Supporting Information

The First Examples of Cofacial Bis(dipyrrins)

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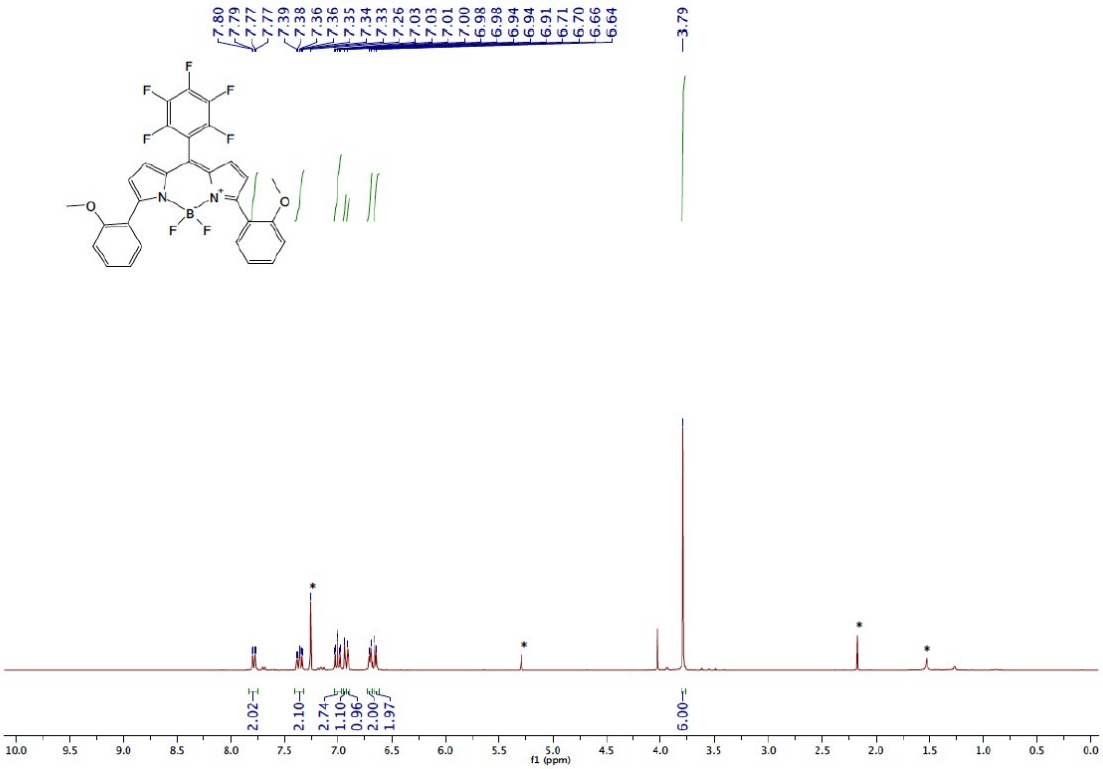


Figure S1. ^{1}H NMR of **BOD-OMe** (**3**) ($CDCl_3$, 298K).

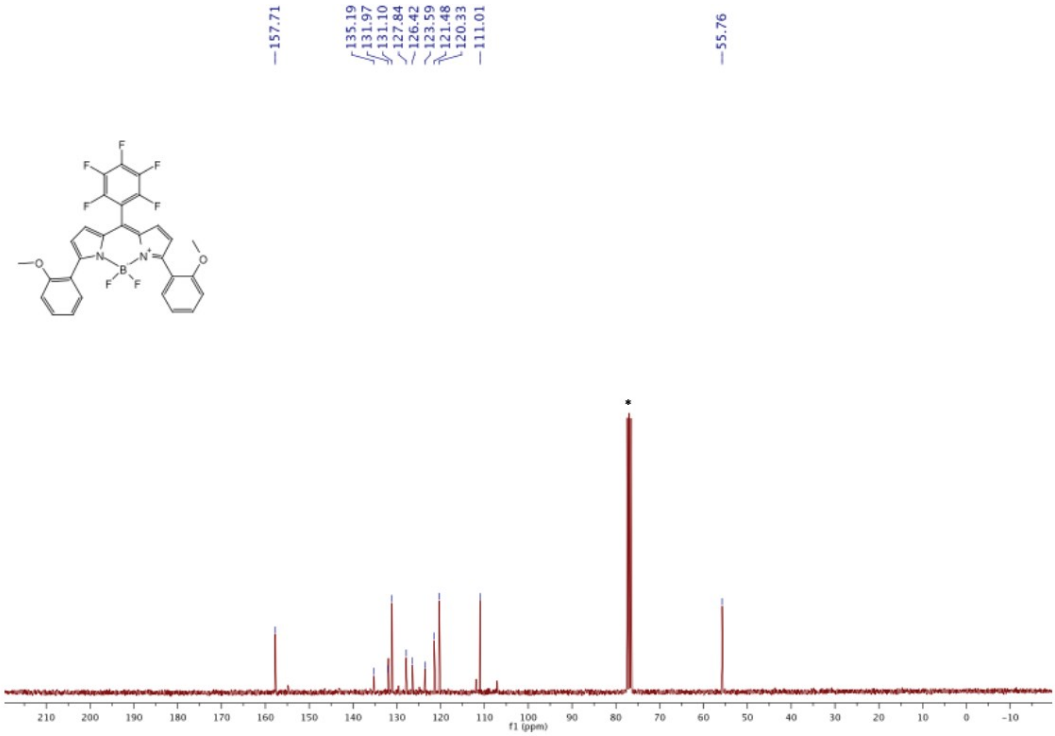


Figure S2. ^{13}C NMR of **BOD-OMe** (**3**) ($CDCl_3$, 298K).

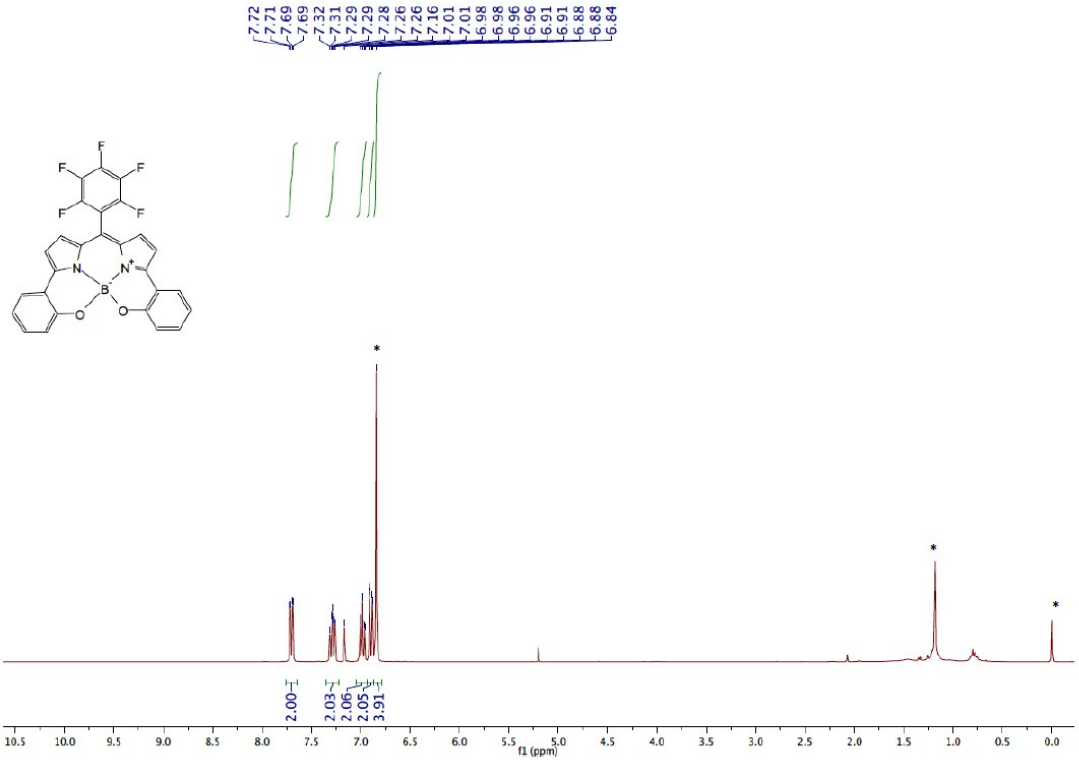


Figure S3. ^{1}H NMR of **BOD-O** (**4**) ($CDCl_3$, 298K).

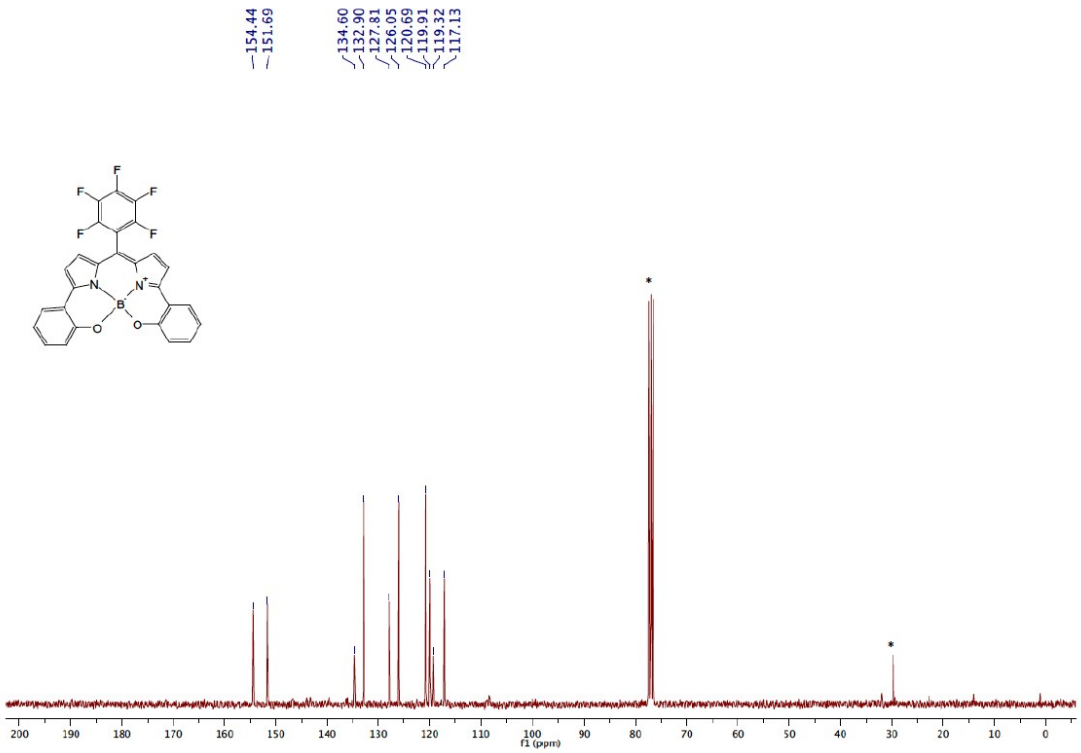


Figure S4. ^{13}C NMR of **BOD-O** (**4**) ($CDCl_3$, 298K).

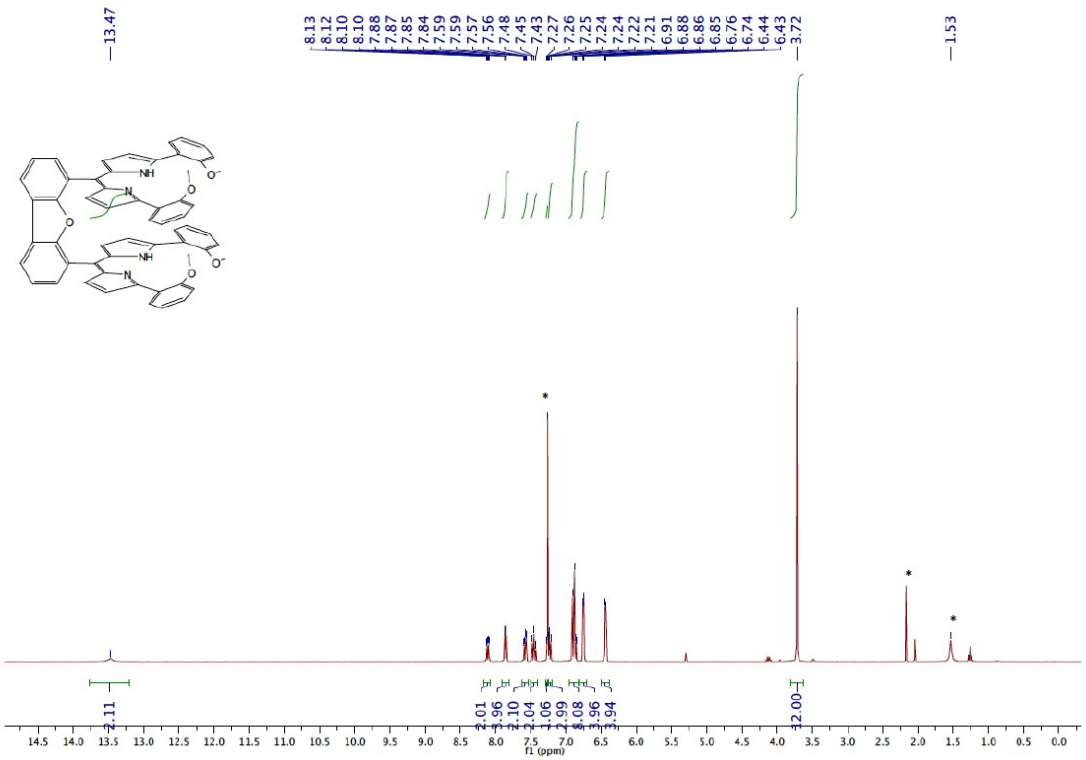


Figure S5. ^{1}H NMR of **5a** ($CDCl_3$, 298K).

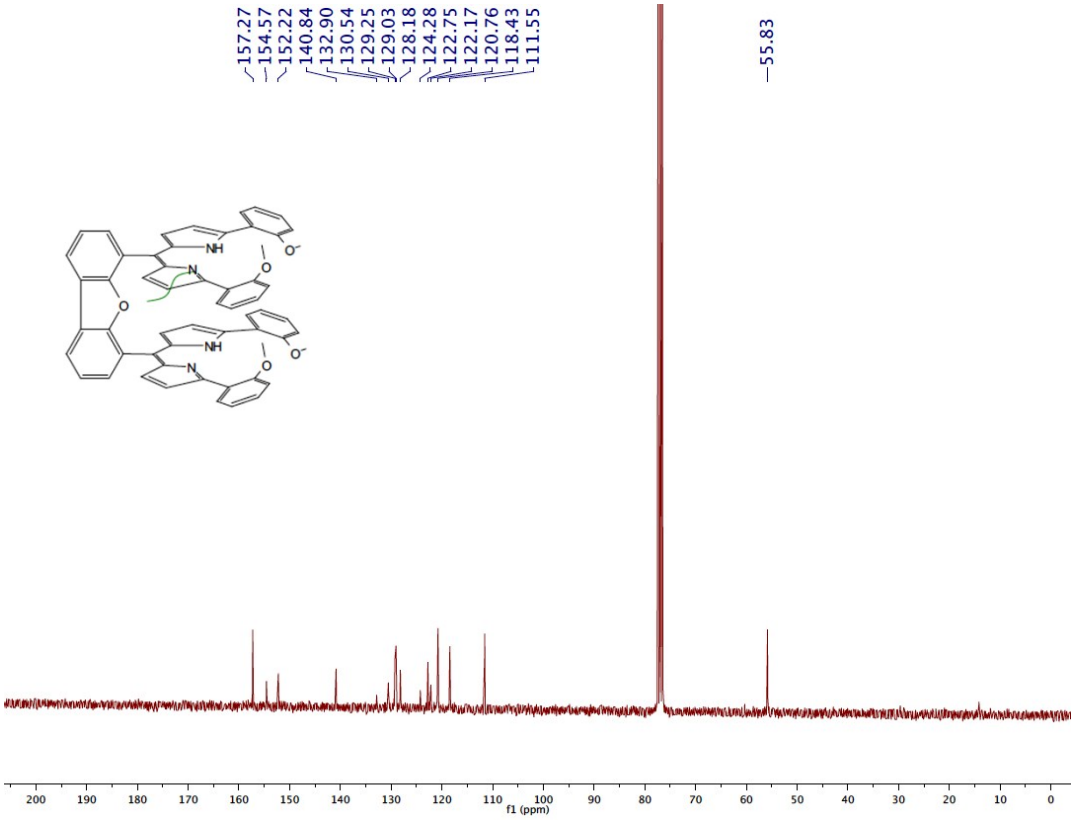


Figure S6. ^{13}C NMR of **5a** ($CDCl_3$, 298K).

