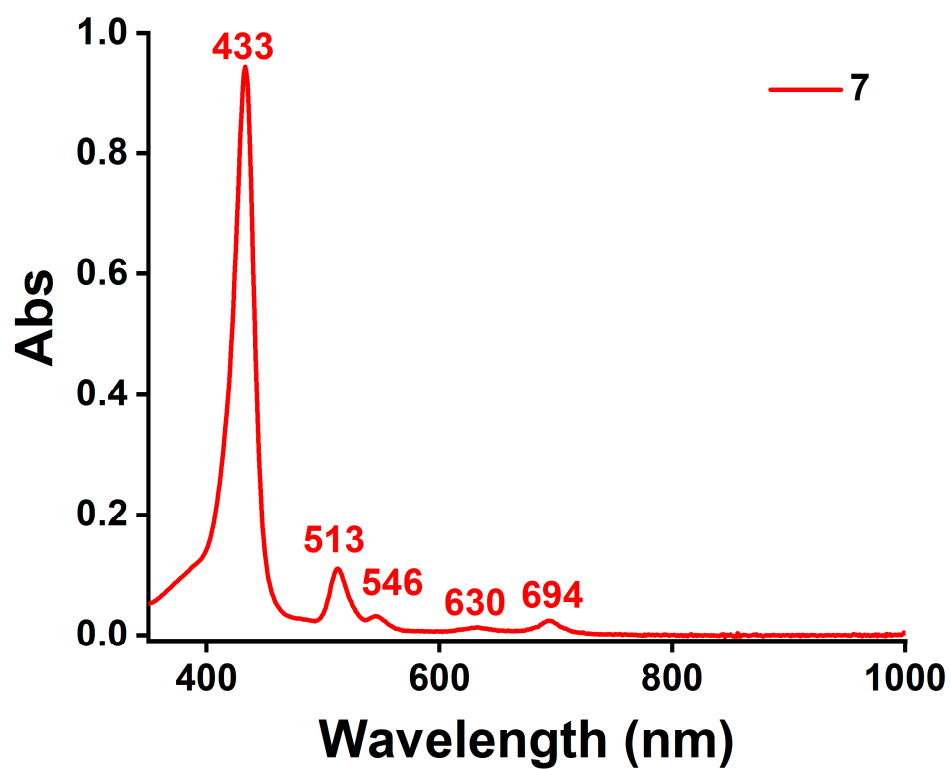
Figure S27: UV-vis absorption spectra of **7** in THF solution.
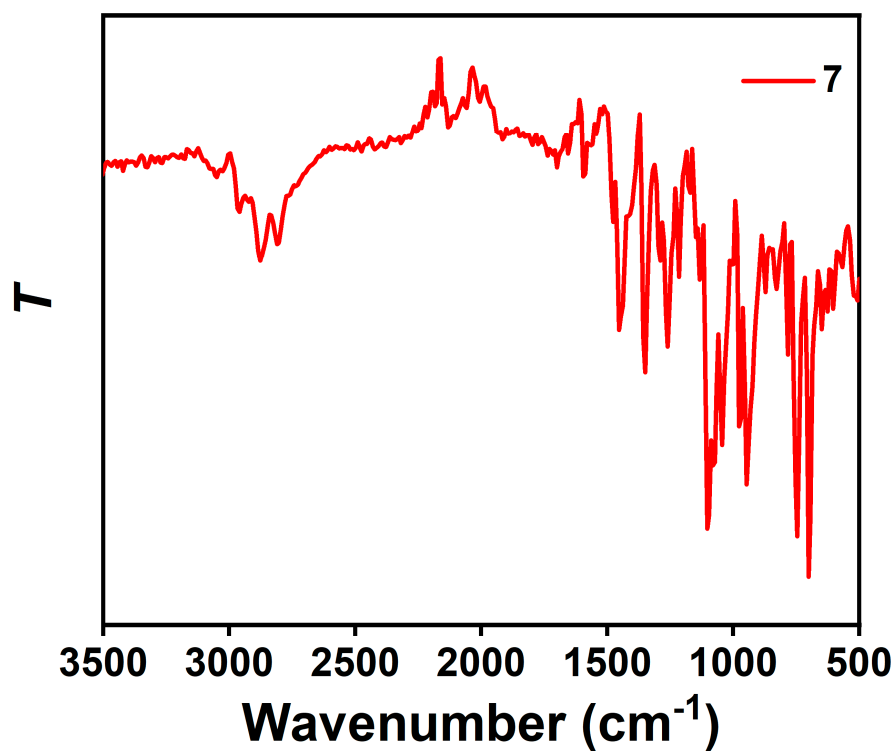
Figure S28: ATR-IR spectrum of **7** in crystalline material.
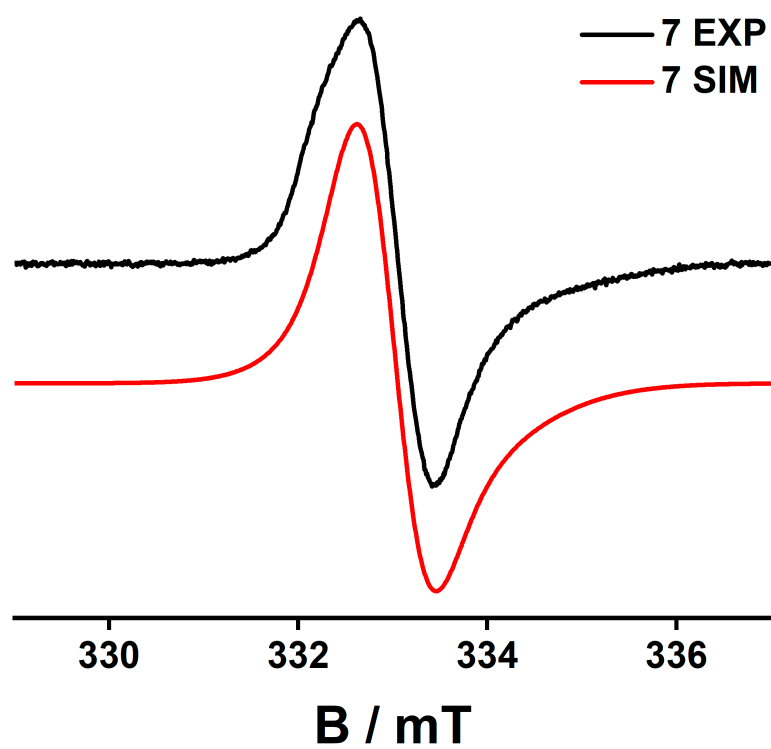
Figure S29: X-band EPR spectrum record at 9.34 GHz, microwave power 1 mW of **7** in 2-MeTHF solution at 106K. The red trace show the simulation with $g = 2.003$.
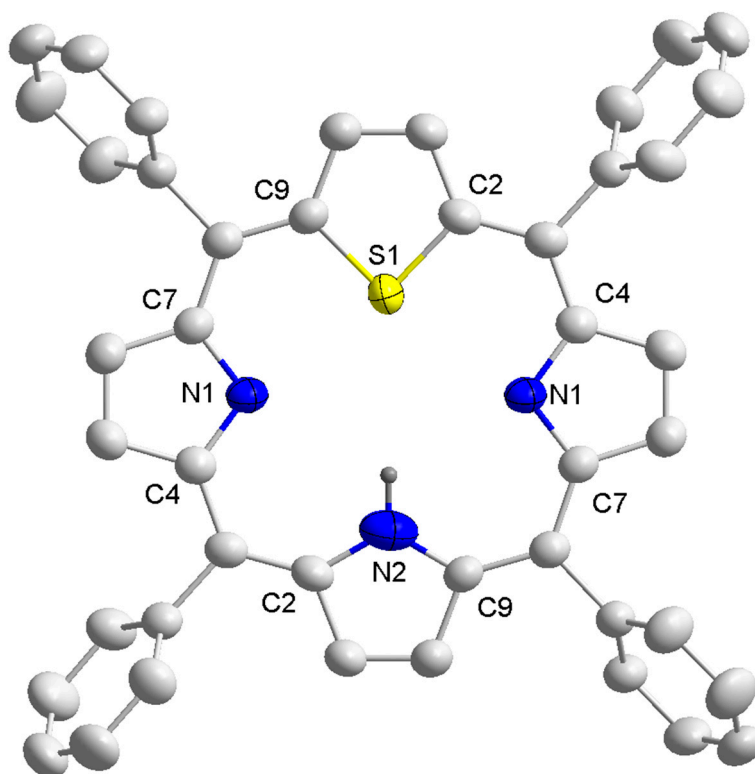
Figure S30: Plot (50% probability thermal ellipsoids) of the molecular structure of **1** (most hydrogen atoms omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C9 1.713(2), S1-C2 1.687(2), N1-C4 1.360(2), N1-C7 1.366(2), N2-C9 1.358(7), N2-C2 1.374(7), ∠ C2-S1-C9 88.46(12), ∠ C4-N1-C7 105.91(15), ∠ C2-N2-C9 120.5(4).
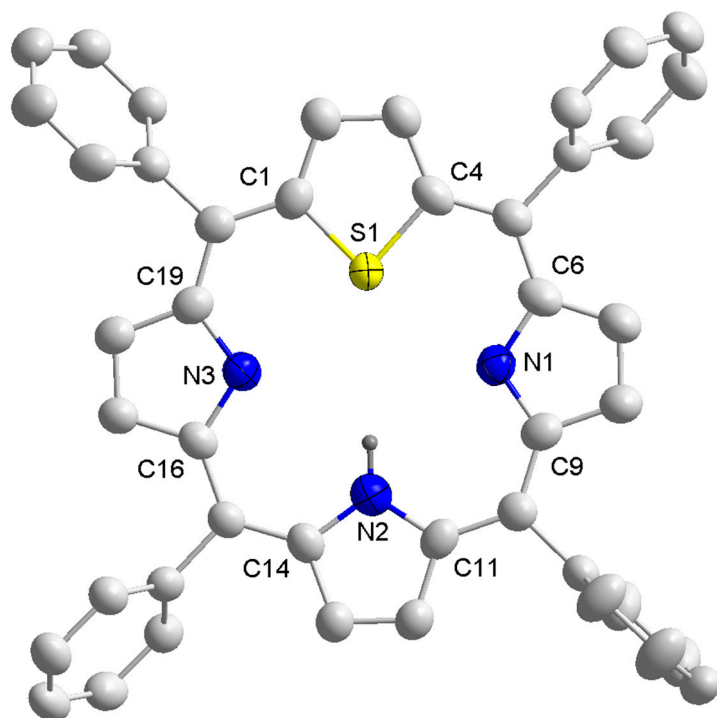
Figure S31: Plot (50% probability thermal ellipsoids) of the molecular structure of **2** (most hydrogen atoms and cation omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C1 1.729(4), S1-C4 1.721(3), N1-C6 1.374(6), N1-C9 1.369(6), N2-C11 1.384(8), N2-C14 1.374(7), N3-C16 1.392(7), N3-C19 1.392(8), ∠ C1-S1-C4 85.72(19), ∠ C6-N1-C9 111.8(4), ∠ C11-N2-C14 111.1(4), ∠ C16-N3-C19 110.7(4).
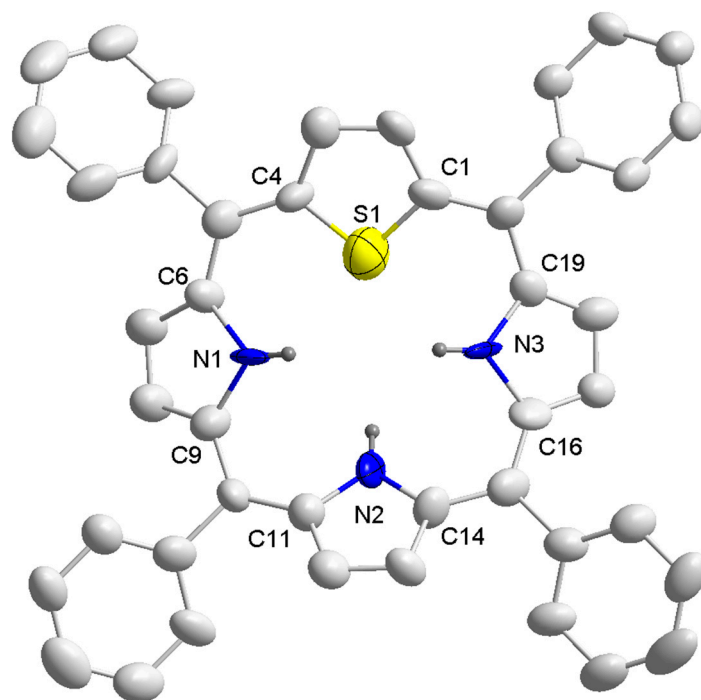
Figure S32: Plot (50% probability thermal ellipsoids) of the molecular structure of **3** (most hydrogen atoms and anion omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C1 1.676(15), S1-C4 1.686(16), N1-C6 1.519(18), N1-C9 1.489(18), N2-C11 1.455(19), N2-C14 1.448(17), N3-C16 1.468(18), N3-C19 1.472(17), $\angle$C1-S1-C4 93.0(8), $\angle$ C6-N1-C9 99.2(11), $\angle$ C11-N2-C14 102.5(12), $\angle$ C16-N3-C19 101.0(12).
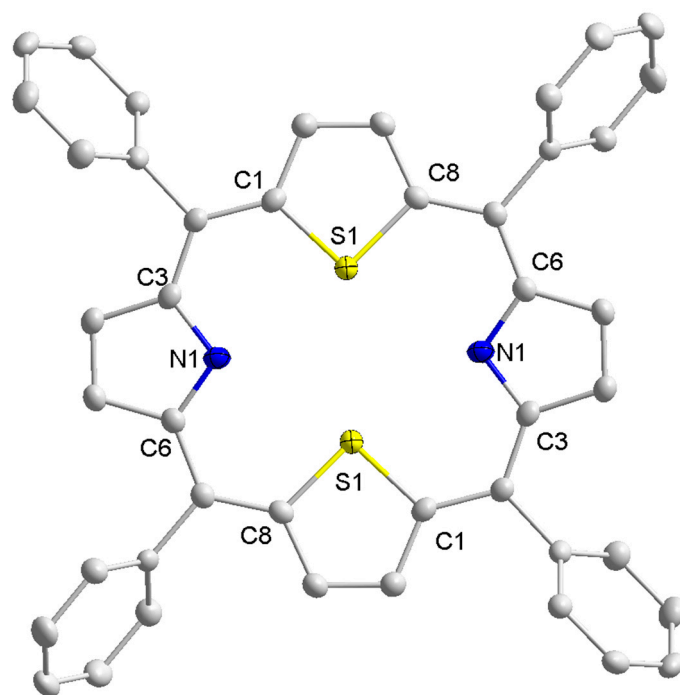
