Supporting Information

Unveiling the Aggregation-Induced Chromic Emission of Triazine Anchored BODIPYs

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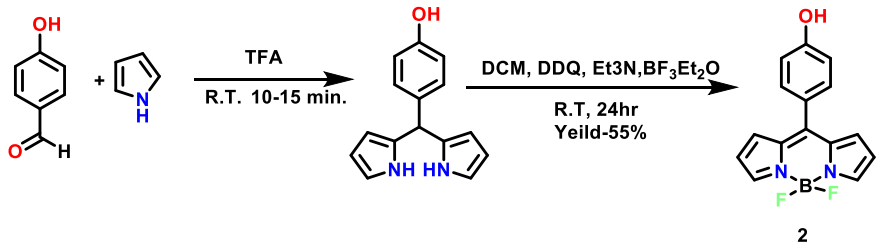
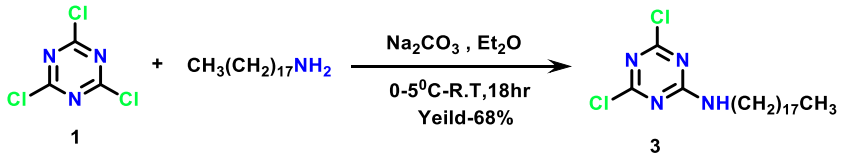
1. General Information

All specified chemicals are obtained from Avra Chemicals, S.D.Fine chemicals, Loba chemicals, Alfa Aesar, Spectrochem and used without further purification. All commercial grade solvents are used after distillation. ^{1}HNMR, ^{13}CNMR were recorded in 400 & 500 MHz VnmrS NMR Agilent. Mass spectra (HR-LCMS), Absorption spectra, Emission Spectra were recorded in the Agilent, UV-1800 SHIMADZU, Jasco Spectrophotometer FP-8200 respectively.

1.1 Exerimental





Compound **2**:

4-hydroxybenzaldehyde (500mg, 4mmol) was dissolved in pyrrole (7ml, 102mmol) under N_2 atmosphere. TFA (2 -3 drops) was added and the reaction mixture was stirred for 10-15 minutes the progress of reaction was monitored by TLC. The reaction was quenched by addition of aqueous solution of 1M NaOH solution followed by extraction with ethyl acetate. The organic layer washes with water and dried over sodium sulphate anhydrous. The solvent and excess pyrrole was evaporated under reduce pressure on rotary evaporator. The residue was purified by column chromatography using (PET: EtOAc, 80:20) System.

The corresponding dipyrromethane (200mg 8.39mmol) dissolved in CH_2Cl_2 and nitrogen was purged for 15min. 3-dichloro-5, 6-dicyano, 1, 4 benzoquinone (DDQ) (226mg 8.39mmol) was added and stirred for 1-2 hrs. at room temperature. To this oxidized dipyrromethene trimethylamine (12.66ml 90.86mmol) was added and stirred for 15-30 minutes after that

BF_3Et_2O (19.05 ml 154.37mmol) was added dropwise. The reaction mixture was then allowed to keep under stirring overnight at room temperature. The completion of reaction was monitored by TLC analysis. The reaction mixture was then extracted with DCM wash with water and dried over sodium sulphate anhydrous. The excess of solvent was then evaporated under reduced pressure. The residue was the purified on column chromatography using (PET: EtOAc , 85:15) System.

Compound **3**:

The 2, 4, 6-trichloro-1, 3, 5 triazine (2.84g, 15.4 mmol) and Na_2CO_3 (1.96g, 18.5mmol) were suspended in Et_2O (50ml). To the stirred and cooled (ice bath) suspension, octadecylamine (4.16g, 15.4mmol) was added within 30 minutes then the ice bath removed and the mixture was stirred at r.t for overnight. After washing with hot EtOAc and evaporation, the residue was submitted to flash column chromatography (PET: EtOAc 95:5) to obtain white solid.

Compound **4**:

To a mixture of 2,4,6-trichloro-1,3,5 triazine (100 mg, 0.542 mmol), OH-BODIPY (276 mg, 0.975 mmol) and $NaHCO_3$ (143 mg, 1.35 mmol) was added dry acetone under a N_2 atmosphere. The reaction started at 0–5°C and was stirred for 2–3 hrs. The progress of the reaction was monitored by TLC. After completion of the reaction, the excess solvent was evaporated under reduced pressure. The obtained crude material was then purified by column chromatography (PET: EtOAc, 90:10) to obtain Compound **4** in 55% yield as an orange–red solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.97 (*s*, 2H), 7.67 (*d*, *J=8.4 Hz,* 2H), 7.39 (*d*, *J=8.4 Hz*, 2H), 6.98 (*d*, *J=3.*8 Hz, 2H), 6.59 (*d*, *J=3.3 Hz,* 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 173.3, 170.7, 152.7, 145.4, 144.7, 134.8, 132.5, 132.0, 131.5, 121.4, 118.9. HR-MS (ESI) (m/z): calcd for $C_{18}H_{10}BCl_2F_2N_5O$ 432.0188; found 432.2209. FTIR (ATR cm^{-1}): 850-550 (C-Cl) 1275-1200 (C-O)

Compound **5**:

Dry THF was added to a mixture of 4,6-dichloro-N-octadecyl-1,3,5-triazin-2-amine (0.5 g, 1.19 mmol), OH-BODIPY (0.340 g, 1.19 mmol) and K_2CO_3 (0.164 g, 1.19 mmol), and the reaction mixture was stirred at 50–55°C for 20 hr. The progress of the reaction was monitored by TLC analysis. After completion of the reaction, the excess solvent was evaporated under reduced

pressure, and the residue obtained was then purified by column chromatography (PET: EtOAc, 90:10) to obtain Compound **5** in 47% yield as an orange–red solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ(ppm): 7.96 (*s*, 2H), 7.61 (*d*, *J=.8.*30 Hz, 2H), 7.39 (*dd*, *J=14.2, 8.1 Hz,* 2H), 7.00 (*dd*, *J=11.4, 3.8 Hz,* 2H), 6.57 (*s*, 2H), 3.50-3.45 (m, 2H), 3.38-3.33 (m, 2H), 1.63-1.52 (m, 2H), 1.23-1.09 (m, 30H), 0.88 (t, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.6, 167.1, 167.0, 153.7, 146.1, 144.3, 134.9, 131.7, 131.6, 121.8, 118.7, 41.5, 41.4, 31.9, 29.6, 26.7, 22.6, 14.1. HRMS (ESI) (m/z): calcd for $C_{36}H_{48}BClF_2N_6O$, 665.3639; found 665.3698. FTIR (ATR cm^{-1}): 850-550 (C-Cl) 1275-1200 (C-O) 3350-3310 (N-H)

Compound **6**:

To a mixture of 2,4,6-dichloro-1,3,5-triazine (100 mg 0.542 mmol), OH-BODIPY (276 mg 0.975 mmol) and Na_2CO_3 (143 mg 1.35 mmol) was added dry THF under a N_2 atmosphere. The reaction was carried out at 50–55°C for 20 hrs. The progress of the reaction was monitored by TLC. After completion of the reaction, the excess solvent was evaporated under reduced pressure. The obtained crude material was then purified using silica gel column chromatography (PET: EtOAc, 80:20) with a mixture as the eluent to obtain Compound **6** in 40% yield as an orange solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.95 (*s*, 4H), 7.62 (*d*, *J=8.08 Hz,* 4H), 7.38 (*d*, *J=8.52 Hz,* 4H), 6.90 (*d*, *J=3.84 Hz,* 4H), 6.51 (*d*, *J=3.08 Hz,* 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 174.2, 172.1, 152.9, 145.3, 144.6, 134.7, 132.1, 131.8, 131.2, 121.5, 118.8. HRMS (ESI) (m/z): calcd for $C_{33}H_{20}B_2ClF_4N_7O_2$ 679.1489; $(M+Na)^+$, found 702.1366. FTIR (ATR cm^{-1}): 850-550 (C-Cl) 1275-1200 (C-O)

Compound **7**:

To a mixture of 4,6-dichloro-N-octadecyl-1,3,5-triazin-2-amine (0.1 g, 0.289 mmol), OH-BODIPY (0.136 g, 0.479 mmol) and K_2CO_3 (0.050 g, 0.479 mmol) in DMSO was added, and the mixture was stirred at 100°C for 24 hr. The progress of the reaction was monitored by TLC analysis. After completion of the reaction, the compound was solvent extracted using ethyl acetate and washed with water, and the organic layer was then dried over anhydrous sodium sulfate. The excess solvent was then evaporated under reduced pressure to obtain a red residue, which was then purified by column chromatography (PET: EtOAc, 75:25) to obtain Compound **7** in 33% yield as an orange–red solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm): 7.94 (*s*, 4H), 7.58 (*d*, *J=8.3 Hz,* 4H),

7.34 (*dd*, *J= 20.6, 7.9 Hz,* 4H), 6.92 (*d*, *J= 4.7 Hz,* 4H), 6.51 (*s*, 4H), 3.45-3.33 (*m*, 2H), 1.62-1.52 (*m*, 2H), 1.43-1.39 (*m*, 2H), 1.23-1.10 (*m*, 30H), 0.88 (*t*, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ (ppm) 172.1, 171.4, 168.3, 154.0, 144.3, 134.7, 131.6, 131.5, 131.4, 121.9, 118.6, 45.8, 41.4, 31.9, 29.7, 29.6, 29.6, 29.5, 29.3, 29.3, 29.3, 26.8, 22.7, 14.1. HRMS (ESI)) (m/z): calcd for $C_{51}H_{58}B_2F_4N_8O_2$, 912.4805 $(M+H)^+$, found 913.4824. FTIR (ATR cm^{-1}): 850-550 (C-Cl) 1275-1200 (C-O) 3350-3310 (N-H)

Compound **8**:

To a mixture of 2,4,6-dichloro-1,3,5 triazine (100 mg 0.542 mmol), OH-BODIPY (477 mg 1.68 mmol) and Na_2CO_3 (229 mg 2.168 mmol) was added dry THF under a N_2 atmosphere. The reaction was carried out at 66°C for 24 hrs. The progress of the reaction was monitored by TLC. After completion of the reaction, the excess solvent was evaporated under reduced pressure. The obtained crude material was then purified using silica gel column chromatography (PET: EtOAc, 70:30) as the eluent to obtain Compound **8** in 35% yield as an orange solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) ^{1}H NMR (400 MHz, $cdcl_3$) δ 7.93(*s*, 6H), 7.61(*d*, *J=8.5 Hz,* 6H), 7.38(d, *J=8.5 Hz,* 6H), 6.85(*d*, *J=4.0 Hz*, 6H), 6.47(*d*, *J=3.8 Hz,* 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 173.5, 153.3, 145.3, 144.6, 134.7, 131.9, 131.6, 131.1, 121.6, 118.7. HRMS (ESI) (m/z): calcd for $C_{48}H_{30}B_3F_6N_9O_3$ 927.2655; $(M+Na)^+$, found 950.2550. FTIR (ATR cm^{-1}): 1275-1200 (C-O).

2. UV- absorption emission spectra of Solvent effect:

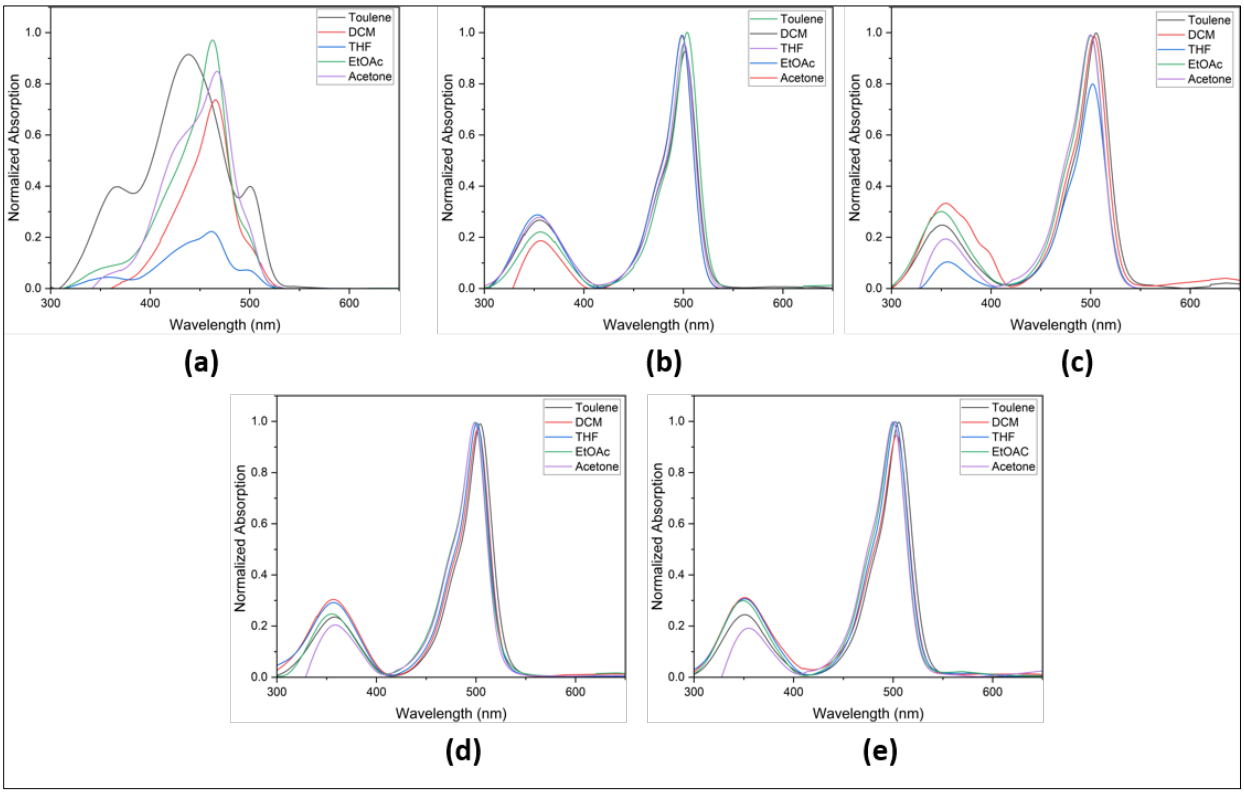


Fig. S1. Normalized absorption spectra (a) (b) (c) (d) and (e) of compounds **4-8** respectively in various solvents. Concentration (10 µm).