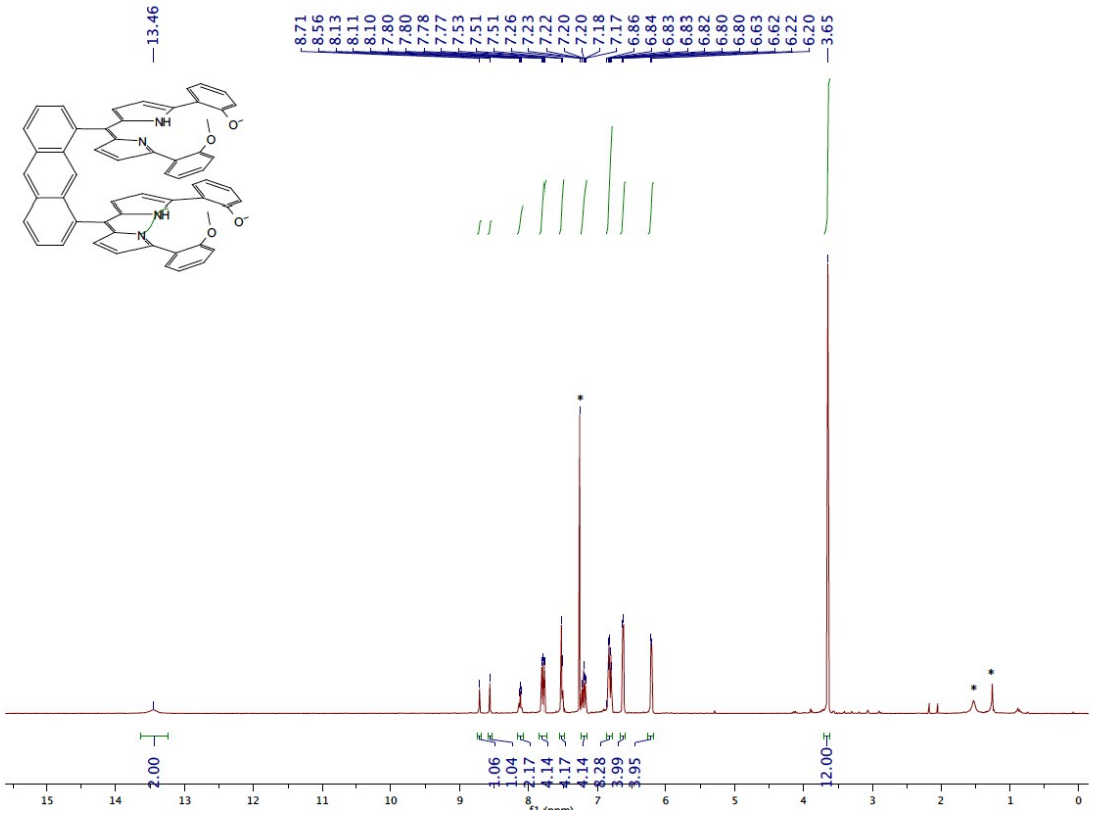


Figure S7. ^{1}H NMR of **6a** ($CDCl_3$, 298K).

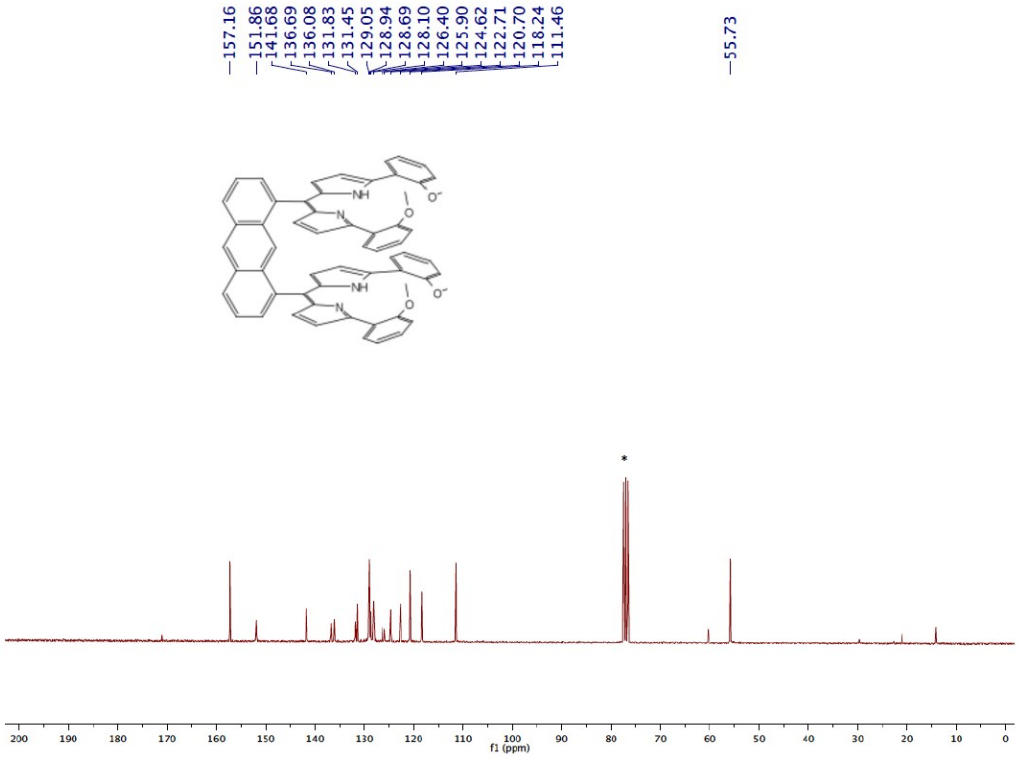


Figure S8. ^{13}C NMR of **6a** ($CDCl_3$, 298K).

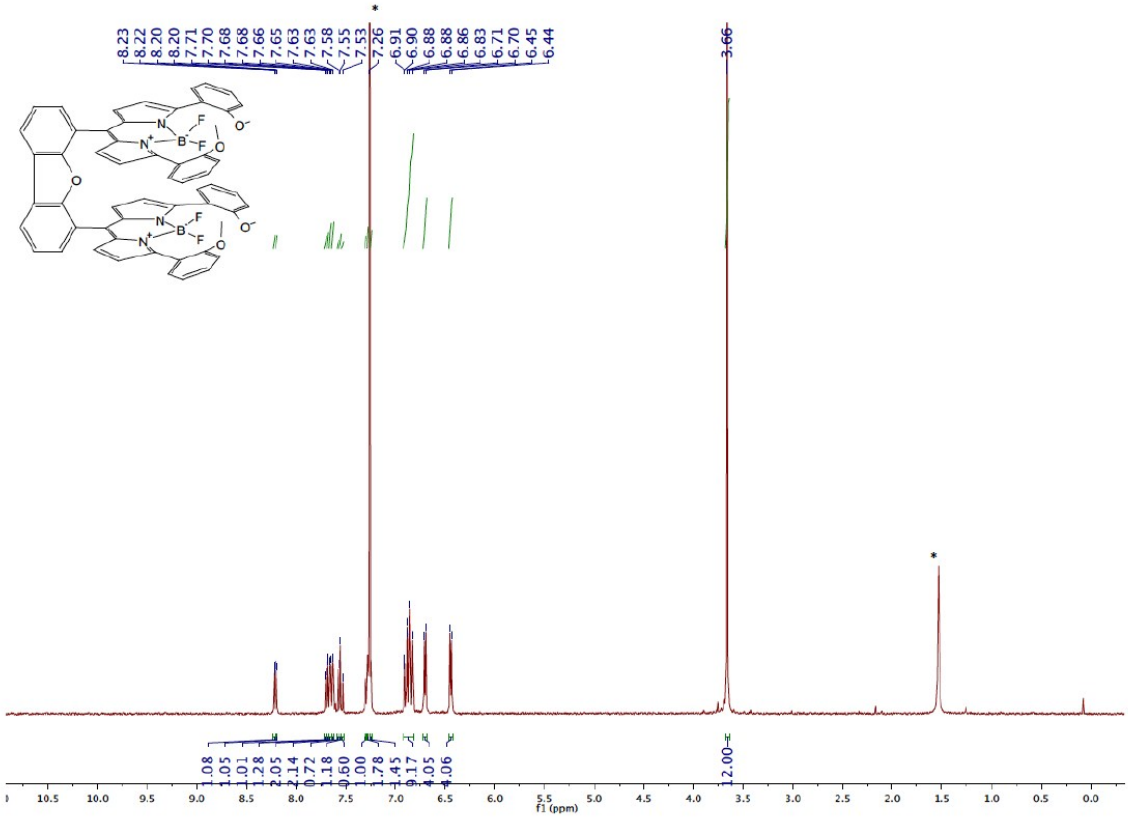


Figure S9. ^{1}H NMR of **DPO-OMe** (**7**) ($CDCl_3$, 298K).

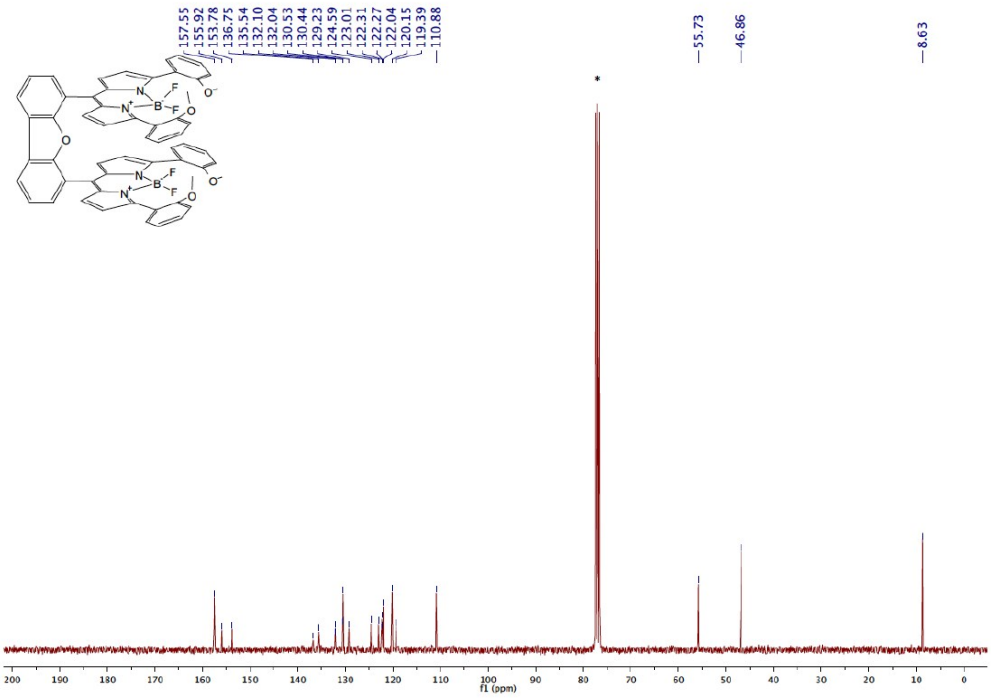


Figure S10. ^{13}C NMR of **DPO-OMe** (**7**) ($CDCl_3$, 298K).

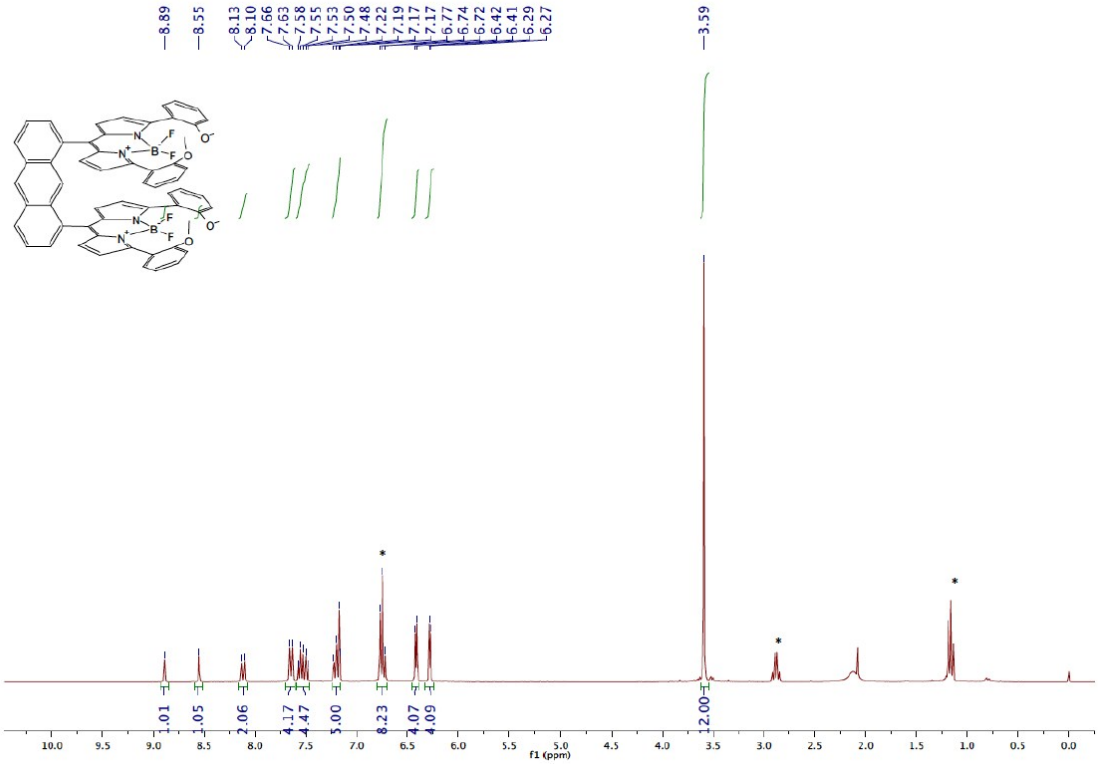


Figure S11. ^{1}H NMR of **DPA-OMe** (**8**) ($CDCl_3$, 298K).

