SUPPORTING INFORMATION FOR

Novel phenomena for aggregation induced emission enhancement: highly fluorescent hydrophobic TPE-BODIPY couples in both organic and aqueous media

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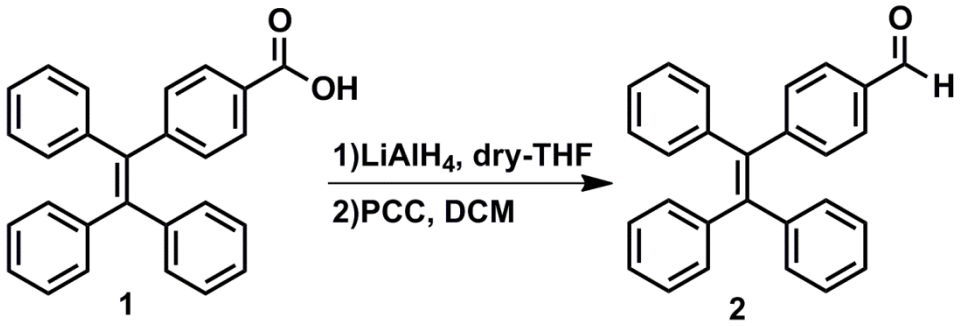
S1. EXPERIMENTAL

S1.1 GENERAL

All chemicals and solvents purchased from Aldrich were used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded using a Bruker DPX-400 in $CDCl_3$ with TMS as internal reference. The THF was further refluxed over metallic sodium in the presence of benzophenone until a persistent blue color was obtained and then it was distilled under an argon atmosphere. Absorption spectrometry was performed using a Shımadzu spectrophotometer. Steady state fluorescence measurements were conducted using a Shımadzu RF-5301PC spectrofluorometer. Fluorescence decays for the lifetime measurements were carried out by means of a LaserStrobe Model TM-3 lifetime fluorophotometer from Photon Technology International (PTI). Column chromatography of all products was performed using Merck Silica Gel 60 (particle size: 0.040–0.063 mm, 230–400 mesh ASTM). Reactions were monitored by thin layer chromatography using fluorescent coated aluminum sheets. Solvents were purchased from Sigma and solvents used for spectroscopy experiments were spectrophotometric grade. TPE-COOH,[1] and TPE-$B(OH)_2$[2] was synthesized according to the literature procedure. SEM images of $(TPE)_3BOD$ was obtained after evaporation of the solvent mixture with conductive carbon adhesive and monitored by Quanta 200 FEG scanning electron microscope. DLS measurements were performed with a Malvern Nano Zetasizer.Confocal Fluorescence Micrsoscope analyses were performed. Fluorescence microscopy images of the dyes were performed at the METU Central Laboratory.

S1.2 SYNTHESIS

Synthesis of TPECOH 2

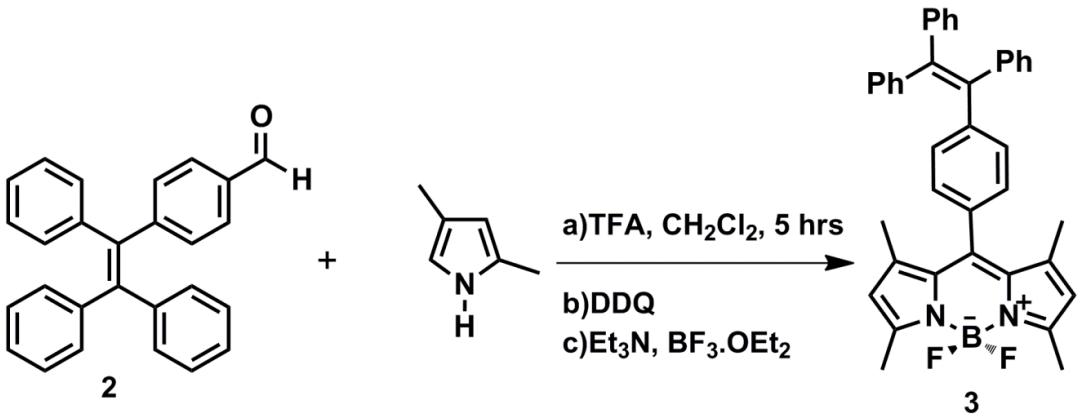


TPE-COOH **1** (490 mg, 1.302 mmol) prepared according to the literature procedure [1] was firstly reduced to TPE-CH_2OH with excess amount of $LiAlH_4$ (494.1 mg, 13.02 mmol) in 20 mL dry-THF. The crude product filtered and washed with methanol and white solute was collected followed by the evaporation of the solvent mixture under reduced pressure. The crude product was, then, used to yield TPE-COH with excess amount of pyridinium choloro

chromate (PCC) (2.81 g, 13.02 mmol) in CH_2Cl_2 (20 ml) without any further purification. After 2 hours, Crude reaction was extracted with basic aqueous solution one times, then three times with acidic aqueous solution. The organic phase was collected and solvent removed by evaporation. **2** was collected after column chromatography with an eluent CH_2Cl_2 (294 mg, 62.5%)

^{1}H NMR (400 MHz, $CDCl_3$) δ; 9.90 (s, 1H), 7.62-7.60 (d, 2H J=8.2 Hz), 7.22-7.20 (d, 2H J=8.2 Hz), 7.11-7.09 (m, 9H), 7.05-7.00 (m, 6H)
^{13}C NMR (100 MHz, $CDCl_3$) δ; 191.8, 150.8, 143.4, 143.3, 143.2, 140.1, 134.6, 132.3, 131.7, 131.6, 131.5, 130.3, 129.8, 129.5, 129.3, 129.0, 128.8, 128.7, 128.3, 127.4, 127.2, 127.1 (overlapping has been observed for some aromatic carbon atoms)
MALDI (TOF) m/z: 361.16102 (**2**+H^+calculated 361.15924, Δ=1.78 ppm)

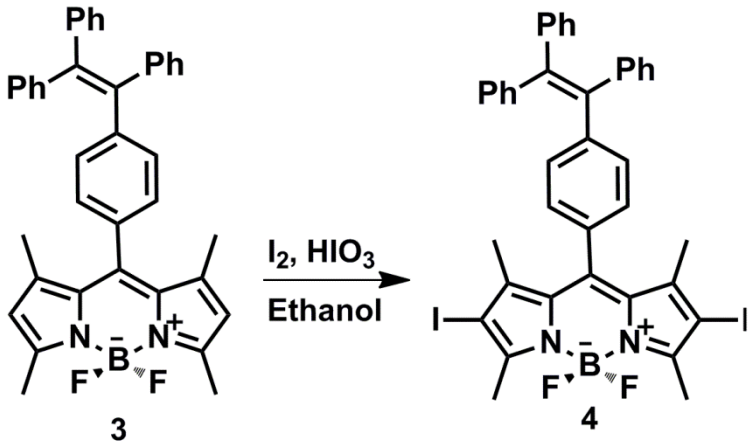
Synthesis of TPE-BOD 3



TPE-Al **2** (200 mg 0.55 mmol,) and 2,4-dimethyl pyrrole **3** (137.12 mg 1.11 mmol,) were dissolved in CH_2Cl_2 (250 ml) and purged with argon in a 500 ml flask. 1 drop of TFA was added as a catalyst and the mixture was stirred at room temperature for 3 hrs. When TLC showed comsumption of the aldehyde was complete, a solution of 166 mg (0.68 mmol) of DDQ (Tetrachloro-1,4-benzoquinone) in 10 mL CH_2Cl_2 was added. After 2 h, Et_3N (3 ml) and $BF_3.OEt_2$ (3 ml) were added. Immediately, after the addition of $BF_3.OEt_2$ bright green fluorescence was observed. Crude product washed three times with water, dried over Na_2SO_4 and concentrated in vacuum. Then crude product purified by silica gel column chromatography using $CHCl_3$/CH_3OH (99/1, v/v). The orange franction which has green fluorescence was collected. Orange solid (86 mg, 28%)

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.19-7.02 (m, 19H), 5.97 (s, 2H), 2.54 (s, 6H), 1.41 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$) δ; 132.42, 132.15, 131.64, 131.44, 131.40, 129.37, 128.12, 128.02, 127.99, 127.96, 127.61, 126.91, 125.74, 121.36, 30.53, 14.88.
MALDI (TOF) m/z: 578.28284 (calculated 578.27049, Δ=12.35 ppm)

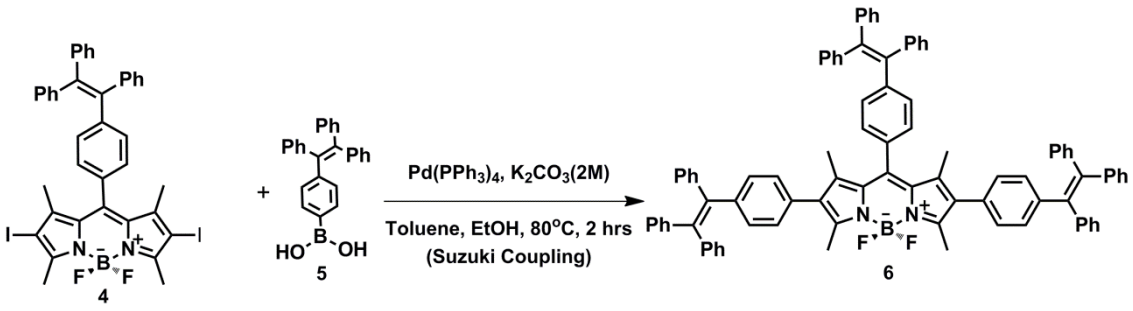
Synthesis of Iodinated TPE-BOD, 4



TPE-BOD **3** (340 mg, 0.58 mmol) was dissolved in ethanol (100ml) and iodine (38 mg, 0.15 mmol) was added to the reaction mixture. Iodic acid (209.2 mg, 1.16 mmol) was dissolved in minimum amount of water and was added to the reaction mixture in a dropwise manner. The reaction temperature was adjusted to 60^0C. The reaction was monitored by TLC and when complete consumption of **3** was seen the reaction was completed. Crude reaction was dissolved in chloroform and extracted with water three times. Then crude product purified by silica gel column chromatography using hexane/$CHCl_3$ (90/10, v/v) to yield 424.56 mg **4** (87%).

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.22-6.98 (m, 19H), 2.62 (s, 6H), 1.42 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$) δ; 156.83, 145.93, 145.42, 143.59, 143.30, 143.28, 142.40, 141.68, 140.05, 132.73, 131.64, 131.43, 131.38, 128.12, 128.07, 128.00, 127.44, 127.13, 127.02, 32.16, 16.24. (overlapping has been observed for some aromatic carbon atoms)

Synthesis of $(TPE)_3$BOD 6

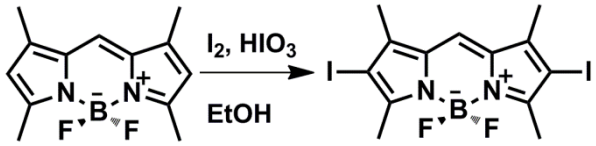


Iodinated-(TPE)BOD **4** (93 mg, 0.11 mmol) and TPE-$B(OH)_2$ **5** (105 mg, 0.28 mmol) was mixed in toluene (50 ml), 2M aqueous K_2CO_3 solution (8 ml) and EtOH (8 ml). The

mixture was stirred for 40 min under argon atmosphere at room temperature. Then, catalytic amount of $Pd(PPh_3)_4$ (12 mg 0.011 mmol) was added and the reaction mixture was stirred at 80°C for 2 h. After cooling to room temperature, the product was concentrated under reduced vacuum and purified by silica gel column chromatography with eluent $CHCl_3$/hexane (85/15, v/v), (109.0 mg, 80%)

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.19-6.99 (m, 53H), 6.88 (d, 4H), 2.47 (s, 6H), 1.30(s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) δ;154.28, 145.30, 143.96, 143.78, 143.66, 143.47, 143.42, 142.68, 142.03, 141.54, 140.93, 140.32, 139.12, 133.66, 133.56, 132.49, 131.91, 131.68, 131.61, 131.58, 131.54, 131.46, 131.40, 129.58, 128.02, 127.98, 127.93, 127.88, 127.74, 126.92, 126.74, 126.69, 126.65, 126.10, 13.56, 13.25. (Overlapping has been observed for some aromatic carbon atoms)
MALDI (TOF) m/z: 1238.55606 (calculated 1238.55219, Δ=3.87 ppm)