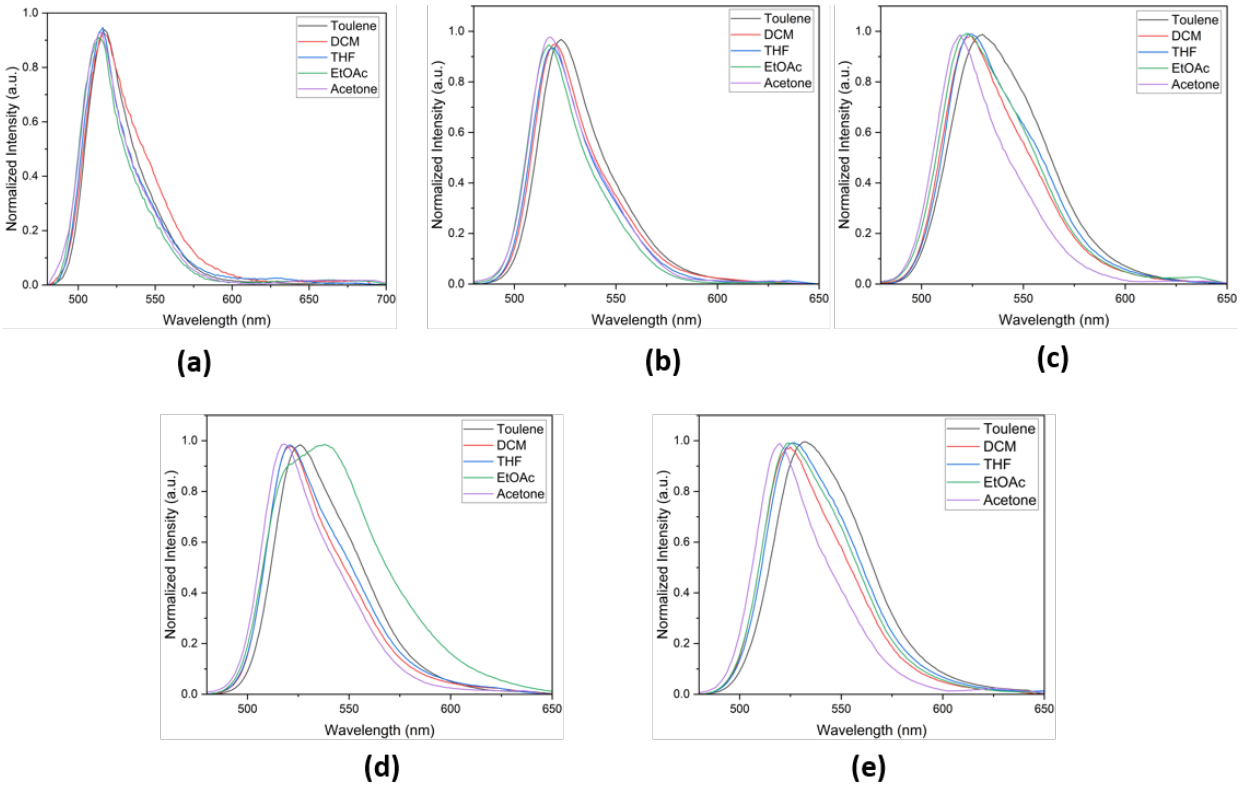


Fig. S2. Normalized emission spectra (a) (b) (c) (d) and (e) of compounds **4-8** respectively in various solvents. Concentration (10 µm), (λ_{ex} = 450 nm) .

3. Fluorescence Lifetime

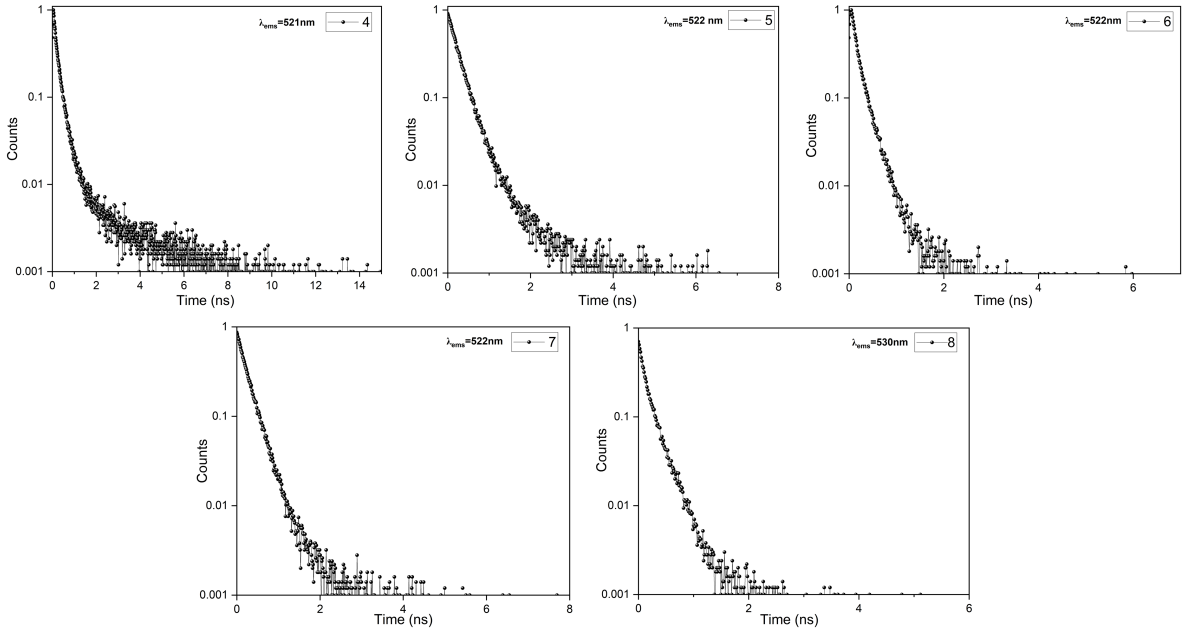


Fig. S3. Fluorescence lifetime profile of compound **4-8** (λ_{ex} = 450 nm) in DMSO (10 μM)

4. Aggregation-induced emission

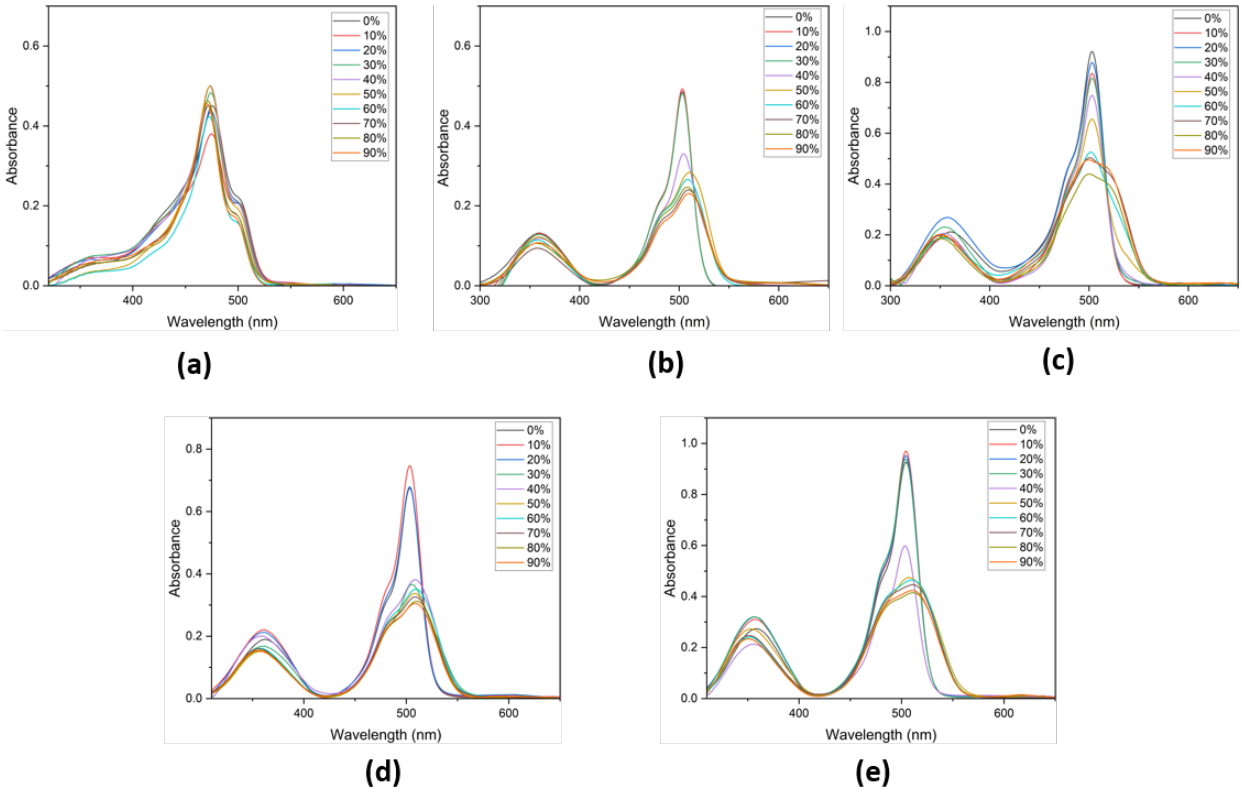


Fig. S4. Absorption spectra with varying water fractions from 0 to 90% in DMSO (a) compound **4** (1×10^{-5} M), (b) compound **5** (1×10^{-5} M), (c) compound **6** (1×10^{-5} M), (d) compound **7** (1×10^{-5} M), and (e) compound **8** (1×10^{-5} M).

5. Linear Fitting plots of Viscosity Vs. Emission Intensity

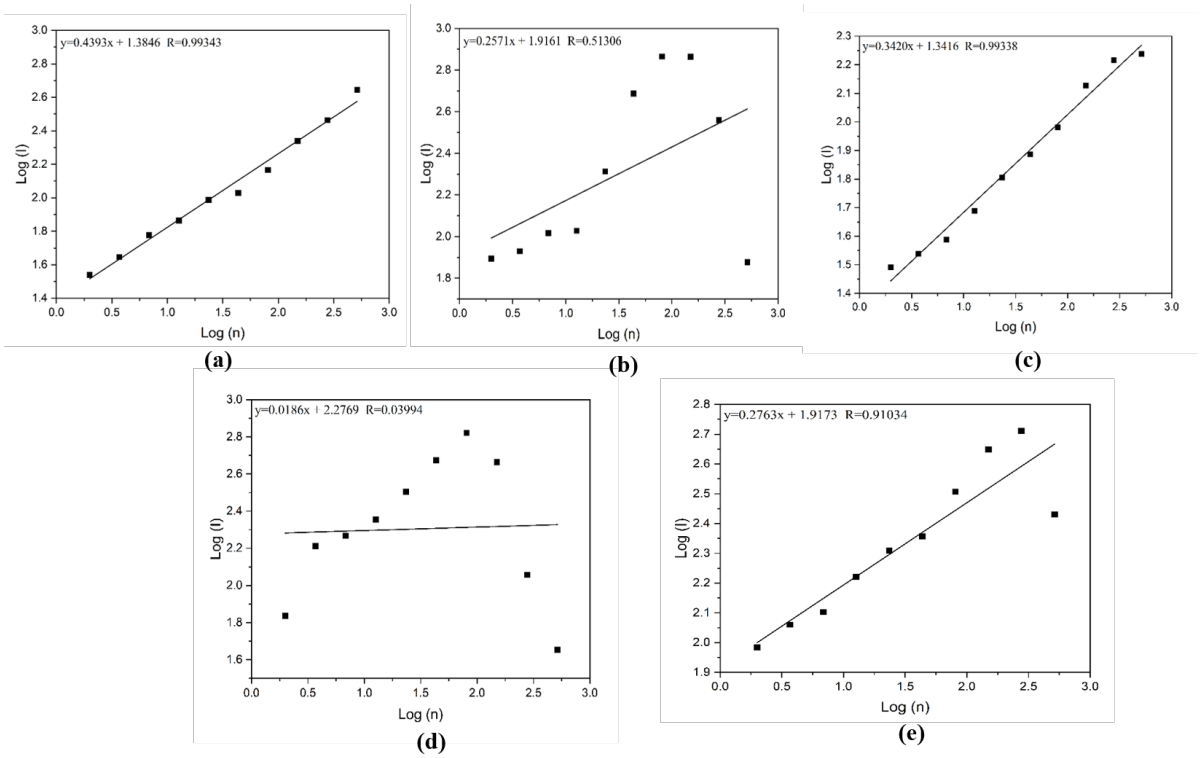


Fig. S5. Linear fitting plots of viscosity vs. emission intensity (a) compound **4**, (b) compound **5**, (c) compound **6**, (d) compound **7**, (e) compound **8**.