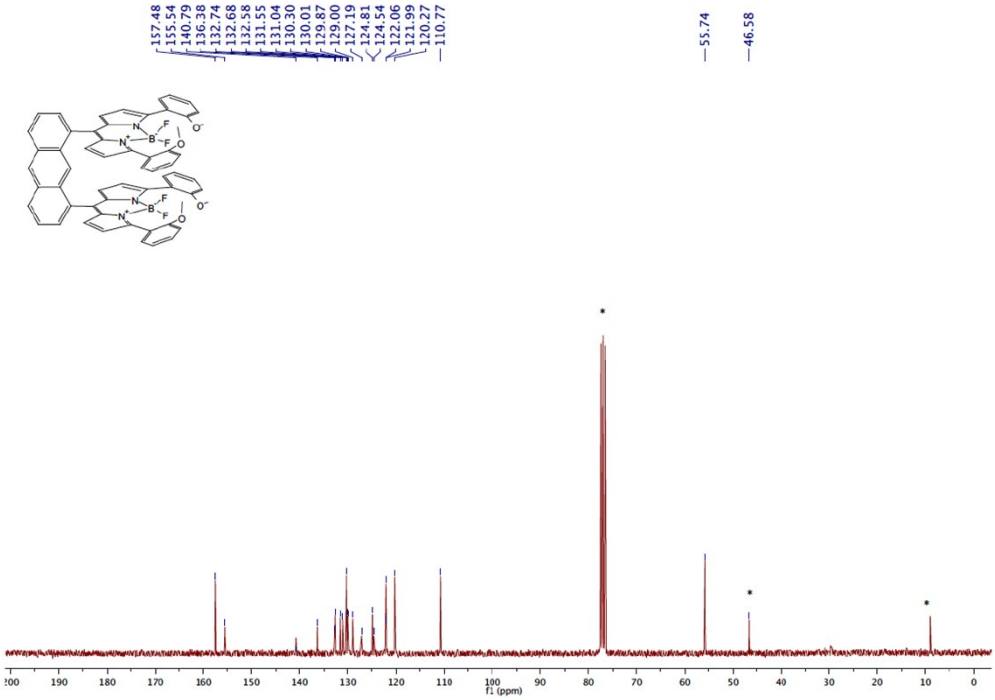


Figure S12. ^{13}C NMR of **DPA-OMe** (**8**) ($CDCl_3$, 298K).

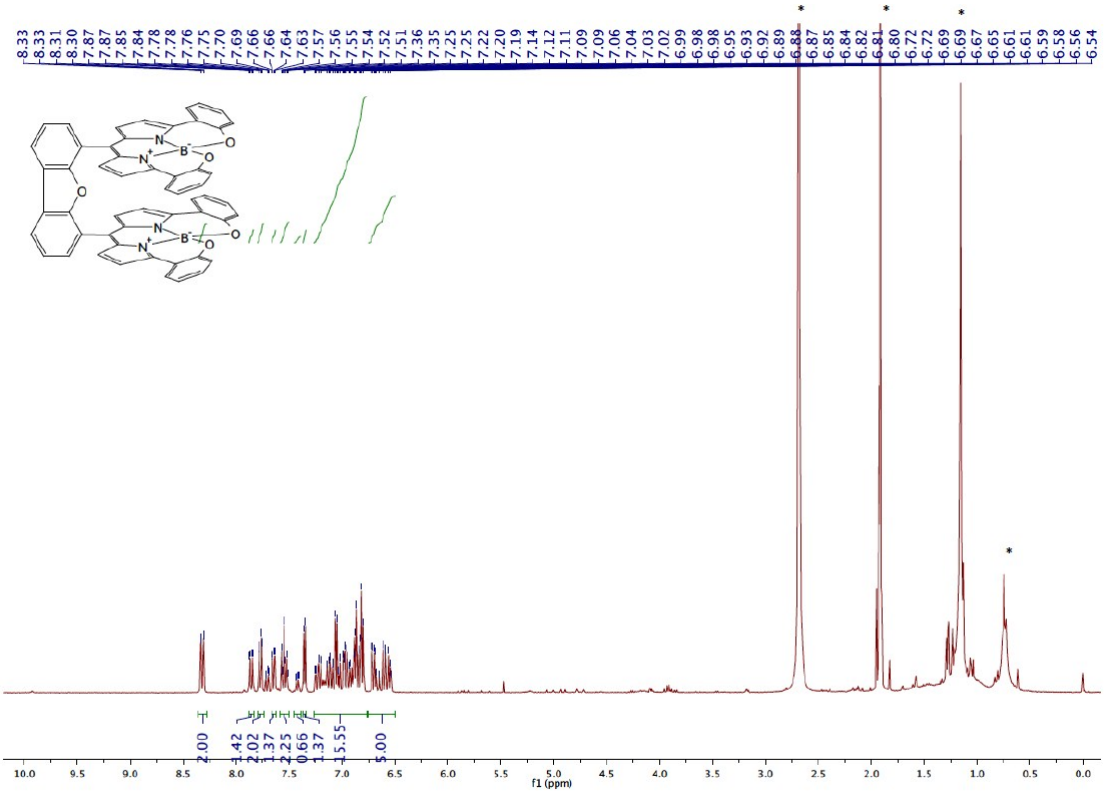


Figure S13. ^{1}H NMR of **DPO-O** (**9**) (d_6-acetone, 298K).

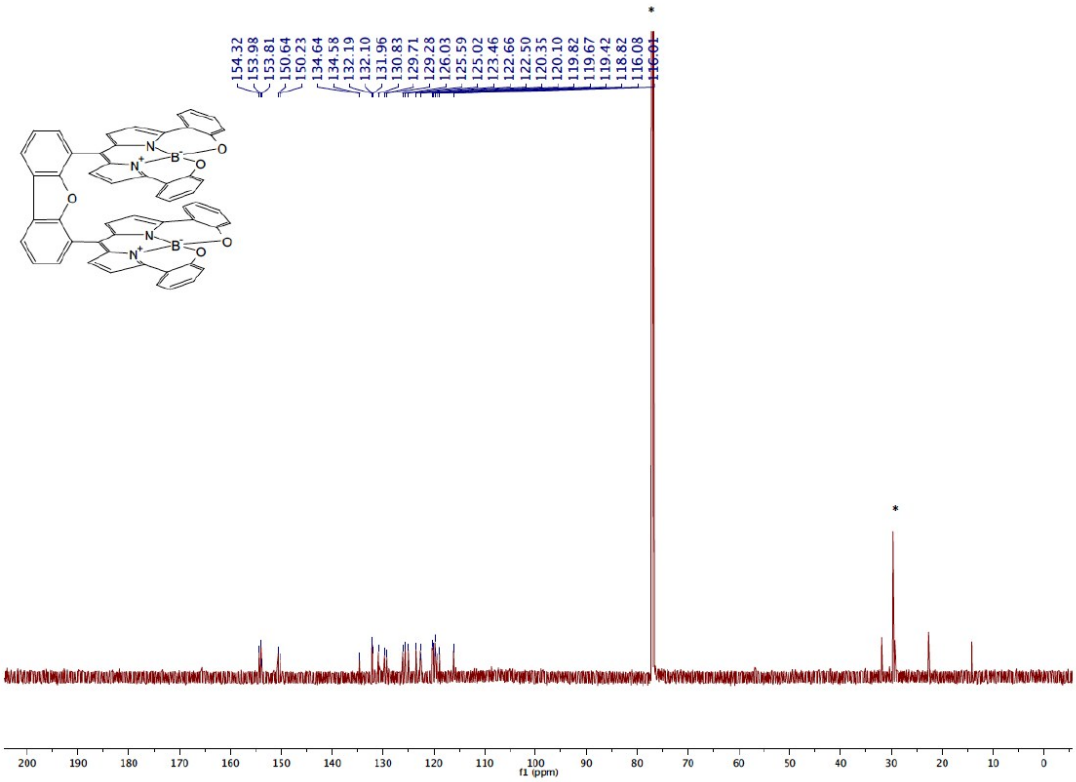


Figure S14. ^{13}C NMR of **DPO-O** (**9**) ($CDCl_3$, 298K).

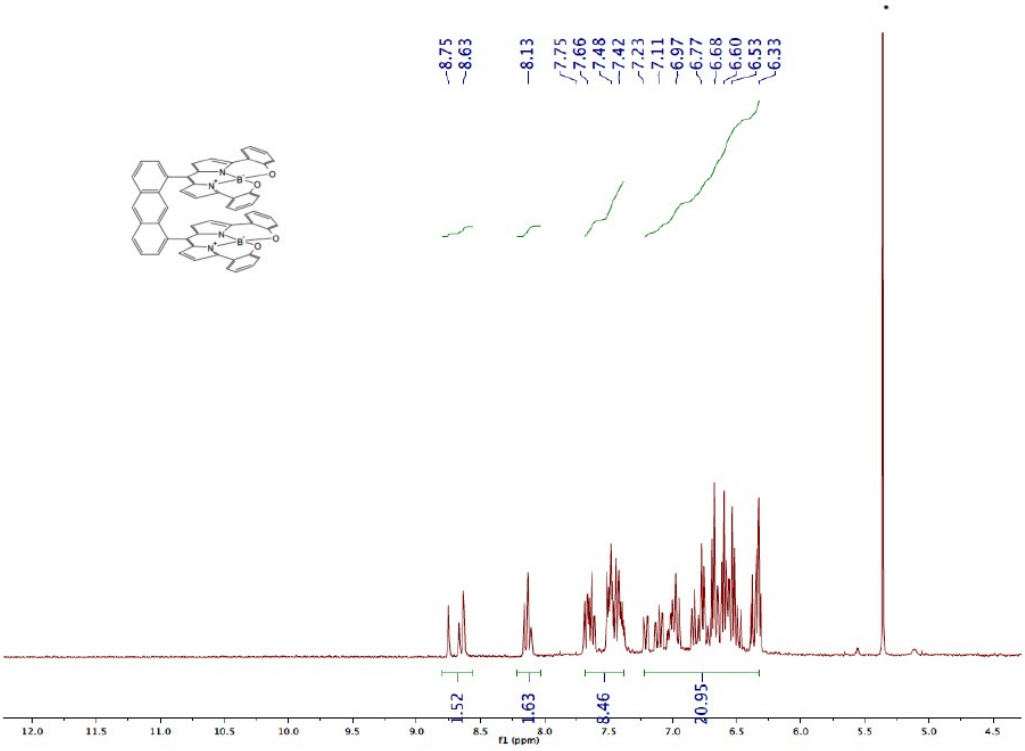


Figure S15. ^{1}H NMR of **DPA-O** (**10**) (d_6-acetone, 298K).

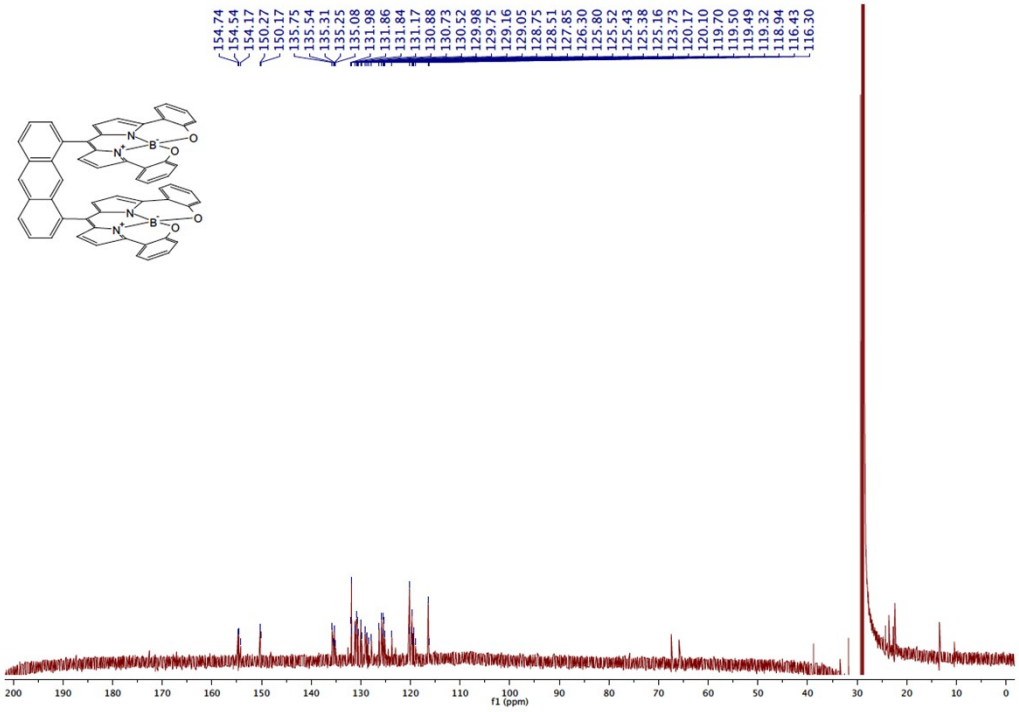
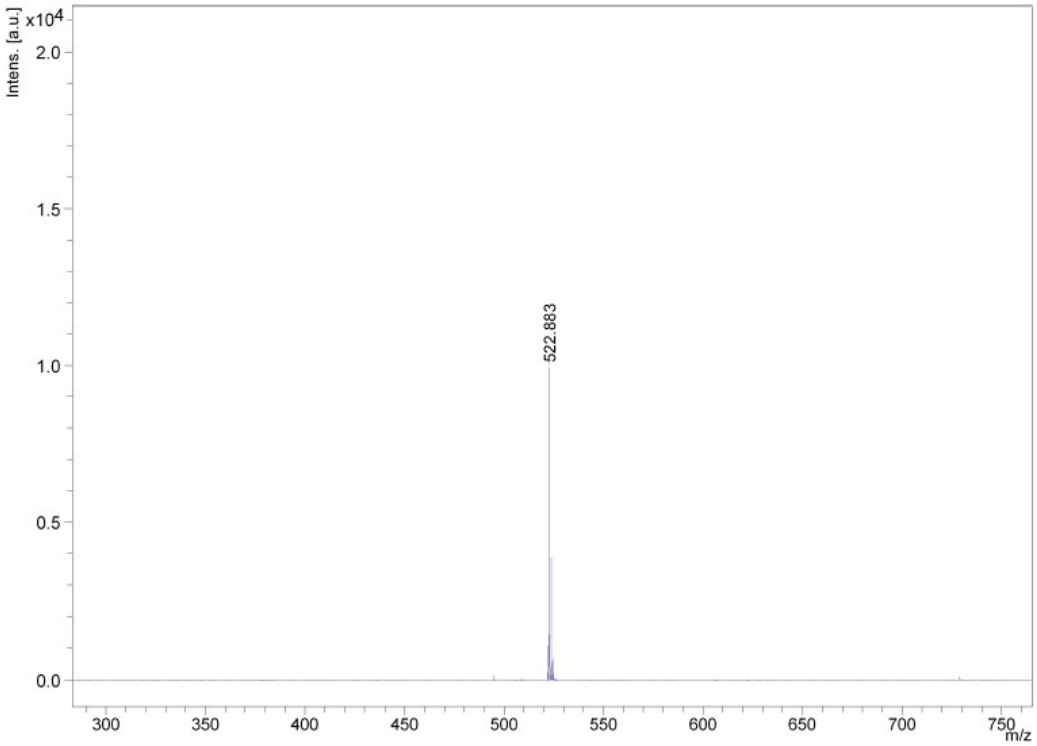
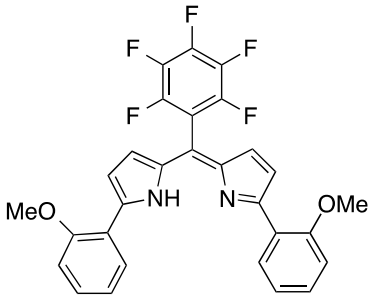


Figure S16. ^{13}C NMR of **DPA-O** (**10**) (d_6-acetone, 298K).