Figure S33: Plot (50% probability thermal ellipsoids) of the molecular structure of **4** (most hydrogen atoms omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C1 1.743(2), S1-C8 1.741(2), N1-C3 1.366(3), N1-C6 1.362(3), $\angle$ C1-S1-C8 91.97(10), $\angle$ C3-N1-C6 106.33(16).
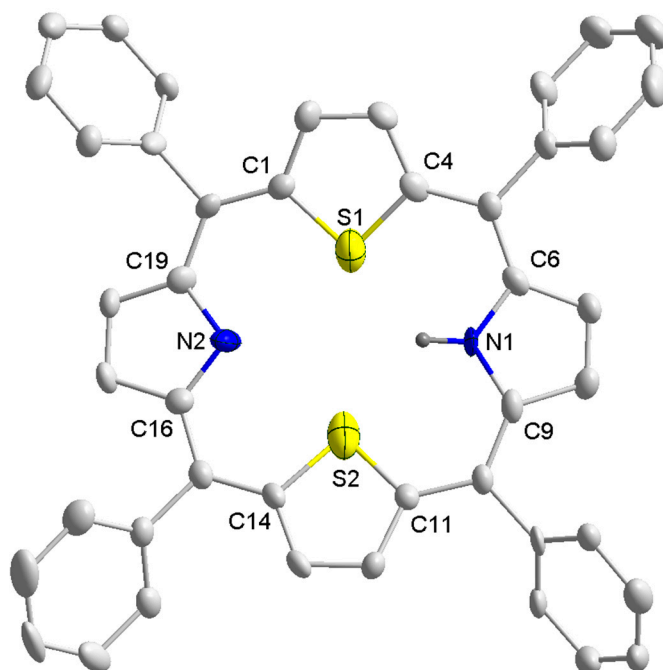
Figure S34: Plot (50% probability thermal ellipsoids) of the molecular structure of **5** (most hydrogen atoms and anion omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C1 1.689(7), S1-C4 1.686(7), S2-C11 1.675(7), S2-C14 1.663(7), N1-C6 1.364(8), N1-C9 1.376(8), N2-C16 1.368(9), N2-C19 1.384(8), ∠C1-S1-C4 92.0(4), ∠C11-S2-C14 92.6(4), ∠C6-N1-C9 109.7(6), ∠C16-N2-C19 104.7(6).
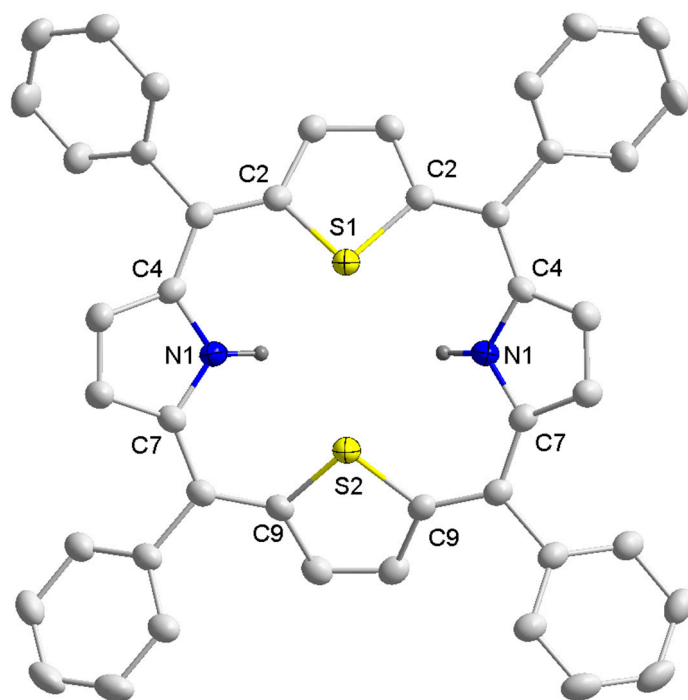
Figure S35: Plot (50% probability thermal ellipsoids) of the molecular structure of **6** (most hydrogen atoms and anion omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C2 1.743(3), S2-C9 1.737(3), N1-C4 1.374(4), N1-C7 1.377(4), ∠C2-S1-C2 92.6(2), ∠C9-S2-C9 93.0(2), ∠C4-N1-C7 110.4(3).
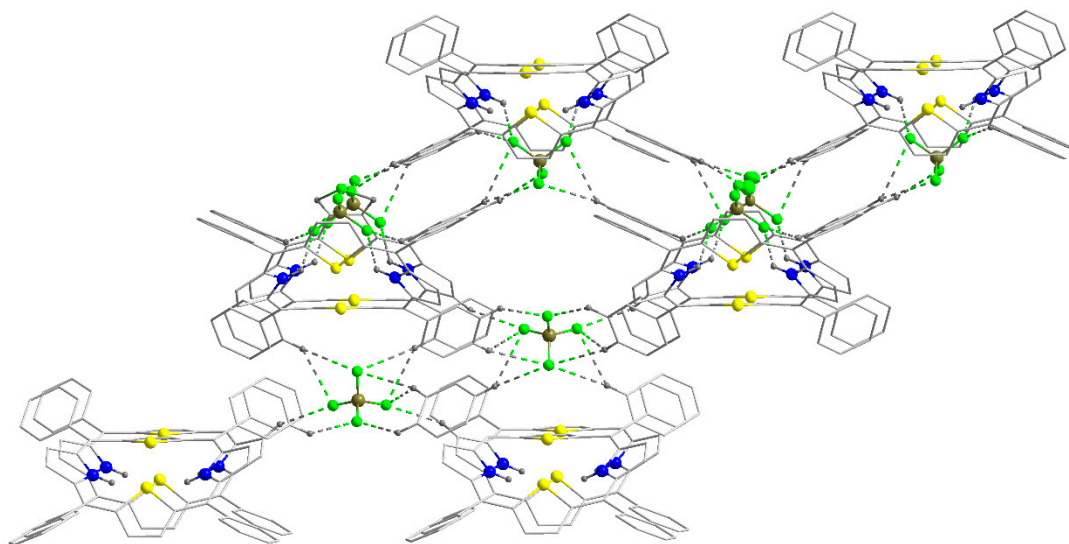
Figure S36: 3D arrangement in the crystal lattice showing interactions with the $C_{(Ph)}$-H⋯BF_4 anion. Solvent molecules and hydrogen atoms are omitted for clarity, except for the NH.
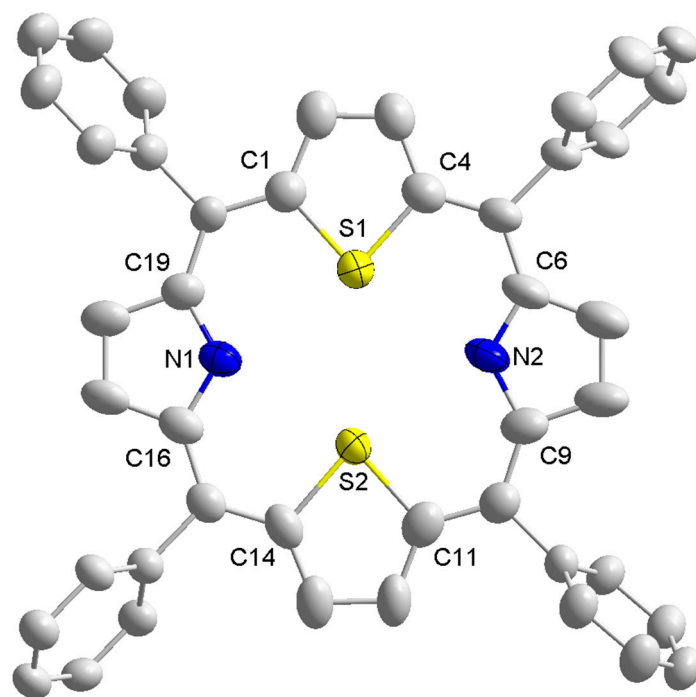
Figure S37: Plot (50% probability thermal ellipsoids) of the molecular structure of **7** (most hydrogen atoms and cation omitted for clarity). Selected bond lengths [Å] and angles [°]: S1-C1 1.805(12), S1-C4 1.769(12), S2-C11 1.808(11), S2-C14 1.837(11), N1-C16 1.340(2), N1-C19 1.330(2), N2-C6 1.294(19), N2-C9 1.370(2), ∠C1-S1-C4 84.1(5), ∠C11-S2-C14 82.6(5), ∠C16-N1-C19 119.6(13), ∠C6-N2-C9 121.2(14).