6. Copies of ^{1}H, ^{13}C NMR and HR-LCMS

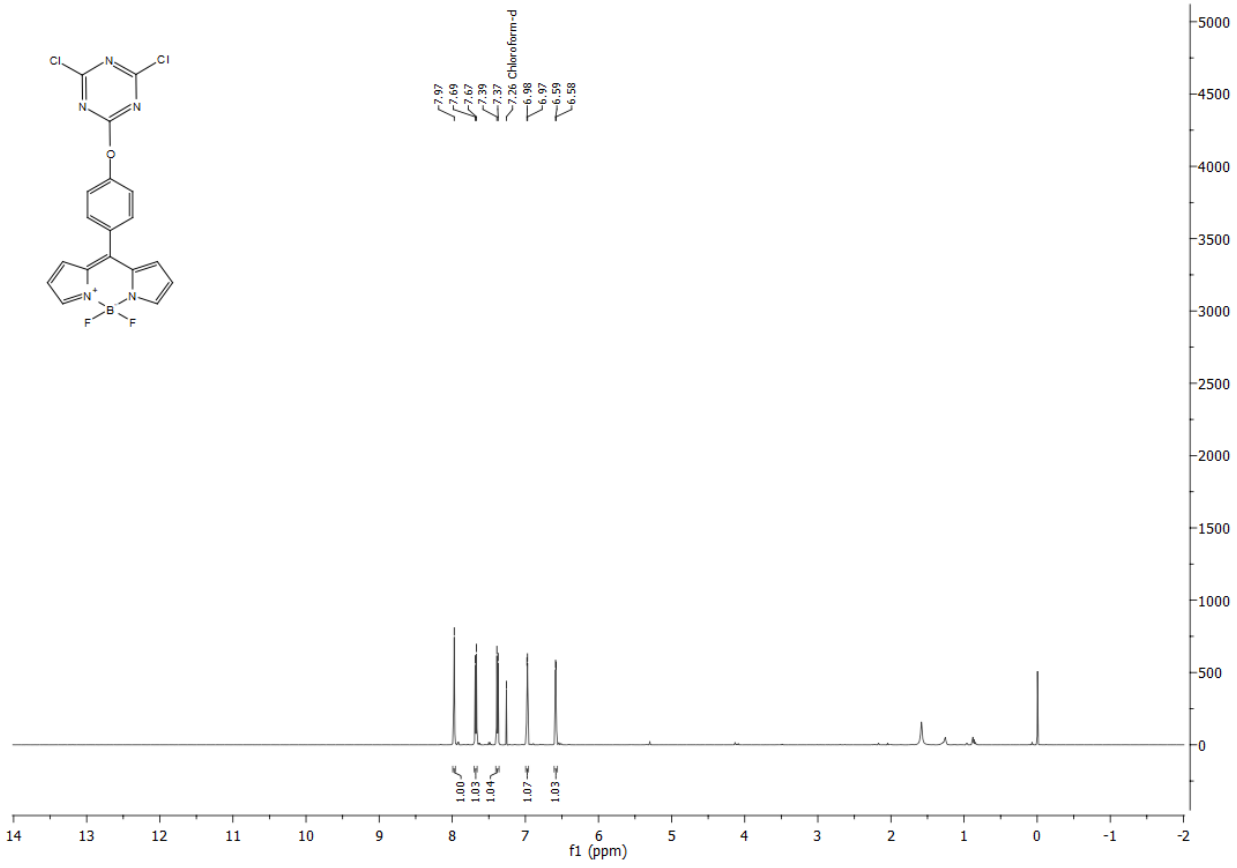


Fig. S6. ^{1}H NMR of Compound **4** $CDCl_3$

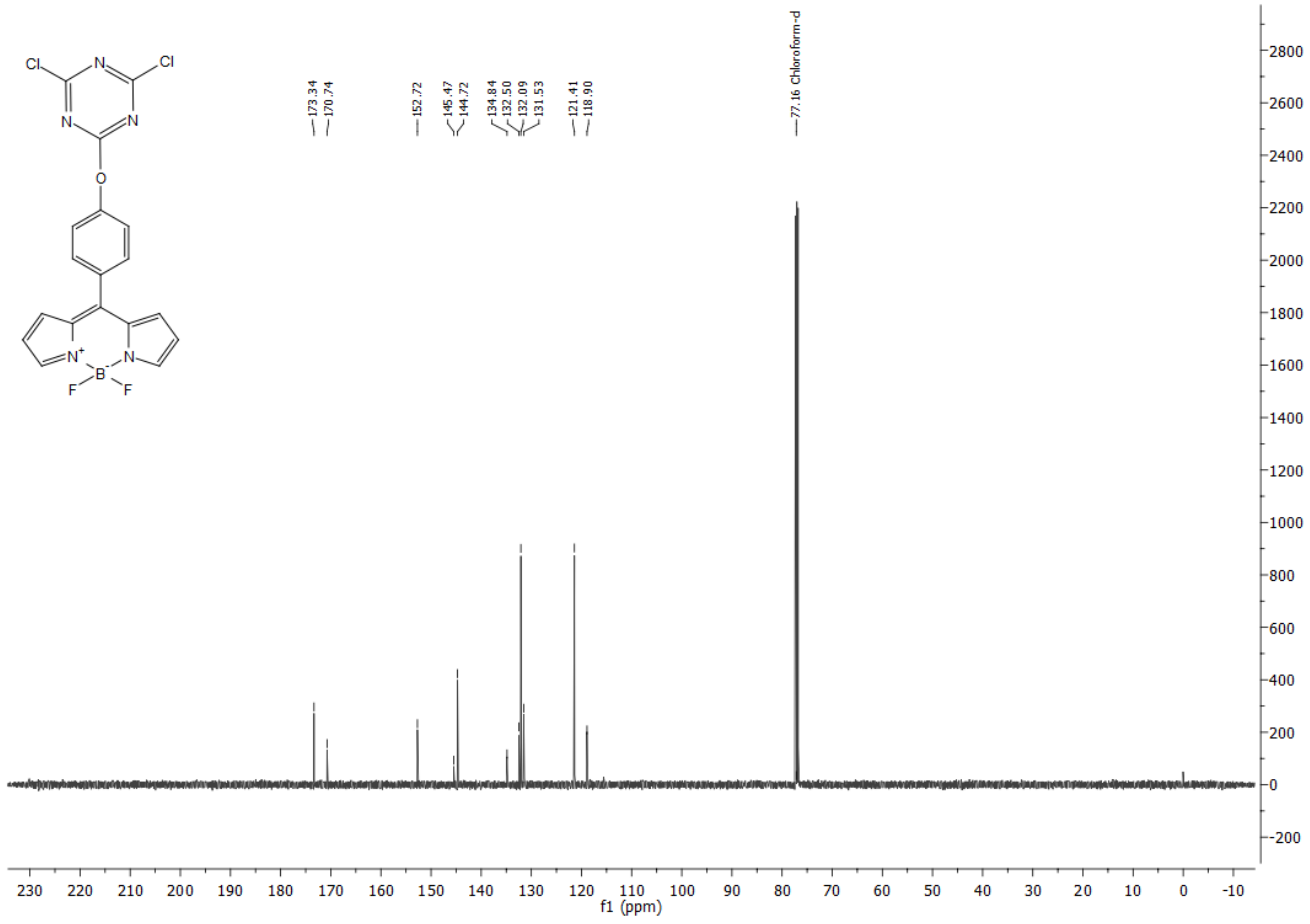


Fig. S7. ^{13}C NMR of Compound **4** $CDCl_3$

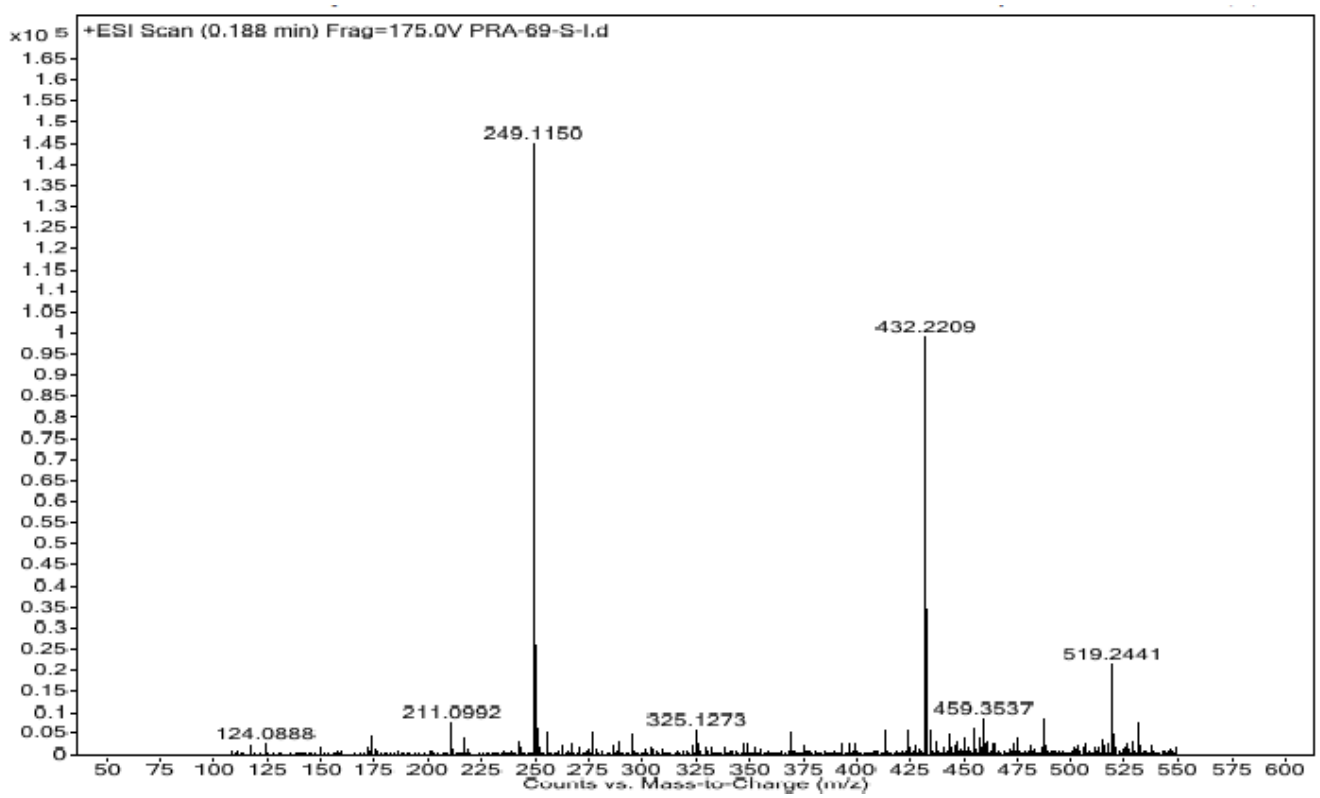


Fig. S8. HRLCMS of Compound **4**, Expected mass: 432.0188, Experimental: 432.22

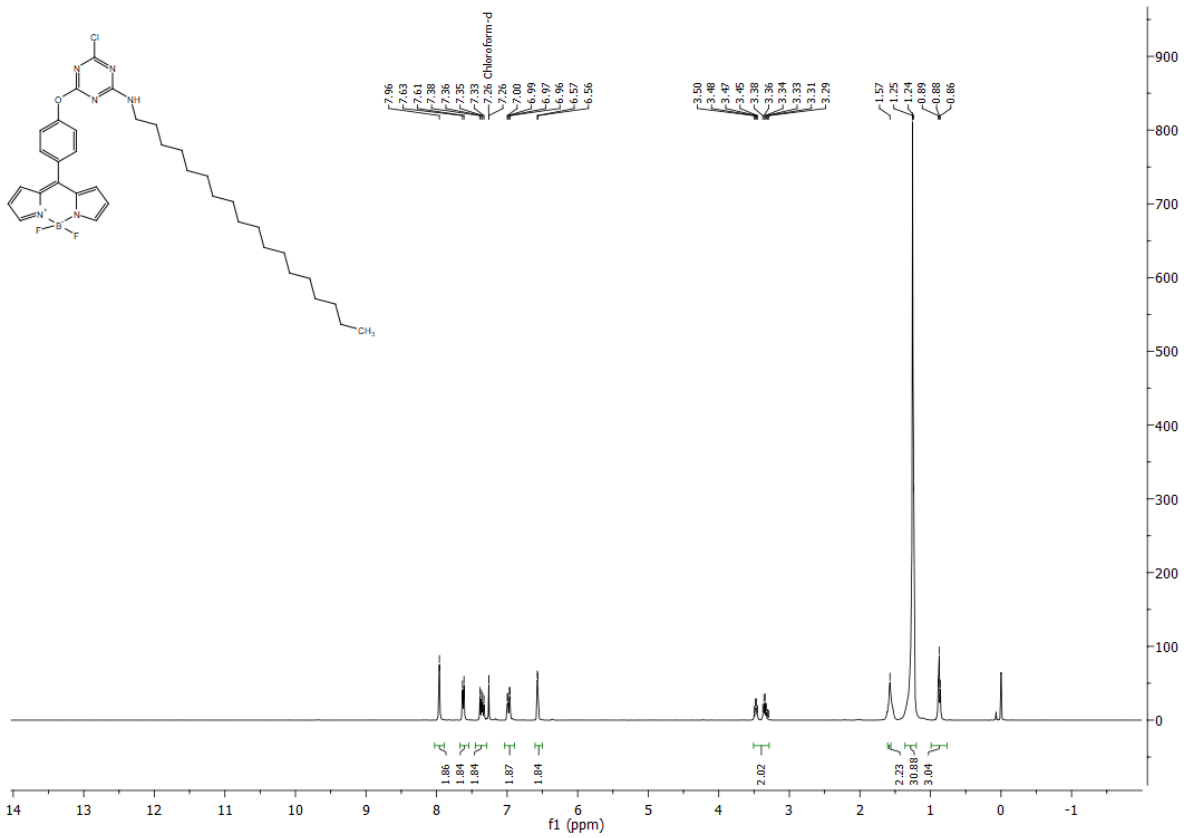


Fig. S9. ^{1}H NMR of Compound **5** $CDCl_3$

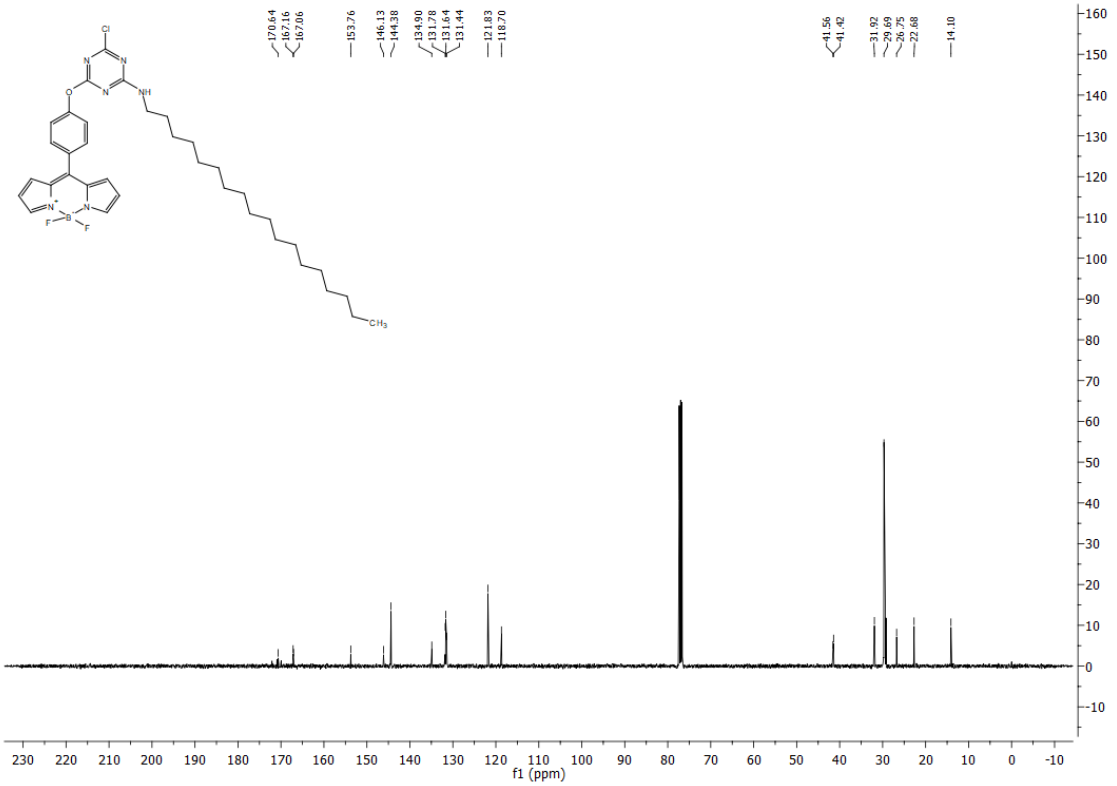


Fig. S10. ^{13}C NMR of Compound **5** $CDCl_3$

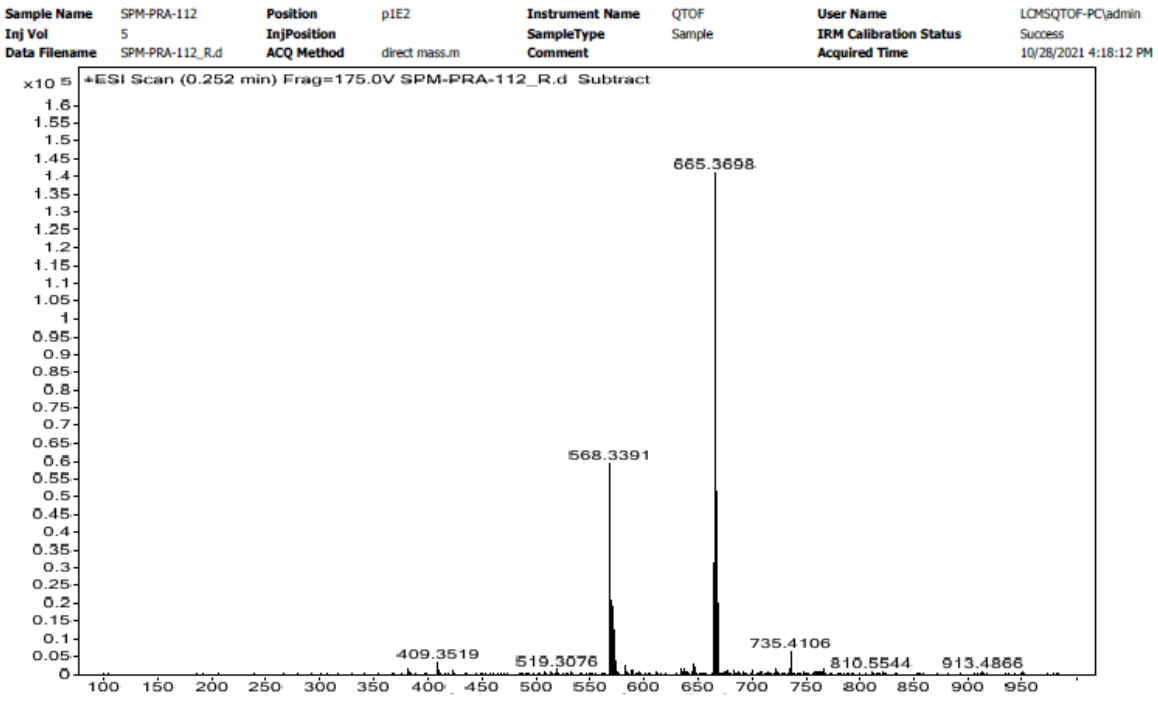


Fig. S11. HRLCMS of Compound **5** Expected mass: 665.3639 , Expermental: 665.3698