1

Chemical Formula: $C_{29}H_{19}F_5N_2O_2$
Exact Mass: 522.1367
Molecular Weight: 522.4750

Figure S17. MALDI-TOF mass spectrum of **1**.

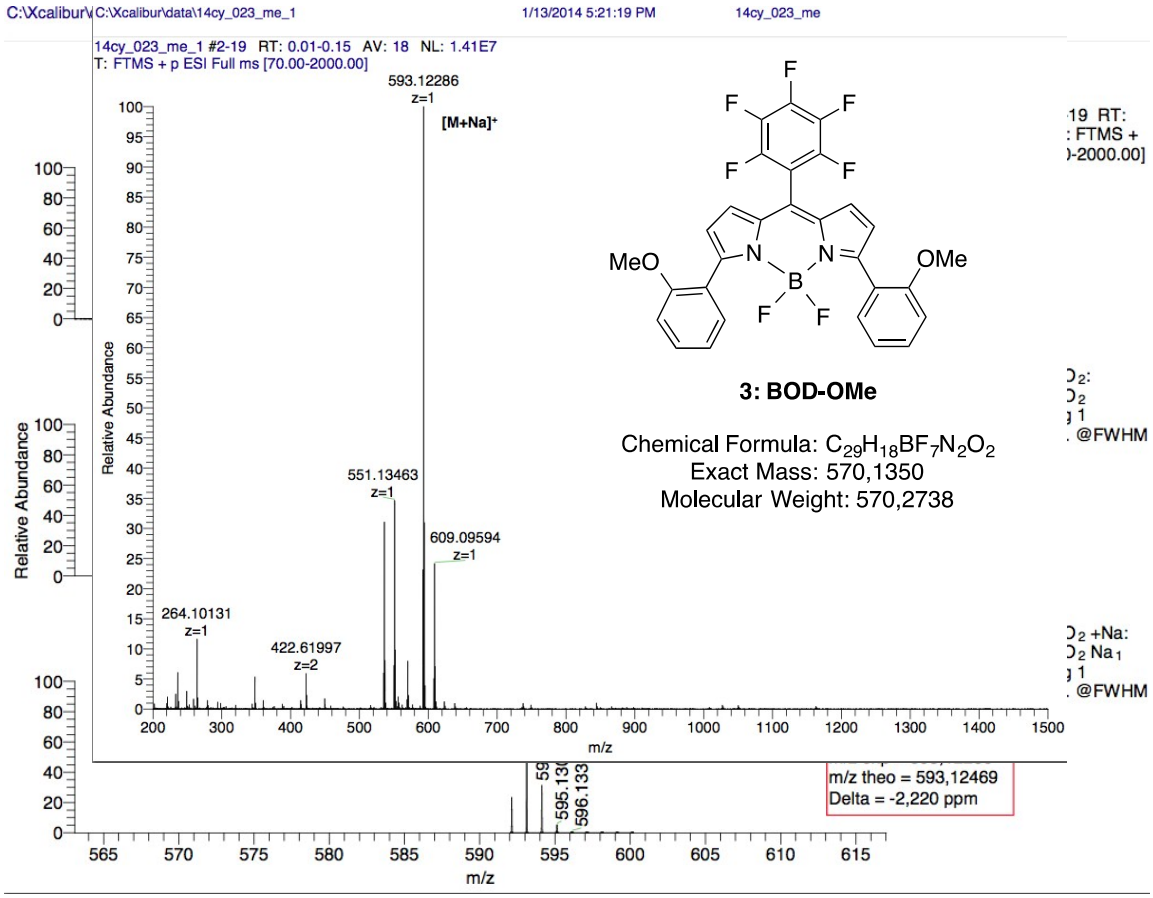
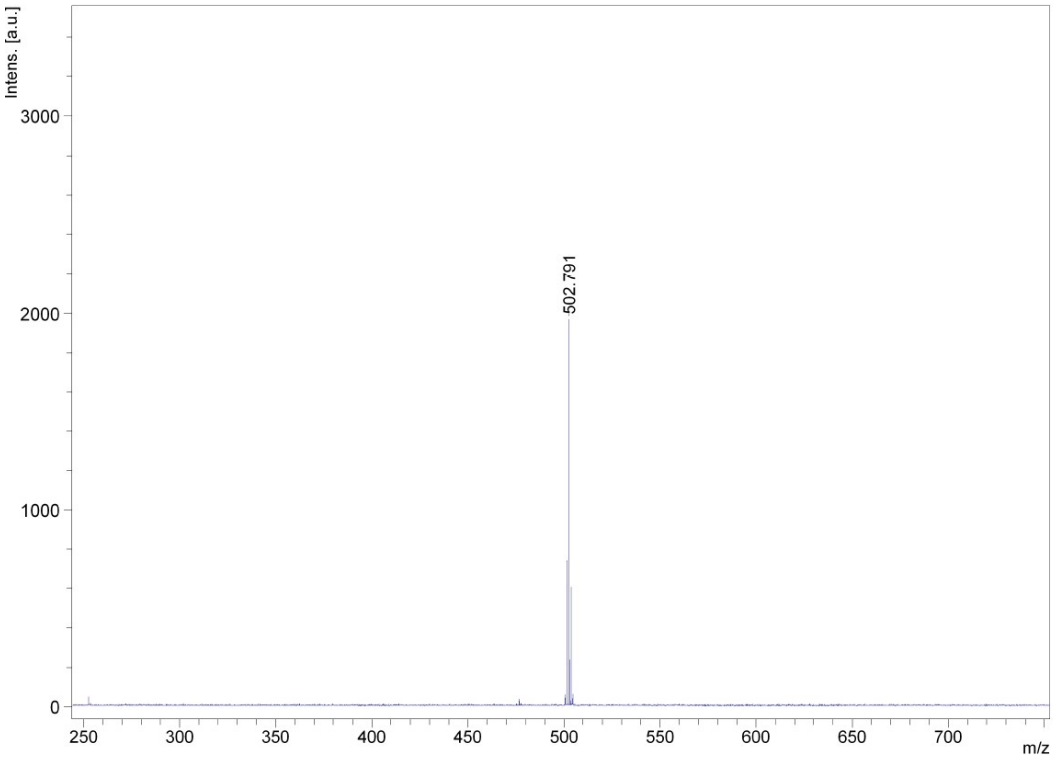
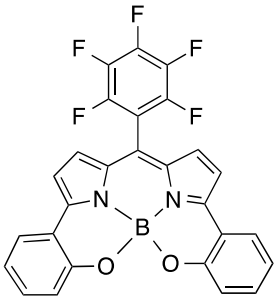


Figure S18. HRMS (ESI) mass spectra of **BOD-OMe (3)**.





4: BOD-O

Chemical Formula: $C_{27}H_{12}BF_5N_2O_2$
Exact Mass: 502.0912
Molecular Weight: 502.2070

Figure S19. MALDI-TOF mass spectrum of **BOD-O (4)**.

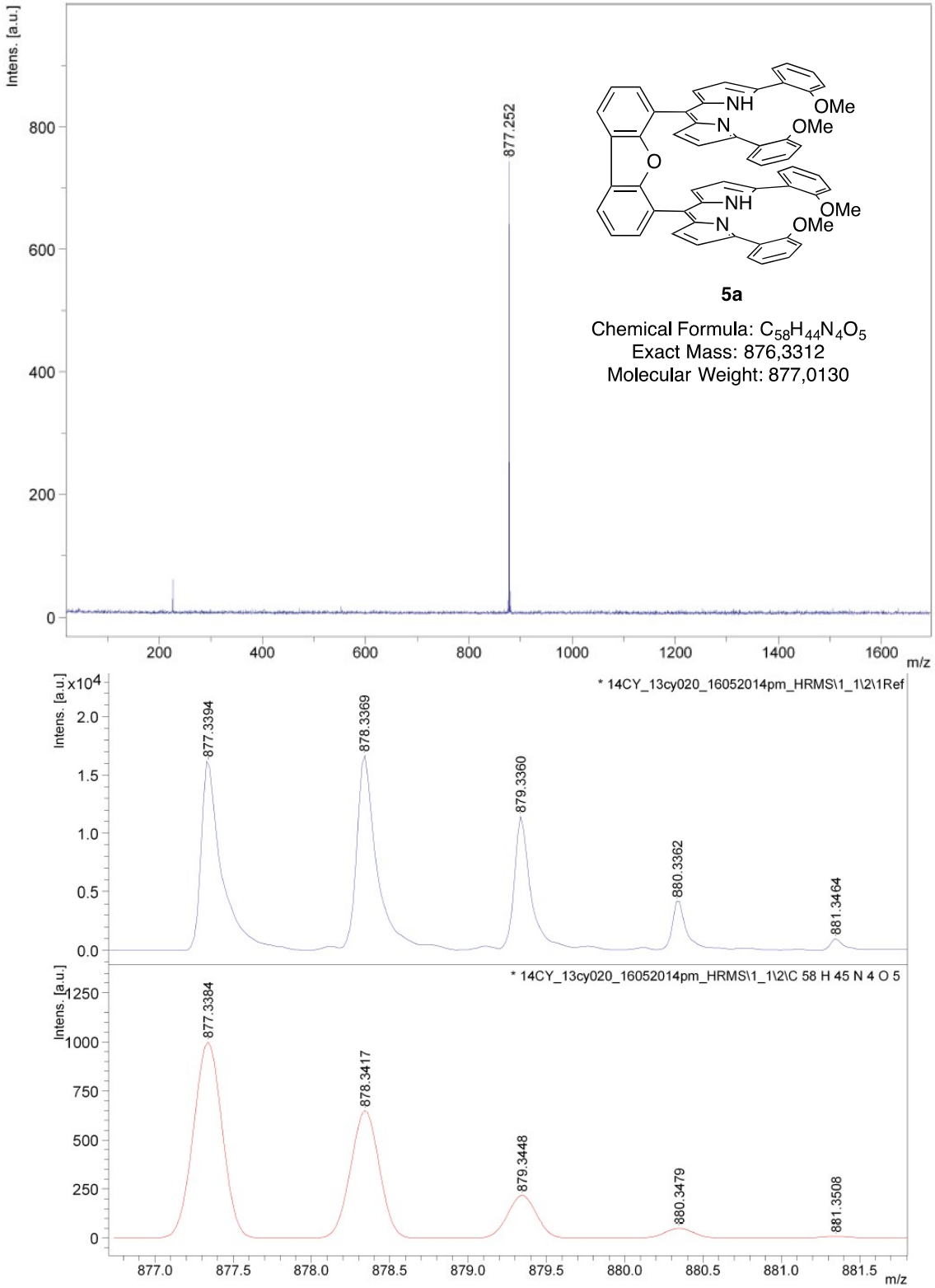
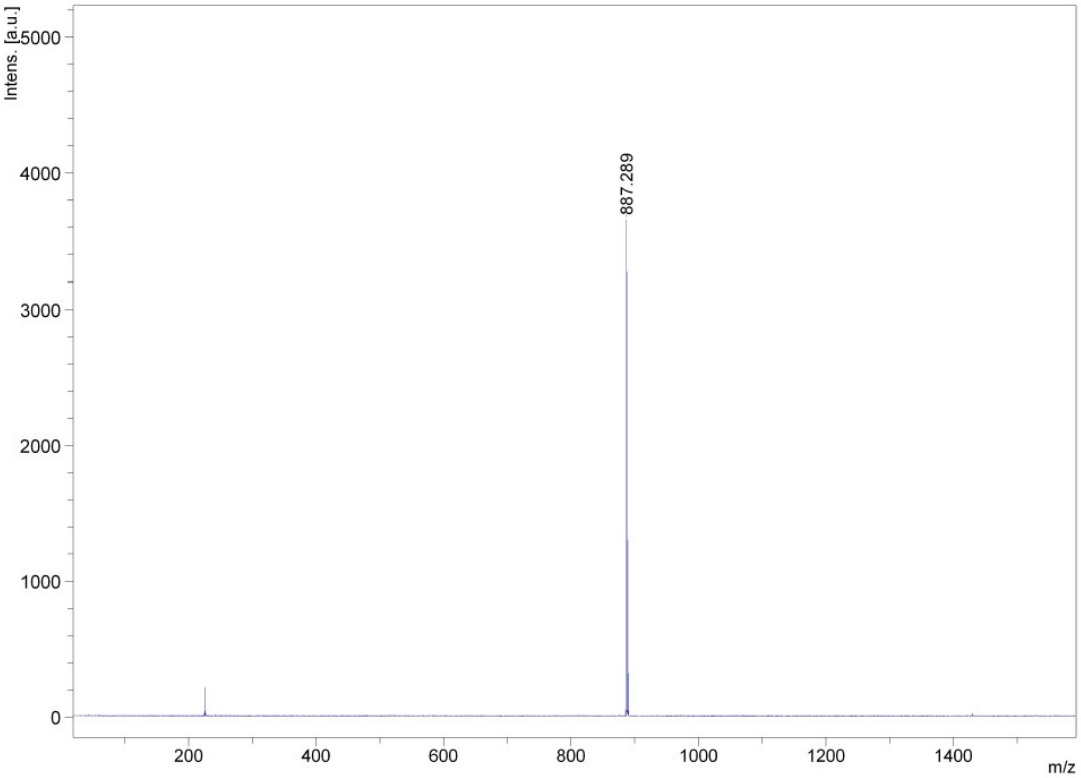
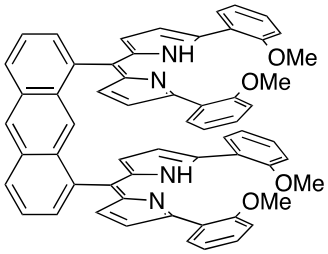


Figure S20. HRMS (MALDI-TOF) mass spectra of **5a**.