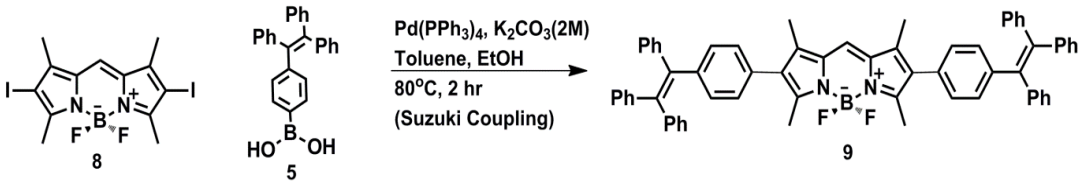
Synthesis of Iodinated-8H-BODIPY 8



Compound **7** (0.100 g, 0.40 mmol) was dissolved in ethanol (100 ml) and iodine (0.26 g, 1.0 mmol) was added to the reaction mixture. Iodic acid (0.14 g, 0.8 mmol) was dissolved in a minimum amount of water and was added to the reaction mixture in a dropwise manner. The reaction temperature was 60^0C. The reaction was monitered by TLC and when complete consumption of **1** was seen the reaction was completed. Crude reaction mixture was dissolved in chloroform and extracted with water three times. Silica-gel column chromatography (hexane/CH2Cl2 4/1) gave **8** as a red solid (150 mg, 75% yield)

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.10 (s, 1H), 2.6 (s, 6H), 2.25 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$) δ; 157.72, 144.35, 132.84, 120.21, 82.03, 15.67, 13.74

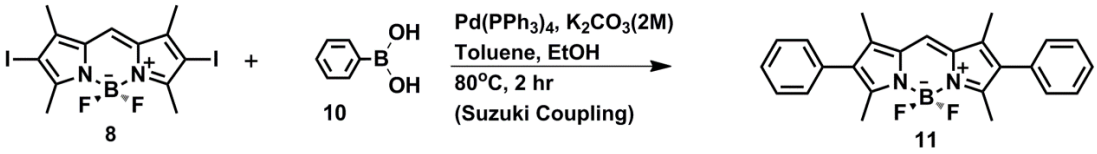
Synthesis of $(TPE)_2BOD$ 9



Iodinated-BODIPY, **8**, (90 mg, 0.18 mmol) and the TPE-$B(OH)_2$, **5**, (169 mg, 0.45 mmol) were added to a mixture of toluene (50 mL), 2M aqueous Na_2CO_3 solution (8 mL) and EtOH (8 ml). The mixture was stirred for 40 min under an argon atmosphere at room temperature. Then the $Pd(PPh_3)_4$ catalyst (catalytic amount) was added and the reaction mixture was stirred at 80°C for 16 h. The reaction mixture was concentrated under vacuum, and the crude product was purified by silica-gel column chromatography with hexane/CH_2Cl_2 (2/1, v/v) as eluent affording a red solid (137.4 mg, yield 84.0%).

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.16-6.98 (m, 39H), 2.50 (s, 6H), 2.00 (s, 6H)
^{13}C NMR (100 MHz, $CDCl_3$) δ; 155.39, 143.71, 143.62, 143.51, 142.51, 141.36, 140.67, 137.09, 133.02, 131.89, 131.75, 131.52, 131.38, 131.34, 128.87, 128.68, 127.73, 127.67, 127.62, 126.52, 126.40, 126.20, 120.06
MALDI (TOF) m/z: 908.40935 (calculated, 908.41134, Δ=1.99 ppm)

Synthesis of $(Ph)_2BOD$, 6.



Experimental procedure, used for the synthesis of compound **9** was repeated for the synthesis of $(Ph)_2BOD$ **11**. $PhB(OH)_2$, **10**, was used as a reagent and the product was purified by column chromatography with $CHCl_3$/Hexane (60/40, v/v).

^{1}H NMR (400 MHz, $CDCl_3$) δ; 7.44 (t, 4H), 7.33 (dd, 2H), 7.33 (dd, 4H), 7.19 (s, 1H), 2.55 (s, 6H), 2.24 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) δ; 133.78, 129.92, 128.65, 127.31, 120.52, 13.68, 10.46 (overlapping has been observed for some aromatic carbon atoms)
MALDI (TOF) m/z: 400.19180 (calculated, 400.19224, Δ=0.44 ppm)

S1.3 Langmuir-Blodgett and spin-coating films of 9

Langmuir-Blodgett (LB) films of **9** were fabricated by a commercially available LB deposition trough (KSV, Minithrough). The pure water used for the subphase was obtained from a KrosClinic (Model: KRS-R-75) and its resistivity was 18.2 MΩcm. The pH of the subphase was 6.3 and the temperature was 22^{o}C. Glass substrates were cleaned by keeping them for 30 min in a piranha solution (3:7 v/v 30% H_2O_2 and H_2SO_4) then substrates were repeatedly washed with deionized water and dried in a hot air oven.

In the Langmuir-Blodgett (LB) film fabrication, surface pressure at the air-water interface was measured by a Wilhelm plate. Floating layer of **9** mixed with SA at the air-water interface was prepared by the moving barrier maintaining constant surface pressure with a precision of ±0.1 mN/m. For LB film deposition, the spreading solution was composed of a mixture of $(TPE)_2BOD$ with SA (0.5 mg/ml) in chloroform. 25 μL of this solution was slowly spread on the air–water interface of a standard LB trough by using Hamilton micro-syringe. After allowing 20 min. to evaporate the chloroform solvent, the monolayer at the air–water interface was slowly and simultaneously compressed by using two compression barriers. The barrier speed was 5 cm^2/min. Y-type deposition of monolayer was achieved by slowly withdrawing the glass slide vertically through the floating monolayer at a speed of 3 mm/min at a constant surface pressure of 25 mN/m. The transfer ratios for the monolayer of **9** mixed with SA were found to be about 1.0±0.1. This value is suitable to fabricate good quality LB films of **9** molecules mixed with SA. To produce spin-coating thin films of **9**, several solutions in THF were prepared and coated onto a cleaned glass slides at 2500 rpm for 30 second by spin-coater

S1.4 Computational Methods

For **9** theoretical computations were carried out using Gaussian 03 program package.[3] Austin model 1 (AM1) [4-6] and density functional theory (DFT) were utilized for this purpose. The optimized geometry and harmonic vibrational frequencies were computed with the AM1 method. At the optimized AM1 geometry a single point energy calculation was performed with the B3LYP functional.[8, 9] In the DFT computation Pople's polarized triple-ζ split valence basis set, 6-311G (d,p), was employed. [10-11]

S1.5 References

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S2 . ADDITIONAL DATA

S2.1 Spectrophotometric studies

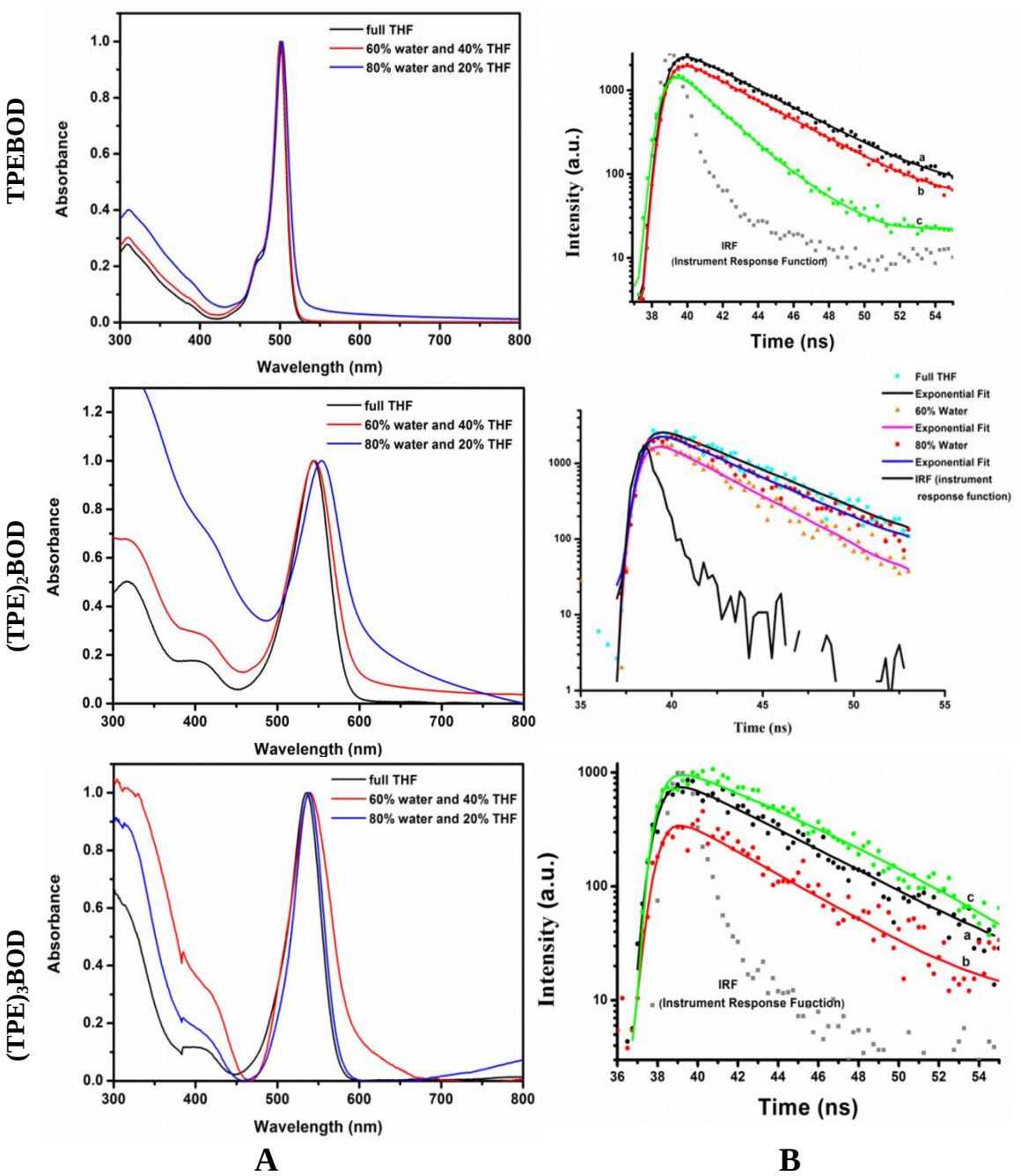

Fig.S1 a) Normalized absorption spectra of fluorophores TPEBOD, $(TPE)_2BOD$, $(TPE)_3BOD$ in THF, 6:4 H_2O/THF and 8:2 H_2O/THF b) Fluorescence Decay Profile of fluorophores

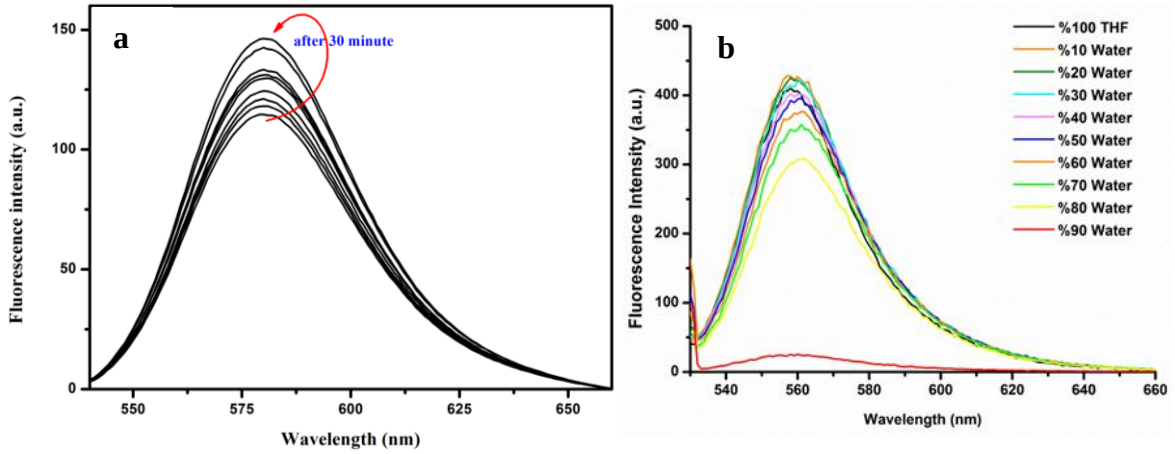

Fig.S2 a) Emission maxima change of **9** with time in 70% water-THF solvent fraction. b) Fluorescence spectrum change of **11** in different water/THF mixture where excitation wavelength is 530 nm

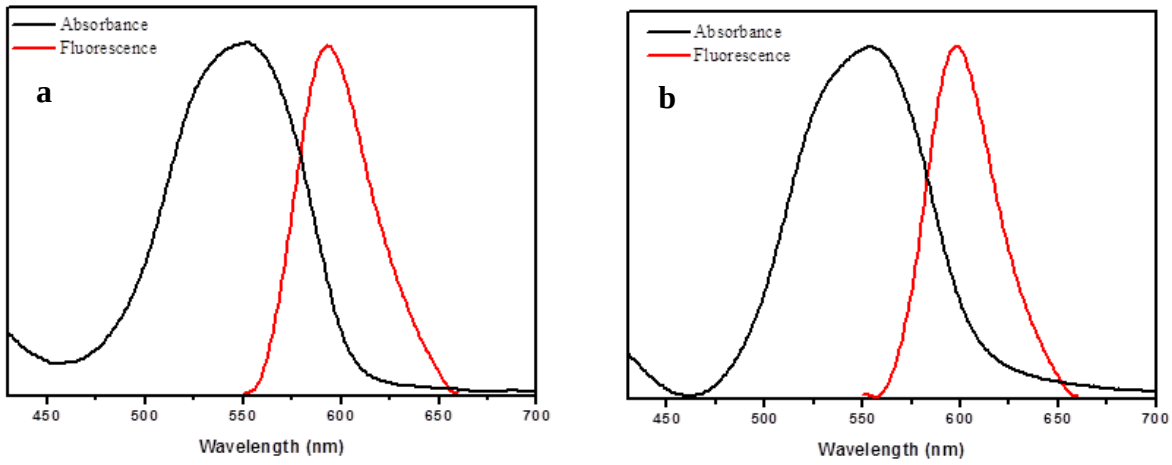

Fig.S3: a) Normalized absorption and emission spectra of $1.0x10^{-3}$ M $(TPE)_2BOD$-LB film. b) Normalized absorption and emission spectra of $1.0x10^{-3}$ M **9** spin-coating film.