Table S1. Crystal data and refinement details for compounds **1**, **2**, **3**, **4**, **5**, **6** and **7**.

| Compound	1	2	3
	HSTTP	[Na(Cryptand)](HSTTP)	(H₃STTP)(BF₄)₂
moiety formula	$C_{44}H_{29}N_3S$	$C_{18}H_{36}N_2NaO_6 \cdot C_{44}H_{29}N_3S \cdot 0.8(C_2H_3N)$	$C_{44}H_{31}N_3S \cdot C_2H_3N \cdot 2(BF_4)$
empirical formula	$C_{44}H_{29}N_3S$	$C_{63.6}H_{67.4}N_{5.8}NaO_6S$	$C_{46}H_{34}B_2F_8N_4S$
T (K)	301	150	150
formula weight	315.88	1064.08	848.45
crystal size [mm³]	0.23×0.17×0.13	0.15×0.13×0.12	0.17×0.16×0.11
crystal system	Monoclinic	Monoclinic	Monoclinic
space group	$P2/c$	$P2/n$	$P2_1$
a [Å]	12.089(4)	11.6796(4)	9.464(3)
b [Å]	11.714(4)	20.8382(9)	21.762(8)
c [Å]	11.761(4)	23.3113(8)	10.031(4)
α [°]	90	90	90
β [°]	101.744(12)	101.3290(10)	107.477(11)
γ [°]	90	90	90
V [Å³]	1630.6(10)	5563.0(4)	1970.6(12)
Z	4	4	2
ρ [g·cm⁻³]	1.287	1.270	1.430
$F(000)$	660	2258	872
μ [mm⁻¹]	0.137	0.124	0.161
T_{min} / T_{max}	0.6538/0.7457	0.0248/ 0.0479	0.0427 / 0.0964
θ-range [°]	2.446-25.749	1.955-25.750	2.129 - 25.000
hkl-range	±14, -13 -14, ±14	±14, -25 -23, -28-27	±11, ±25, ±11
measured refl.	15601	46281	13531
unique refl. [R_{int}]	3123 [0.0451]	10643 [0.0576]	6622 [0.1686]
observed refl. ($I > 2(I)$)	2263	7558	2690
data / restr / param.	3123/1/230	10643/942/983	6622/235/548
goodness-of-fit (F^2)	1.055	1.056	1.010
R_1, wR_2 ($I > 2(I)$)	0.0425/0.0926	0.0689/0.1670	0.1006/0.2209
R_1, wR_2 (all data)	0.0677/0.1085	0.0980/0.1876	0.2298/0.3073
res. el. dens. [e·Å⁻³]	-0.302/0.516	-0.464/0.684	-0.510/0.491

Compound	4	5	6
	S_2TTP	$(HS_2TTP)SbCl_6$	$(H_2S_2TTP)(BF_4)_2$
moiety formula	$C_{44}H_{28}N_2S_2$	$C_{44}H_{29}N_2S_2 \cdot SbCl_6 \cdot C_4H_8O \cdot CH_3CN$	$C_{22}H_{15}NS \cdot 2(B_{0.5}F_2)$
empirical formula	$C_{44}H_{28}N_2S_2$	$C_{50}H_{40}Cl_6N_3OS_2Sb$	$C_{22}H_{15}BF_4NS$
T (K)	150	150	150
formula weight	648.80	1097.42	412.22
crystal size [mm³]	0.28×0.2×0.18	0.2×0.18×0.15	0.12×0.12×0.1
crystal system	Monoclinic	Triclinic	Orthorhombic
space group	$P2/c$	P-1	$Pnma$
a [Å]	11.9829(5)	12.9291(8)	32.1452(15)
b [Å]	11.5801(4)	13.9689(10)	16.9625(7)
c [Å]	11.7140(6)	14.0358(9)	8.2039(3)
α [°]	90	103.380(5)	90
β [°]	102.426(2)	94.423(5)	90
γ [°]	90	100.957(5)	90
V [Å³]	1587.39(12)	2401.6(3)	4473.3(3)
Z	2	2	8
ρ [g·cm⁻³]	1.357	1.518	1.224
$F(000)$	676	1108	1688
μ [mm⁻¹]	0.205	1.036	0.184
T_{min} / T_{max}	0.6871 / 0.7457	0.8824/ 1.0000	0.7030 / 0.7457
θ-range [°]	2.474 - 25.743	3.230 - 25.750	2.401 - 25.749
hkl-range	±14, -14 - 13, ±14	±15, -16 - 17, -16 - 17	-34 - 39, -19 - 20, -9 - 10
measured refl.	20693	18452	34773
unique refl. [R_{int}]	3031 [0.0607]	9159 [0.0557]	4424 [0.0847]
observed refl. ($I > 2(I)$)	2476	5507	3201
data / restr / param.	3031/0/217	9154/18/569	4424/6/274
goodness-of-fit (F^2)	1.054	1.030	1.105
R_1, wR_2 ($I > 2(I)$)	0.0400/0.0873	0.0766/0.1592	0.0626/0.1746
R_1, wR_2 (all data)	0.0548/0.0973	0.1357/0.1852	0.0867/0.1946
res. el. dens. [e·Å⁻³]	-0.342/0.669	-0.982/1.139	-0.546/0.617

Compound	7
	[K(Cryptand)]S_2TTP
moiety formula	$C_{44}H_{28}N_2S_2 \cdot C_{18}H_{36}KN_2O_6 \cdot 0.5[C_4H_8O] \cdot 0.5[C_4H_8O]$
empirical formula	$C_{62}H_{64}KN_4O_6S_2$
T (K)	150
formula weight	1064.39
crystal size [mm³]	0.14×0.12×0.1
crystal system	Triclinic
space group	P-1
a [Å]	12.951(10)
b [Å]	17.598(13)
c [Å]	26.63(2)
α [°]	88.81(2)
β [°]	76.54(3)
γ [°]	86.89(3)
V [Å³]	5893(8)
Z	4
ρ [g·cm⁻³]	1.200
$F(000)$	2252
μ [mm⁻¹]	0.213
T_{min} / T_{max}	0.6296/0.7441
θ-range [°]	1.942 - 17.353
hkl-range	±10, ±14, ±22
measured refl.	47351
unique refl. [R_{int}]	7244 [0.1110]
observed refl. ($I > 2(I)$)	5127
data / restr / param.	7244/2728/1896
goodness-of-fit (F^2)	1.054
R_1, wR_2 ($I > 2(I)$)	0.0520/0.1162
R_1, wR_2 (all data)	0.0827/0.1346
res. el. dens. [e·Å⁻³]	-0.278/0.290

The ZINDO/S method was used to calculate the excitation energies and absorption spectra for the x-ray geometries of the compound **1-7**. RHF for **1**, **3**, **4-6** and UHF for **2** and **7** DFT calculations, ZINDO/S semiempirical method, TightSCF instruction, DIIS approximation using the auxiliary TightSCF basis set. (! RHF ZINDO/S TightSCF DIIS NoRICO).

(a)   (b)

HOMO(112)   LUMO(113)

-6.4940 eV   -1.7162 eV
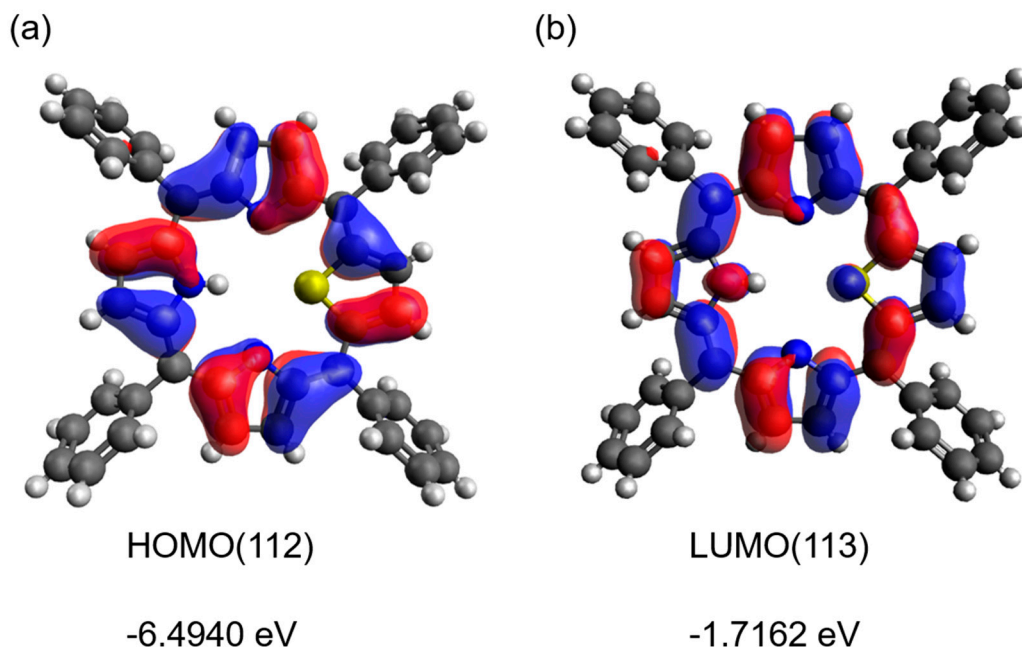
Figure S38: HOMO (a) and LUMO (b) plot for the compound **1**.