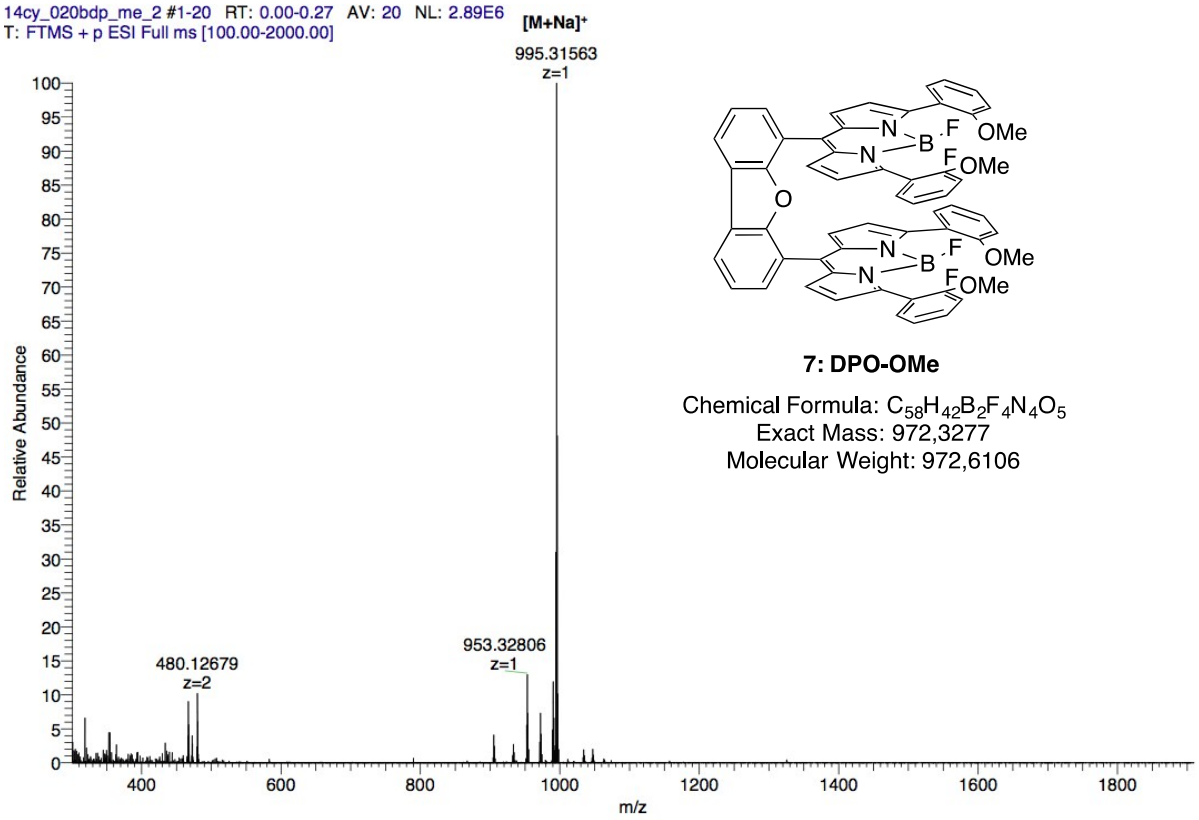




6a

Chemical Formula: $C_{60}H_{46}N_4O_4$
Exact Mass: 886.3519
Molecular Weight: 887.0520

Figure S21. MALDI-TOF mass spectrum of **6a**.



7: DPO-OMe

Chemical Formula: $C_{58}H_{42}B_2F_4N_4O_5$
Exact Mass: 972,3277
Molecular Weight: 972,6106

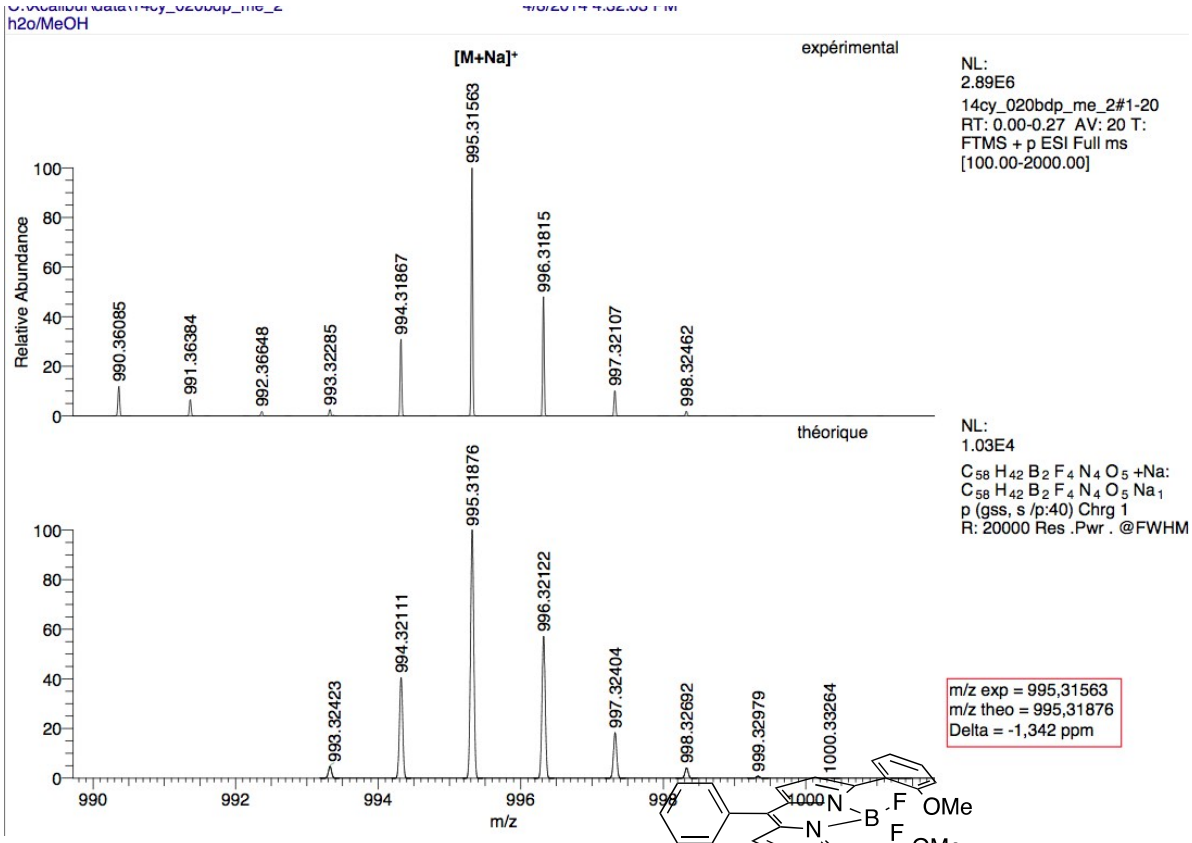
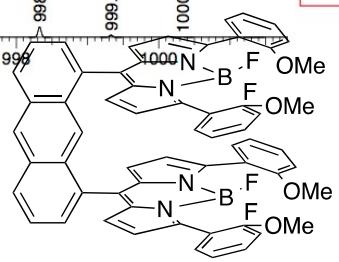
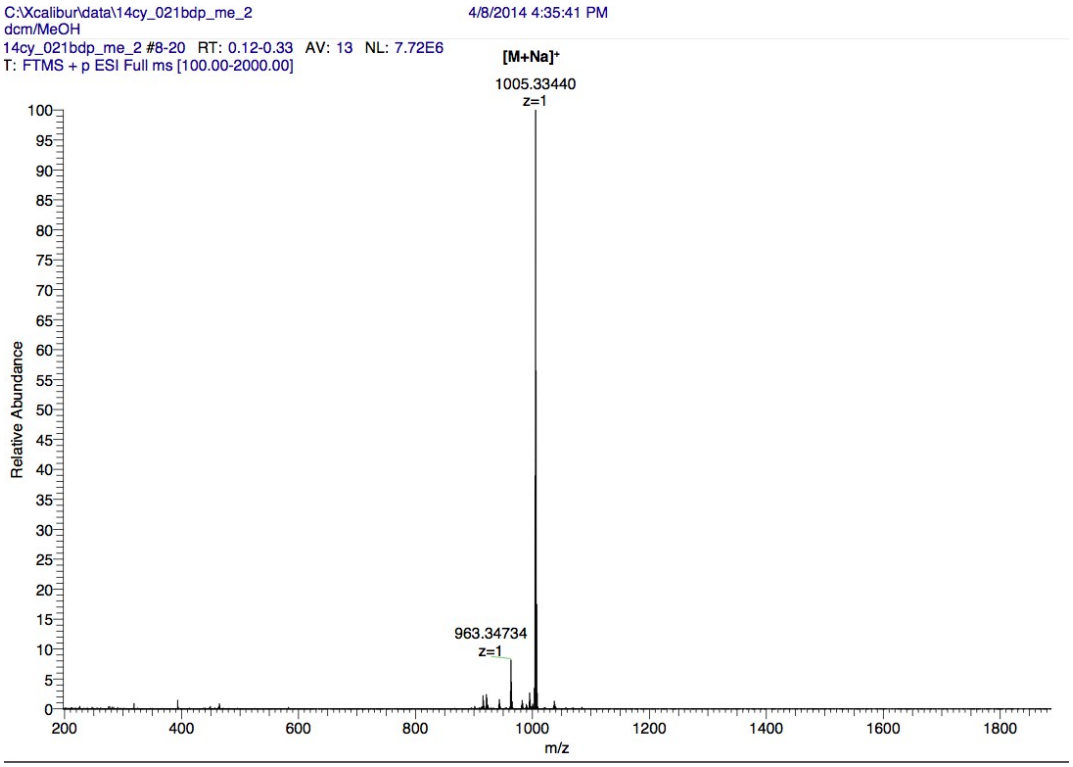


Figure S22. HRMS (ESI) mass spectra of **DPO-OMe (7)**.



8: DPA-OMe

Chemical Formula: $C_{60}H_{44}B_2F_4N_4O_4$
Exact Mass: 982,3485
Molecular Weight: 982,6496



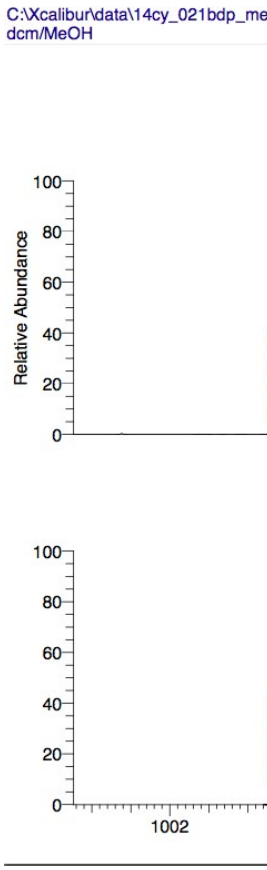


Figure S23. HRMS (ESI) mass spectra of **DPA-OMe (8)**.

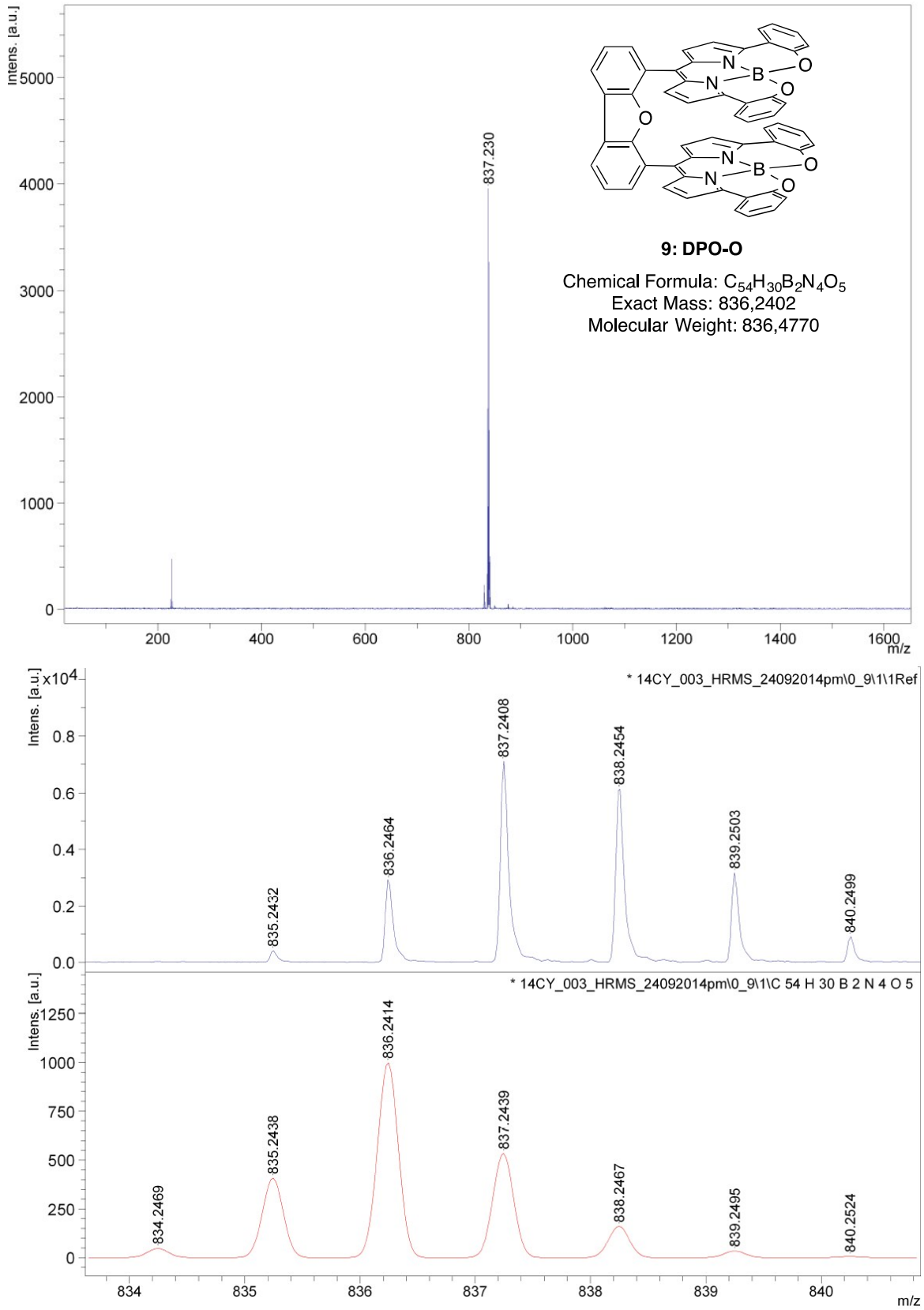
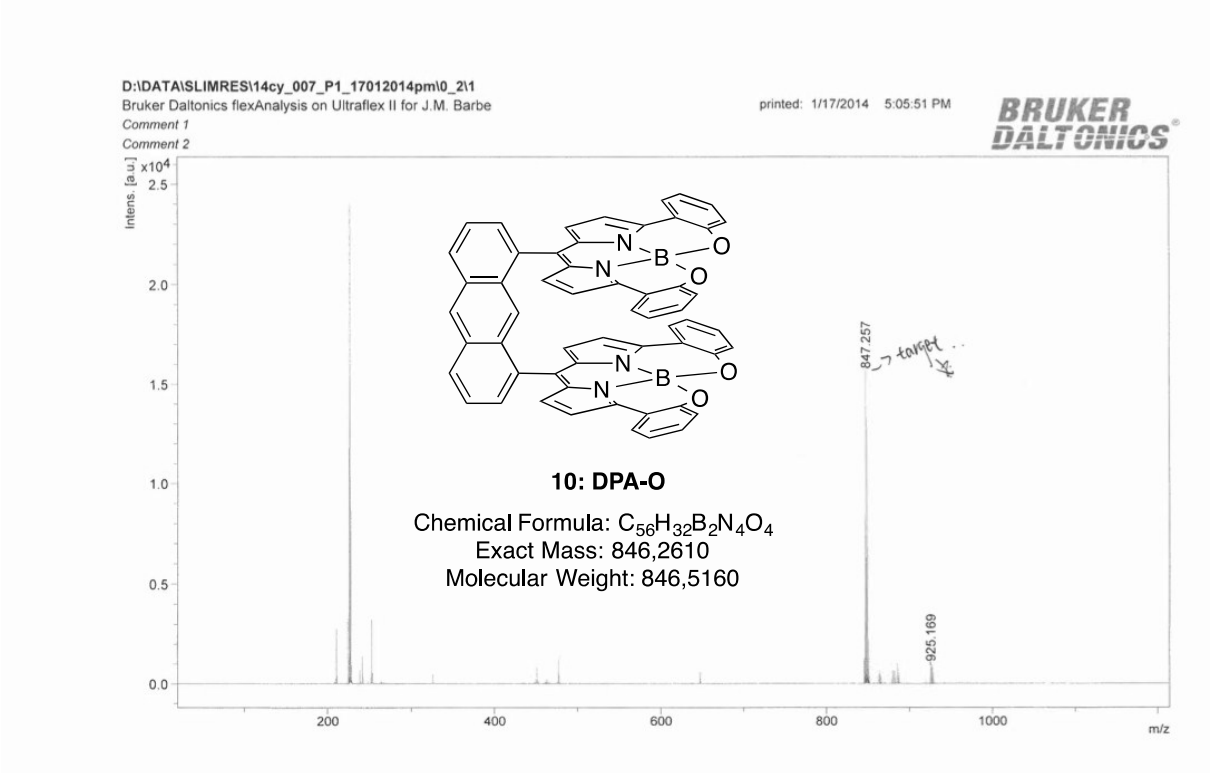


Figure S24. HRMS (MALDI-TOF) mass spectra of **DPO-O (9)**.