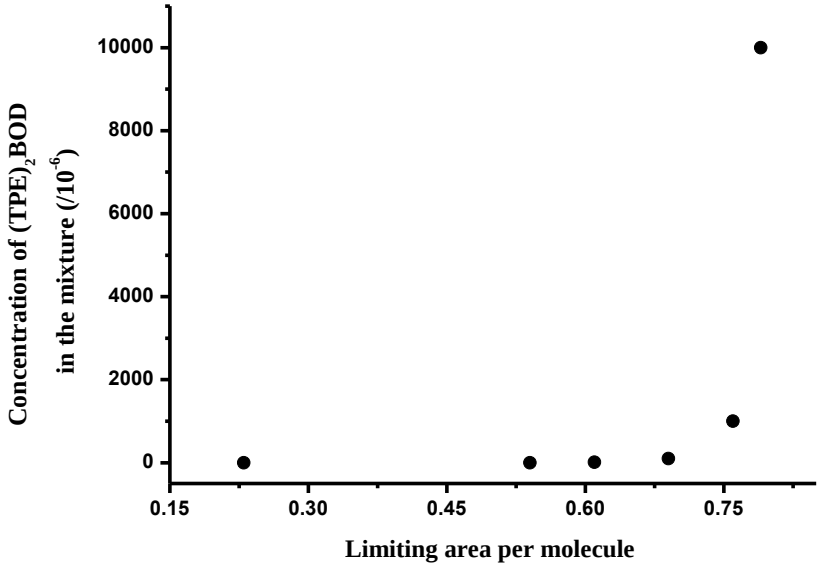

Fig.S5: Plot of the $(TPE)_2BOD$ concentration in the mixture versus limiting area of SA.

S2.2 DLS analysis

			Diam. (nm)	% Intensity	Width (nm)
Z-Average (d.nm):	754,3	Peak 1:	873,1	100,0	231,5
PdI:	0,167	Peak 2:	0,000	0,0	0,000
Intercept:	0,918	Peak 3:	0,000	0,0	0,000
Result quality	Refer to quality report				

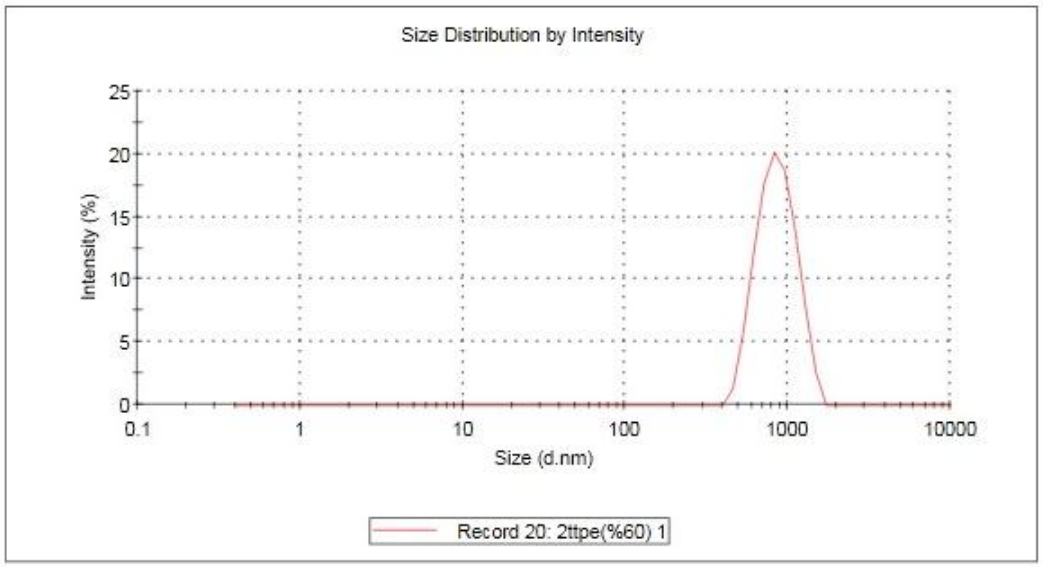

Fig.S6: Results of DLS analysis of **9** in 60% water-THF

			Diam. (nm)	% Intensity	Width (nm)
Z-Average (d.nm):	285,9	Peak 1:	388,1	100,0	214,1
PdI:	0,252	Peak 2:	0,000	0,0	0,000
Intercept:	0,955	Peak 3:	0,000	0,0	0,000
Result quality	Good				

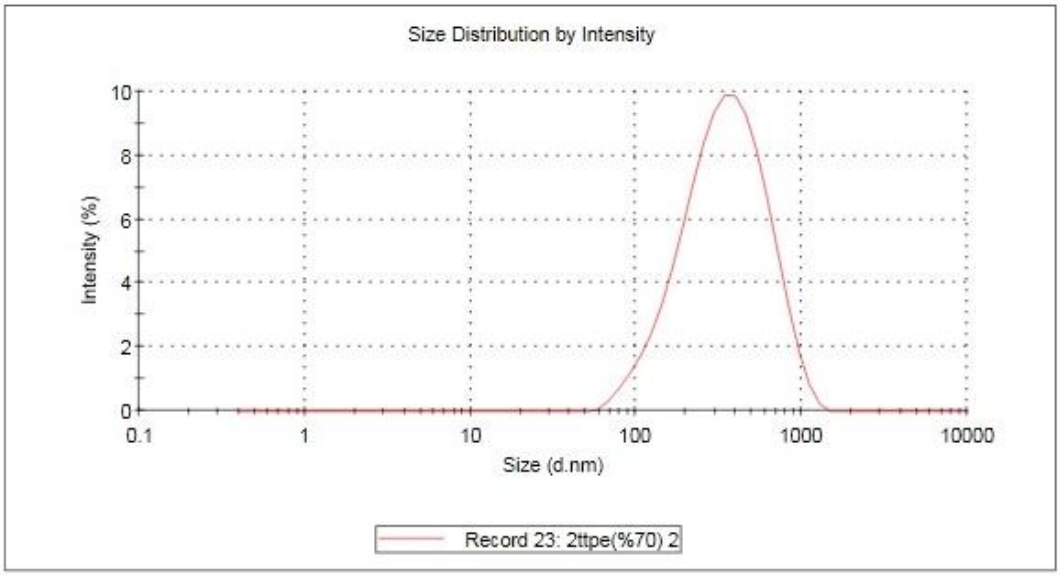

Fig.S7: Results of DLS analysis of **9** in 70% water-THF

			Diam. (nm)	% Number	Width (nm)
Z-Average (d.nm):	370,0	Peak 1:	267,9	100,0	135,4
PdI:	0,219	Peak 2:	0,000	0,0	0,000
Intercept:	0,941	Peak 3:	0,000	0,0	0,000
Result quality	Good				

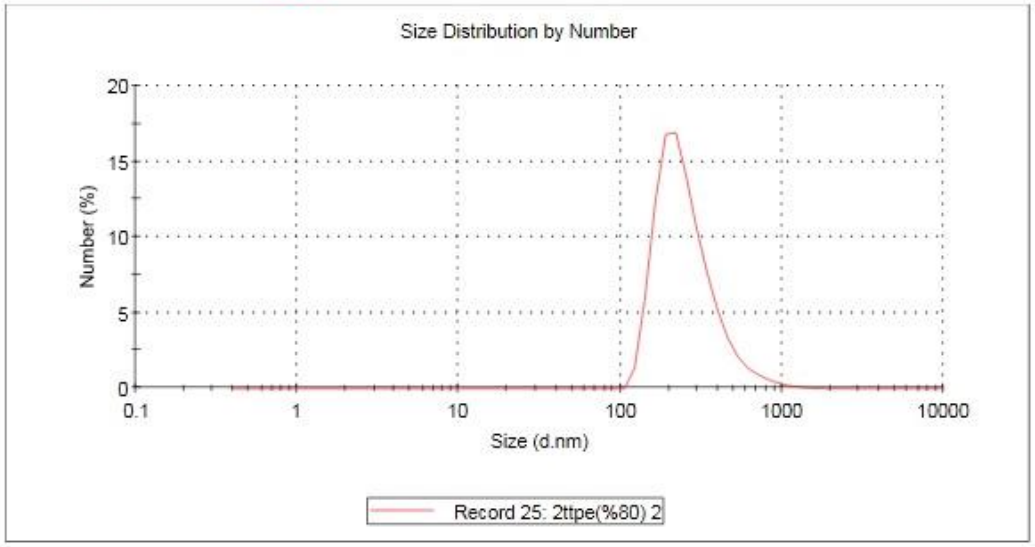

Fig.S8: Results of DLS analysis of **9** in 80% water-THF

		Diam. (nm)	% Intensity	Width (nm)
Z-Average (d.nm): 765,9	Peak 1:	860,9	100,0	236,5
PdI: 0,115	Peak 2:	0,000	0,0	0,000
Intercept: 0,963	Peak 3:	0,000	0,0	0,000
Result quality Good				

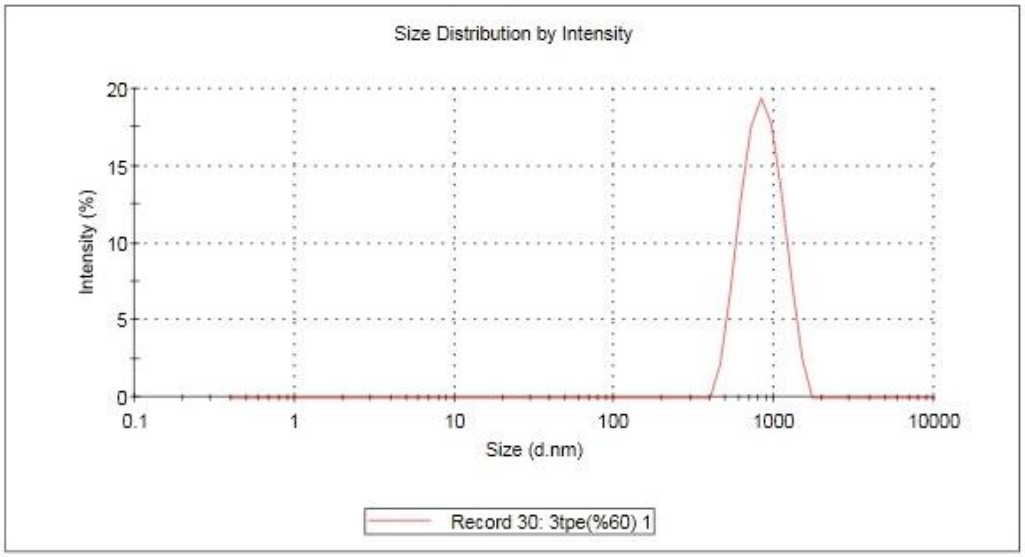

Fig.S9: Results of DLS analysis of **6** in 60% water-THF

		Diam. (nm)	% Intensity	Width (nm)
Z-Average (d.nm): 327,9	Peak 1:	354,5	94,7	151,8
PdI: 0,238	Peak 2:	4511	5,3	873,6
Intercept: 0,943	Peak 3:	0,000	0,0	0,000
Result quality Good				