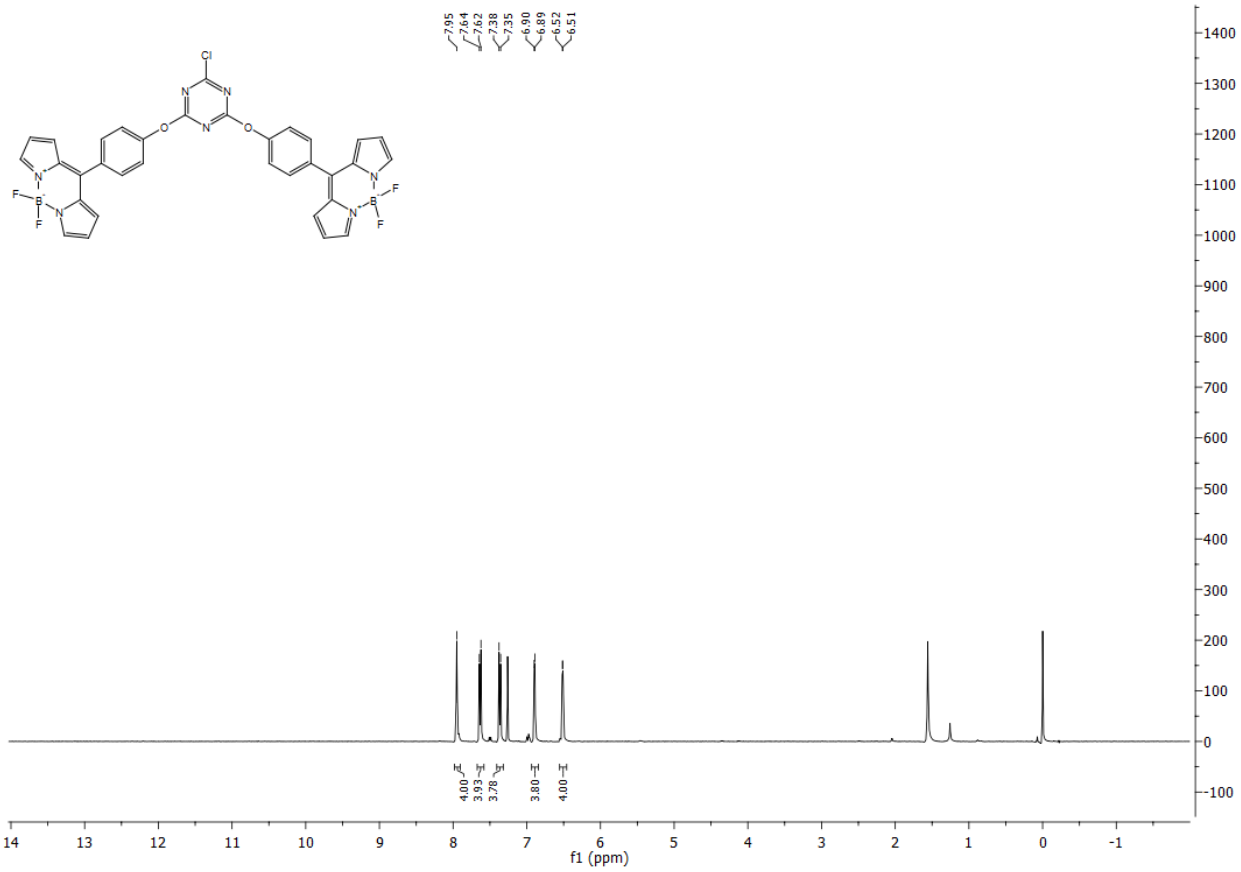


Fig. S12. ^{1}H NMR of Compound **6** $CDCl_3$

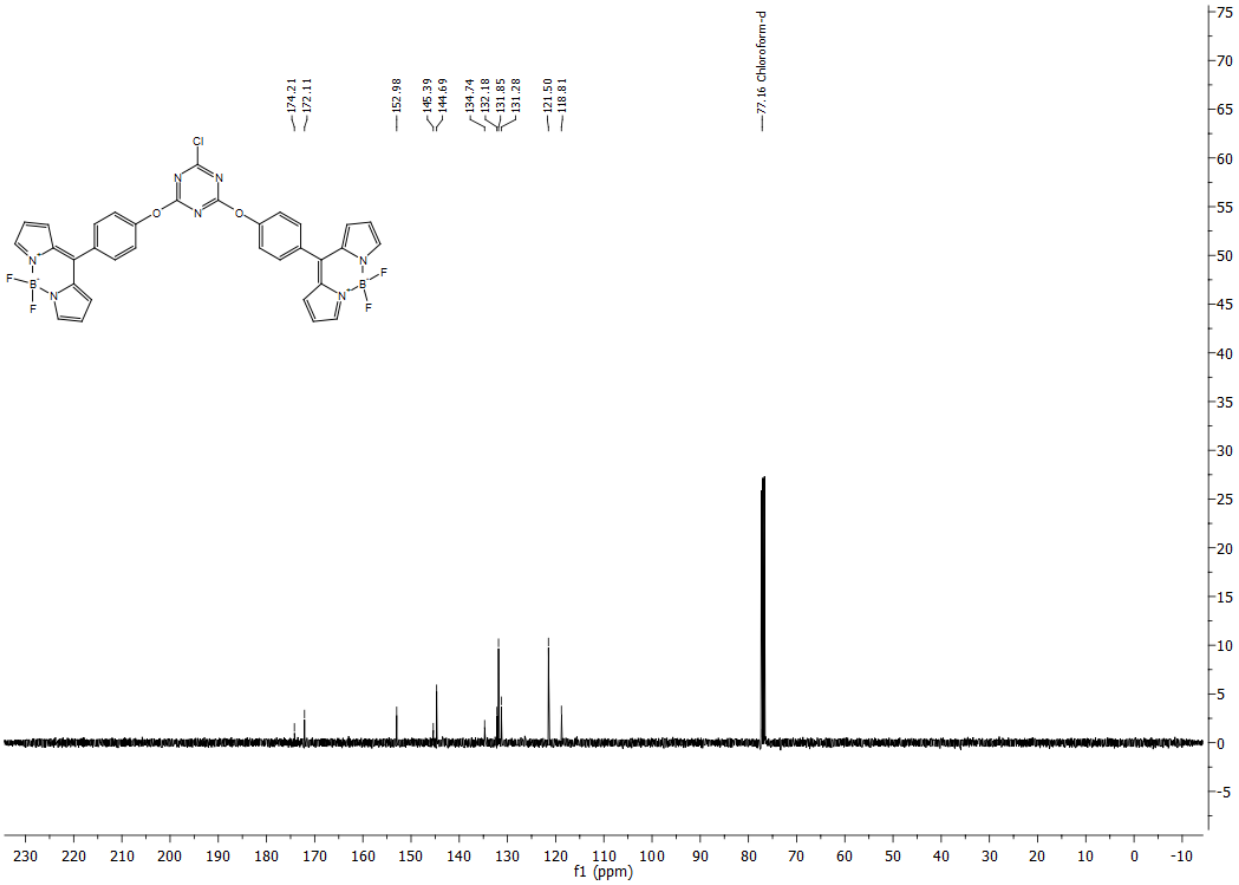


Fig. S13. ^{13}C NMR of Compound **6** $CDCl_3$

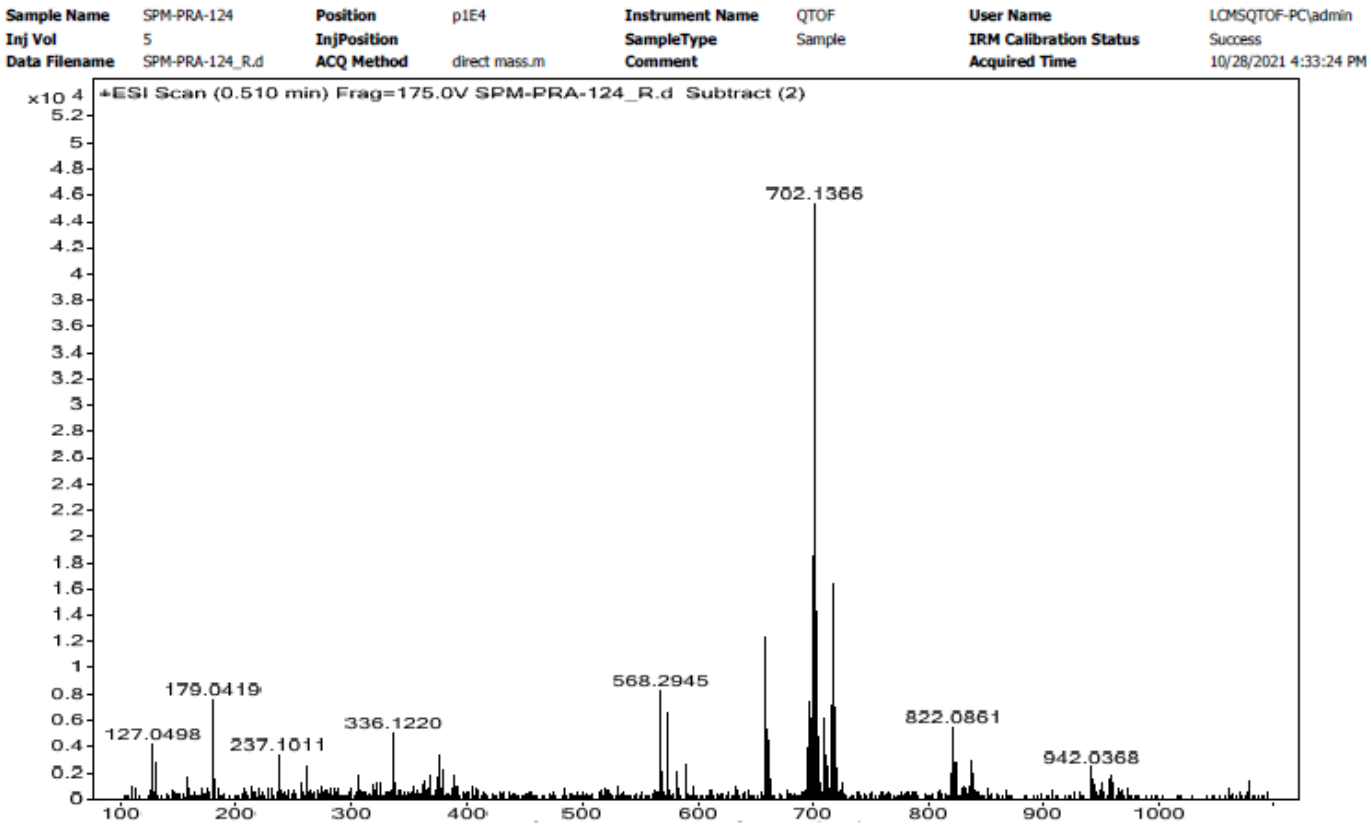


Fig. S14. HRLCMS of Compound **6** Expected mass: 679.1489, Experimental: 702.1366 (679.63+23)