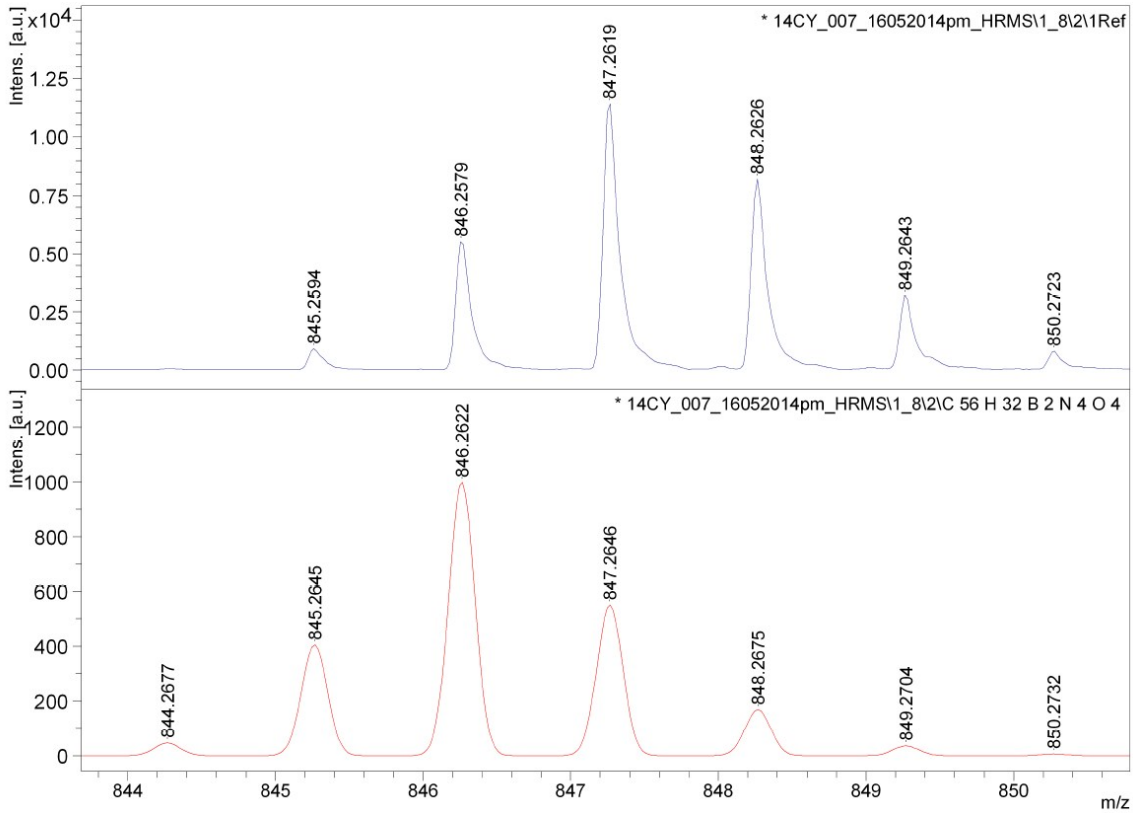


Figure S25. HRMS (MALDI/TOF) mass spectra of **DPA-O (10)**.

Calculation Procedure

All density functional theory (DFT) and time dependent density functional theory (TD-DFT) calculations were performed with Gaussian 09 [1] at the Université de Sherbrooke with the Mammouth supercomputer supported by *Le Réseau Québécois De Calculs Hautes Performances*. The DFT geometry optimisations as well as TD-DFT calculations [2-11] were carried out using the B3LYP method. A 6-31g* basis set was applied to all atoms [12-17]. All calculations were carried out in a THF solvent field. The calculated absorption spectra were obtained from GaussSum 2.1 [18].

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3. Hohenberg P and Kohn W. *J. Phys. Rev.* 1965; **140**: A1133–1138.
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16. Dobbs KD and Hehre WJ. *J. Comput. Chem.* 1987; **8**: 861–879.
17. Dobbs KD and Hehre WJ. *J. Comput. Chem.* 1987; **8**: 880–893.
18. O'Boyle NM, Tenderholt AL and Langner KM. *J. Comp. Chem.* 2008; **29**: 839–845.

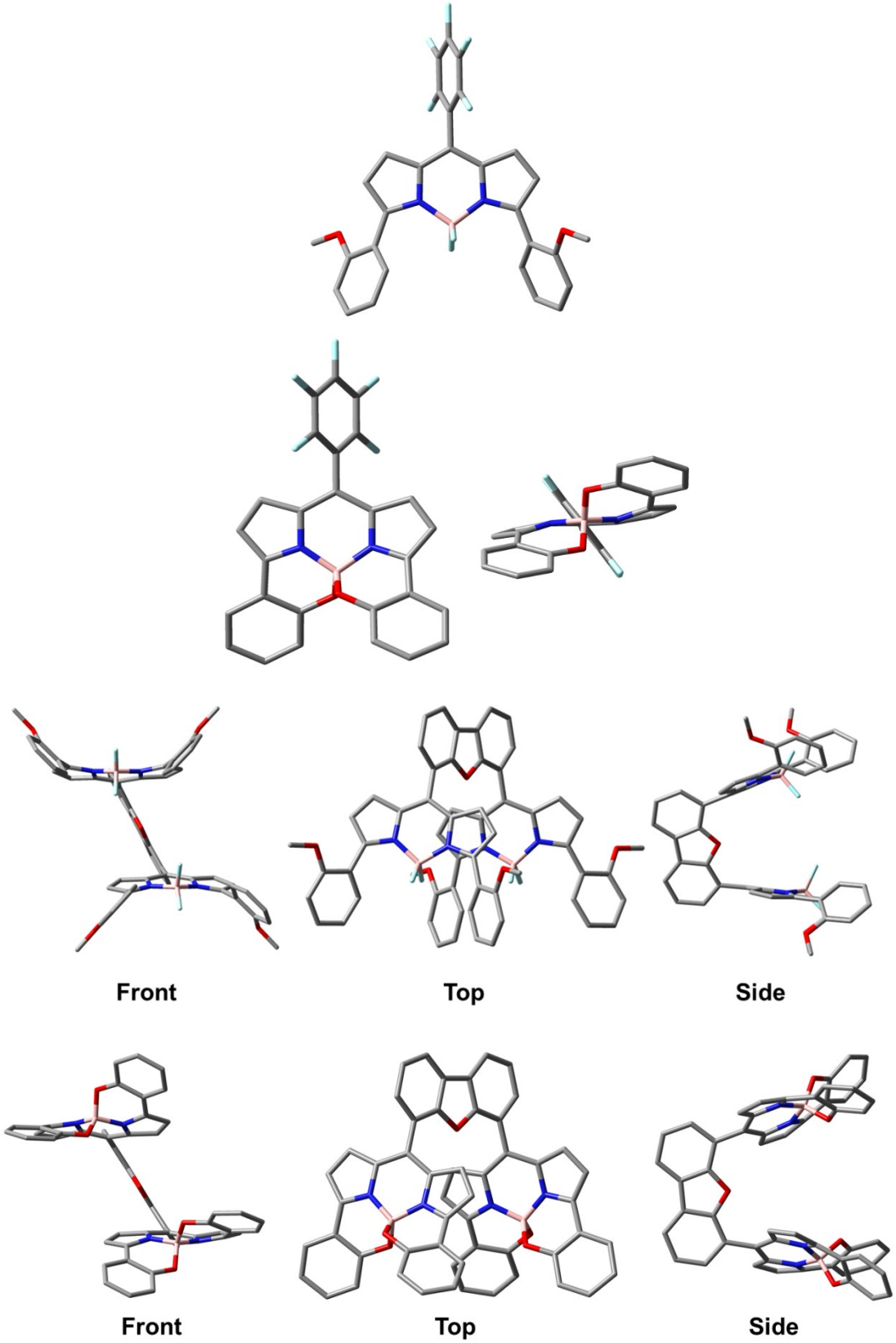

Figure S26. Optimized geometries (DFT, B3LYP) for **BOD-OMe (3)** (first) **BOD-O (4)** (second), **DPO-OMe (7)** (third) and **DPO-O (9)** (fourth).

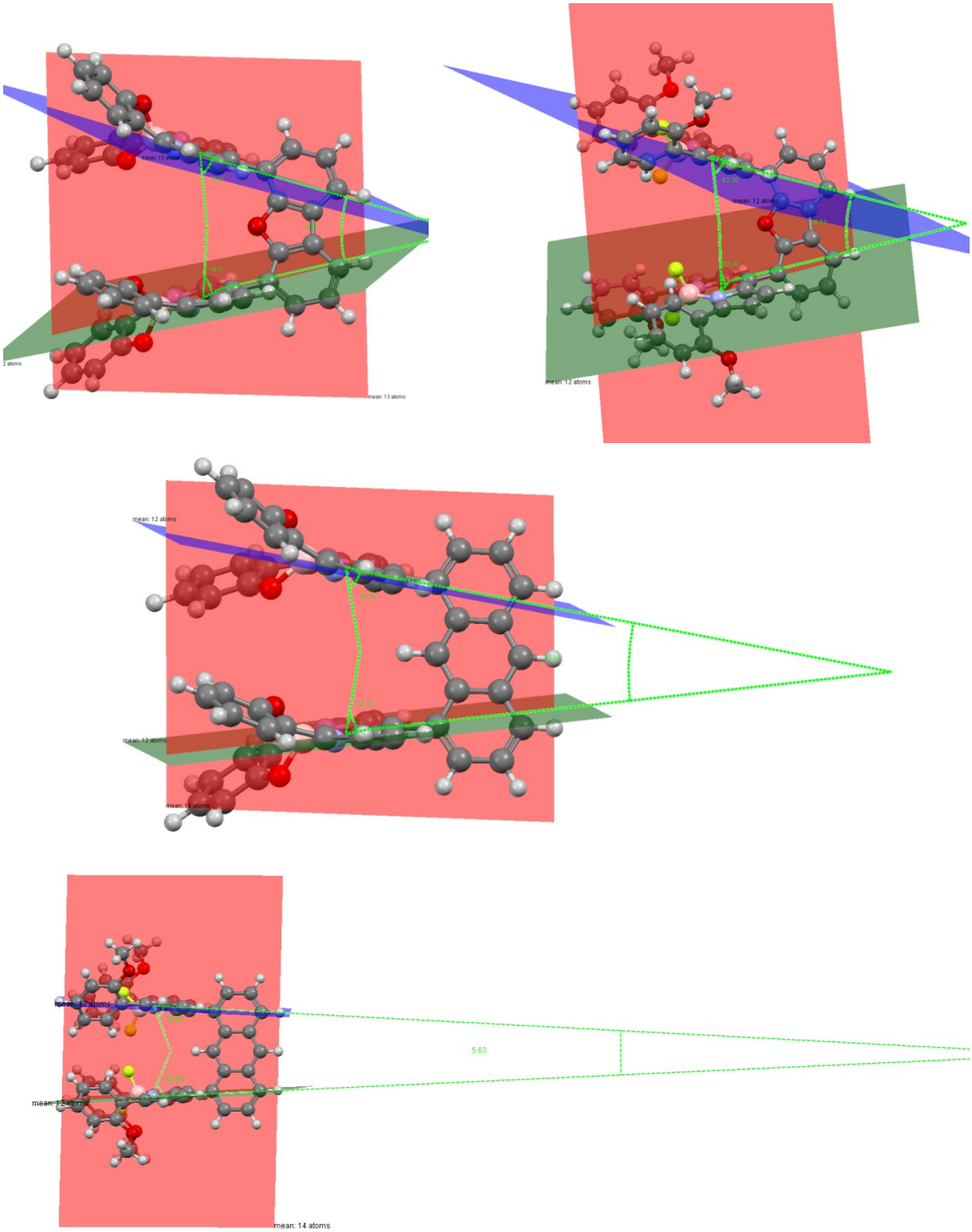

Figure S27. Optimized geometries (DFT, B3LYP) for **DPO-O (9)** (top, left), **DPO-OMe (7)** (top, right), **DPA-O (10)** (middle) and **DPA-OMe (8)** (bottom) showing select structural parameters.

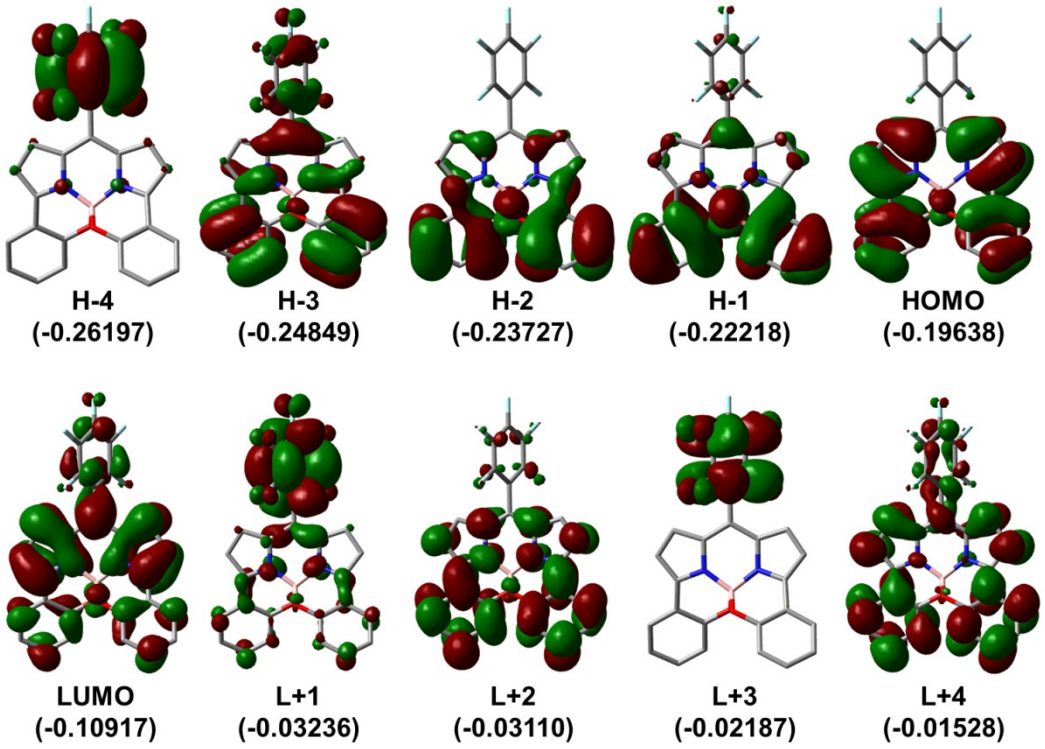

Figure S28. Representations of the frontier MOs for **BOD-O (4).** The energies are in a.u.