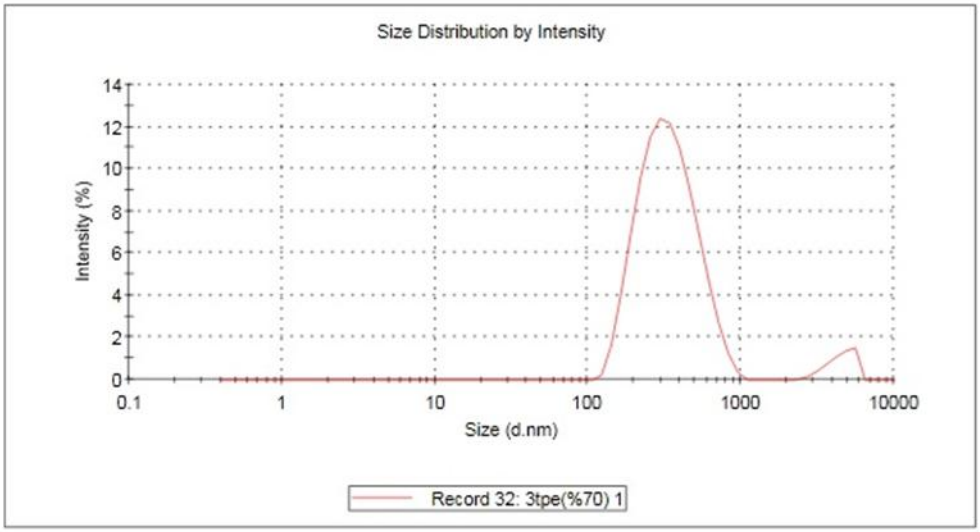

Fig.S10: Results of DLS analysis of **6** in 70% water-THF

		Diam. (nm)	% Number	Width (nm)
Z-Average (d.nm): 321,6	Peak 1:	205,2	100,0	111,3
PdI: 0,222	Peak 2:	0,000	0,0	0,000
Intercept: 0,966	Peak 3:	0,000	0,0	0,000