(a)   (b)

HOMO(113)   LUMO(114)

-3.1608 eV   2.4348 eV
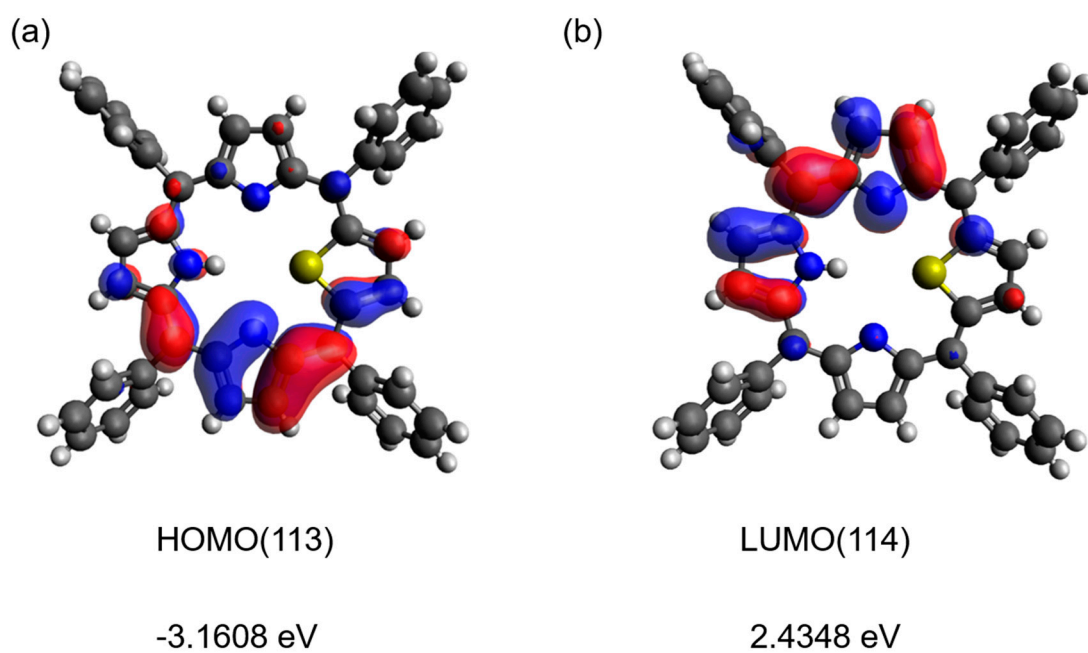
Figure S39: HOMO (a) and LUMO (b) plot for the compound **2**.

(a)

(b)

HOMO(112)

LUMO(113)

-11.6699 eV

-7.6293 eV
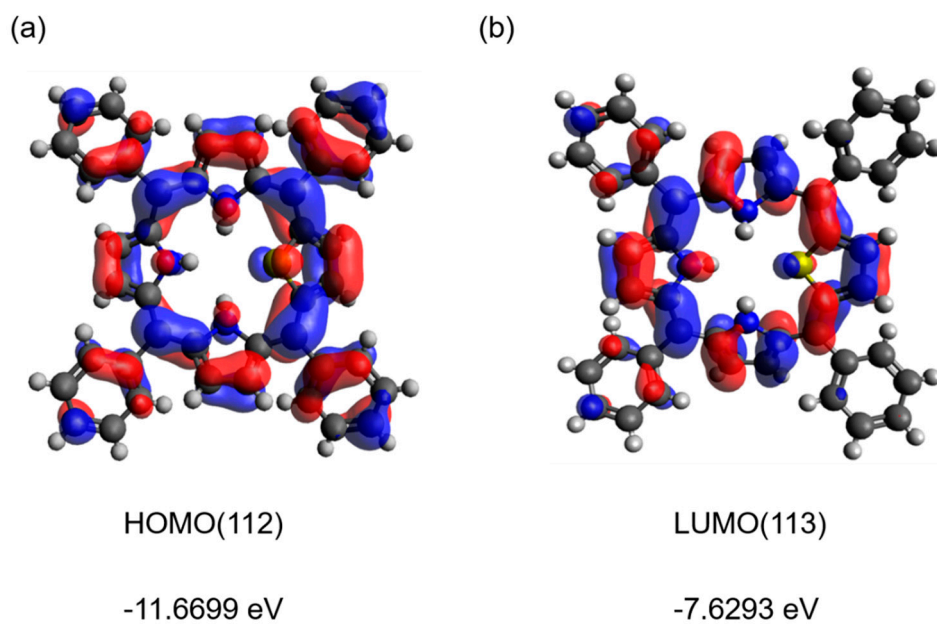
Figure S40: HOMO (a) and LUMO (b) plot for the compound **3**.

(a)

(b)

HOMO(112)

LUMO(113)

-6.4706 eV

-1.9008 eV
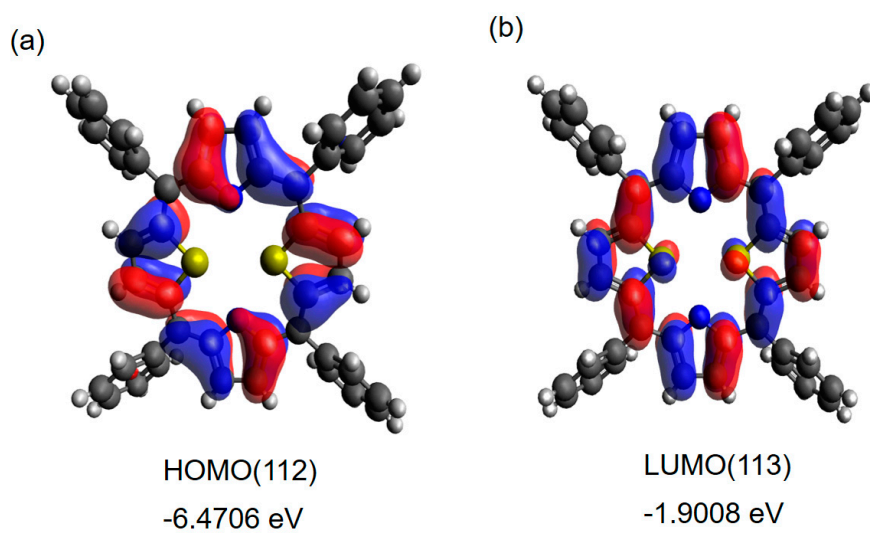
Figure S41: HOMO (a) and LUMO (b) plot for the compound **4**.

(a)   (b)

HOMO(112)   LUMO(113)

-9.3081 eV   -4.8609 eV
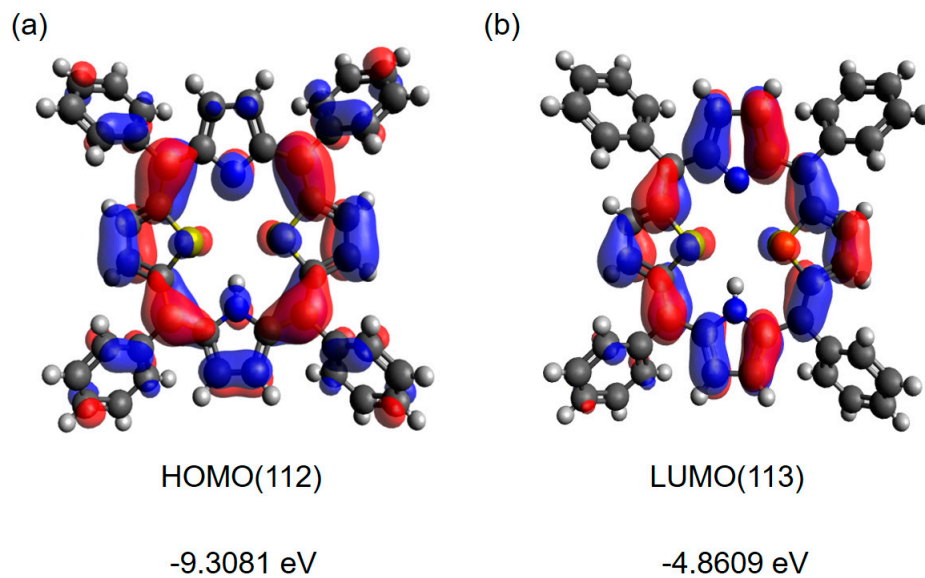
Figure S42: HOMO (a) and LUMO (b) plot for the compound **5**.

(a)   (b)

HOMO(112)   LUMO(113)

-11.7472 eV   -7.7915 eV
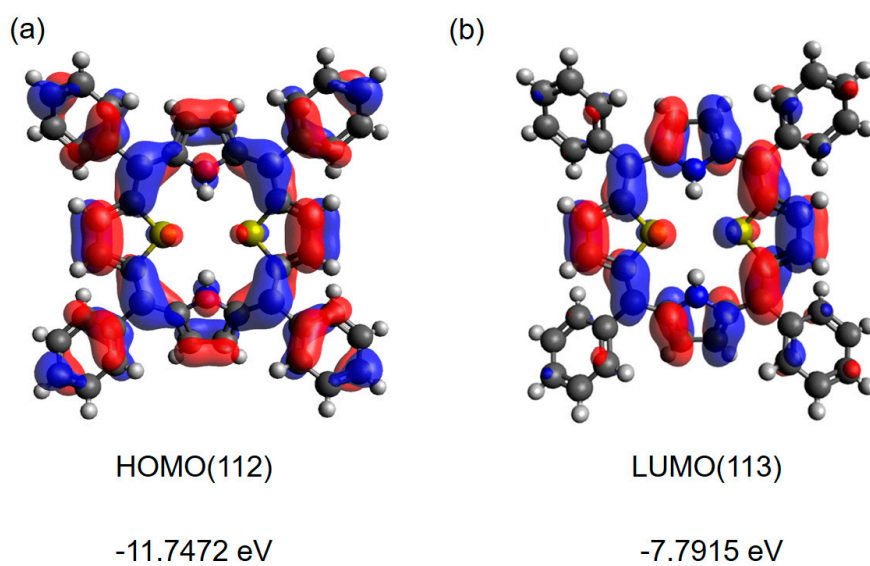
Figure S43: HOMO (a) and LUMO (b) plot for the compound **6**.

(a)   (b)

HOMO(113)   LUMO(114)