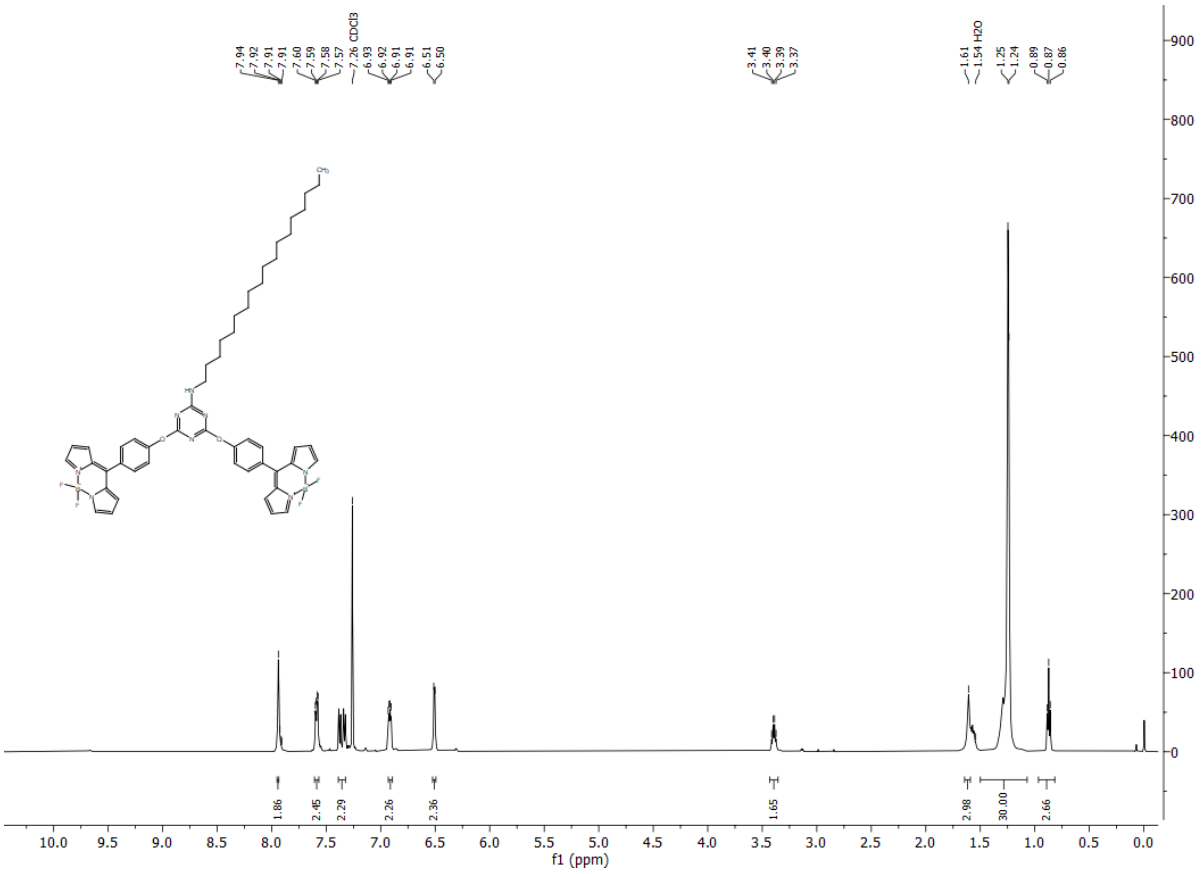


Fig. S15. ^{1}H NMR of Compound **7** $CDCl_3$

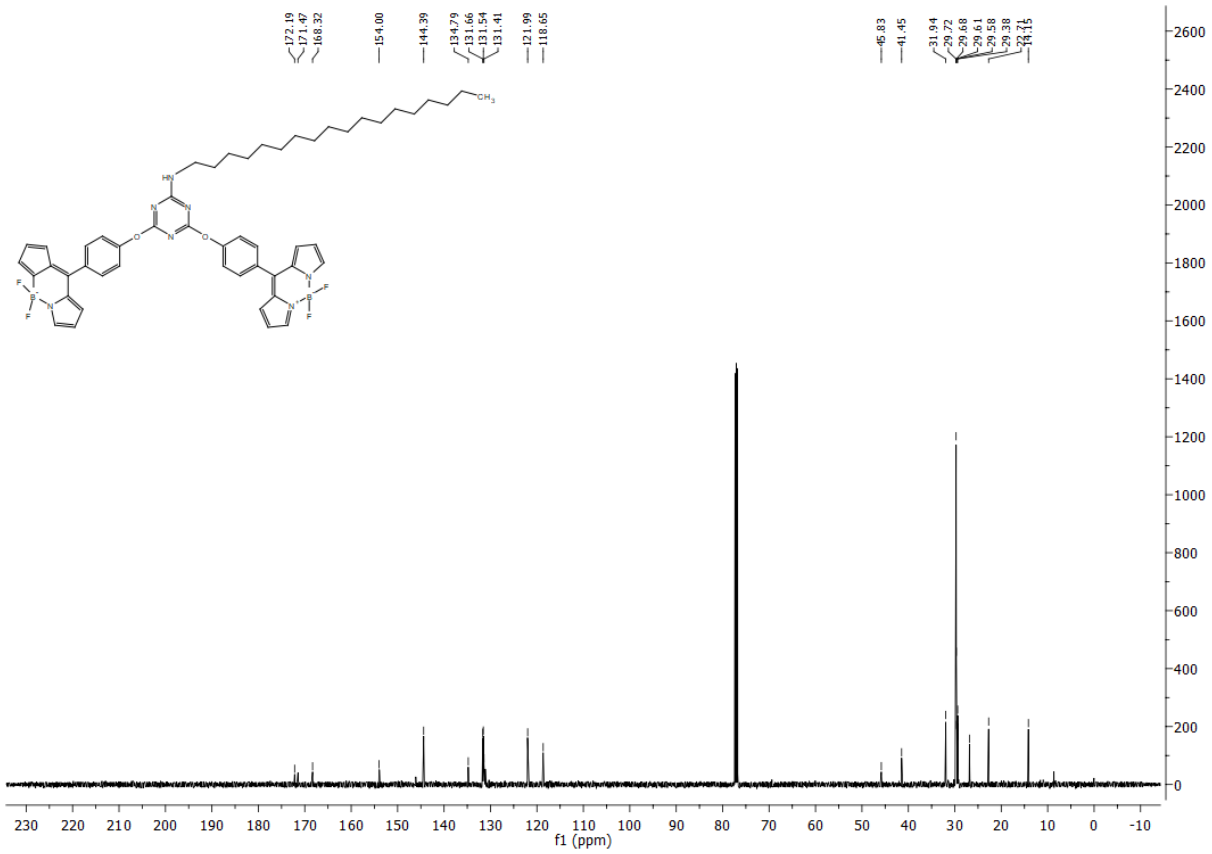


Fig. S16. ^{13}C NMR of Compound **7** $CDCl_3$

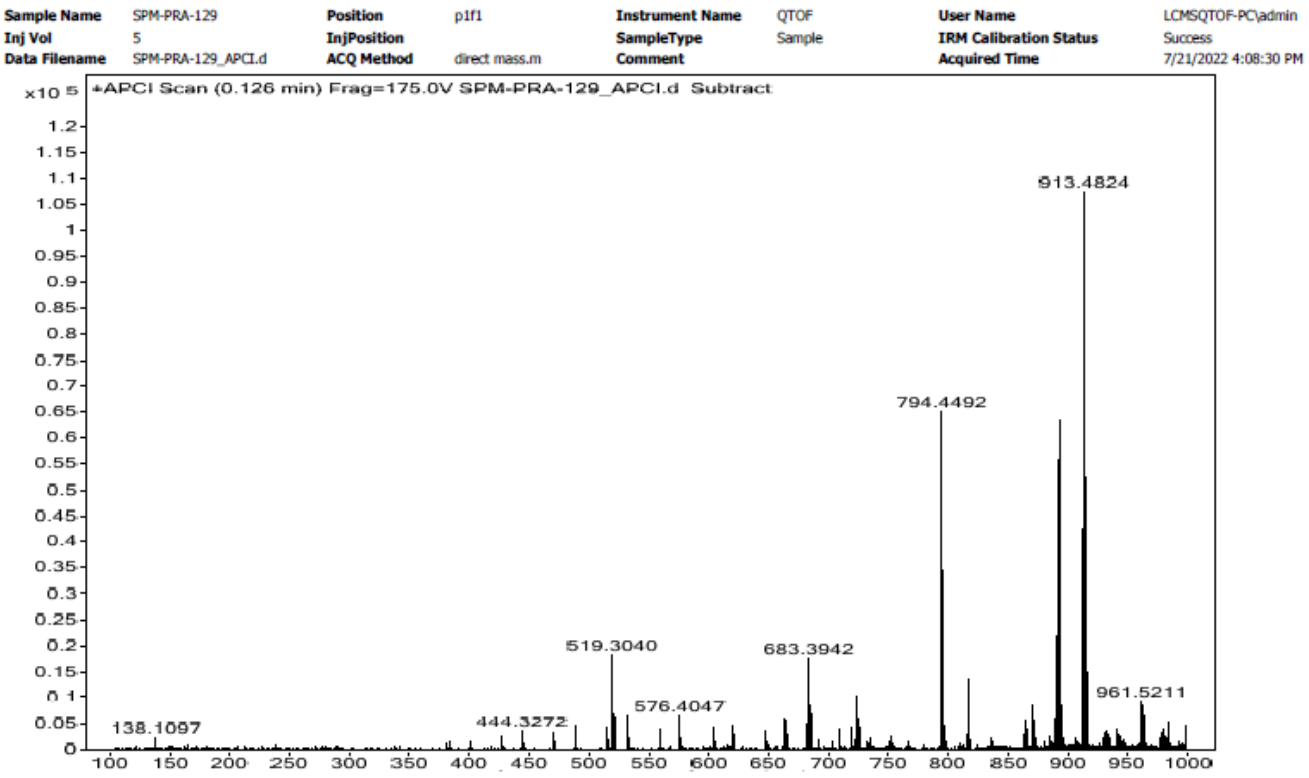


Fig. S17. HRLCMS of Compound **7** Expected mass: 912.4805, Experimental: 913.4824 (912.69+1)

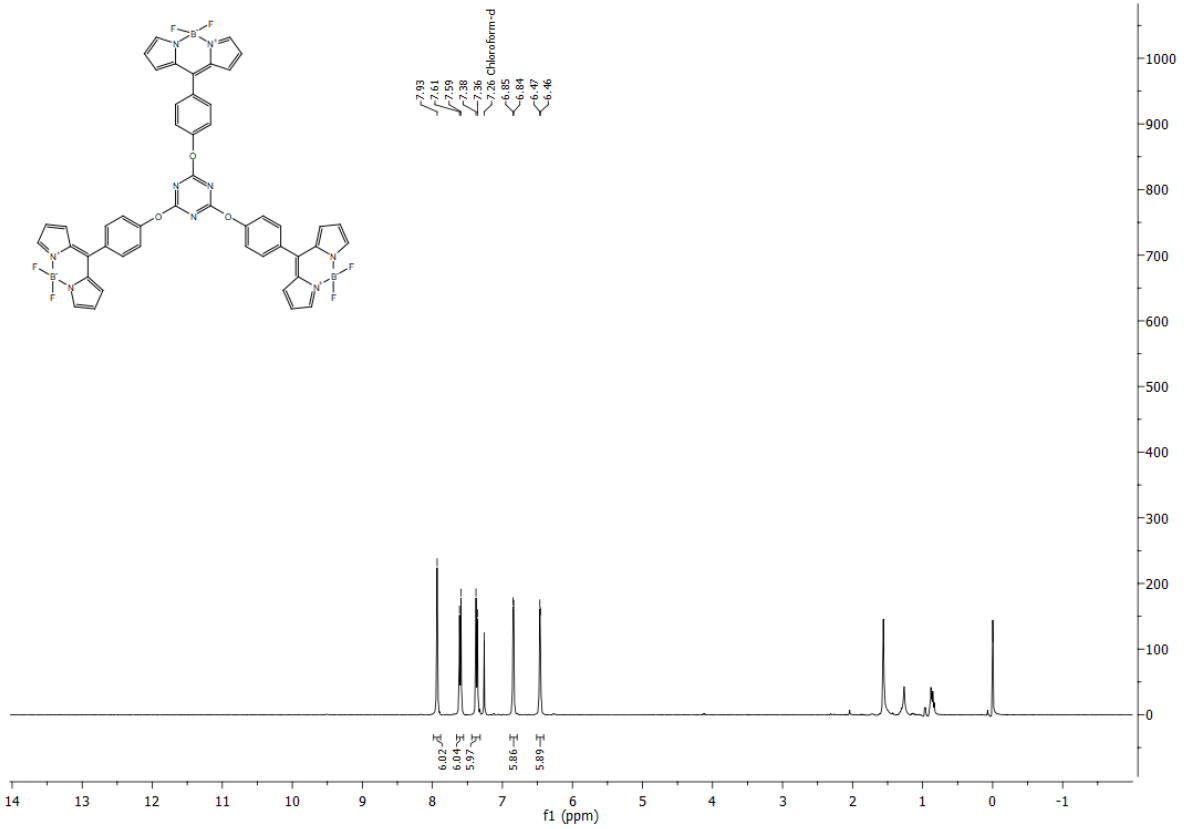


Fig. S18. ^{1}H NMR of Compound **8** $CDCl_3$

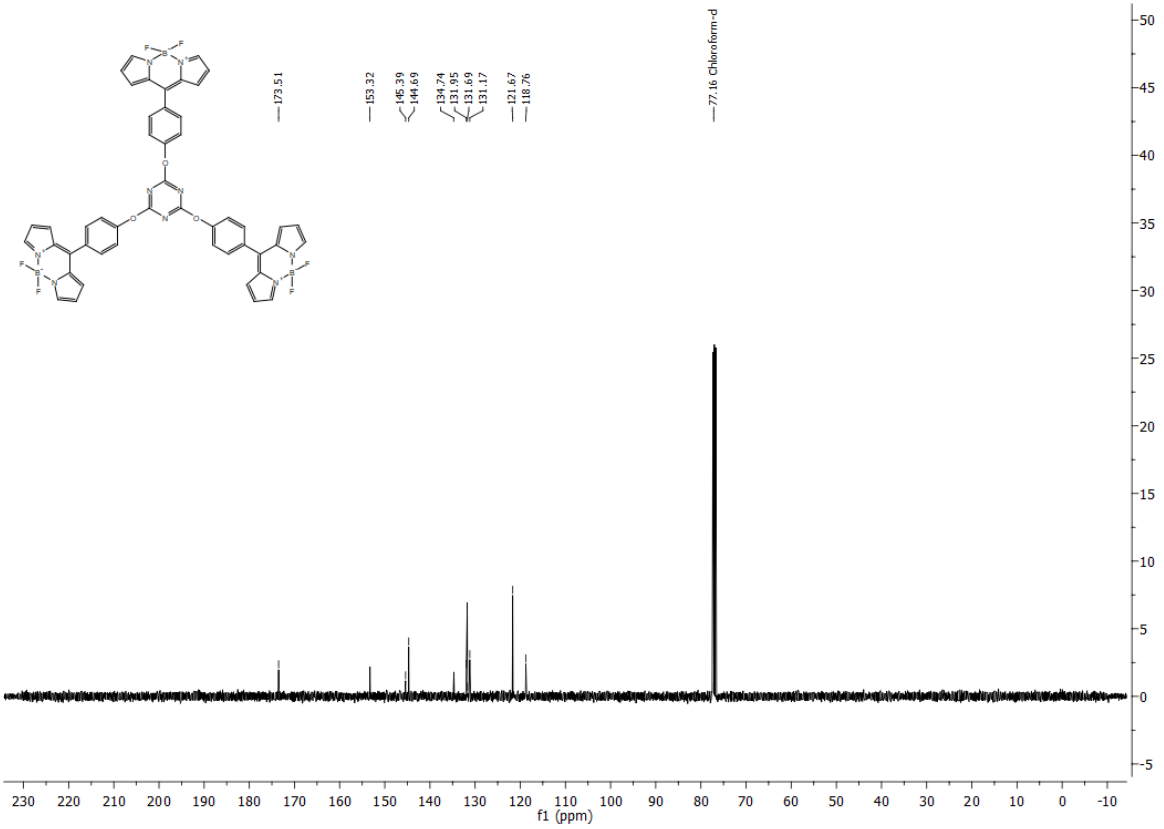


Fig. S19. ^{13}C NMR of Compound **8** $CDCl_3$

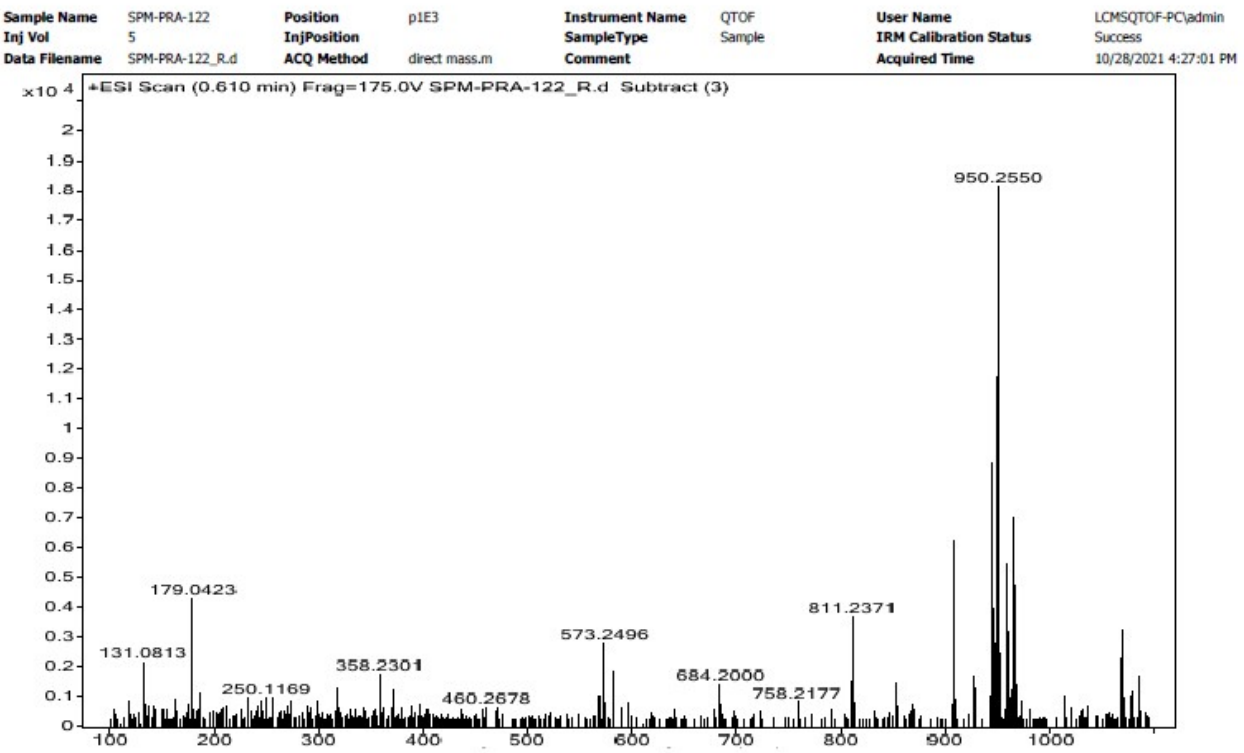


Fig. S20. HRLCMS of Compound **8** Expected mass: 927.2655, Experimental: 950.2550 (927.25+23)