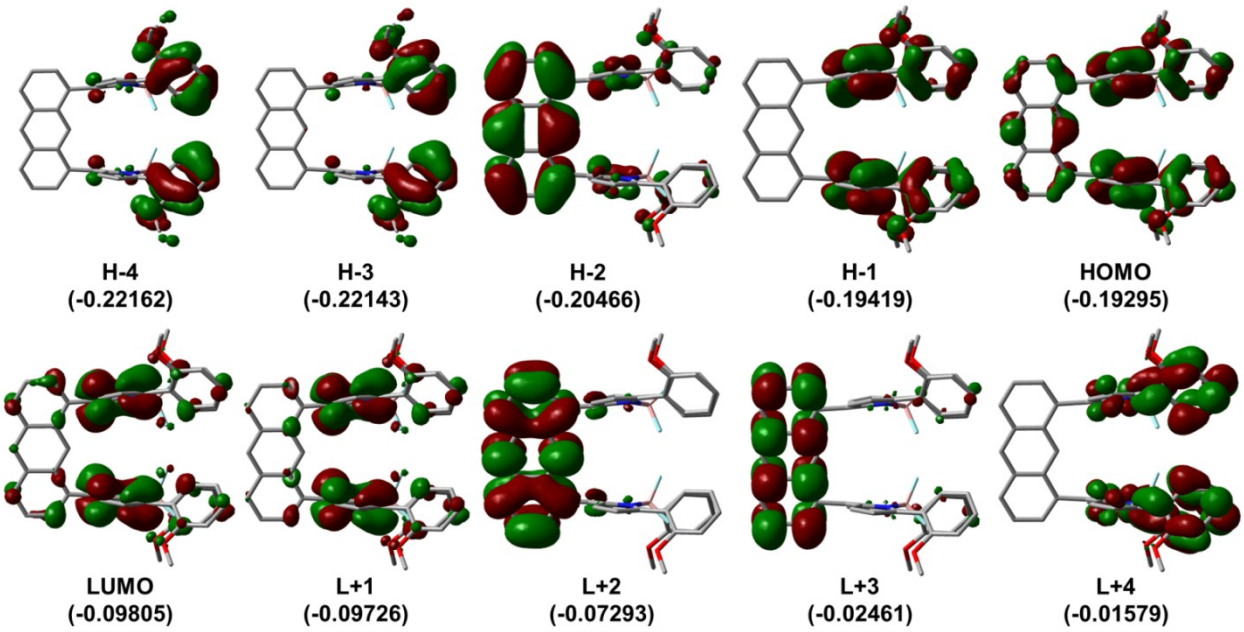

Figure S29. Representations of the frontier MOs for **DPA-OMe (8).** The energies are in a.u.

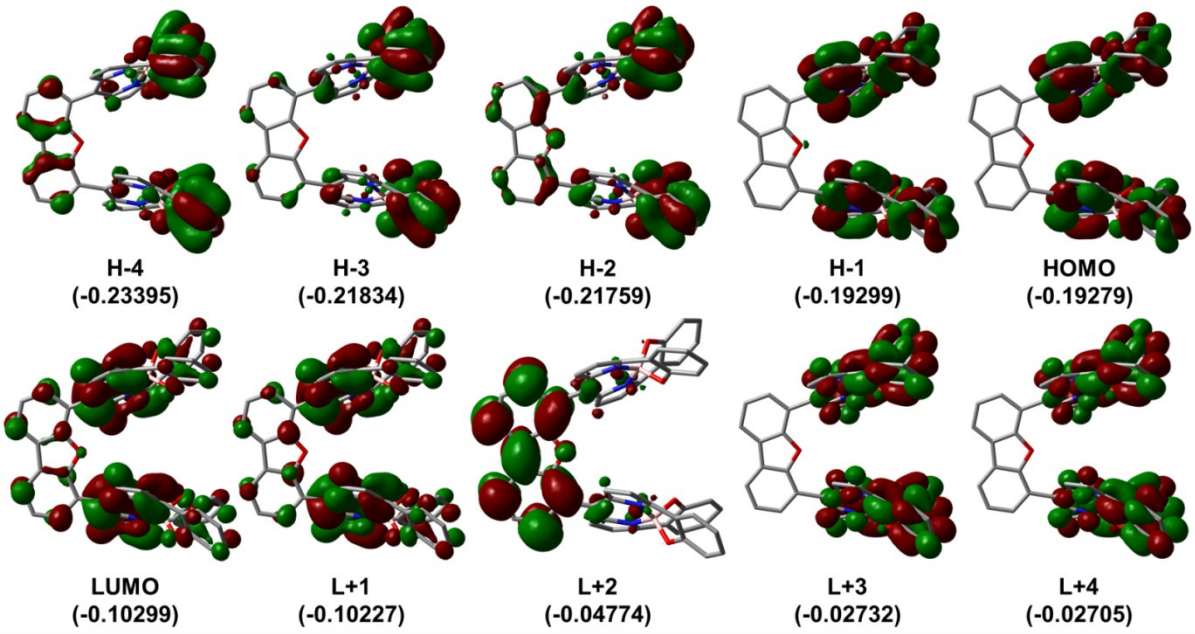

Figure S30. Representations of the frontier MOs for **DPO-O (9).** The energies are in a.u.

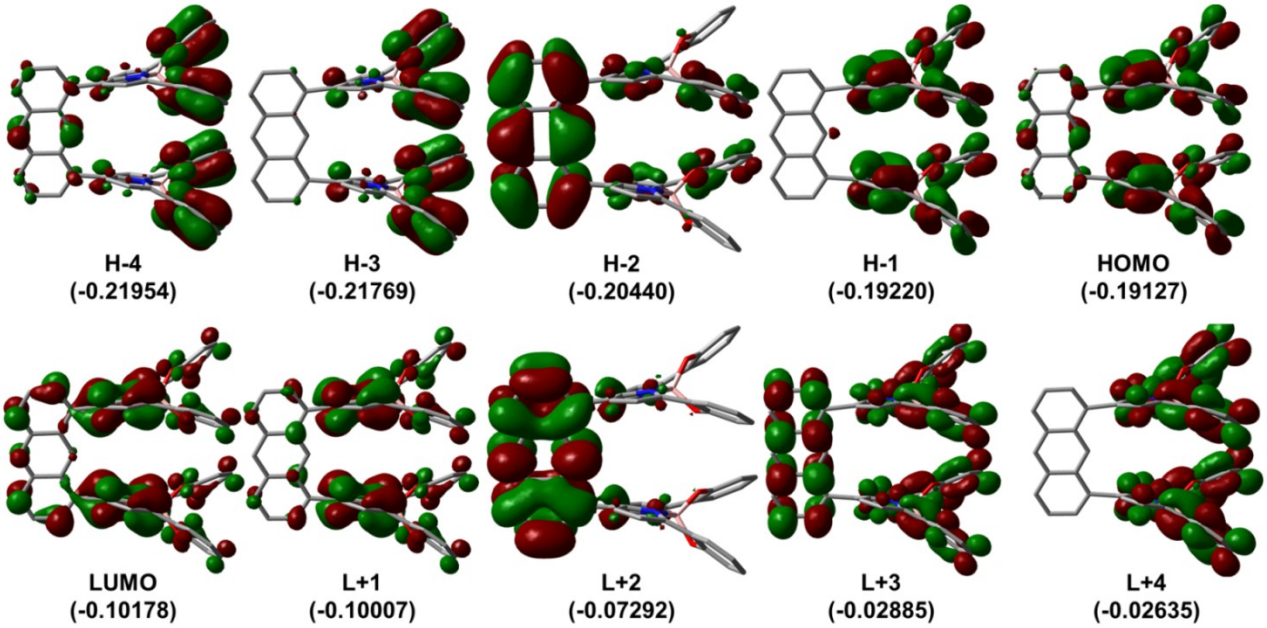

Figure S31. Representations of the frontier MOs for **DPA-O (10).** The energies are in a.u.

Table 1. Percent distribution of the molecular orbitals over selected molecular fragments of **DPA-OMe (8)**.

Molecular Fragment	H-4	H-3	H-2	H-1	HOMO	LUMO	L+1	L+2	L+3	L+4
Anthracene	0.9	1.5	**77.6**	1.9	12.6	13.3	7.9	**92.0**	**88.7**	1.2
BODIPY 1	**49.4**	**49.4**	11.2	**49.1**	**43.6**	**43.2**	**46.2**	4.0	5.7	**49.2**
BODIPY 2	**49.6**	**49.2**	11.2	**49.0**	**43.8**	**43.5**	**45.9**	4.0	5.7	**49.6**

Table 2. Percent distribution of the molecular orbitals over selected molecular fragments of **DPO-O (9)**.

Molecular Fragment	H-4	H-3	H-2	H-1	HOMO	LUMO	L+1	L+2	L+3	L+4
Dibenzofuran	9.3	3.9	8.6	2.9	5.0	12.7	10.1	**86.0**	1.9	3.8
BODIPY 1	**45.1**	**48.1**	**45.7**	**48.6**	**47.4**	**43.6**	**45.0**	7.0	**49.1**	**48.0**
BODIPY 2	**45.6**	**48.0**	**45.7**	**48.5**	**47.5**	**43.6**	**45.0**	7.0	**49.0**	**48.1**

Table 3. Percent distribution of the molecular orbitals over selected molecular fragments of **DPA-O (10)**.

Molecular Fragment	H-4	H-3	H-2	H-1	HOMO	LUMO	L+1	L+2	L+3	L+4
Anthracene	7.8	2.2	**72.8**	3.9	9.1	17.8	9.0	**86.9**	**43.2**	3.0
BODIPY 1	**46.1**	**48.9**	13.6	**48.0**	**45.5**	**41.1**	**45.5**	6.6	**28.4**	**48.5**
BODIPY 2	**46.1**	**48.9**	13.6	**48.0**	**45.5**	**41.1**	**45.5**	6.6	**28.4**	**48.5**

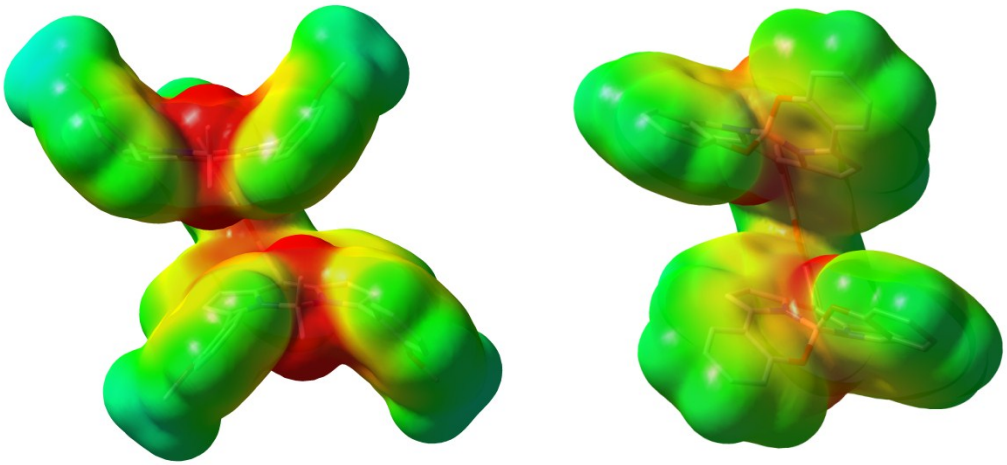

Figure S32. Electronic density map (DFT) for **DPA-OMe (8)** and **DPA-O (10)**. The red and blue areas are respectively the electron rich and poor segments of the molecule.

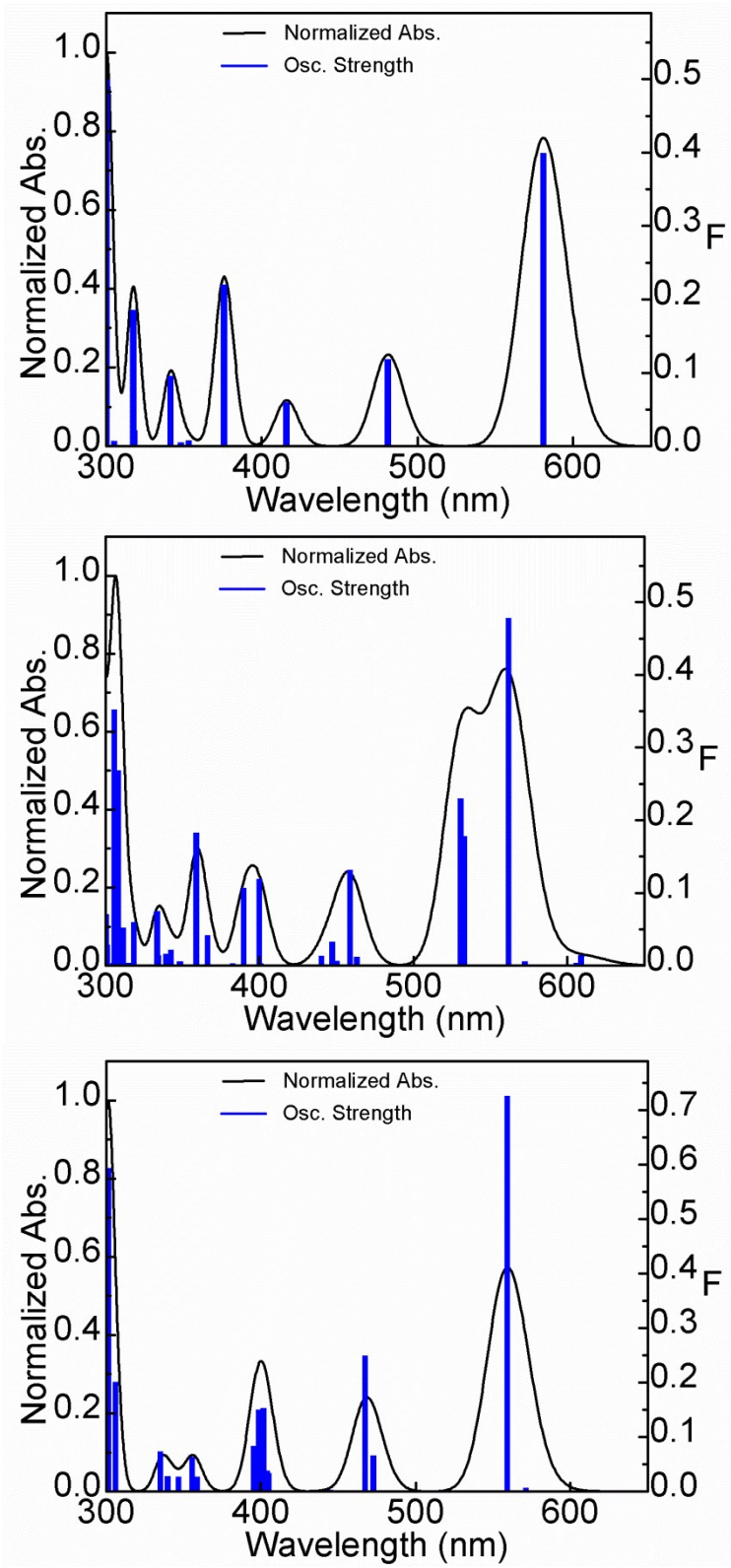

Figure S33. Graphs reported the computed oscillator strength (F) as a function of the calculated positions of the first 75 electronic transitions for **BOD-O (4)** (top), **DPA-O (10)** (middle) and **DPO-O (9)** (bottom).