-3.0995 eV   2.9035 eV
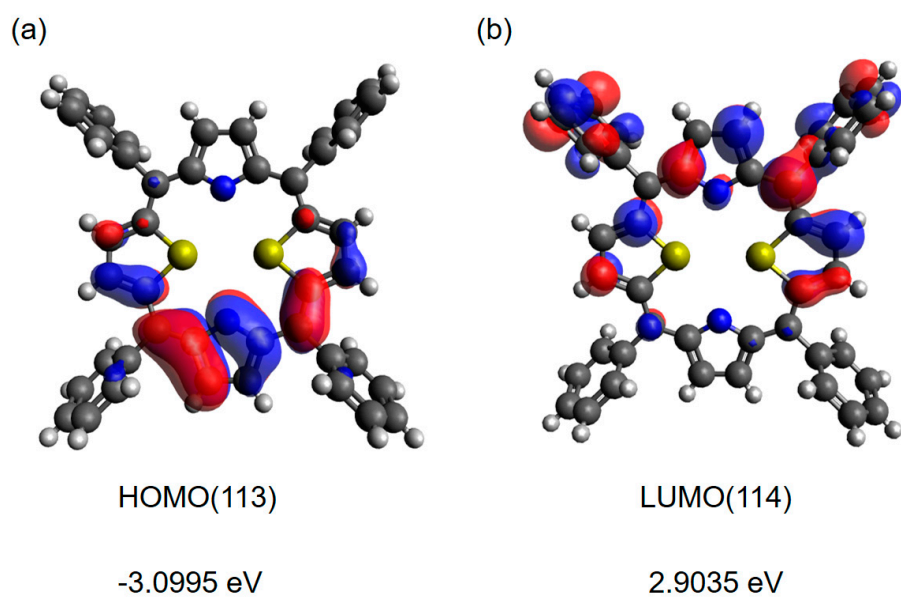
Figure S44: HOMO (a) and LUMO (b) plot for the compound **7**.
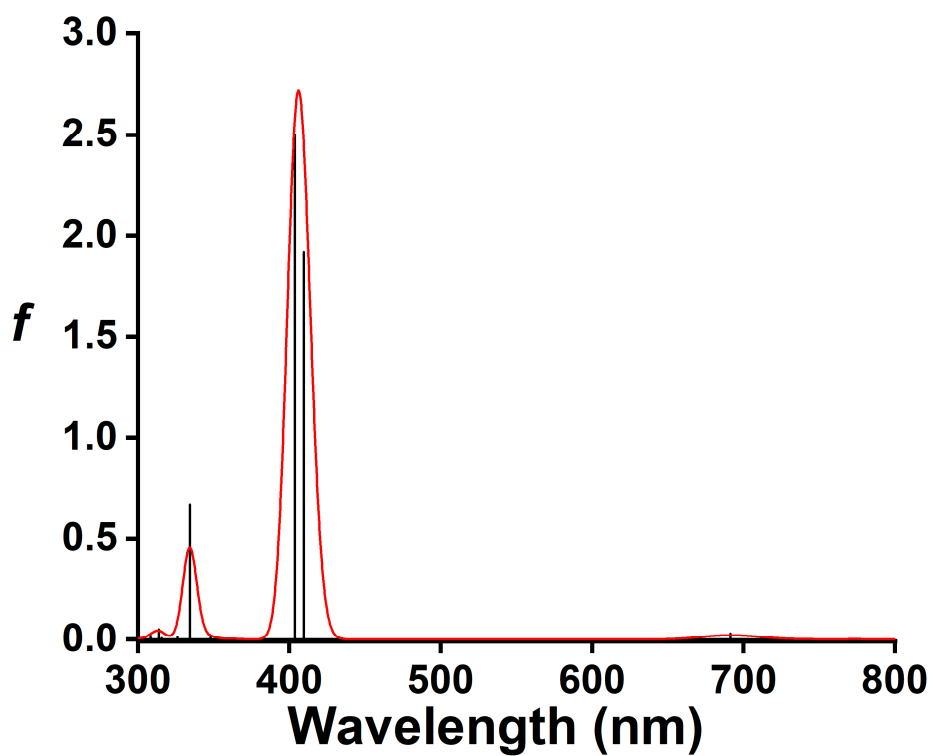
Figure S45: Calculated absorption spectra of the compound **1** obtained using the ZINDO/S method.
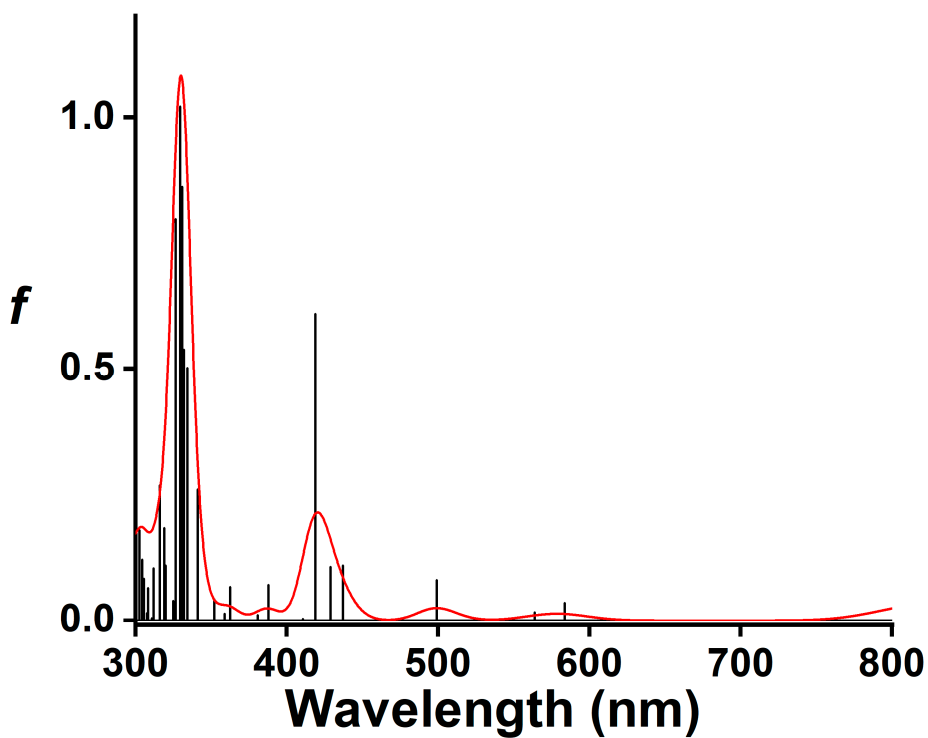
Figure S46: Calculated absorption spectra of the compound **2** obtained using the ZINDO/S method.
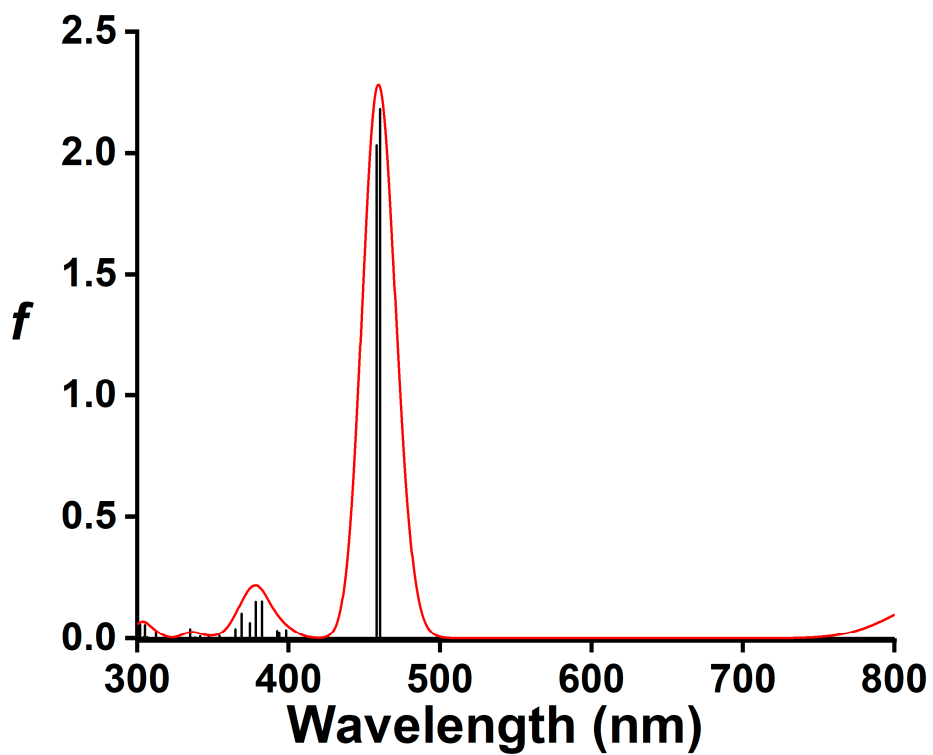
Figure S47: Calculated absorption spectra of the compound **3** obtained using the ZINDO/S method.
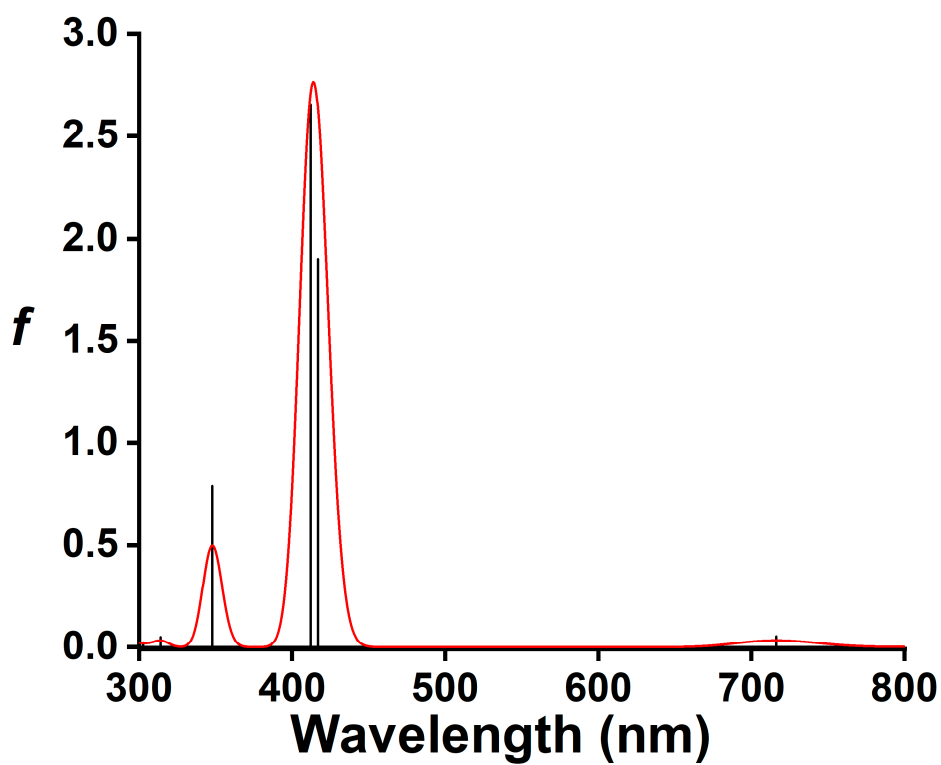
Figure S48: Calculated absorption spectra of the compound **4** obtained using the ZINDO/S method.
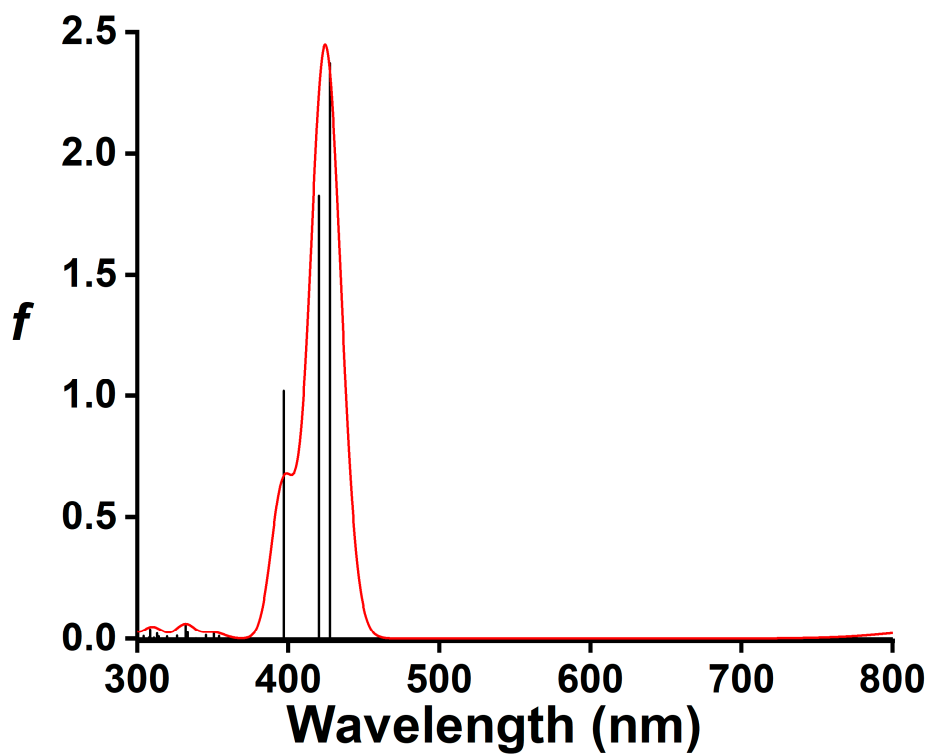
Figure S49: Calculated absorption spectra of the compound **5** obtained using the ZINDO/S method.
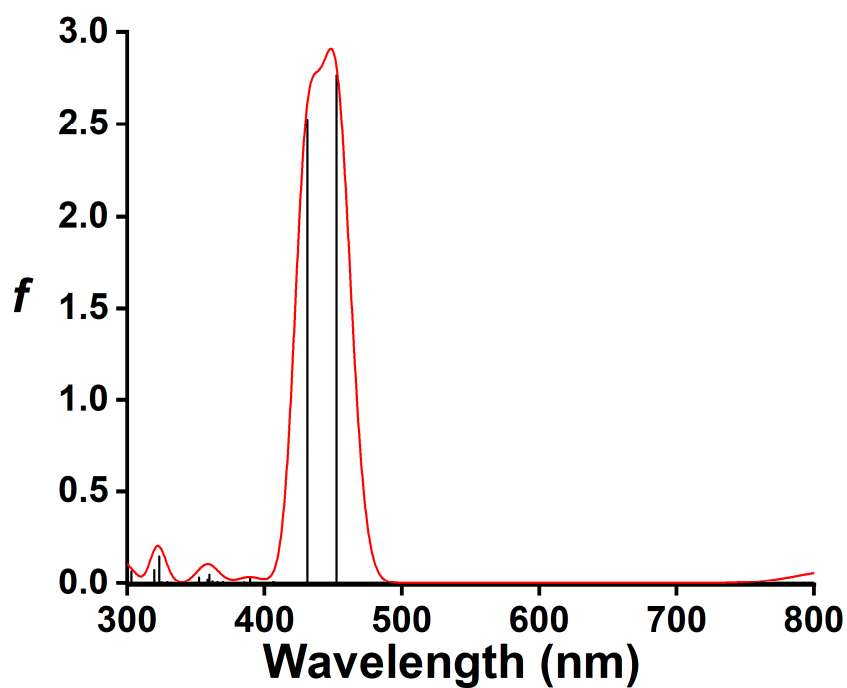
Figure S50: Calculated absorption spectra of the compound **6** obtained using the ZINDO/S method.
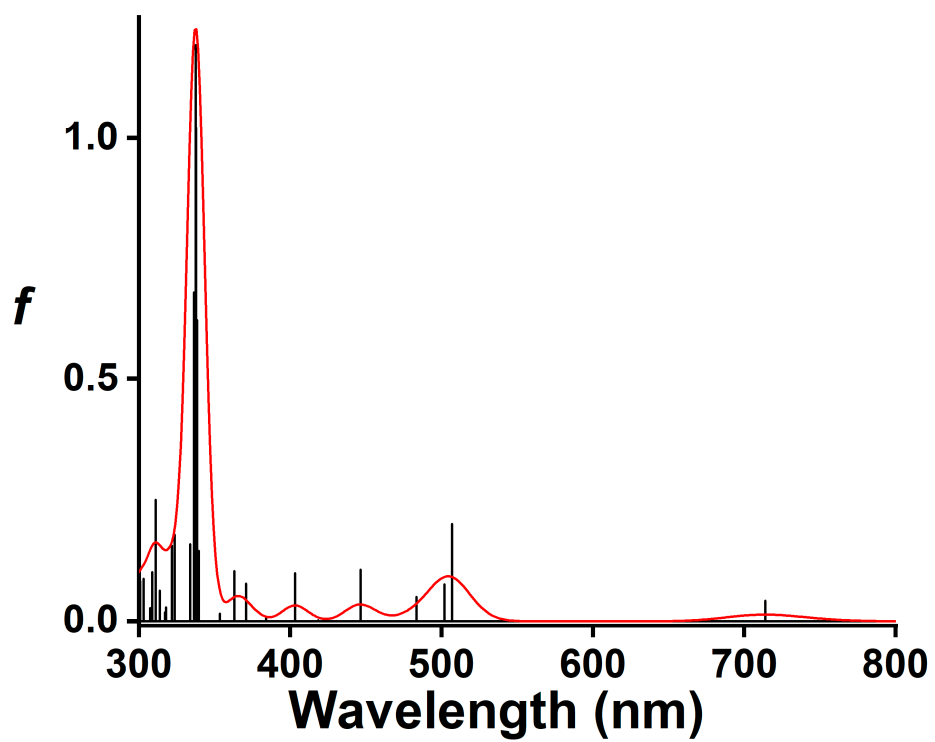
Figure S51: Calculated absorption spectra of the compound **7** obtained using the ZINDO/S method.