7. Copies of FTIR spectra:

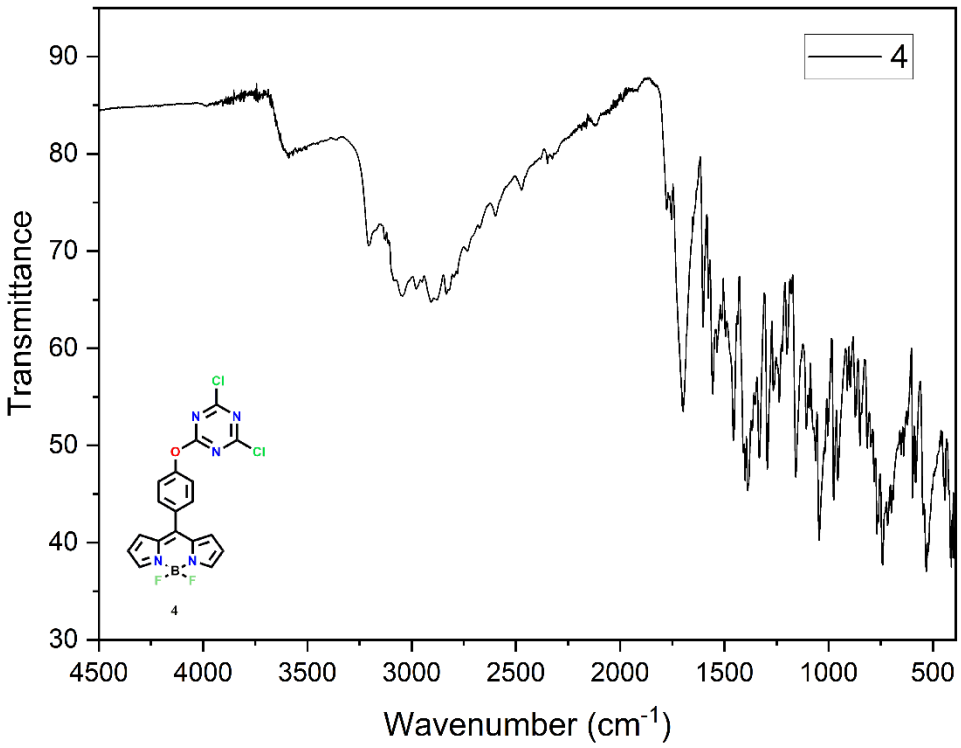


Fig. S21. FTIR spectra of compound **4**

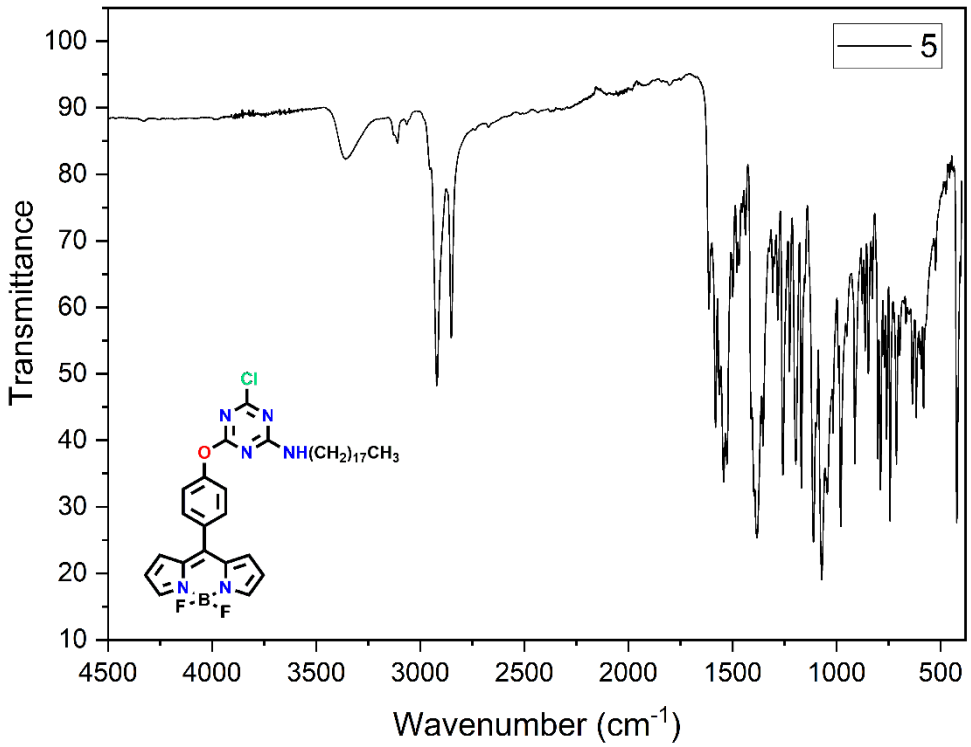


Fig. S22. FTIR spectra of compound **5**

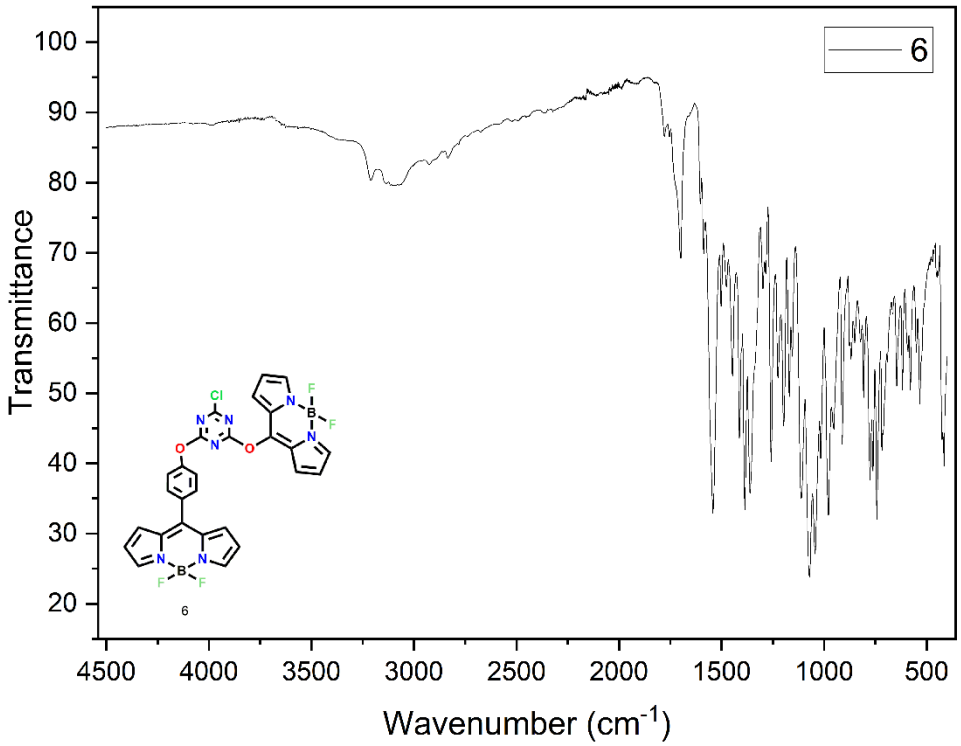


Fig. S23. FTIR spectra of compound **6**

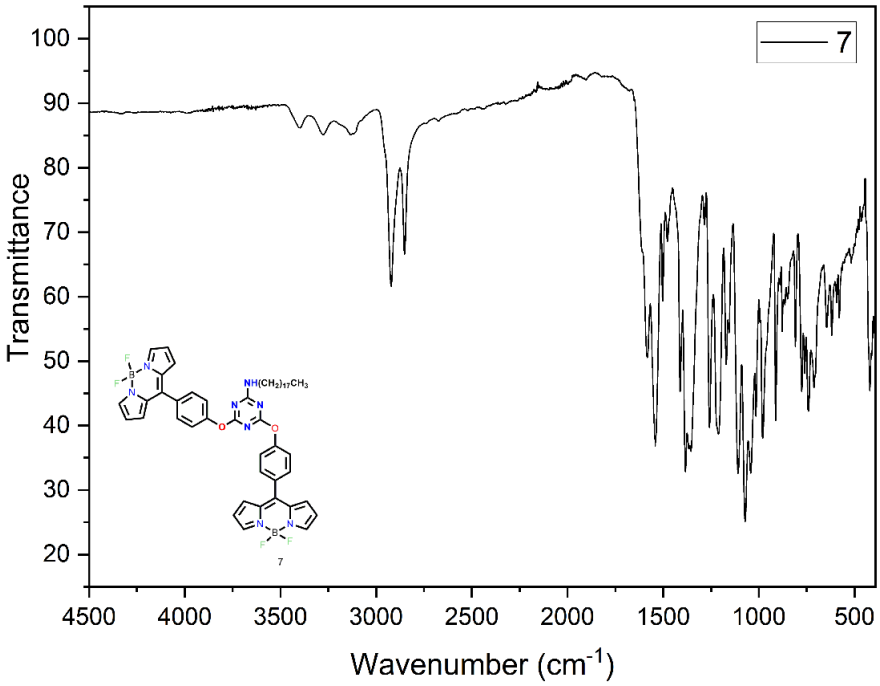


Fig. S24. FTIR spectra of compound **7**

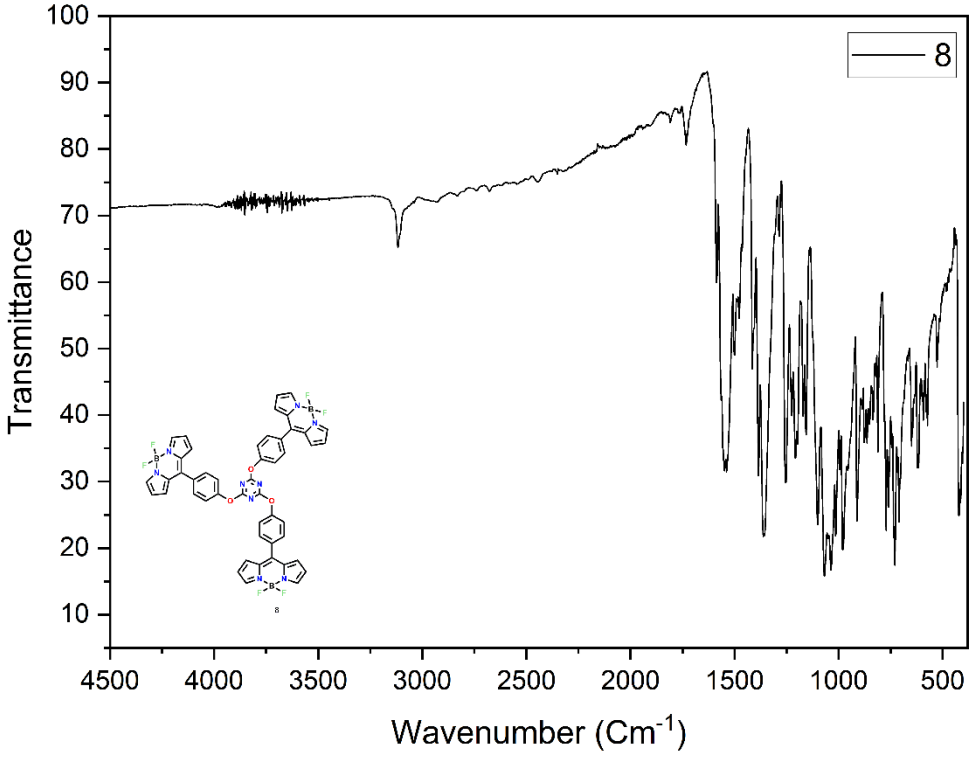


Fig. S25. FTIR spectra of compound **8**

8. Relative quantum yield (φ):

The relative fluorescent quantum yield is calculated by using equation given below.

$$\varphi_{f,s} = \varphi_{f,r} \times \frac{m_s}{m_r} \times \frac{\eta_s}{\eta_r}$$

Where $\varphi_{f,}$ and $\varphi_{f,}$ the fluorescence quantum yield of sample and reference fluorophore respectively. '*m*' represents the obtained slope optical density (abs.) vs. integrated fluorescence area. 'η' represents the refractive index of the respective solvent. The subscript *s* and *r* refer to sample and reference respectively.

The absorbance property of samples and reference was measured and kept within an optical density of 0.01-0.1 in solvent, 5 measurements were carried out on different concentration maintaining the optical density below 0.1 to minimize the error. Fluorescence spectra of same solutions were measured and integrated fluorescence area was calculated from the area under the curve. Further, integrated fluorescence area *vs* optical density as a function of solution absorbance plotted to obtain the slope and the quantum yield is calculated using the obtained gradients and refractive index in equation mentioned above. The obtained integrated fluorescence area *vs* optical density (abs) graph for Compound 4 **(a)**, 5 **(b)**, 6 **(c)**, 7 **(d)**, 8 **(e) and** Reference standard, Qunine sulfate **(f)** are given in (**Fig. S26)**

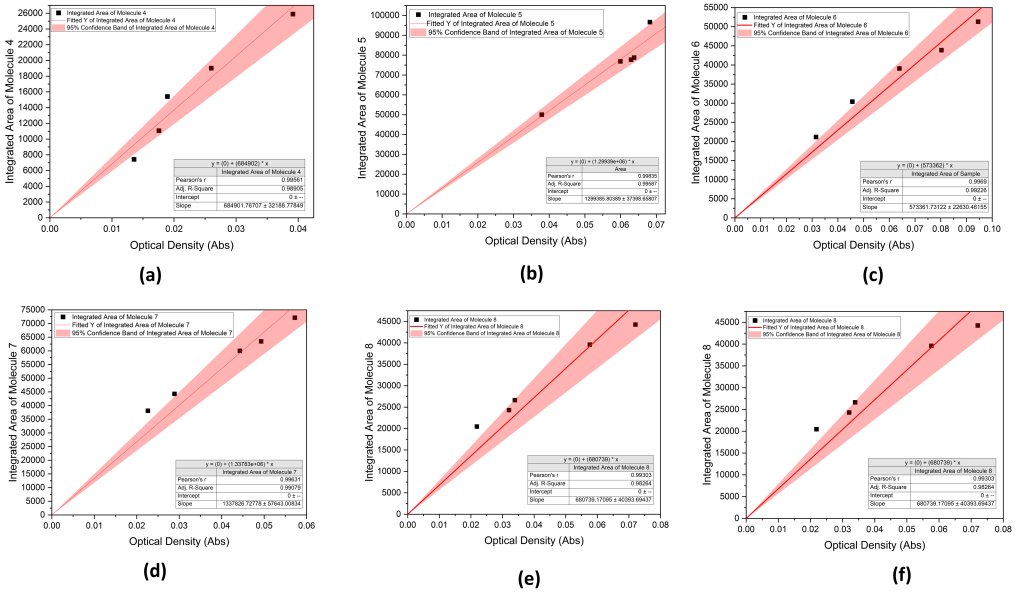


Fig. S26. Linear Fit plots of integrated fluorescence intensity vs. optical density (Abs.) **a-e** of compound **4-8** respectively and **f** of Quinine Sulfate Ref. Std.

9. Computational study:

S1-Calculation of the Molecular Reactivity Descriptors

Formulations of these RDs (A, I, μ, η, S, ω^{+}, ω^{-}, ω, $\Delta\omega^{\pm}$, ΔE_n, ΔE_e, and χ) are done by Koopmans's theorem[1] with conceptual aspects of DFT under finite difference approximations.[2–7] Ionisation energy (I) and electron affinity (A) tends to equality with that of energy of frontier orbitals under said approximations. Expressions for chemical potential (μ) and electronegativity (χ) have been rewritten in terms of HOMO and LUMO.[8] Parr et.al[9] have derived expressions for the electrophilicity (ω). These equalities were further validated by Janak.[10] Following equations **(1-9)** employed to calculate the reactivity descriptors.