Result quality Good

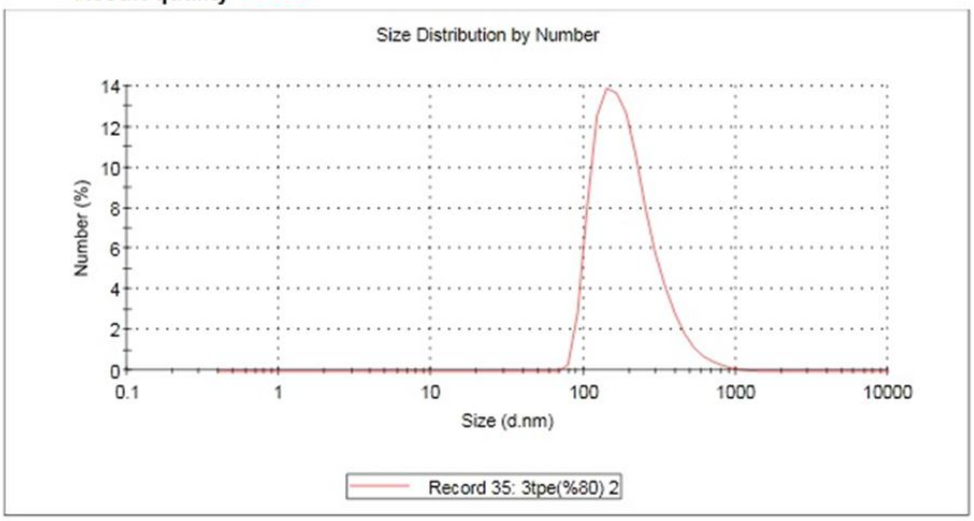

Fig.S11: Results of DLS analysis of **6** in 80% water-THF

S2.2 ^{1}H and ^{13}C NMR spectra and HRMS spectrum

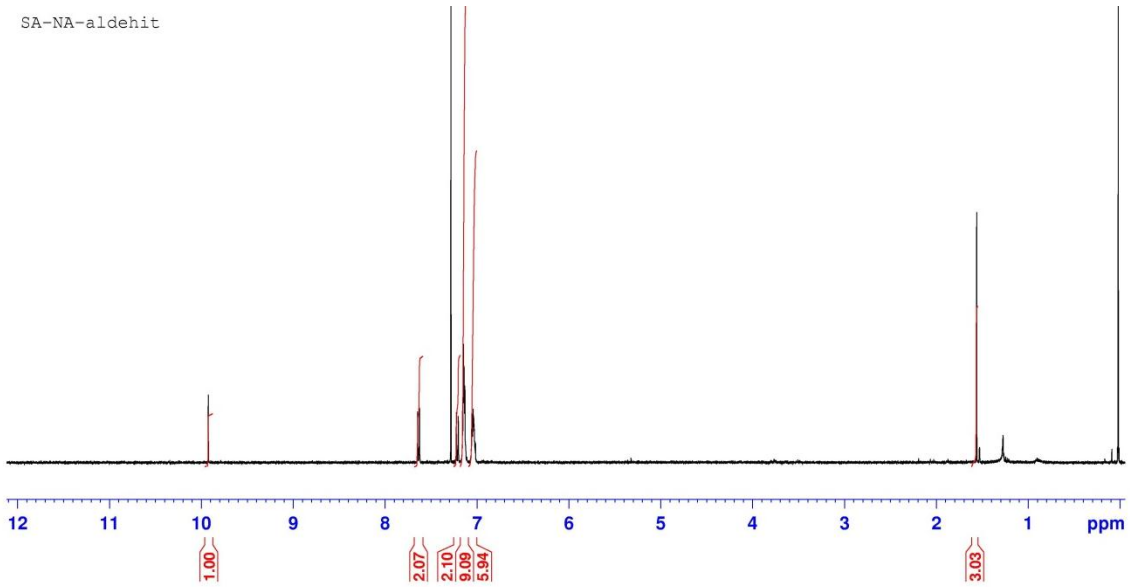

Fig.S12 ^{1}H NMR spectra of the TPE-Al **2**

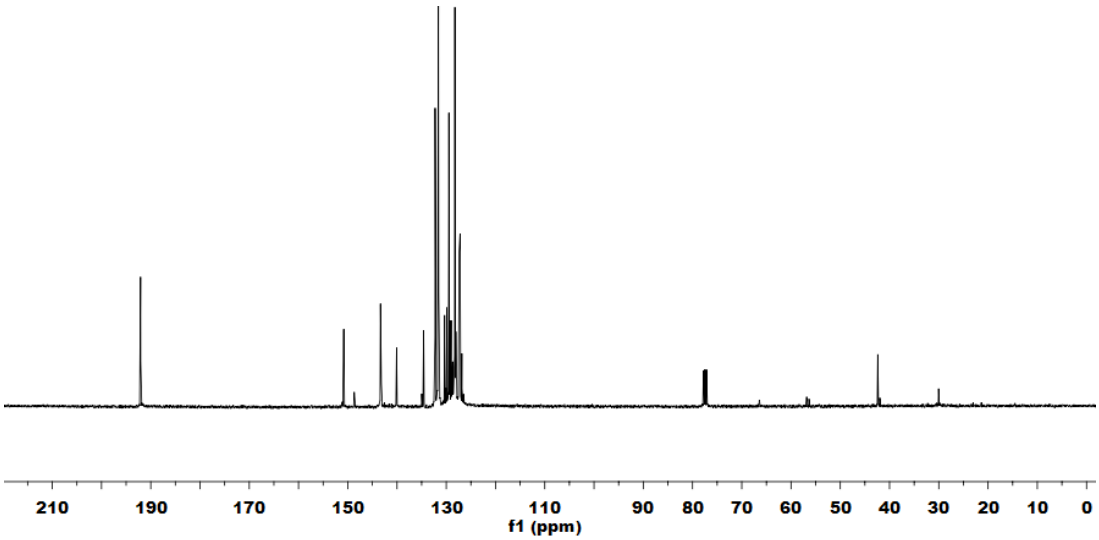

Fig.S13 ^{13}C NMR spectra of the compound **2**

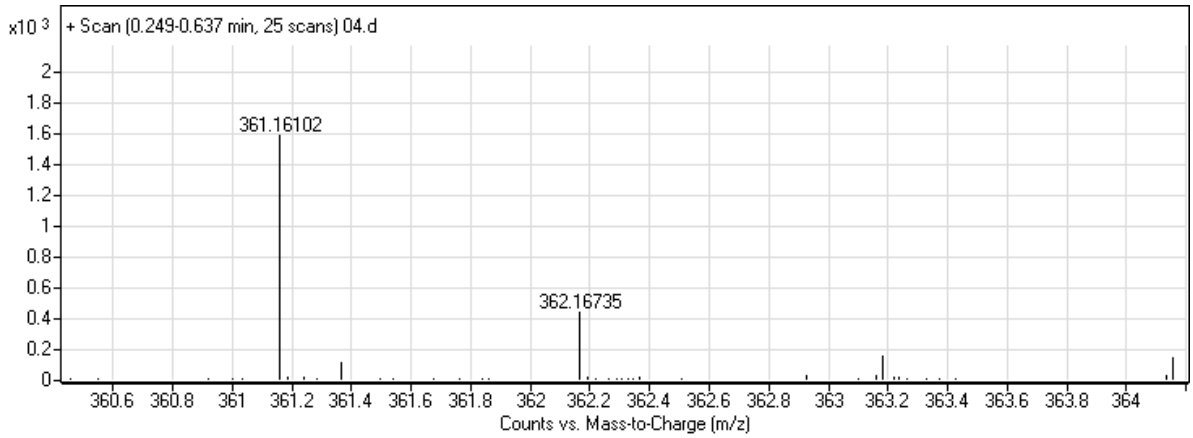

Fig.S14 MALDI-TOF Analysis of the compound **2**

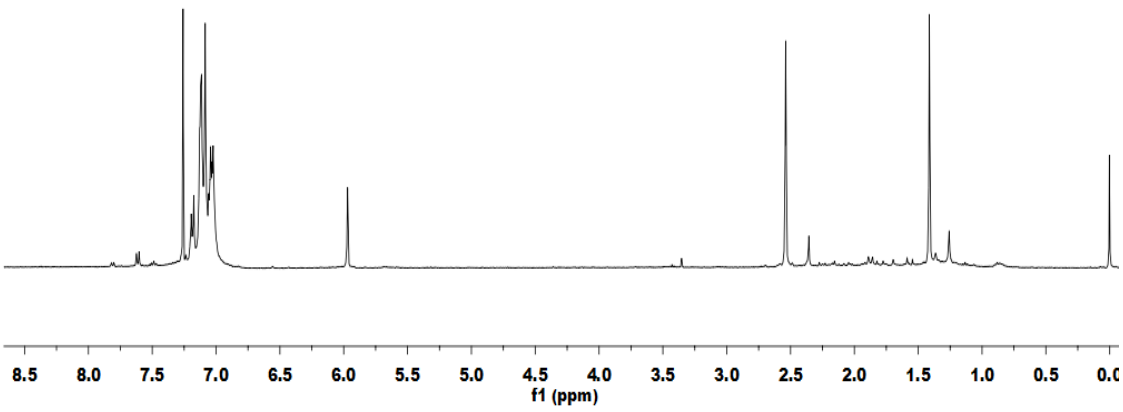

Fig.S15 ^{1}H NMR spectra of the TPEBOD **3**

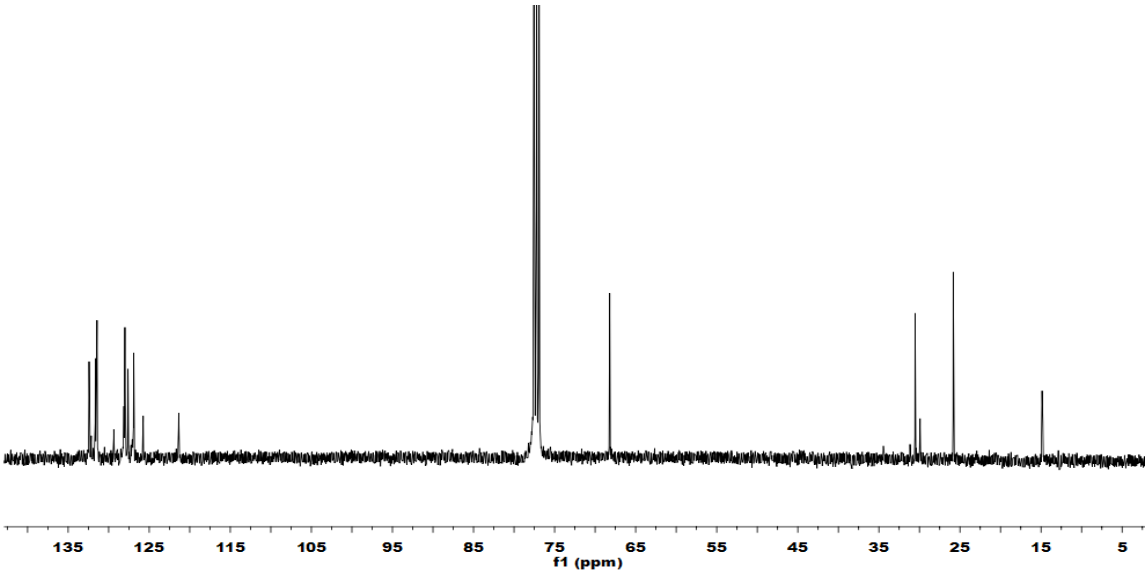

Fig.S16 ^{13}C NMR spectra of the compound **3**

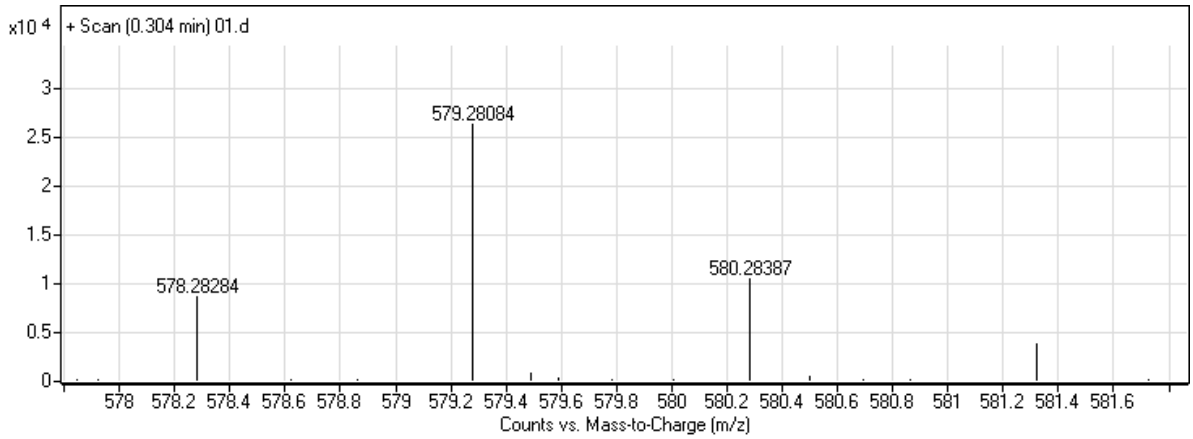

Fig.S17 MALDI-TOF Analysis of the compound **3**

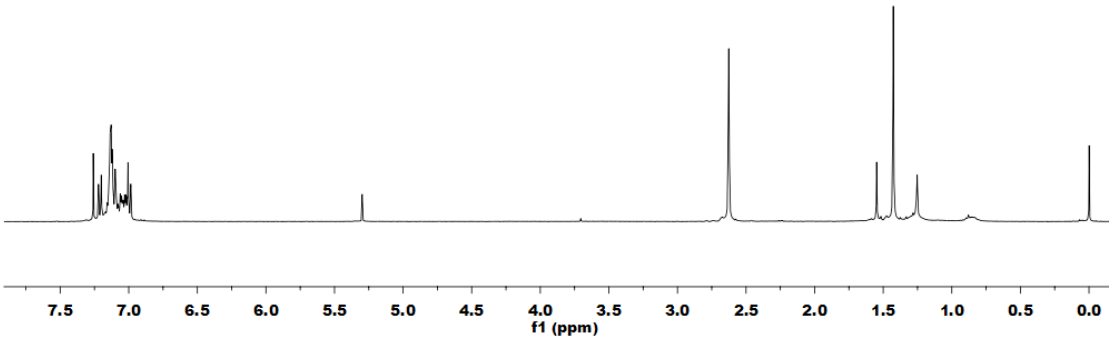

Fig.S18 ^{1}H NMR spectra of iodinated TPEBOD **4**

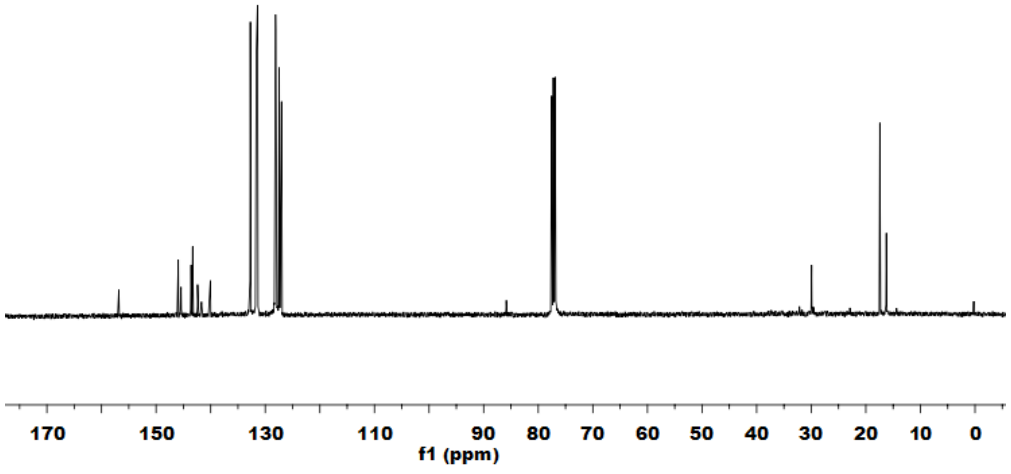

Fig.S19 ^{13}C NMR spectra of the compound **4**

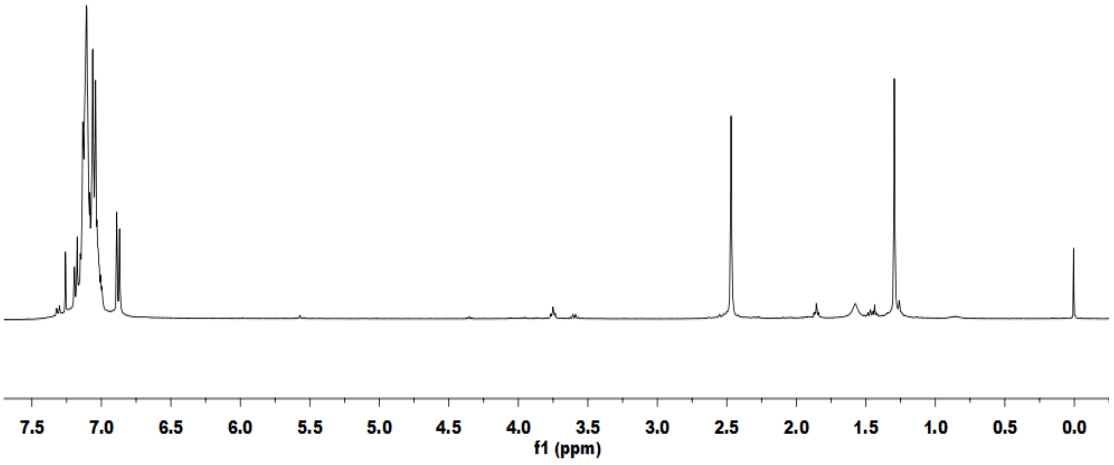

Fig.S20 ^{1}H NMR spectra of iodinated $(TPE)_3BOD$ **6**

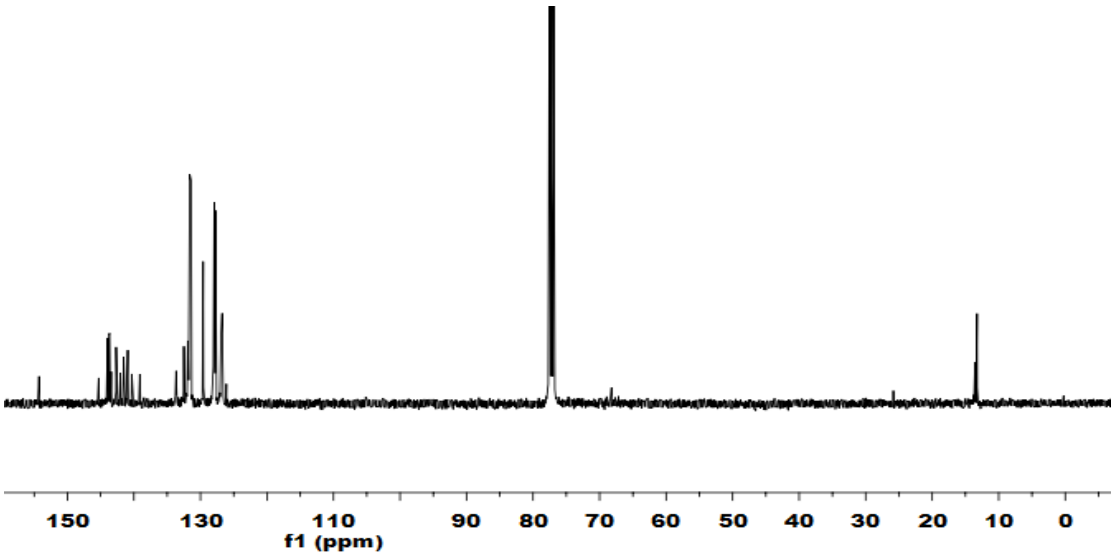

Fig.S21 ^{13}C NMR spectra of the compound **6**

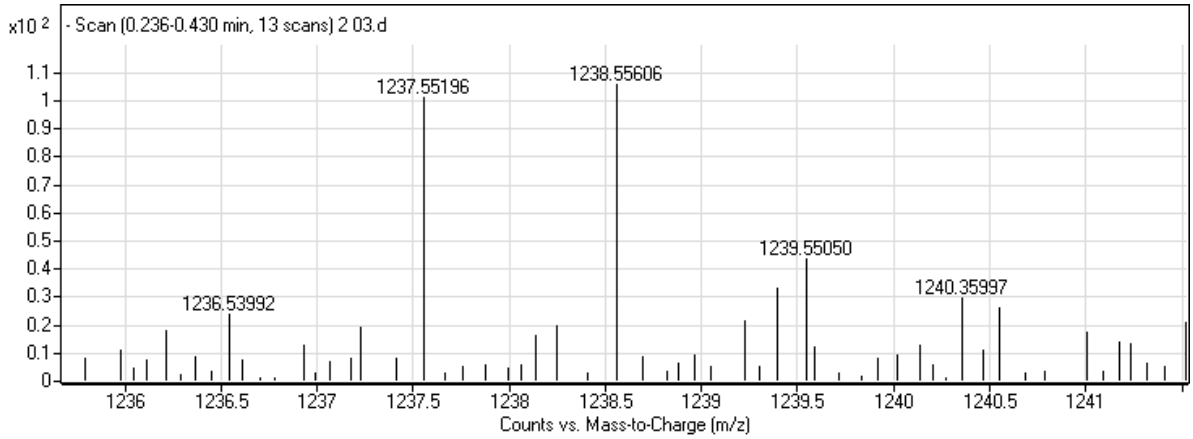

Fig.S22 MALDI-TOF Analysis of the compound **6**

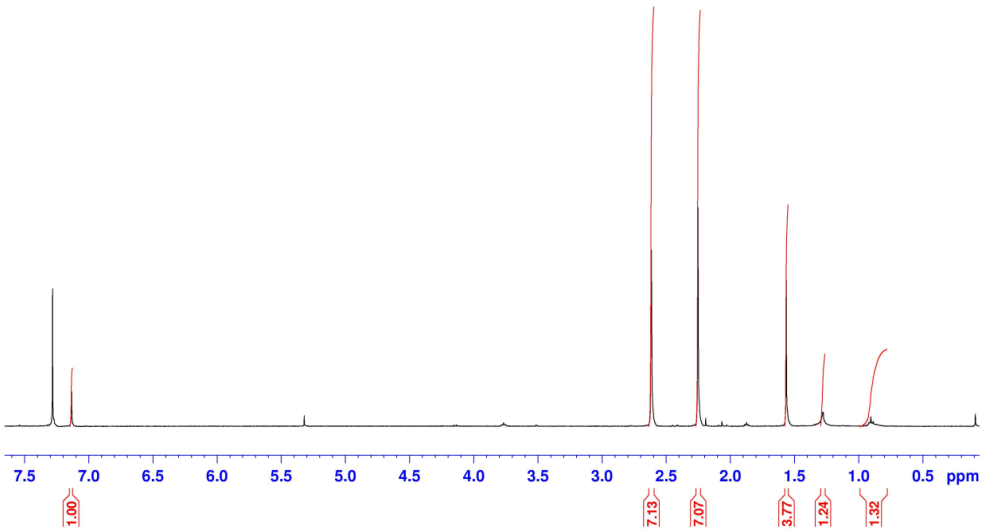

Fig.S23 ^{1}H NMR spectra of the Iodinated-8H-BODIPY **8**

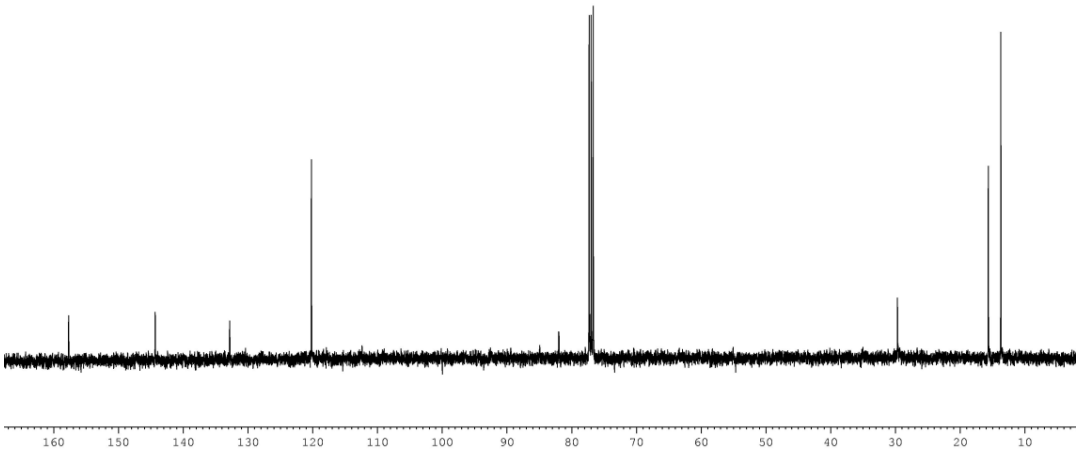

Fig.S24 ^{13}C NMR spectra of the compound **8**

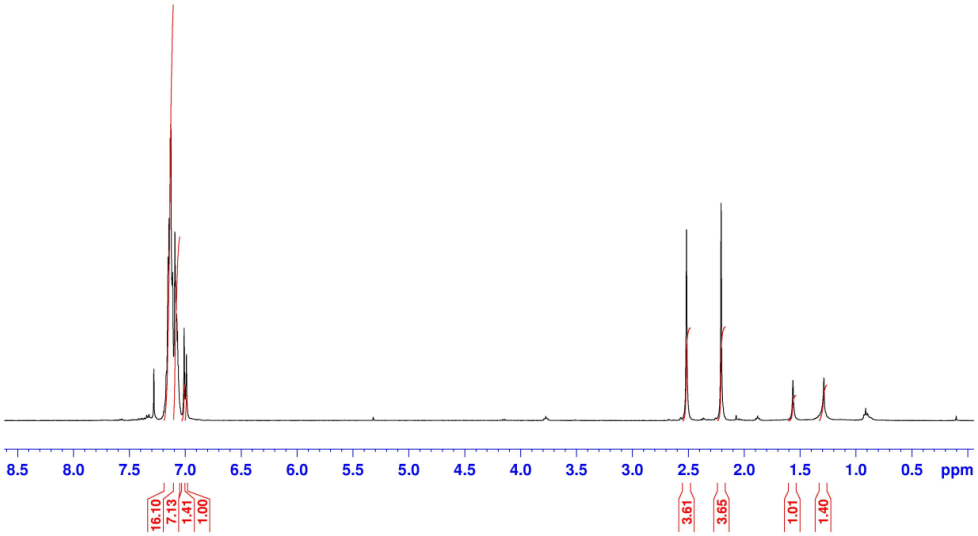

Fig.S25 ^{1}H NMR spectra of $(TPE)_2BOD$ **9**

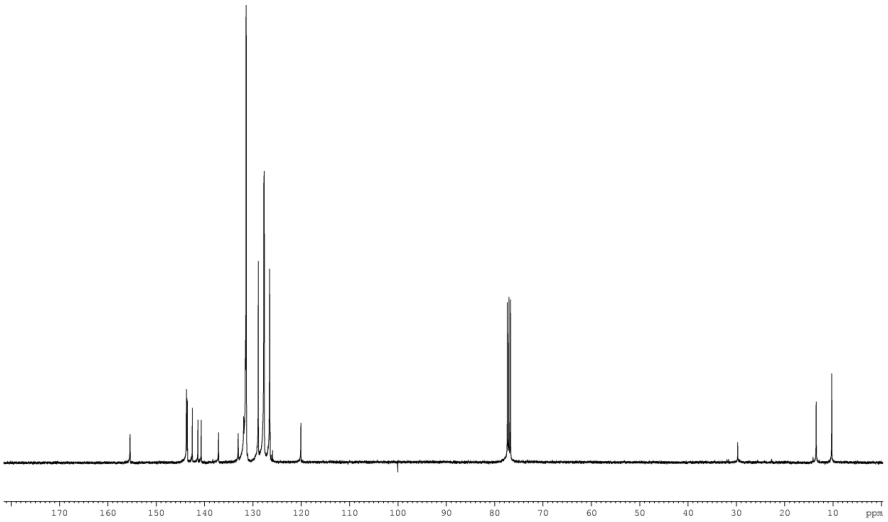

Fig.S26 ^{13}C NMR spectra of the compound **9**

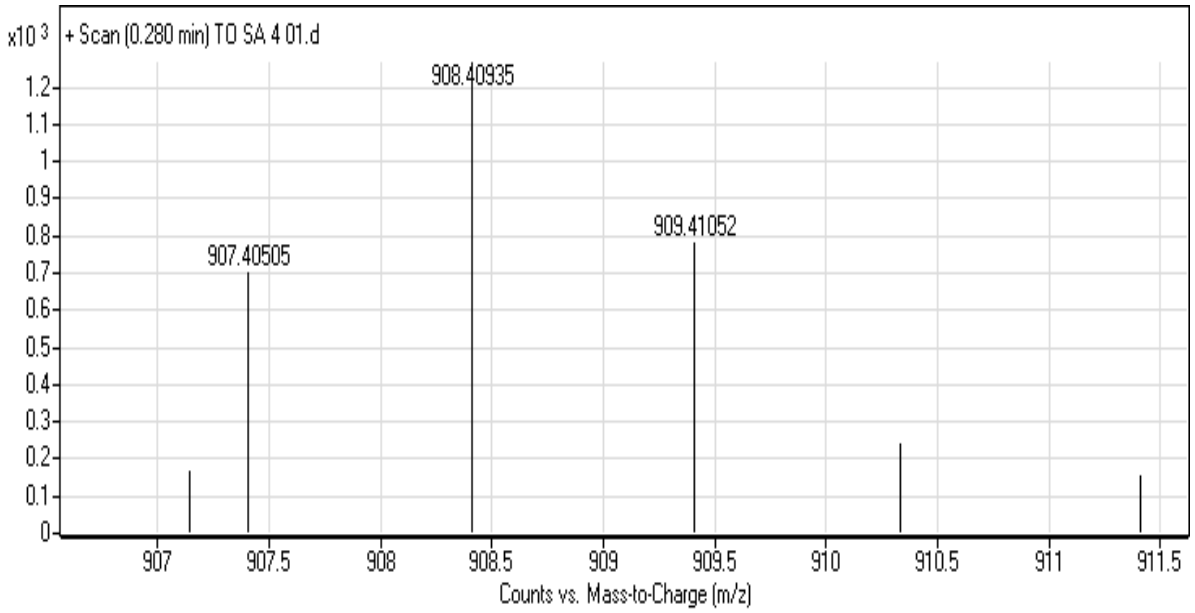

Fig.S27 MALDI-TOF Analysis of the compound **9**

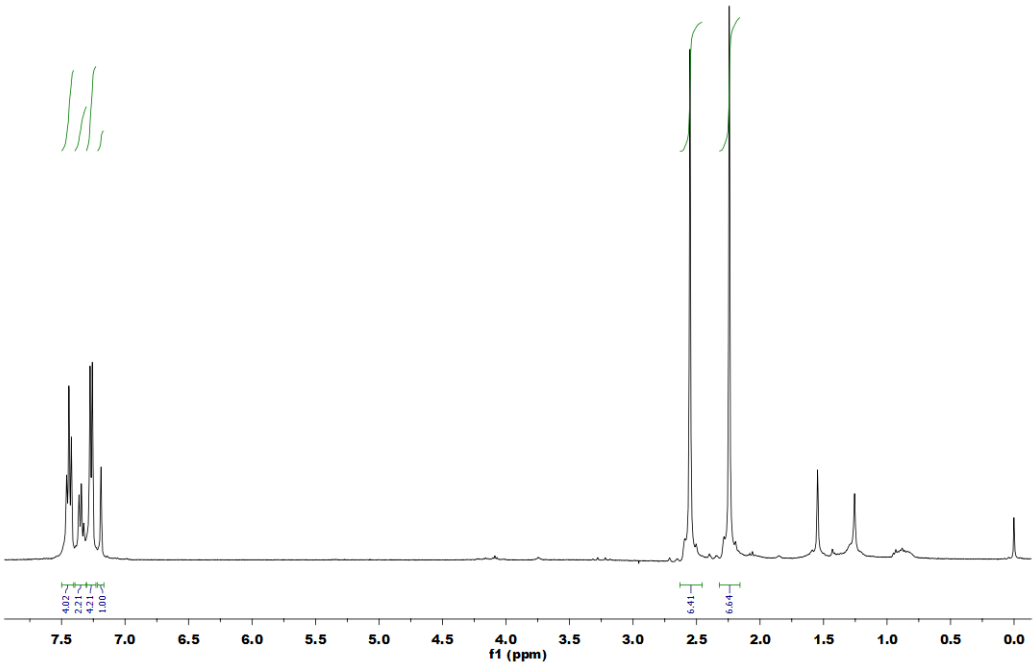

Fig.S28 ^{1}H NMR spectra of $(Ph)_2$BOD **11**

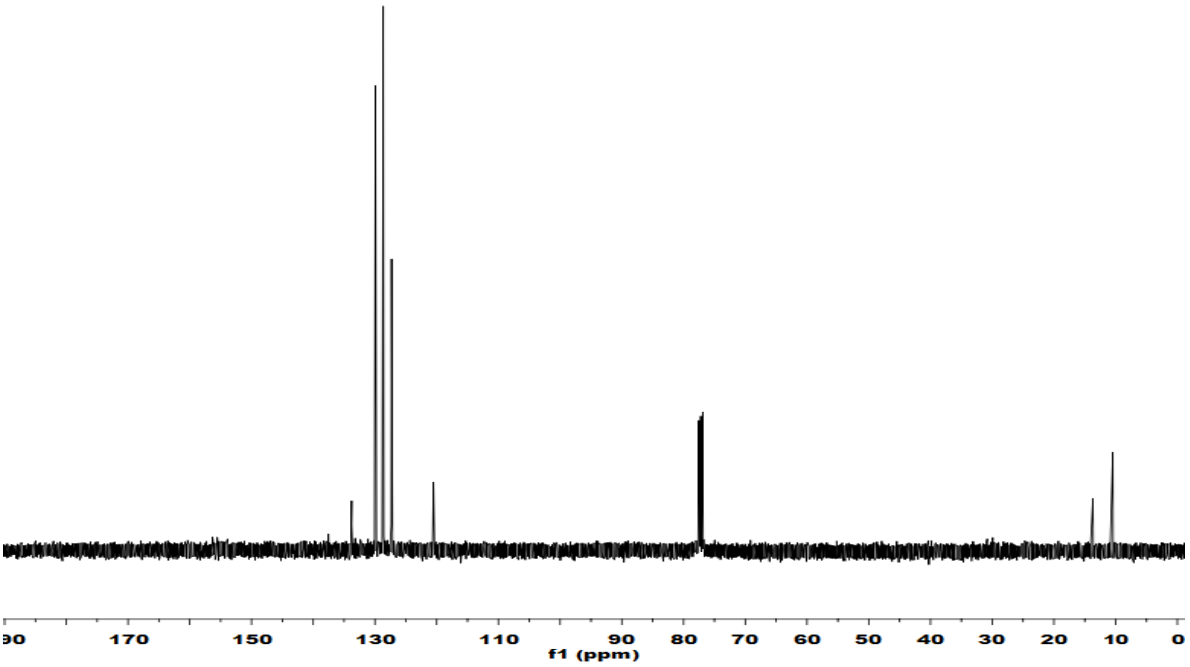

Fig.29 ^{13}C NMR spectra of the compound **11**

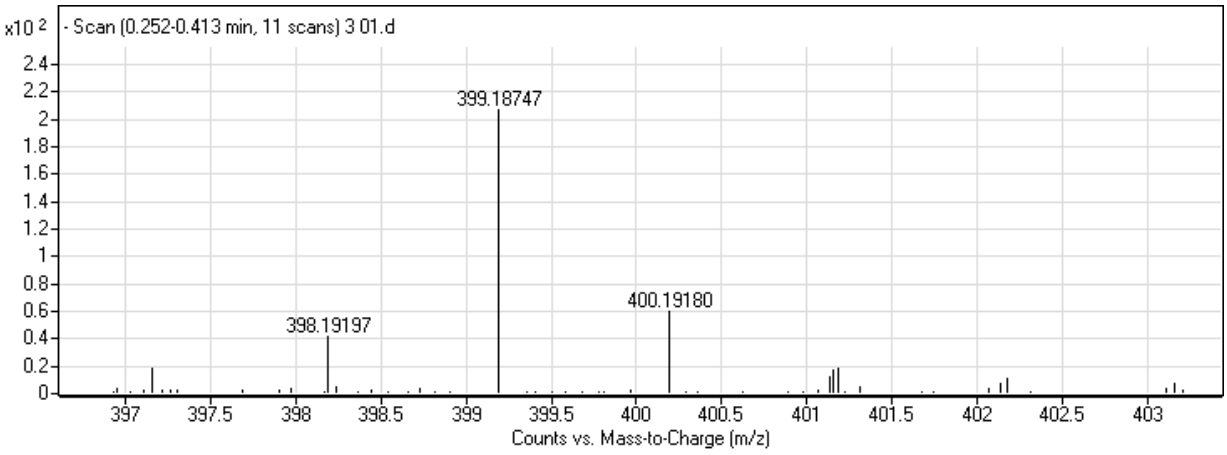

Fig.S30 MALDI-TOF Analysis of the compound **11**

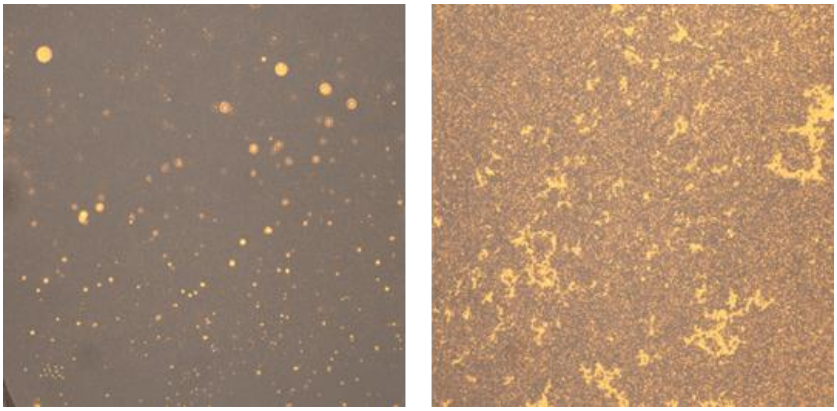

Fig. S31. Confocal Fluoresce microscope images of **9** (10µM) in a) %60 water-THF b) %80 water-THF. The excitation wavelength is 514 nm.

S2.3 Cartesian Coordinates of the fluorophores

Optimized geometry of 9 at AM1 level:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.826919	-0.141291	0.051481
2	6	0	3.491301	1.015099	0.481817
3	7	0	4.907420	1.114662	0.473414
4	5	0	5.893533	-0.018490	-0.004412
5	6	0	3.565799	-1.242825	-0.401801
6	7	0	4.984682	-1.229125	-0.443589
7	9	0	6.708581	-0.371168	0.965818
8	9	0	6.636931	0.398114	-1.006329
9	6	0	3.128363	-2.540516	-0.890763
10	6	0	5.416786	-2.423904	-0.921720
11	6	0	4.278469	-3.266333	-1.210748

12	6	0	2.969473	2.272826	0.991865
13	6	0	4.068577	3.087712	1.274173
14	6	0	5.259508	2.339425	0.941019