Table S2: Selected Results of ZINDO/S Calculations for Low-Energy π-π* Transitions of compounds **1-7**.

compound	λ (nm)	f	Composition (weight %)[a]
1	691	0.03	H-1⟶L+1 (33) H⟶L (53)
	409	1.92	H-1⟶L (30) H ⟶L+1 (40)
	403	2.50	H-1 ⟶L+1 (48) H⟶L (30)
2	584	0.034	S-8⟶S (25) S-2⟶S (15)
	564	0.016	S-8⟶S (15) S-2⟶S (18)
	499	0.080	S-1 ⟶L (20) S ⟶L (29)
	437	0.11	S ⟶L (12) S-1 ⟶L (13) S-1 ⟶ L+5 (12)
	429	0.11	S-5⟶S (12)
	419	0.61	S⟶L+5 (18) S-5 ⟶H (10)
3	460	2.18	H-1⟶L (45) H⟶L+1 (26)
	458	2.03	H-1⟶L+1 (51) H⟶L (14)
4	716	0.054	H-1⟶L+1 (30) H⟶L (57)
	416	1.90	H-1⟶L (31) H⟶L+1 (44)
	412	2.66	H-1⟶L+1 (56) H ⟶L (29)
5	427	2.37	H-1⟶L (39) H⟶L+1 (45)
	420	1.83	H-1⟶L+1 (44) H⟶L (21)
	397	1.02	H-10⟶L (13) H-7⟶L (25) H-1⟶L+1 (12) H⟶L (12)
6	452	2.77	H-1⟶L (54) H⟶L+1 (37)
	431	2.53	H-1⟶L+1 (63) H⟶L (24)

	714	0.04	S-1 ⟶S (95)
	507	0.20	S-2 ⟶S (28)
	502	0.08	S-2 ⟶S (67)
	483	0.05	S-7 ⟶S (16)
7			S-5 ⟶S (13)
	446	0.11	S ⟶L+5 (13)
			S-1 ⟶L+4 (14)
			S-1 ⟶L+5 (11)
	403	0.10	S-4 ⟶S (37)

ᵃ H = HOMO; L = LUMO, S = SOMO

Compound **1** xyz

S	0.502864542	1.456987544	0.106190056
C	2.032947421	2.224476954	0.047762723
C	−0.214573202	2.979590459	−0.010009788
C	3.188552868	1.429472567	0.045533293
C	1.974101372	3.635001850	−0.028075222
C	−1.610234470	3.066649098	0.017441030
C	0.692469048	4.067430941	−0.079896405
C	3.191700419	0.025684319	0.016754368
C	4.509757213	2.129202568	0.004785380
H	2.736714491	4.211999682	−0.061550347
C	−2.485594079	1.966647382	0.028203126
C	−2.209364095	4.437091006	0.037865502
H	0.438880356	4.959688233	−0.152051994
N	2.066114276	−0.738447476	0.145796029
C	4.336463397	−0.812592235	−0.257701244
C	4.858481168	2.943344177	−1.061791899
C	5.418784863	1.960356997	1.033776455
N	−2.085379627	0.679513812	−0.155974300
C	−3.914606442	2.021464980	0.287026696
C	−2.987910539	4.875653717	−1.012308817
C	−1.979758739	5.315835584	1.085203002
C	2.466329009	−2.025575416	−0.038389657
C	3.895547738	−2.080588275	−0.297327186
H	5.212874899	−0.527544808	−0.383290623
H	4.253762070	3.075772722	−1.755538159
C	6.089375709	3.558744782	−1.105958478
H	5.200512409	1.424674936	1.762279361
C	6.657453397	2.587648016	0.984128646
C	−3.210959869	−0.084611407	−0.026927956
H	−4.422955350	2.783758864	0.448268419
C	−4.355530451	0.753468317	0.247412152
H	−3.166037162	4.302132024	−1.723477726
C	−3.508548418	6.157919264	−1.022485422
H	−1.458415162	5.043872129	1.806541933
C	−2.512993236	6.588202571	1.074776159
C	1.591503215	−3.125197509	−0.027338548
H	4.404216303	−2.842508559	−0.458279180
H	6.313794014	4.098279489	−1.829870924
C	6.984579045	3.378225793	−0.083662892
H	7.265258546	2.471090346	1.678433943
C	−3.207284124	−1.488020978	−0.055430811
H	−5.231613945	0.468795113	0.373279862
C	−3.265386700	7.011678587	0.014349113

H	−4.026231516	6.441061900	−1.740390228
H	−2.360289506	7.161098098	1.791590520
C	0.195841947	−3.038138869	0.000112270
C	2.190434538	−4.495661082	−0.047760319
H	7.816060973	3.792986664	−0.117176144
C	−2.051672776	−2.283018788	−0.057655558
C	−4.528688937	−2.187761062	−0.014672377
H	−3.610786965	7.874412204	0.000304047
C	−0.711400772	−4.125989435	0.070009408
N	−0.721533922	−2.015138588	−0.031493765
C	2.968780514	−4.934233875	1.002424521
C	1.960628995	−5.374410113	−1.095095558
C	−1.993033096	−3.693560344	0.018188225
C	−4.877619262	−3.001919330	1.051910741
C	−5.437914607	−2.018931526	−1.043669011
H	−0.458010382	−5.018268392	0.142167698
H	−0.450497544	−1.199567351	−0.034206497
H	3.147306180	−4.361098643	1.713355706
C	3.489823056	−6.216884937	1.012376345
H	1.439682012	−5.102827167	−1.816656133
C	2.494254186	−6.647164185	−1.084895042
H	−2.755838615	−4.270573265	0.051670734
H	−4.272495500	−3.134733389	1.745432219
C	−6.108109139	−3.617705449	1.095852538
H	−5.219245559	−1.483629973	−1.772393560
C	−6.676186547	−2.646603054	−0.994242846
C	3.246987177	−7.070258455	−0.024172039
H	4.007834161	−6.499653349	1.730559482
H	2.341889983	−7.219677965	−1.801413446
H	−6.332199438	−4.156865933	1.820043315
C	−7.002978568	−3.436805661	0.073839966
H	−7.283655901	−2.529681796	−1.688264689
H	3.592181073	−7.933008731	−0.010121135
H	−7.834658797	−3.851588196	0.107355918