$$\mu = -\frac{(I+A)}{2} \approx \frac{(E_L + E_H)}{2} = -\chi \quad \textbf{(1)}$$

$$\eta = \frac{(I-A)}{2} \approx \frac{(E_L - E_H)}{2} \approx (E_L - E_H) \quad \textbf{(2)}$$

$$S = (1/\eta) \approx \frac{1}{(E_L - E_H)} \quad \textbf{(3)}$$

$$\omega^{-} = \frac{(3I + A)^2}{16(I - A)} \approx \frac{(3E_H + E_L)^2}{16(E_L - E_H)} \quad \textbf{(4)}$$

$$\omega^{+} = \frac{(I + 3A)^2}{16(I - A)} \approx \frac{(E_H + 3E_L)^2}{16(E_L - E_H)} \quad \textbf{(5)}$$

$$\omega = \frac{\mu 2}{2\eta} \approx \frac{\chi^2}{2\eta} \approx \frac{(I + A)^2}{2(I - A)} \approx \frac{(E_L + E_H)^2}{2(E_L - E_H)} \quad \textbf{(6)}$$

$$\Delta\omega^{\pm} = \omega^{\pm(-\omega^{-})} = \omega^{+} + \omega^{-} \quad \textbf{(7)}$$

$$\Delta E_n = -A + \omega = \frac{(\mu + \eta)}{2\eta} \quad \textbf{(8)}$$

$$\Delta E_e = I + \omega = \frac{(\mu - \eta)}{2\eta} \quad \textbf{(9)}$$

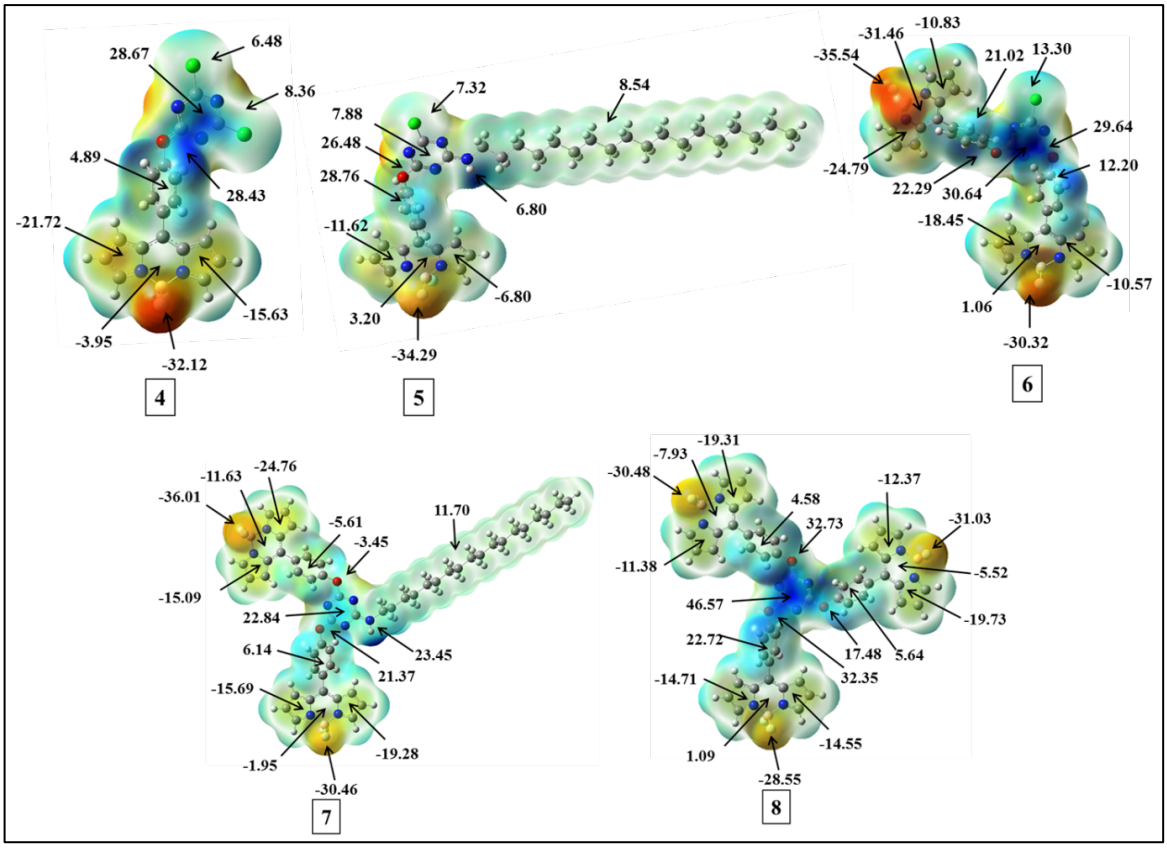


Fig. S27. Qunatitative molecular electrostatic potential (MEP) plots (all values are given in kcal/mol) of synthesized BODIPYs

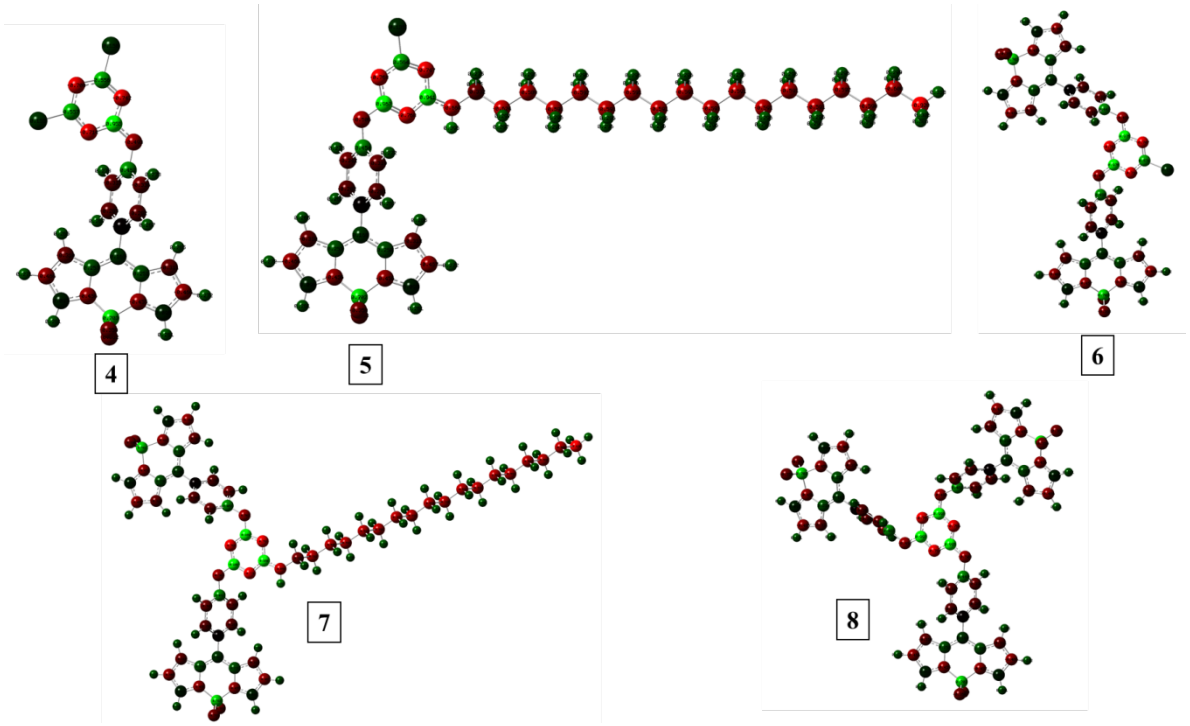


Fig. S28. Mullikens Charge analysis of BODIPY **4, 5, 6, 7,** and **8** using 6-31G (d, p) basis set

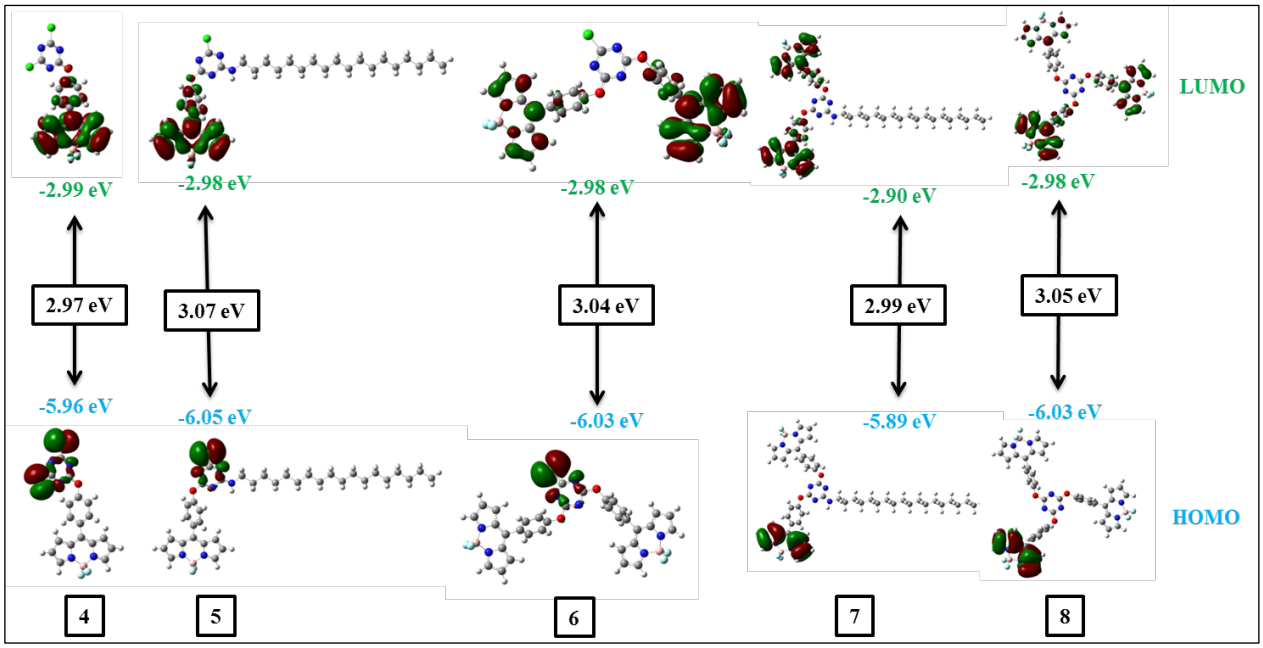


Fig. S29. Computed HOMO-LUMO energy gap of synthesized BODIPYs

TABLE S1: Chemical potential(μ) , absolute hardness(η) , global electrophilicity index(ω), net electrophilicity (Δω±), nucleofugality (ΔEn), electrofugality (ΔEe) and electronegativity (χ) of synthesized BODIPYs using gas phase B3LYP/6-31 G(d, p)

Compounds	**Molecular Reactivity Descriptors**						
	μ(eV)	η(eV)	ω	Δω±	ΔEn	ΔEe	χ
BODIPY **4**	-4.5233	3.055	3.349	13.777	3.294	86.617	4.523
BODIPY **5**	-4.4304	3.075	3.191	13.150	2.824	87/713	4.430
BODIPY **6**	-4.5086	3.046	3.337	13.728	3.258	86.922	4.508
BODIPY **7**	-4.3891	2.973	3.239	13.329	2.980	80.587	4.389
BODIPY **8**	-4.5082	3.052	3.330	13.701	3.237	87.209	4.508

S2- Cartesian coordinates of **BODIPYs 4, 5, 6, 7** and **8**

BODIPY-4

0 1

N	5.09033100	-1.33613900	-0.20066300
N	3.61232400	0.50341700	0.14451800
N	5.96609400	0.84676100	0.17280400
C	3.87506200	-0.78647300	-0.08636800
C	4.70317600	1.24920900	0.26060100
C	6.07314600	-0.46319400	-0.05888300
O	2.87041000	-1.65824300	-0.21402200
C	1.53645500	-1.23082900	-0.16848300
C	0.75487800	-1.68876100	0.88573300
C	0.99579400	-0.47040500	-1.20100800
C	-0.60095300	-1.36949900	0.91149000
H	1.20802000	-2.28481700	1.67010400
C	-0.35646000	-0.14464500	-1.15922700
H	1.62096000	-0.14321900	-2.02384200
C	-1.17383400	-0.58805600	-0.10499300
H	-1.21719600	-1.70816300	1.73705900
H	-0.79205600	0.43687900	-1.96422200
C	-3.16947100	3.35097000	-0.33097200
C	-2.26366900	2.30156700	-0.26682300
C	-4.45621200	2.78037300	-0.24899800
C	-3.01949000	1.10134100	-0.16232800
N	-4.36985500	1.44654400	-0.14748100

C	-2.61594000	-0.24168000	-0.06712700
C	-3.57735100	-1.26085700	0.05034000
B	-5.57227600	0.47214900	0.11485000
N	-4.93698100	-0.96182000	0.10706100
C	-3.44211100	-2.67635600	0.04993400
C	-4.72162600	-3.20980800	0.11711600
C	-5.61365100	-2.11839100	0.14592800
F	-6.12543400	0.74040800	1.35274000
F	-6.50607500	0.57861400	-0.89649700
H	-2.94951300	4.40508100	-0.41910100
H	-1.18564200	2.36462300	-0.28130700
H	-5.42093300	3.26893300	-0.24807600
H	-2.50915300	-3.21640900	-0.01570000
H	-4.99925300	-4.25387000	0.13036000
H	-6.69428300	-2.12012600	0.18422200
Cl	7.69008400	-1.08530700	-0.18933000
Cl	4.45232100	2.94334900	0.56185800

BODIPY-5

0 1

N	-5.22317200	5.15963800	0.39146100
N	-4.34289200	2.99387500	-0.09162900
N	-2.88648000	4.89914300	0.00203100
C	-5.32134300	3.83658500	0.18968500
C	-3.12359400	3.57939600	-0.17824800
C	-3.97660400	5.59192300	0.28059900
O	-6.58895700	3.38329700	0.28342000

C	-6.86501100	2.02115300	0.20739600
C	-7.65532800	1.58191600	-0.85044100
C	-6.46427800	1.14871800	1.21782300
C	-8.05033600	0.24720400	-0.89992500
H	-7.95256200	2.28570000	-1.62007700
C	-6.85029400	-0.18608900	1.15384400
H	-5.86536400	1.51507800	2.04363300
C	-7.65165100	-0.65722500	0.09820900
H	-8.65175400	-0.10439900	-1.73107200
H	-6.55655400	-0.86835200	1.94416100
C	-5.20047700	-4.32961700	0.15187700
C	-5.67473600	-3.02451300	0.15085400
C	-6.33105500	-5.17030300	0.11957800
C	-7.09411000	-3.09396700	0.12882100
N	-7.45491900	-4.43907600	0.10656500
C	-8.06606100	-2.07935400	0.04730300
C	-9.42338100	-2.41736000	-0.09743000
B	-8.91648300	-5.00453200	0.07678600
N	-9.82739500	-3.75001300	-0.16514100
C	-10.58673100	-1.60495900	-0.18896500
C	-11.67240800	-2.45818800	-0.32980800
C	-11.16055200	-3.77132600	-0.30445400
F	-9.05266800	-5.90616700	-0.96029600
F	-9.22970900	-5.57661300	1.29603600
H	-4.17039700	-4.65574200	0.15995400
H	-5.09377200	-2.11421400	0.14271800
H	-6.37991800	-6.25024100	0.09724900

H	-10.60257400	-0.52615400	-0.14586000
H	-12.71310300	-2.18666400	-0.43263100
H	-11.68981800	-4.71220500	-0.36745600
Cl	-3.74263700	7.30977300	0.53380400
N	-2.08405000	2.77347200	-0.45853500
H	-2.32732200	1.81188400	-0.65048200
C	-0.70854800	3.21522600	-0.66496800
C	0.28255200	2.09660300	-0.33867200
H	-0.54084700	4.08541100	-0.02646100
H	-0.57034600	3.55092400	-1.70280600
C	1.73847300	2.53115700	-0.54520900
H	0.13195600	1.77456100	0.69958800
H	0.06998900	1.22295600	-0.97218000
C	2.75359300	1.41628800	-0.26474700
H	1.86926500	2.88889500	-1.57599500
H	1.95291200	3.39095400	0.10429100
H	2.60951100	1.04176100	0.75850000
H	2.55151900	0.56537700	-0.93068400
C	4.20945500	1.86507600	-0.44028000
C	5.23223200	0.75066000	-0.18731300
H	4.41234400	2.70515900	0.23895400
H	4.34756400	2.25901400	-1.45723400
C	6.68666500	1.21257500	-0.33962400
H	5.08455900	0.34402200	0.82333200
H	5.04052600	-0.08193600	-0.87912100
C	7.71510800	0.09922500	-0.10566500
H	6.83039100	1.63253800	-1.34541500

H	6.87897400	2.03714500	0.36155800
H	7.56485200	-0.32983300	0.89533500
H	7.53143700	-0.71970600	-0.81577900
C	9.16790700	0.57146400	-0.24098700
C	10.20086000	-0.54028900	-0.01968500
H	9.35173600	1.38493400	0.47535300
H	9.31542700	1.00945400	-1.23854100
C	11.65217900	-0.06026900	-0.14298800
H	10.04896100	-0.98457800	0.97441900
H	10.02336900	-1.34973600	-0.74216900
C	12.68866200	-1.17030500	0.07019400
H	11.80221500	0.38982800	-1.13477400
H	11.82953800	0.74565400	0.58347800
H	12.53573800	-1.62468100	1.05957900
H	12.51580900	-1.97344600	-0.66042600
C	14.13875700	-0.68456400	-0.04481700
C	15.17784300	-1.79313900	0.16308700
H	14.31140700	0.11626900	0.68839700
H	14.29040700	-0.22636400	-1.03264400
C	16.62706900	-1.30351800	0.05371000
H	15.02427200	-2.25420900	1.14927000
H	15.00827300	-2.59208000	-0.57289500
C	17.66794500	-2.41081800	0.25804700
H	16.77977300	-0.83989900	-0.93145300
H	16.79650300	-0.50611300	0.79144400
H	17.51488000	-2.87682300	1.24213600
H	17.50160000	-3.20735800	-0.48150600