15	6	0	1.746745	-3.001956	-1.022805
16	6	0	6.828064	-2.810662	-1.118301
17	1	0	4.339885	-4.276119	-1.604269
18	6	0	1.560775	2.620307	1.175153
19	1	0	4.063325	4.098351	1.670173
20	6	0	6.641510	2.837561	1.088917
21	1	0	1.175428	-2.331652	-1.716018
22	1	0	1.713271	-4.045065	-1.423791
23	1	0	1.231040	-2.982623	-0.027762
24	1	0	7.379935	-2.776291	-0.143677
25	1	0	6.881480	-3.845146	-1.535355
26	1	0	7.332041	-2.101088	-1.824074
27	1	0	1.069767	1.901916	1.881613
28	1	0	1.457372	3.654891	1.586031
29	1	0	1.014097	2.564988	0.198145
30	1	0	7.159765	2.847071	0.095464
31	1	0	6.626970	3.873090	1.506536
32	1	0	7.224921	2.170557	1.774745
33	6	0	1.359832	-0.200835	0.074692
34	6	0	0.619404	0.201528	-1.044264
35	6	0	0.690750	-0.666672	1.214820
36	6	0	-0.771879	0.134263	-1.024131
37	1	0	1.138344	0.571618	-1.941761
38	6	0	-0.699204	-0.737961	1.228515

39	1	0	1.266712	-0.980693	2.098780
40	6	0	-1.445303	-0.337982	0.109891
41	1	0	-1.349857	0.463007	-1.902596
42	1	0	-1.222301	-1.117284	2.120625
43	6	0	-2.909209	-0.455350	0.129871
44	6	0	-3.741039	0.562475	-0.190282
45	6	0	-3.398394	-1.780587	0.544989
46	6	0	-3.876955	-1.983640	1.845909
47	6	0	-3.353760	-2.859133	-0.348805
48	6	0	-4.308760	-3.248124	2.243654
49	1	0	-3.916044	-1.140766	2.551672
50	6	0	-3.786831	-4.120967	0.054361
51	1	0	-2.974284	-2.706962	-1.370032
52	6	0	-4.264467	-4.317738	1.350047
53	1	0	-4.686176	-3.399879	3.265644
54	1	0	-3.750374	-4.963060	-0.652314
55	1	0	-4.605453	-5.314354	1.666015
56	6	0	-3.256981	1.906396	-0.547076
57	6	0	-2.866000	2.806651	0.452533
58	6	0	-3.226695	2.310645	-1.888645
59	6	0	-2.445171	4.091396	0.111981
60	1	0	-2.891655	2.496738	1.507699
61	6	0	-2.803641	3.595762	-2.223164
62	1	0	-3.543485	1.611823	-2.677093
63	6	0	-2.412431	4.487681	-1.224589
64	1	0	-2.139841	4.793463	0.901771
65	1	0	-2.781669	3.906801	-3.278041

66	1	0	-2.080603	5.501769	-1.490938
67	6	0	-5.204037	0.430069	-0.197596
68	6	0	-5.990864	1.352212	0.508040
69	6	0	-5.831619	-0.589981	-0.924667
70	6	0	-7.379681	1.247592	0.492643
71	1	0	-5.501708	2.161969	1.071236
72	6	0	-7.222004	-0.686027	-0.943395
73	1	0	-5.219105	-1.322428	-1.473158
74	6	0	-7.998072	0.230038	-0.234306
75	1	0	-7.988813	1.971890	1.053029
76	1	0	-7.705852	-1.489424	-1.517983
77	1	0	-9.094794	0.151137	-0.248301

Optimized geometry of 6 at AM1 level:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.100743	-0.824474	0.052089
2	6	0	1.106765	-1.535584	0.043255
3	7	0	1.143088	-2.952885	-0.029646
4	5	0	-0.122117	-3.889740	-0.109194
5	6	0	-1.318382	-1.516059	-0.009951
6	7	0	-1.374204	-2.932556	-0.084671
7	9	0	-0.150997	-4.726499	0.905218
8	9	0	-0.103802	-4.610675	-1.209173

9	6	0	-2.687310	-1.025685	-0.012394
10	6	0	-2.676132	-3.314174	-0.131259
11	6	0	-3.522344	-2.143270	-0.087662
12	6	0	2.482161	-1.067193	0.100064