Compound **2** xyz

```
C   -1.30798    7.64991    9.25689
C   -2.63767    7.70347    9.75518
C   -0.57922    8.70016    8.66832
S   -0.49553    6.12706    9.36409
H   -3.18721    8.47877    9.75166
C   -3.01451    6.49089   10.23700
H   -3.85636    6.29978   10.63241
C   -1.95644    5.54296   10.06260
C   -1.98203    4.18181   10.37689
C   -0.92852    3.27222   10.11449
C   -3.23550    3.63897   10.97277
C   -0.93265    1.87231   10.35083
N    0.28101    3.53833    9.52226
H   -1.63515    1.38314   10.76301
C    0.23792    1.34427    9.88889
H    0.48904    0.42889    9.92875
C    1.01780    2.39973    9.33666
C    2.27001    2.26220    8.70626
C    3.03104    3.29514    8.14901
C    2.83537    0.86895    8.60684
C    4.30100    3.16199    7.51747
N    2.73078    4.64483    8.10284
H    4.77495    2.34844    7.39345
C    4.71884    4.38894    7.12250
H    5.53845    4.57649    6.67964
C    3.73177    5.35229    7.47884
C    3.77133    6.73053    7.22307
C    2.73264    7.65387    7.49895
C    5.00362    7.27545    6.56387
C    2.76196    9.06128    7.27678
N    1.47470    7.38297    8.02970
H    3.49592    9.54610    6.91804
C    1.57584    9.60016    7.65895
H    1.34681   10.52106    7.61342
C    0.72686    8.55346    8.14215
C   -1.20978   10.03797    8.58604
C   -3.26502    3.12740   12.25688
C   -4.42236    3.63022   10.23929
H   -2.46576    3.10766   12.77055
C   -4.44924    2.63916   12.81026
H   -4.45346    2.31077   13.70164
C   -5.60390    2.63041   12.07928
H   -6.40495    2.27901   12.45115
```

```
C   -5.59614    3.14032   10.78717
H   -6.39762    3.15288   10.27767
H   -4.42578    3.96570    9.35061
C    3.64169    0.35029    9.60158
C    2.54714    0.07168    7.52707
H    3.85807    0.88554   10.35593
C    4.13711   -0.94126    9.51312
H    4.68929   -1.28228   10.20756
C    3.83791   -1.72749    8.43564
H    4.17354   -2.61551    8.38048
C    3.04975   -1.22320    7.43770
H    2.84423   -1.75937    6.68051
H    1.99718    0.40924    6.83027
C    6.22879    7.29462    7.22855
C    4.94757    7.79390    5.27542
H    6.29140    6.93474    8.10563
C    7.35690    7.83037    6.62878
H    8.18337    7.83798    7.09772
C    7.28700    8.35195    5.35702
H    8.05884    8.72635    4.94893
C    6.07676    8.32569    4.67610
H    6.02373    8.67457    3.79405
H    4.12460    7.78321    4.80054
C   -1.60148   10.72042    9.74832
C   -1.45563   10.65436    7.35884
H   -1.43929   10.32877   10.59851
C   -2.21734   11.94883    9.67426
H   -2.47710   12.39214   10.47330
C   -2.46289   12.54668    8.45141
H   -2.89356   13.39225    8.40544
C   -2.07066   11.89153    7.29233
H   -2.22581   12.29583    6.44668
H   -1.19684   10.21747    6.55619
H    1.99695    5.00329    8.42928
```

Compound **3** xyz

S	−0.102488450	1.805531432	−0.427933192
C	−1.371240693	2.762767857	0.135637141
C	1.065115928	2.866975417	0.134501267
C	−0.891576534	3.976050260	0.744504482
C	−2.692680601	2.331047120	−0.082151930
C	0.473358704	4.002086784	0.766297474
C	2.425243889	2.585317356	−0.081007179
H	−1.449371937	4.664528503	1.085452897
C	−2.993358165	0.961539263	−0.370808847
C	−3.832506028	3.293126455	0.021715665
H	0.977724715	4.703257403	1.161748143
C	2.852251221	1.256445332	−0.446438739
C	3.480377612	3.651472549	0.040280353
N	−2.090200668	−0.149873455	0.137443747
C	−4.085229910	0.417207385	−1.130328574
C	−3.729571078	4.591175331	−0.467707610
C	−5.001727642	2.879322300	0.649772720
N	2.112282643	0.082699154	0.043803911
C	4.012816793	0.868840994	−1.195778156
C	3.201790102	4.979695380	−0.259361948
C	4.736232910	3.296520531	0.518388994
H	−1.356225483	−0.112156549	0.621673943
C	−2.816646213	−1.321807944	−0.426315556
C	−3.956432293	−0.946581792	−1.147705844
H	−4.776379989	0.917290022	−1.547041754
H	−2.930042325	4.874008407	−0.896214657
C	−4.793390201	5.472982247	−0.326498711
C	−6.066318785	3.761378033	0.787696474
H	−5.072454251	1.992188274	0.982462963
H	1.364668911	0.045547793	0.506530508
C	2.960498581	−1.008819323	−0.454764783
H	4.630998551	1.458473058	−1.610283992
C	4.073107917	−0.503156952	−1.205516815
H	2.342420981	5.222465645	−0.586428746
C	4.177389927	5.952873590	−0.083105478
C	5.714195223	4.269001020	0.695818596
H	4.928116788	2.388459536	0.724332684
C	−2.328014864	−2.637380654	−0.154098377
H	−4.551798691	−1.545635458	−1.583370015
H	−4.722631360	6.360068838	−0.661703117
C	−5.961795830	5.057639909	0.299900918
H	−6.865028240	3.477724566	1.216726408
C	2.632743989	−2.358421277	−0.151520035

H	4.739303491	−1.027517679	−1.635487745
H	3.988086472	6.860323077	−0.288393212
C	5.434029650	5.597953058	0.394072471
H	6.572404966	4.026655685	1.022013284
C	−0.972996946	−2.926616491	0.181623801
C	−3.350757184	−3.731770978	0.001123965
H	−6.690650861	5.661268016	0.395047284
C	1.285482748	−2.784448830	0.204067202
C	3.720110690	−3.372277579	−0.048975844
H	6.102055040	6.262191651	0.515806604
N	0.119692220	−2.104271562	−0.315648738
C	−0.463089387	−3.997981316	0.924021428
C	−4.628935658	−3.444117193	0.465753244
C	−3.005403100	−5.038726685	−0.323313502
C	0.920735776	−3.919096489	0.954905805
C	4.964832812	−2.993877465	0.442607468
C	3.476029653	−4.702490949	−0.371274832
H	0.079583630	−1.377236088	−0.809958229
H	−0.984568497	−4.673546269	1.341735241
H	−4.862592807	−2.551251643	0.689632146
C	−5.563413887	−4.463511245	0.603734644
C	−3.941649315	−6.058323700	−0.185454313
H	−2.132962669	−5.235465100	−0.639802659
H	1.509369163	−4.516706149	1.397988317
H	5.132451186	−2.085382407	0.663009733
C	5.963983449	−3.945131457	0.611916145
C	4.475180147	−5.653735849	−0.201961993
H	2.625347855	−4.960730121	−0.706244549
H	−6.436812257	−4.266744261	0.921113429
C	−5.220014558	−5.770269860	0.277429694
H	−3.707182119	−6.950957718	−0.408321376
H	6.814484325	−3.686829531	0.946838646
C	5.718923955	−5.274982650	0.288792263
H	4.307387567	−6.562164982	−0.422418169
H	−5.859441753	−6.466988556	0.372295018
H	6.402113622	−5.925789993	0.404688796

Compound **4** xyz

S	−0.155420139	−1.518761386	−0.127478883
C	−1.513193393	−2.610726341	−0.099518009
C	0.981397273	−2.833150670	−0.019667883
C	−2.850219731	−2.159960405	−0.084263213
C	−1.066367781	−3.951443972	−0.003903412
C	2.374737799	−2.645013062	−0.026952126
C	0.293692142	−4.068422169	0.056795053
C	−3.205377020	−0.797886840	−0.054621021
C	−3.946200508	−3.171211309	−0.014882801
H	−1.655144814	−4.697584808	0.016119102
C	2.986143729	−1.373732323	−0.016802449
C	3.253069453	−3.850898225	−0.042214963
H	0.738184727	−4.904148638	0.143007198
N	−2.301051384	0.215889484	−0.196725844
C	−4.521695655	−0.255873609	0.253487183
C	−4.015921657	−4.082668198	1.037118179
C	−4.932125547	−3.202174644	−0.996731890
N	2.300852382	−0.216354170	0.196972410
C	4.386872182	−1.087343323	−0.301991300
C	4.165948370	−4.065550359	0.984549236
C	3.171234365	−4.792245542	−1.065522866
C	−2.986342731	1.373267637	0.017049015
C	−4.387128391	1.086847423	0.302104251
H	−5.320849671	−0.750603992	0.392809747
H	−3.344030577	−4.080697008	1.708159422
C	−5.058748206	−4.989444091	1.109630709
H	−4.895418143	−2.589200873	−1.721855946
C	−5.970473737	−4.123204882	−0.922312068
C	3.205179126	0.797416673	0.054875877
H	5.070091398	−1.721291438	−0.485970069
C	4.521430436	0.255380676	−0.253371068
H	4.243705614	−3.428447355	1.685107259
C	4.959888947	−5.195147982	0.996906916
H	2.556846411	−4.660024517	−1.777691821
C	3.976751764	−5.920709530	−1.056531289
C	−2.374585590	2.645434979	0.026893589
H	−5.070038109	1.721246828	0.486098795
H	−5.102311489	−5.601466501	1.834345449
C	−6.034204102	−5.006341009	0.132269274
H	−6.636652699	−4.142892389	−1.599255139
C	2.850370832	2.160387803	0.084196385
H	5.320898766	0.750551561	−0.392685631
H	5.577115501	−5.331328936	1.706681814

C	4.861788574	−6.130292694	−0.017570544
H	3.919177606	−6.549205366	−1.766277505
C	−0.981237161	2.833575100	0.019597891
C	−3.252963151	3.850877008	0.042472695
H	−6.749755972	−5.628663520	0.186299453
C	1.513344495	2.611153739	0.099451182
C	3.946315821	3.171187126	0.015137368
H	5.399935447	−6.913191435	−0.000167697
S	0.155571241	1.519188783	0.127412056
C	−0.293664465	4.068790104	−0.057125946
C	−4.165966600	4.065475161	−0.984563861
C	−3.171251487	4.792164864	1.065516532
C	1.066404468	3.951808941	0.003569355
C	4.015913545	4.082584553	−1.037127678
C	4.932117435	3.202090999	0.996722391
H	−0.738198763	4.904081260	−0.143017212
H	−4.243847268	3.428312696	−1.685385949
C	−4.960030601	5.195013322	−0.997185606
H	−2.556988065	4.659889857	1.777413131
C	−3.976889224	5.920582690	1.056257209
H	1.655139789	4.697514465	−0.016132281
H	3.343902127	4.080567203	−1.708436667
C	5.058619756	4.989314285	−1.109907954
H	4.895280683	2.589074034	1.721581865
C	5.970332083	4.123070222	0.922033377
H	−5.576860022	5.331253447	−1.706359269
C	−4.861542105	6.130220172	0.017896254
H	−3.918928051	6.549146145	1.766599534
H	5.102565860	5.601396493	−1.834031194
C	6.034449463	5.006273967	−0.131951855
H	6.636902877	4.142814561	1.599564783
H	−5.400471258	6.913281483	0.000452076
H	6.749229171	5.628750602	−0.186018240