C	19.11691300	-1.91941700	0.15265900
C	20.15004400	-3.03179700	0.35491500
H	19.28382200	-1.12566400	0.89353800
H	19.26936300	-1.45219100	-0.82984700
H	20.04419700	-3.49603500	1.34207500
H	20.03251500	-3.82282100	-0.39454500
H	21.17282000	-2.64909900	0.27598000

BODIPY-6

0 1

N	-0.51103300	4.37708400	0.33826000
N	-0.86084200	2.02377300	0.14167700
N	1.35232400	2.89792000	0.28110000
C	-1.27970900	3.28223200	0.22875500
C	0.46795100	1.90332700	0.17398200
C	0.77930900	4.09572400	0.35651600
O	-2.59209100	3.55047800	0.19895900
O	0.89891100	0.63603400	0.09955800
C	-3.52483300	2.50841200	0.13777100
C	-4.24160800	2.34593900	-1.04222600
C	-3.79336500	1.73677700	1.26440500
C	-5.24722200	1.38330400	-1.09748000
H	-4.00974600	2.96704200	-1.90037200
C	-4.78990900	0.76792400	1.19629500
H	-3.23366400	1.89713000	2.17893300
C	-5.53205800	0.57848500	0.01752500
H	-5.80068000	1.23652100	-2.01845600

H	-5.01604100	0.16748700	2.07067300
C	2.26467400	0.33622800	0.05694700
C	2.76411200	-0.47539700	1.06965300
C	3.06299200	0.73968900	-1.01022200
C	4.09432700	-0.88548800	1.01868800
H	2.11400400	-0.77449300	1.88440300
C	4.39473100	0.33828700	-1.04448100
H	2.65065800	1.35826100	-1.79853500
C	4.92997500	-0.48017400	-0.03454500
H	4.49673100	-1.50249200	1.81451800
H	5.02381900	0.64027800	-1.87462900
C	-5.30782000	-3.76476000	0.76753600
C	-5.05259500	-2.41088000	0.59942100
C	-6.68877400	-3.94646100	0.54875400
C	-6.29189100	-1.78634300	0.28958500
N	-7.27408600	-2.77425300	0.26536300
C	-6.59564200	-0.45401600	-0.04102200
C	-7.89823100	-0.10568500	-0.43880300
B	-8.79800700	-2.55750300	-0.03359500
N	-8.90553900	-1.06640600	-0.51244100
C	-8.46239900	1.14620000	-0.80781800
C	-9.79664000	0.91923200	-1.11555500
C	-10.02950700	-0.45662700	-0.91478600
F	-9.20881100	-3.41465300	-1.03487700
F	-9.53761400	-2.72761000	1.12190200
H	-4.59750500	-4.54377200	1.00405000
H	-4.09765000	-1.91013900	0.66140000

H	-7.27091000	-4.85731700	0.57612100
H	-7.93635300	2.08900600	-0.82973500
H	-10.52921000	1.64399000	-1.44019000
H	-10.94633900	-1.01813600	-1.03082500
C	8.60078200	1.96046700	-0.24196500
C	7.29655500	1.49064600	-0.17752700
C	9.43760300	0.82657000	-0.28914800
C	7.36156500	0.06997800	-0.19731300
N	8.70462100	-0.29534900	-0.26343100
C	6.35141700	-0.90090000	-0.08293900
C	6.68932400	-2.26329800	0.00289000
B	9.26503900	-1.75909300	-0.30480500
N	8.02098900	-2.67366000	-0.02189000
C	5.87736400	-3.42525900	0.11101900
C	6.73162500	-4.51793400	0.16803500
C	8.04358800	-4.01044600	0.07772100
F	9.77015900	-2.03946000	-1.56075600
F	10.21883300	-1.92709000	0.67917200
H	8.92990500	2.98954400	-0.24084900
H	6.39185900	2.07541500	-0.09947700
H	10.51686600	0.77495200	-0.33142100
H	4.79778800	-3.43576300	0.13442300
H	6.46133400	-5.56018700	0.25749800
H	8.98369100	-4.54472100	0.06935800
Cl	1.86585000	5.45172600	0.49820800

BODIPY-7

0 1

N	-0.88501700	0.45548000	1.81511700
N	-2.99769700	0.89879600	0.79762700
N	-2.37927200	-1.34962100	1.29602900
C	-1.82114600	1.25130900	1.31081200
C	-3.19664800	-0.42387200	0.82829600
C	-1.21732800	-0.84836800	1.79060500
O	-1.47388700	2.55775900	1.32700200
O	-4.39851100	-0.78412500	0.32212000
C	-2.35291200	3.55775300	0.92709600
C	-1.86887600	4.47166600	-0.00576500
C	-3.61148800	3.72174300	1.50519600
C	-2.65460800	5.56107300	-0.37188500
H	-0.88530000	4.31793700	-0.43587300
C	-4.39701700	4.80329400	1.12095400
H	-3.97140400	3.01065600	2.23798300
C	-3.93330300	5.74075600	0.18082100
H	-2.28842300	6.26276900	-1.11329900
H	-5.37305300	4.94200900	1.57323600
C	-4.74540400	-2.12150800	0.16935600
C	-5.90739800	-2.55083400	0.80470400
C	-4.03542600	-2.97154800	-0.67805800
C	-6.36633100	-3.84827400	0.59211400
H	-6.43881500	-1.86658000	1.45697000
C	-4.49133100	-4.27122400	-0.87299900
H	-3.14221900	-2.61677900	-1.17829200
C	-5.66414500	-4.72969900	-0.24626800

H	-7.26151700	-4.19126100	1.09926900
H	-3.95276200	-4.93289300	-1.54287700
C	-8.02736900	5.80054100	-1.46755600
C	-6.78565100	5.45198400	-0.95363400
C	-8.06795100	7.20882700	-1.50719600
C	-6.09195100	6.66164100	-0.67695600
N	-6.92123300	7.72147600	-1.03828200
C	-4.78189700	6.88828900	-0.21701700
C	-4.27735500	8.20034400	-0.15314600
B	-6.58027000	9.24596500	-0.91521800
N	-5.05716700	9.28819200	-0.54210000
C	-3.01807400	8.69951600	0.27679800
C	-3.04964300	10.07922800	0.12285200
C	-4.32642800	10.40070600	-0.37900900
F	-6.79766600	9.87842700	-2.12385900
F	-7.32299800	9.81901100	0.10135200
H	-8.81398800	5.13576600	-1.79424500
H	-6.39055100	4.45737800	-0.80863400
H	-8.85721400	7.86071500	-1.85552200
H	-2.20399100	8.10123500	0.65789300
H	-2.26151900	10.78390900	0.34585100
H	-4.74461000	11.37000200	-0.61328800
C	-3.60204900	-8.58943700	0.35311300
C	-3.96191200	-7.25066000	0.27454100
C	-4.70578100	-9.33233000	-0.11140100
C	-5.28168800	-7.20097300	-0.25035700
N	-5.70271800	-8.51059900	-0.47036100

C	-6.14675900	-6.11295700	-0.47000400
C	-7.47067900	-6.34165200	-0.88581700
B	-7.09894300	-8.95464100	-1.02813000
N	-7.94843400	-7.63671600	-1.08070900
C	-8.52445600	-5.43833600	-1.19422600
C	-9.62707500	-6.20159700	-1.55243700
C	-9.22712900	-7.55088800	-1.47440400
F	-6.96021400	-9.46914900	-2.30403600
F	-7.68038300	-9.86790300	-0.17057900
H	-2.66947000	-9.00050500	0.71199800
H	-3.37609100	-6.39427200	0.57373100
H	-4.82342000	-10.40420600	-0.19157900
H	-8.45635200	-4.36125500	-1.16024100
H	-10.60524400	-5.84760500	-1.84439600
H	-9.79435900	-8.44519500	-1.69307500
N	-0.35376700	-1.74627100	2.30453300
H	-0.63937000	-2.71020800	2.21233200
C	0.97615100	-1.43192200	2.81315100
C	2.08199100	-1.58019900	1.75960700
H	1.17217700	-2.09216800	3.66585600
H	0.94711000	-0.40626200	3.18643300
C	3.47033200	-1.23805000	2.31297600
H	2.07911200	-2.60828800	1.37186400
H	1.84590800	-0.92406600	0.91293600
C	4.59184300	-1.40406000	1.28005800
H	3.46647500	-0.20316700	2.68241900
H	3.68494200	-1.87172200	3.18557400

H	4.60911000	-2.44545800	0.92842100
H	4.36388800	-0.79031200	0.39725600
C	5.97817200	-1.02519300	1.81499500
C	7.10139000	-1.20877700	0.78711800
H	6.20133600	-1.62695900	2.70760600
H	5.96197200	0.02093000	2.15220500
C	8.48483600	-0.80374100	1.31034500
H	7.12826100	-2.25913800	0.46352800
H	6.86851700	-0.62176100	-0.11278500
C	9.60911500	-0.99868900	0.28572200
H	8.45889300	0.24951900	1.62431800
H	8.71514600	-1.38288300	2.21603000
H	9.64231200	-2.05445100	-0.01922400
H	9.37260000	-0.42927700	-0.62452700
C	10.99032300	-0.57652100	0.80131300
C	12.11514900	-0.77831000	-0.22139700
H	11.22536200	-1.14110700	1.71495000
H	10.95766900	0.48092600	1.10037000
C	13.49500200	-0.34589500	0.28934200
H	12.15218600	-1.83715900	-0.51501300
H	11.87637100	-0.21961600	-1.13768200
C	14.61993600	-0.55158400	-0.73248000
H	13.45830000	0.71388000	0.57961300
H	13.73302800	-0.90186300	1.20748200
H	14.65892200	-1.61208300	-1.01983300
H	14.37983500	0.00120000	-1.65199800
C	15.99917000	-0.11376900	-0.22467300

C	17.12390600	-0.32148100	-1.24630300
H	16.23897400	-0.66523200	0.69572000
H	15.96041300	0.94718300	0.06102400
C	18.50307700	0.11823800	-0.74000100
H	17.16341500	-1.38270100	-1.53090100
H	16.88322200	0.22876300	-2.16718500
C	19.62763900	-0.08983100	-1.76150100
H	18.46363600	1.17957900	-0.45572900
H	18.74373900	-0.43177600	0.18107000
H	19.66777900	-1.15105800	-2.04652700
H	19.38823400	0.46063600	-2.68275600
C	21.00728900	0.34893100	-1.25559600
C	22.12401900	0.13865000	-2.28247600
H	21.24704200	-0.20220500	-0.33603400
H	20.96743800	1.40910800	-0.97047800
H	22.21147000	-0.91743900	-2.56219800
H	21.93100300	0.70674700	-3.19963000
H	23.09484400	0.45986500	-1.89118300

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N	-0.05493700	1.34158000	-0.03885600
N	1.28840000	-0.62788900	0.01074200
N	-1.08922200	-0.80714000	-0.05066200
C	1.11187100	0.68804700	-0.00095200
C	0.13890200	-1.31149800	-0.01871100
C	-1.10641300	0.53064100	-0.06046400

O	-2.34750600	1.04310000	-0.11257500
O	2.17740800	1.50626400	0.04237800
O	0.30942900	-2.64442200	-0.02467600
C	3.48083500	1.00561300	0.02625200
C	4.30882100	1.38096000	1.07938400
C	3.96776500	0.26255000	-1.04688300
C	5.64774600	0.99768100	1.06465200
H	3.90010600	1.96511300	1.89650900
C	5.30248300	-0.12972000	-1.04544300
H	3.31305100	-0.00585600	-1.86699400
C	6.16215900	0.22991300	0.00737300
H	6.29535300	1.27287500	1.88987000
H	5.69322000	-0.69861000	-1.88198100
C	-2.57494700	2.42043900	-0.10240100
C	-2.17091200	3.22814100	0.95844000
C	-3.32936800	2.93302100	-1.15333700
C	-2.51314200	4.57678200	0.94732300
H	-1.59568700	2.81066000	1.77559400
C	-3.68068100	4.28050300	-1.14807300
H	-3.63091200	2.27605300	-1.96169500
C	-3.27382200	5.12338100	-0.10105000
H	-2.21107400	5.21196200	1.77288800
H	-4.25239200	4.68957600	-1.97378600
C	-0.79698500	-3.49897800	-0.00460700
C	-1.04706500	-4.26042700	-1.14094700
C	-1.55002900	-3.65875400	1.15526600
C	-2.07582900	-5.19934300	-1.11753400

H	-0.44044700	-4.11355200	-2.02776900
C	-2.58496800	-4.58878200	1.16613800
H	-1.32542000	-3.06595700	2.03457300
C	-2.86147300	-5.37413600	0.03324300
H	-2.28917200	-5.78533100	-2.00476000
H	-3.17075100	-4.72959600	2.06796300
C	7.95604300	-3.78897200	-0.43083300
C	7.10425700	-2.70055400	-0.30247900
C	9.27035200	-3.28638500	-0.34621700
C	7.91987100	-1.54486900	-0.15780700
N	9.25159300	-1.95591300	-0.18266800
C	7.58461200	-0.18876800	0.00250300
C	8.59844900	0.77550600	0.14400500
B	10.50256300	-1.05594100	0.11500000
N	9.94200600	0.40758700	0.16345600
C	8.53466100	2.19481100	0.19925000
C	9.84056700	2.66122900	0.26140900
C	10.67684600	1.52673300	0.23225900
F	11.03962700	-1.39983700	1.34159100
F	11.43114500	-1.17185400	-0.90022600
H	7.68275800	-4.82588000	-0.56309100
H	6.02435600	-2.71001200	-0.30037700
H	10.20977200	-3.82059400	-0.38438300
H	7.62880100	2.78216100	0.17128900
H	10.17067700	3.68898000	0.30746100
H	11.75667000	1.47289400	0.24934500
C	-7.15349500	-4.83222100	0.91527000

C	-5.79282500	-4.67348600	0.69199400
C	-7.43097300	-6.20611500	0.76315200
C	-5.26023400	-5.96297400	0.41679900
N	-6.30951400	-6.87840900	0.46790200
C	-3.96251700	-6.36758700	0.05798200
C	-3.71302100	-7.70695200	-0.29020800
B	-6.20395600	-8.42397000	0.22495900
N	-4.73849400	-8.65091900	-0.28920600
C	-2.51277000	-8.36816300	-0.66900700
C	-2.83508200	-9.69691100	-0.90831000
C	-4.21586200	-9.82941200	-0.65722800
F	-6.38926900	-9.10560500	1.41332500
F	-7.11611200	-8.81355500	-0.73561200
H	-7.87627700	-4.06308900	1.14629600
H	-5.23027200	-3.75153900	0.69600300
H	-8.37575000	-6.72565500	0.84517900
H	-1.53922100	-7.90667300	-0.74193300
H	-2.16990100	-10.48941100	-1.21949000
H	-4.83901500	-10.71129100	-0.71455000
C	-0.69267600	8.69730800	0.12817500
C	-1.21305600	7.41180100	0.07057200
C	-1.79206300	9.57977700	0.11586500
C	-2.62925800	7.53426800	0.03481200
N	-2.94137800	8.89191700	0.06131800
C	-3.63588700	6.56131700	-0.09715200
C	-4.97898100	6.95259500	-0.24121500
B	-4.38110800	9.51195000	0.03312500

N	-5.33498400	8.30005800	-0.25839200
C	-6.16879400	6.18618500	-0.37647200
C	-7.22254000	7.08243100	-0.49151600
C	-6.66516800	8.37445400	-0.40833400
F	-4.68808300	10.05739300	1.26585500
F	-4.47137400	10.44865800	-0.97716900
H	0.34834800	8.98472000	0.16027800
H	-0.66393000	6.48253800	0.03239400
H	-1.80096100	10.66088600	0.13538400
H	-6.22267600	5.10769300	-0.37854000
H	-8.27105300	6.85257600	-0.61457900
H	-7.16045700	9.33524300	-0.43846100

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