13	6	0	3.301720	-2.197912	0.060498
14	6	0	2.439514	-3.355201	-0.020276
15	6	0	-3.112772	0.372167	0.052591
16	6	0	-3.160613	-4.706475	-0.213159
17	6	0	2.925120	0.324095	0.182961
18	6	0	2.904842	-4.755013	-0.083027
19	1	0	-2.700018	0.947092	-0.816518
20	1	0	-4.228053	0.448769	0.036265
21	1	0	-2.733094	0.853444	0.991022
22	1	0	-2.814710	-5.291483	0.677768
23	1	0	-4.276647	-4.716385	-0.249422
24	1	0	-2.756492	-5.206499	-1.130910
25	1	0	2.512465	0.811391	1.104112
26	1	0	4.041040	0.384148	0.214477
27	1	0	2.558543	0.904592	-0.703101
28	1	0	2.552678	-5.239713	-1.029956
29	1	0	4.020562	-4.783990	-0.047438
30	1	0	2.492185	-5.341867	0.777751
31	6	0	-0.092475	0.642109	0.126209
32	6	0	-0.070916	1.407894	-1.046523
33	6	0	-0.112360	1.285566	1.371253
34	6	0	-0.073853	2.799070	-0.974276
35	1	0	-0.051787	0.909022	-2.027607

36	6	0	-0.121335	2.675745	1.438815
37	1	0	-0.125444	0.689455	2.296567
38	6	0	-0.101682	3.447252	0.267338
39	1	0	-0.044989	3.396592	-1.899460
40	1	0	-0.150819	3.179214	2.418113
41	6	0	-0.148907	4.912413	0.358275
42	6	0	0.728070	5.725187	-0.274748
43	6	0	-1.231155	5.424945	1.214971
44	6	0	-0.956512	5.865187	2.516279
45	6	0	-2.551957	5.441055	0.746630
46	6	0	-1.989915	6.319247	3.334499
47	1	0	0.078341	5.856558	2.889200
48	6	0	-3.580962	5.896122	1.569052
49	1	0	-2.774478	5.091868	-0.272495
50	6	0	-3.302259	6.335437	2.863264
51	1	0	-1.766820	6.666338	4.354152
52	1	0	-4.615295	5.907389	1.195064
53	1	0	-4.115868	6.693880	3.510495
54	6	0	1.848081	5.215288	-1.083028
55	6	0	3.021248	4.765514	-0.463411
56	6	0	1.765435	5.218520	-2.482064
57	6	0	4.093729	4.319924	-1.234694
58	1	0	3.093860	4.764577	0.634225
59	6	0	2.840253	4.770494	-3.247860
60	1	0	0.850980	5.581354	-2.974487
61	6	0	4.005234	4.320763	-2.626348
62	1	0	5.012129	3.968401	-0.741880

63	1	0	2.768937	4.775069	-4.345534
64	1	0	4.852633	3.969307	-3.232828
65	6	0	0.657324	7.190784	-0.204268
66	6	0	1.795146	7.926915	0.157450
67	6	0	-0.525582	7.871200	-0.521697
68	6	0	1.744856	9.317882	0.209164
69	1	0	2.729727	7.396277	0.396512
70	6	0	-0.568910	9.263602	-0.476029
71	1	0	-1.424746	7.298540	-0.797485
72	6	0	0.563983	9.989041	-0.109210
73	1	0	2.640330	9.886997	0.498849
74	1	0	-1.501640	9.789138	-0.728088
75	1	0	0.527126	11.087418	-0.071376
76	6	0	4.840467	-2.250152	0.094080
77	6	0	5.511875	-2.249870	1.317062
78	6	0	5.562940	-2.297861	-1.098105
79	6	0	6.905466	-2.296606	1.347743
80	1	0	4.942028	-2.211474	2.256765
81	6	0	6.956926	-2.345610	-1.067568
82	1	0	5.033920	-2.298271	-2.062089
83	6	0	7.628257	-2.344852	0.155073
84	1	0	7.434768	-2.295753	2.311659
85	1	0	7.526286	-2.383636	-2.007705
86	6	0	-5.061756	-2.170787	-0.120089
87	6	0	-5.783006	-2.261486	1.070728
88	6	0	-5.735011	-2.104927	-1.339899
89	6	0	-7.177181	-2.286994	1.041601