Compound **5** xyz

C	−4.344745199	3.862495042	0.869253575
H	−4.482888347	3.157403776	1.490860812
C	−3.299483262	3.784627744	−0.050576981
C	−5.186363069	4.974320064	0.877912117
C	−2.361523381	2.629326789	−0.018085976
C	−3.136753023	4.810212961	−0.985745170
C	−5.005095055	5.984391153	−0.049686985
H	−5.884009517	5.037586312	1.519357283
C	−2.947089722	1.339976655	−0.087427848
C	−0.989924016	2.870243885	0.050862348
H	−2.435094832	4.762324999	−1.625392217
C	−3.995400533	5.899207146	−0.986527116
H	−5.579087424	6.740409202	−0.042191757
C	−4.262943176	0.970671519	−0.500559691
N	−2.297309330	0.167152928	0.223055029
C	−0.364809875	4.094705968	0.371770512
S	0.141158767	1.674200868	−0.266092296
H	−3.888917272	6.586984202	−1.633620818
C	−4.376205452	−0.368388517	−0.443519482
H	−4.945621583	1.572230346	−0.770959717
C	−3.131546214	−0.893111982	0.016070084
H	−1.466544899	0.109209577	0.509683601
H	−0.835853761	4.895204937	0.572775433
C	0.979020113	3.992640450	0.358801586
C	1.418453070	2.706738533	−0.005706638
H	−5.147411382	−0.874313697	−0.668904510
C	−2.742750034	−2.242684330	0.152229851
H	1.566460874	4.709447029	0.570956304
C	2.735984274	2.236612304	−0.144833944
C	−1.408645588	−2.670464874	0.226173117
C	−3.815965726	−3.293406207	0.167516896
C	3.079401416	0.876638423	−0.322814296
C	3.822707547	3.220110252	0.044631078
S	−0.149910469	−1.633176420	−0.201468042
C	−0.945452924	−3.944780316	0.604977839
C	−3.715805892	−4.382493261	−0.685453220
C	−4.941522704	−3.183394580	0.979130347
C	4.414157428	0.350634613	−0.635554391
N	2.181682915	−0.150350941	−0.199771900
C	4.839456163	2.980279730	0.961370048
C	3.851120084	4.424465251	−0.661547610
C	1.008284083	−2.831320247	0.076183004
C	0.416355057	−4.021287019	0.501604565

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H	−1.505628615	−4.656060169	0.893961617
H	−2.954868141	−4.472002196	−1.248922838
C	−4.714609994	−5.341521534	−0.725242538
C	−5.920131070	−4.167403924	0.936638969
H	−5.039722845	−2.437091163	1.559011317
H	5.201775739	0.853264460	−0.806148696
C	4.291214654	−0.987273415	−0.632216825
C	2.941867668	−1.298804771	−0.330230819
H	4.858660391	2.165573779	1.449444696
C	5.836607776	3.943147806	1.160911726
C	4.845759705	5.368428362	−0.420513166
H	3.185964523	4.601702245	−1.315868560
C	2.373803741	−2.572532744	−0.133051431
H	0.910137081	−4.810040493	0.699591507
H	−4.642315819	−6.082425166	−1.316482410
C	−5.801482038	−5.218521159	0.086764557
H	−6.677653786	−4.104882358	1.507060819
H	4.985214190	−1.613033682	−0.801698404
H	6.536443964	3.765755593	1.777998690
C	5.823087515	5.123077619	0.491849385
H	4.841669037	6.189804280	−0.895800712
C	3.308375234	−3.753870897	−0.076885776
H	−6.484202821	−5.877659417	0.058322305
H	6.493014904	5.774462476	0.659653452
C	3.122328508	−4.835078717	−0.928649153
C	4.346637157	−3.778777469	0.843307257
H	2.402439621	−4.834301644	−1.548194832
C	3.999270955	−5.937260597	−0.871391041
H	4.479485702	−3.045815814	1.432881219
C	5.193595274	−4.878852862	0.901329642
C	5.013507982	−5.957943130	0.051130275
H	3.887932445	−6.664169972	−1.471972187
H	5.903770944	−4.890405416	1.532478645
H	5.591621867	−6.710252254	0.107394350

Compound **6** xyz

S	−0.029088924	1.633081293	−0.224022406
C	1.211121713	2.762137847	0.252032030
C	−1.308433140	2.717513348	0.252032266
C	2.577494476	2.496811752	0.062287249
C	0.612386944	3.945803631	0.742522332
C	−2.664493412	2.403969526	0.062287741
C	−0.751929087	3.921639871	0.742522460
C	3.533979559	3.625361110	0.054298270
C	3.078999639	1.193112293	−0.154810986
H	1.115885822	4.692908916	1.047301608
C	−3.660282149	3.497941650	0.054298944
C	−3.119458244	1.083329776	−0.154810405
H	−1.281508189	4.650448040	1.047301833
C	4.768168538	3.515504880	0.708543891
C	3.223135307	4.808152635	−0.617398428
N	2.402508835	0.044214269	0.176339758
C	4.291695568	0.776598571	−0.774351303
C	−4.889746790	3.344451003	0.708544796
C	−3.391457312	4.690999847	−0.617397808
N	−2.402647562	−0.040891120	0.176340208
C	−4.316584377	0.624135062	−0.774350496
H	4.990426777	2.719652324	1.175076481
C	5.659637293	4.573812838	0.675389021
H	2.384965280	4.895034959	−1.057480495
C	4.127156705	5.859081420	−0.643765296
H	1.614958429	0.020889221	0.568664599
C	3.130435763	−1.064452962	−0.192845695
H	4.963874988	1.354059010	−1.117720451
C	4.329244541	−0.581681698	−0.792850258
H	−5.083623288	2.541228175	1.175077425
C	−5.818072633	4.370528100	0.675390097
H	−2.556829688	4.807509529	−1.057480032
C	−4.332066617	5.709257892	−0.643764503
H	−1.614705056	−0.036312198	0.568664901
C	−3.090798548	−1.174638878	−0.192845112
H	−5.008730987	1.177431564	−1.117719517
C	−4.305951183	−0.734621919	−0.792849448
H	6.497703752	4.496166297	1.117026140
C	5.349120799	5.737534013	0.005880325
H	3.913134734	6.660864684	−1.106683098
C	2.671399721	−2.389575905	0.005585603
H	5.031481242	−1.116827326	−1.146624701
H	−6.652803826	4.263254200	1.117027373

C	−5.548900041	5.544516302	0.005881346
H	−4.146511255	6.518118175	−1.106682342
C	−2.585065896	−2.482674549	0.005586096
H	−4.988737266	−1.294298050	−1.146623762
H	5.969088023	6.456397880	−0.011268991
C	1.307870873	−2.690840789	0.200846280
C	3.653006243	−3.497666016	0.010567774
H	−6.193884433	6.240976278	−0.011267851
C	−1.211673981	−2.735465110	0.200846516
C	−3.526767738	−3.624828880	0.010568447
S	0.029663934	−1.670626377	−0.382297461
C	0.748317210	−3.835716799	0.829699322
C	3.327984099	−4.729780158	−0.565651961
C	4.911229311	−3.327449000	0.599312551
C	−0.611859471	−3.859807246	0.829699449
C	−3.158248652	−4.844659531	−0.565651353
C	−4.790159199	−3.499272842	0.599313460
H	1.278296710	−4.525011180	1.213432352
H	2.481084281	−4.851926234	−0.979923925
C	4.236887710	−5.767197244	−0.532625577
H	5.146075369	−2.495598963	0.990157768
C	5.818433259	−4.385229480	0.607890068
H	−1.117037624	−4.567435576	1.213432576
H	−2.307494716	−4.936738016	−0.979923477
C	−4.029785810	−5.913610471	−0.532624802
H	−5.054254891	−2.676259693	0.990158724
C	−5.659276667	−4.588514217	0.607891144
H	4.007407251	−6.606092288	−0.912200904
C	5.485759214	−5.595280617	0.050443209
H	6.674791448	−4.267990110	1.002556615
H	−3.770682895	−6.743852087	−0.912200175
C	−5.283901757	−5.786024914	0.050444218
H	−6.519189312	−4.501672172	1.002557851
H	6.107369565	−6.313742755	0.062352252
H	−5.879620490	−6.526047487	0.062353376

Compound **7** xyz

```
C     4.99220    10.22441    3.05074
C     6.34993     9.79815    3.13879
C     4.37741    10.96629    2.04332
S     3.95309     9.81633    4.46993
H     7.00946     9.96187    2.47449
C     6.57519     9.12779    4.29383
H     7.41395     8.75387    4.53530
C     5.42032     9.04839    5.09406
C     5.30899     8.45967    6.34492
C     4.14315     8.41852    7.09595
C     6.50838     7.79872    6.94575
C     3.92109     7.82114    8.36235
N     2.95849     8.87142    6.83180
H     4.58453     7.39058    8.88949
C     2.59917     7.95938    8.71196
H     2.21126     7.64821    9.52160
C     1.90481     8.63778    7.67865
C     0.54310     8.95378    7.64239
C    -0.05494     9.68158    6.63238
C    -0.29034     8.46081    8.78707
C    -1.42149    10.01278    6.52361
S     1.03645    10.20980    5.29089
H    -2.08346     9.74617    7.15124
C    -1.68487    10.76430    5.40743
H    -2.53945    11.11428    5.18074
C    -0.51434    10.94763    4.63827
C    -0.35473    11.63328    3.42108
C     0.84479    11.70272    2.69076
C    -1.55835    12.35974    2.87982
C     1.04684    12.25079    1.41142
N     2.07017    11.24988    2.96269
H     0.38128    12.69490    0.89756
C     2.32975    12.05241    1.01519
H     2.69885    12.32276    0.18333
C     3.03758    11.37227    2.05109
C     5.22272    11.39069    0.89347
C     5.83048    10.49435    0.03626
C     5.47308    12.73484    0.67075
H     5.69211     9.56265    0.16082
C     6.63731    10.92497   -0.99965
H     7.04032    10.29183   -1.58253
C     6.85606    12.26587   -1.19129
H     7.41069    12.56081   -1.90329
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C    6.27691   13.17260   -0.35221
H    6.42963   14.10146   -0.47722
H    5.07350   13.37761    1.24570
C    6.58247    6.43155    6.93798
C    7.53564    8.50465    7.51808
H    5.88024    5.93137    6.53845
C    7.65208    5.76848    7.49478
H    7.68922    4.81961    7.47209
C    8.65385    6.47275    8.08006
H    9.38336    6.01816    8.48238
C    8.61051    7.84518    8.08524
H    9.31833    8.34130    8.48062
H    7.50867    9.45449    7.52259
C   -0.65172    7.14000    8.85958
C   -0.64459    9.27952    9.81779
H   -0.42671    6.56009    8.14126
C   -1.33306    6.63243    9.93951
H   -1.56078    5.71022    9.97401
C   -1.67671    7.46694   10.96765
H   -2.15777    7.12937   11.71373
C   -1.33157    8.77914   10.91585
H   -1.55984    9.35730   11.63568
H   -0.41879   10.20197    9.78457
C   -2.71250   11.71324    2.47840
C   -1.53242   13.74531    2.77623
H   -2.75804   10.76687    2.54444
C   -3.79525   12.39794    1.98635
H   -4.57302   11.92518    1.71383
C   -3.75590   13.76949    1.88794
H   -4.50083   14.25098    1.54769
C   -2.61879   14.43713    2.29453
H   -2.58656   15.38536    2.23926
H   -0.75456   14.22158    3.04222
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