90	1	0	-5.251914	-2.314167	2.032189
91	6	0	-7.129627	-2.129438	-1.369144
92	1	0	-5.166714	-2.033259	-2.278532
93	6	0	-7.850761	-2.220592	-0.178684
94	1	0	-7.745733	-2.359115	1.980133
95	1	0	-7.660196	-2.077081	-2.331032
96	6	0	9.167009	-2.396533	0.189302
97	6	0	9.889975	-1.253030	0.109997
98	6	0	-9.390176	-2.248697	-0.210491
99	6	0	-10.095055	-1.092883	-0.148798
100	6	0	-9.537362	0.190563	-0.791718
101	6	0	-9.333922	0.248309	-2.170757
102	6	0	-9.235728	1.295317	0.004575
103	6	0	-8.828323	1.410354	-2.753202
104	1	0	-9.571100	-0.623095	-2.798167
105	6	0	-8.730895	2.458134	-0.578014
106	1	0	-9.396177	1.250038	1.091468
107	6	0	-8.527031	2.515775	-1.956656
108	1	0	-8.667352	1.455728	-3.840090
109	1	0	-8.493547	3.329171	0.050027
110	1	0	-8.128450	3.431918	-2.416125
111	6	0	-11.458427	-1.062800	0.566683
112	6	0	-12.635797	-1.195950	-0.169892
113	6	0	-11.516251	-0.902554	1.951069
114	6	0	-13.870695	-1.168173	0.477778
115	1	0	-12.589901	-1.321499	-1.261392
116	6	0	-12.751408	-0.875735	2.599205

117	1	0	-10.588391	-0.797774	2.531780
118	6	0	-13.928555	-1.008372	1.862817
119	1	0	-14.798779	-1.272488	-0.102805
120	1	0	-12.796675	-0.749787	3.690792
121	1	0	-14.902342	-0.986560	2.373268
122	6	0	-10.131135	-3.594848	-0.312753
123	6	0	-10.611829	-4.034504	-1.546490
124	6	0	-10.321596	-4.374617	0.827963
125	6	0	-11.283413	-5.253351	-1.639279
126	1	0	-10.462187	-3.419155	-2.445487
127	6	0	-10.992499	-5.594323	0.735144
128	1	0	-9.942643	-4.028335	1.800389
129	6	0	-11.473521	-6.033716	-0.498181
130	1	0	-11.662880	-5.599663	-2.611580
131	1	0	-11.142161	-6.209118	1.634645
132	1	0	-12.003020	-6.994725	-0.571597
133	6	0	9.178406	0.106989	-0.014968
134	6	0	8.896188	0.633305	-1.275847
135	6	0	8.815955	0.812584	1.132339
136	6	0	8.252265	1.865260	-1.389302
137	1	0	9.182756	0.077141	-2.180171
138	6	0	8.170947	2.044467	1.019027
139	1	0	9.038151	0.397828	2.126188
140	6	0	7.889188	2.570940	-0.241518
141	1	0	8.030346	2.280465	-2.383109
142	1	0	7.884920	2.600380	1.923805
143	1	0	7.381435	3.542246	-0.331222

144	6	0	11.428378	-1.313824	0.144964
145	6	0	12.148174	-1.451316	-1.042243
146	6	0	12.102172	-1.231327	1.363464
147	6	0	13.541421	-1.506967	-1.010801
148	1	0	11.616639	-1.517101	-2.002652
149	6	0	13.495882	-1.285988	1.394999
150	1	0	11.535024	-1.122781	2.299247
151	6	0	14.215553	-1.423923	0.208160
152	1	0	14.108814	-1.615970	-1.946472
153	1	0	14.026887	-1.220505	2.355842
154	1	0	15.314085	-1.467766	0.232697
155	6	0	9.886678	-3.752301	0.314077
156	6	0	10.193850	-4.265552	1.574510
157	6	0	10.231323	-4.467209	-0.832951
158	6	0	10.846124	-5.493123	1.687776
159	1	0	9.922692	-3.701325	2.478591
160	6	0	10.882918	-5.695635	-0.719798
161	1	0	9.989139	-4.062918	-1.826443
162	6	0	11.190472	-6.208601	0.540287
163	1	0	11.088834	-5.897441	2.681212
164	1	0	11.154165	-6.259280	-1.624344
165	1	0	11.704710	-7.176504	0.629844

S2.5 Calculated electronic excitation energies with the first 20 excited states of fluorophores and oscillator strengths in THF and water.

TPEBOD 3 in THF

B3LYP/6-311G* (THF)										
Excited State	Excitation energy (nm)	oscillator strength	Gaussian Comment		My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
1	435,57	0,5636	152 ->153	0.59701	HOMO -> LUMO	0,10895	152	153	C39H33BF2N2	304
2	430,88	0,0025	151 ->153	0.69590		2.9646804011975 eV				152
3	363,20	0,0332	150 ->153	0.66377						
4	335,77	0,0535	148 ->153	0.65985						
5	331,53	0,0002	152 ->154	0.69523						
6	326,11	0,0056	149 ->153	0.55133						
7	318,89	0,0018	147 ->153	0.53634						
8	309,57	0,0017	146 ->153	0.57471						
9	306,80	0,6434	151 ->154	0.66535	HOMO-1 -> LUMO+1					
10	306,07	0,0113	145 ->153	0.47199						
11	303,42	0,0022	145 ->153	0.51227						
12	297,52	0,0033	143 ->153	0.48866						
13	291,27	0,0053	152 ->155	0.65438						
14	289,49	0,0010	142 ->153	0.54097						
15	276,78	0,0994	151 ->155	0.66004						
16	272,36	0,0001	152 ->156	0.67183						
17	267,98	0,0314	151 ->156	0.54101						
18	264,16	0,0028	152 ->157	0.63524						
19	262,52	0,0023	151 ->157	0.45796						
20	261,86	0,0032	141 ->153	0.65515						

TPEBOD 3 in water

B3LYP/6-311G* (H2O)										
Excited State	Excitation energy (nm)	oscillator strength	Gaussian Comment		My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
1	439,04	0,0012	151 ->153	0.69604		0,10918	152	153	C39H33BF2N2	304
2	433,02	0,5465	152 ->153	0.59563	HOMO -> LUMO	2.970939019759 eV				152
3	363,36	0,0319	150 ->153	0.65013						
4	334,61	0,0542	146 ->153	0.65893						
5	330,47	0,0074	149 ->153	0.53964						
6	325,96	0,0002	152 ->154	0.69481						
7	323,14	0,0026	148 ->153	0.55722						
8	313,04	0,0016	147 ->153	0.59767						
9	310,22	0,0016	145 ->153	0.47985						
10	307,18	0,0060	145 ->153	0.49151						
11	306,15	0,6373	151 ->154	0.66540	HOMO-1 -> LUMO+1					
12	300,83	0,0030	143 ->153	0.48324						
13	291,94	0,0008	152 ->155	0.64576						
14	286,47	0,0052	152 ->155	0.64576						
15	276,22	0,0984	151 ->155	0.65909						
16	269,19	0,0006	152 ->156	0.66122						
17	267,92	0,0278	151 ->156	0.54729						
18	264,60	0,0016	141 ->153	0.68008						
19	262,49	0,0063	151 ->157	0.46776						
20	261,28	0,0120	152 ->160	0.10340						

$(TPE)_2BOD$ 9 in THF

B3LYP/6-31G* (THF)										
Excited State	Excitation energy (nm)	oscillator strength	Gaussian		Comment	My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
1	444,16	0,9378	326 -> 327	0.59625		HOMO -> LUMO	0,10789	326	327	C91H69BF2N2	652
2	427,59	0,0008	325 -> 327	0.69684			2.9358363330445 eV				326
3	369,64	0,0714	321 -> 327	0.55497							
4	363,94	0,0107	324 -> 327	0.61013							
5	356,16	0,0030	323 -> 327	0.64174							
6	346,83	0,0001	322 -> 327	0.67013							
7	341,75	0,0476	319 -> 327	0.61117							
8	331,42	0,0003	326 -> 328	0.69625							
9	324,04	0,0099	318 -> 327	0.55024							
10	320,26	0,0006	316 -> 327	0.49412							
11	317,68	0,0031	317 -> 327	0.50094							
12	316,77	0,0005	312 -> 327	0.41530							
13	314,76	0,0001	315 -> 327	0.45897							
14	309,95	0,0000	320 -> 327	0.54432							
15	308,86	0,0004	308 -> 327	0.40820							
16	307,69	0,0030	310 -> 327	0.54710							
17	305,36	0,0000	313 -> 327	0.56167							
18	303,64	0,0005	314 -> 327	0.44353							
19	303,34	0,0020	306 -> 327	0.36881							
20	302,52	0,0001	309 -> 327	0.56519							

$(TPE)_2BOD$ 9 in water

Excitation energy (nm)	oscillator strength	Gaussian		Comment	My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
442,19	0,9174	326 -> 327	0.59333		HOMO -> LUMO	0,10815	326	327	C91H69BF2N2	652
439,46	0,0086	325 -> 327	0.69442			2.9429112931575 eV				326
372,59	0,0245	324 -> 327	0.64073							
367,43	0,0536	321 -> 327	0.56302							
359,80	0,0041	323 -> 327	0.63554							
349,58	0,0000	322 -> 327	0.67073							
340,66	0,0481	318 -> 327	0.43405							
330,40	0,0129	320 -> 327	0.55506							
323,94	0,0010	326 -> 328	0.47822							
323,93	0,0001	326 -> 328	0.50514							
323,18	0,0032	314 -> 327	0.39792							
320,32	0,0010	318 -> 327	0.40722							
317,60	0,0001	312 -> 327	0.50143							
313,53	0,0027	311 -> 327	0.56259							
313,03	0,0000	319 -> 327	0.51155							
311,58	0,0005	307 -> 327	0.36291							
309,51	0,0023	308 -> 327	0.41856							
309,17	0,0007	313 -> 327	0.50610							
307,54	0,0005	309 -> 327	0.49893							
307,17	0,0016	308 -> 327	0.41044							

$(TPE)_3BOD$ 6 in THF

B3LYP/6-31G* (THF)										
Excited State	Excitation energy (nm)	oscillator strength	Gaussian Comment		My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
1	521,78	0,8964	239 -> 240	0.61919	HOMO -> LUMO	0,0978	239	240	C65H51BF2N2	478
2	464,08	0,0112	238 -> 240	0.69069		2.66127345789 eV				239
3	419,20	0,5652	237 -> 240	0.64780						
4	372,03	0,2571	236 -> 240	0.65980						
5	364,67	0,0255	235 -> 240	0.67122						
6	335,54	0,0025	234 -> 240	0.63477						
7	335,33	0,0013	233 -> 240	0.63544						
8	330,59	0,6468	239 -> 241	0.65931						
9	328,18	0,0073	239 -> 242	0.66404						
10	317,93	0,0001	232 -> 240	0.55100						
11	317,87	0,0001	231 -> 240	0.55159						
12	314,44	0,0029	228 -> 240	0.59162						
13	314,12	0,0008	227 -> 240	0.59502						
14	311,49	0,001	230 -> 240	0.63799						
15	311,45	0,0007	229 -> 240	0.63806						
16	309,00	0,0093	226 -> 240	0.60725						
17	308,60	0,0016	225 -> 240	0.62165						
18	302,60	0,0064	238 -> 241	0.55676						
19	302,23	0,5335	238 -> 242	0.53437						
20	297,87	0,0007	224 -> 240	0.49008						

$(TPE)_3BOD$ 6 in water

B3LYP/6-31G* (H2O)										
Excited State	Excitation energy (nm)	oscillator strength	Gaussian Comment		My Comment	E (homo-lumo)	HOMO	LUMO	stoichiometry	Nelectron
1	518,77	0,8585	239 -> 240	0.61932	HOMO -> LUMO	0,0982	239	240	C65H51BF2N2	478
2	464,11	0,0106	238 -> 240	0.69129		2.67215801191 eV				239
3	418,42	0,5820	237 -> 240	0.64636						
4	371,02	0,2736	236 -> 240	0.65864						
5	363,99	0,0255	235 -> 240	0.67129						
6	335,43	0,0034	233 -> 240	0.46480						
7	335,37	0,0000	234 -> 240	0.46507						
8	329,47	0,6568	239 -> 241	0.65794						
9	326,82	0,0070	239 -> 242	0.66187						
10	318,42	0,0001	232 -> 240	0.62349						
11	318,29	0,0002	231 -> 240	0.62188						
12	314,84	0,0038	228 -> 240	0.59249						
13	314,48	0,0008	227 -> 240	0.59465						
14	312,51	0,0003	230 -> 240	0.62969						
15	312,49	0,0005	229 -> 240	0.63190						
16	309,78	0,0109	226 -> 240	0.58226						
17	309,33	0,0019	225 -> 240	0.60190						
18	302,37	0,0008	238 -> 241	0.55697						
19	301,98	0,5071	238 -> 242	0.53297						
20	298,18	0,0005	224 -> 240	0.54345						