Table 4. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **BOD-OMe (3)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	533.5	0.6403	HOMO→LUMO (96)
2	452.8	0.0826	H-1→LUMO (99)
3	421.0	0.0845	H-2→LUMO (95)
4	362.9	0.0483	H-4→LUMO (77), H-3→LUMO (21)
5	359.1	0.1597	H-4→LUMO (21), H-3→LUMO (75)
6	346.9	0.0013	H-5→LUMO (99)
7	337.4	0.0443	H-6→LUMO (94)
8	323.7	0.035	H-8→LUMO (94)
9	318.7	0.0469	H-7→LUMO (86)
10	313.0	0.0168	HOMO→L+1 (98)
11	288.4	0.151	HOMO→L+2 (92)
12	279.1	0.2537	HOMO→L+3 (91)
13	266.6	0.0039	HOMO→L+4 (91)
14	256.0	0.0062	H-1→L+1 (93)
15	253.6	0.0135	H-1→L+2 (30), H-1→L+3 (16), HOMO→L+6 (21)
16	252.8	0.0155	H-9→LUMO (11), H-2→L+2 (12), H-1→L+4 (15), HOMO→L+5 (31)
17	246.5	0.0078	H-2→L+1 (94)
18	245.4	0.2013	H-9→LUMO (66)
19	240.8	0.0275	H-1→L+2 (47), HOMO→L+6 (27)
20	240.7	0.0044	HOMO→L+7 (89)
21	237.7	0.0369	H-5→L+1 (13), H-1→L+3 (42), HOMO→L+6 (33)
22	236.6	0.0021	H-10→LUMO (13), H-2→L+2 (26), HOMO→L+5 (36)
23	235.4	0.0147	H-12→LUMO (20), H-10→LUMO (40), H-2→L+2 (11)
24	234.1	0.0263	H-8→L+2 (11), H-5→L+1 (43), H-1→L+3 (21)
25	231.9	0.0161	H-2→L+2 (37), H-1→L+4 (51)
26	229.9	0.0007	H-11→LUMO (83), H-10→LUMO (12)
27	229.3	0.0244	H-12→LUMO (27), H-10→LUMO (12), H-2→L+3 (33)
28	228.9	0.0016	H-13→LUMO (17), H-12→LUMO (20), H-2→L+3 (38), H-1→L+4 (10)
29	227.9	0.0071	H-13→LUMO (72), H-12→LUMO (10)
30	226.2	0.0252	H-2→L+4 (70)
31	225.3	0.0026	H-4→L+1 (74), H-3→L+1 (19)
32	224.2	0.0041	H-4→L+1 (19), H-3→L+1 (76)
33	221.3	0.0002	H-14→LUMO (83), H-12→LUMO (10)
34	217.6	0.0136	H-6→L+1 (95)
35	216.1	0.0144	H-3→L+2 (47), H-3→L+3 (13), H-1→L+5 (21)
36	213.5	0.0063	H-4→L+2 (73), HOMO→L+8 (15)
37	212.7	0.0261	H-3→L+4 (13), H-1→L+6 (29), HOMO→L+8 (28)
38	210.1	0.0379	H-4→L+3 (25), H-3→L+2 (21), H-3→L+3 (25)
39	209.8	0.0603	H-4→L+3 (26), H-3→L+2 (15), H-3→L+3 (11)

40	209.3	0.0106	H-15→LUMO (67)
41	208.8	0.0024	H-7→L+1 (82)
42	207.9	0.1781	H-4→L+3 (35), H-1→L+6 (17), HOMO→L+8 (18)
43	207.7	0.0421	H-16→LUMO (18), H-6→L+2 (45), H-4→L+4 (15)
44	207.1	0.0028	H-1→L+7 (90)
45	206.6	0.0343	H-16→LUMO (18), H-3→L+3 (18), H-2→L+6 (10), H-1→L+5 (31)
46	206.3	0.0119	H-16→LUMO (47), H-15→LUMO (12)
47	205.6	0.0124	H-5→L+2 (31), H-5→L+7 (50)
48	204.6	0.0174	H-2→L+5 (56), H-1→L+6 (18)
49	204.0	0.0065	H-6→L+2 (21), H-6→L+3 (42), H-4→L+4 (17)
50	203.9	0.003	H-17→LUMO (14), H-8→L+1 (29), H-5→L+2 (13), H-5→L+7 (16)
51	201.9	0.0111	H-17→LUMO (45), H-7→L+2 (16), H-3→L+4 (14)
52	201.7	0.1402	H-17→LUMO (24), H-7→L+2 (17), H-3→L+4 (17)
53	201.6	0.0326	H-6→L+3 (16), H-4→L+4 (11), H-2→L+6 (43)
54	200.7	0.005	H-5→L+2 (10), H-5→L+3 (20), H-2→L+7 (43)
55	200.6	0.0076	H-19→LUMO (42), H-18→LUMO (11), H-2→L+7 (28)
56	200.2	0.0252	H-19→LUMO (10), H-5→L+3 (31), H-2→L+7 (23)
57	198.8	0.0415	H-6→L+3 (16), H-4→L+4 (30)
58	198.0	0.0496	H-19→LUMO (18), H-18→LUMO (54)
59	196.9	0.0274	H-7→L+2 (34), H-7→L+3 (39)
60	196.7	0.0159	H-8→L+7 (35), H-3→L+7 (11)
61	196.0	0.0239	H-8→L+7 (16), HOMO→L+9 (47)
62	194.7	0.0726	H-6→L+4 (80)
63	193.7	0.0004	H-5→L+4 (97)
64	193.1	0.0008	H-8→L+2 (35), H-8→L+3 (29), H-8→L+7 (10)
65	191.4	0.0228	H-20→LUMO (17), H-1→L+8 (28)
66	190.9	0.0387	H-7→L+3 (10), H-3→L+5 (10), H-1→L+8 (30)
67	190.6	0.0319	H-20→LUMO (63), H-7→L+4 (11)
68	188.5	0.0643	H-21→LUMO (11), H-4→L+5 (40)
69	188.3	0.0036	H-26→LUMO (11), H-21→LUMO (48), H-4→L+5 (16)
70	187.6	0.0031	H-9→L+1 (11), H-4→L+5 (12), H-4→L+6 (10), H-3→L+5 (10)
71	187.1	0.035	H-6→L+5 (11), H-4→L+6 (54)
72	186.4	0.0463	H-22→LUMO (63)
73	185.8	0.0212	H-9→L+1 (19), H-8→L+4 (52)
74	185.6	0.0873	H-7→L+4 (36)
75	185.5	0.2365	H-9→L+1 (11), H-3→L+6 (15)

Table 5. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **BOD-O (4)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	580.8	0.3993	HOMO→LUMO (99)
2	480.9	0.1187	H-1→LUMO (98)
3	415.8	0.0594	H-2→LUMO (98)
4	375.7	0.2197	H-3→LUMO (92)
5	353.0	0.0076	H-5→LUMO (84), H-4→LUMO (15)
6	348.1	0.0047	H-5→LUMO (15), H-4→LUMO (84)
7	341.3	0.0954	H-6→LUMO (90)
8	318.0	0.0212	HOMO→L+1 (99)
9	317.3	0.1853	H-7→LUMO (81), HOMO→L+2 (17)
10	305.1	0.0068	H-8→LUMO (85), HOMO→L+4 (13)
11	300.2	0.4992	H-7→LUMO (15), HOMO→L+2 (72)
12	293.1	0.0458	HOMO→L+3 (94)
13	276.1	0.0326	H-8→LUMO (10), HOMO→L+4 (82)
14	272.3	0.0725	H-1→L+2 (79), HOMO→L+6 (14)
15	264.4	0.0114	H-1→L+1 (67), HOMO→L+5 (16)
16	258.4	0.0014	H-9→LUMO (97)
17	257.2	0.0005	H-2→L+2 (19), H-1→L+1 (30), HOMO→L+5 (36)
18	251.1	0.004	H-11→LUMO (58), H-10→LUMO (35)
19	247.9	0.1228	H-1→L+2 (13), H-1→L+3 (15), HOMO→L+6 (55)
20	246.7	0.0361	H-1→L+3 (72), HOMO→L+6 (14)
21	245.4	0.0002	HOMO→L+7 (92)
22	243.9	0.0852	H-2→L+2 (25), H-1→L+4 (56)
23	241.6	0.0006	H-2→L+2 (40), HOMO→L+5 (38)
24	239.4	0.0437	H-2→L+1 (89)
25	238.8	0.0347	H-11→LUMO (24), H-10→LUMO (51), H-1→L+4 (12)
26	233.2	0.0056	H-7→L+3 (15), H-4→L+1 (46), H-3→L+3 (20), H-1→L+3 (11)
27	232.3	0.0122	H-12→LUMO (92)
28	229.0	0.0171	H-3→L+2 (70), H-1→L+5 (12)
29	227.8	0.0178	H-3→L+1 (87)
30	225.8	0.0001	H-2→L+3 (99)
31	225.0	0.0184	H-3→L+2 (11), H-2→L+4 (77)
32	219.9	0.02	H-5→L+2 (28), HOMO→L+8 (51)
33	217.8	0.2032	H-1→L+5 (71)
34	217.5	0.0017	H-5→L+2 (11), H-3→L+4 (20), H-1→L+6 (53)
35	217.3	0.0104	H-5→L+1 (95)
36	214.5	0.0105	H-6→L+1 (91)
37	213.8	0.0158	H-6→L+2 (80)
38	212.7	0.0065	H-1→L+7 (87)
39	212.2	0.0004	H-4→L+2 (91)
40	211.8	0.0258	H-7→L+3 (12), H-4→L+1 (12), H-3→L+3 (71)

41	211.3	0.0056	H-5→L+2 (44), H-3→L+4 (25), HOMO→L+8 (12)
42	209.9	0.0053	H-13→LUMO (84), H-2→L+6 (11)
43	209.8	0.1067	H-3→L+4 (39), H-2→L+5 (18), H-1→L+6 (22)
44	205.8	0.0002	H-5→L+3 (93)
45	203.7	0.0048	H-14→LUMO (68), H-4→L+7 (10)
46	203.5	0.0006	H-6→L+3 (88)
47	203.3	0.0044	H-4→L+7 (75)
48	203.1	0.0251	H-7→L+2 (34), H-6→L+3 (10), H-2→L+6 (32)
49	202.0	0.1	H-8→L+2 (46), H-7→L+1 (11), H-2→L+5 (27)
50	201.2	0.0262	H-14→LUMO (11), H-7→L+1 (40), H-4→L+3 (26)
51	200.7	0.003	H-8→L+1 (26), H-7→L+2 (32), H-5→L+4 (18)
52	199.9	0.0541	H-8→L+1 (21), H-2→L+6 (16), HOMO→L+9 (42)
53	199.7	0.0558	H-8→L+1 (33), H-5→L+4 (47)
54	198.5	0.0326	H-15→LUMO (36), H-6→L+4 (50)
55	197.9	0.0062	H-7→L+7 (11), H-3→L+5 (15), H-3→L+7 (15), H-1→L+8 (29)
56	197.9	0.0001	H-4→L+4 (58), H-1→L+8 (15)
57	197.7	0.0041	H-7→L+7 (11), H-4→L+4 (27), H-3→L+7 (27), H-1→L+8 (11)
58	196.8	0.013	H-2→L+5 (10), H-2→L+7 (67)
59	195.9	0.1757	H-15→LUMO (37), H-6→L+4 (28), H-2→L+7 (12)
60	195.4	0.0116	H-16→LUMO (72)
61	195.0	0.0052	H-3→L+6 (40), H-2→L+7 (18)
62	194.8	0.1628	H-16→LUMO (10), H-7→L+2 (11), H-2→L+6 (10), H-1→L+8 (15), HOMO→L+9 (20)
63	193.8	0.2642	H-17→LUMO (18), H-8→L+2 (11), H-3→L+6 (16), H-2→L+5 (12), HOMO→L+10 (16)
64	192.7	0.0025	H-18→LUMO (80)
65	191.5	0.003	H-17→LUMO (68)
66	190.7	0.0371	H-3→L+5 (47), H-1→L+8 (10)
67	190.1	0	H-8→L+3 (96)
68	188.6	0.0313	H-7→L+4 (64), HOMO→L+10 (15)
69	186.3	0.0766	H-8→L+4 (27), H-6→L+5 (22), H-5→L+6 (39)
70	186.3	0.0024	H-6→L+6 (38), H-5→L+5 (13), HOMO→L+10 (25)
71	185.4	0.1292	H-5→L+5 (37), H-3→L+6 (14), H-2→L+8 (26)
72	185.4	0.139	H-8→L+4 (52), H-5→L+6 (23)
73	183.2	0.0493	H-21→LUMO (21), H-20→LUMO (31), H-19→LUMO (28)
74	182.8	0.0985	H-9→L+2 (49), H-7→L+1 (10), H-4→L+3 (11)
75	182.2	0.1187	H-7→L+3 (24), H-7→L+7 (31), H-3→L+7 (18)

Table 6. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **DPO-OMe (7)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	565.0	0.0005	H-1→LUMO (43), HOMO→LUMO (11), HOMO→L+1 (37)
2	565.0	0.0022	H-1→LUMO (11), H-1→L+1 (37), HOMO→LUMO (43)
3	534.9	0.0213	H-1→LUMO (45), HOMO→L+1 (53)
4	525.0	1.1673	H-1→L+1 (53), HOMO→LUMO (45)
5	438.5	0.1145	H-3→LUMO (46), H-2→L+1 (53)
6	435.1	0.169	H-3→L+1 (41), H-2→LUMO (58)
7	413.5	0.0018	H-3→LUMO (52), H-2→L+1 (42)
8	413.3	0.0007	H-3→L+1 (56), H-2→LUMO (39)
9	409.1	0.0064	H-5→LUMO (50), H-4→L+1 (47)
10	408.5	0.0661	H-5→L+1 (43), H-4→LUMO (52)
11	396.9	0.0093	H-6→LUMO (86)
12	395.9	0.0211	H-6→L+1 (81)
13	393.6	0.0299	H-7→L+1 (73), H-5→L+1 (10), H-4→LUMO (10)
14	392.3	0.0875	H-7→LUMO (77)
15	384.9	0.0045	H-7→L+1 (14), H-6→LUMO (11), H-5→L+1 (39), H-4→LUMO (32)
16	384.7	0.0056	H-7→LUMO (16), H-6→L+1 (12), H-5→LUMO (33), H-4→L+1 (35)
17	357.4	0.0028	H-11→L+1 (45), H-10→LUMO (50)
18	357.2	0.0681	H-11→LUMO (48), H-10→L+1 (44)
19	351.6	0.0251	HOMO→L+2 (95)
20	351.4	0.0009	H-1→L+2 (96)
21	347.5	0.0302	H-9→L+1 (19), H-8→LUMO (74)
22	345.3	0.1732	H-9→LUMO (23), H-8→L+1 (67)
23	334.3	0.0012	H-9→LUMO (66), H-8→L+1 (26)
24	333.9	0.0012	H-9→L+1 (66), H-8→LUMO (20)
25	332.8	0.0203	H-13→L+1 (38), H-12→LUMO (49)
26	331.8	0.0816	H-13→LUMO (22), H-12→L+1 (36), H-11→L+1 (19), H-10→LUMO (18)
27	331.6	0.0007	H-11→LUMO (44), H-10→L+1 (45)
28	331.6	0.0499	H-13→LUMO (27), H-12→L+1 (10), H-11→L+1 (32), H-10→LUMO (26)
29	316.1	0.0013	H-15→L+1 (42), H-14→LUMO (51)
30	315.4	0.1069	H-15→LUMO (49), H-14→L+1 (44)
31	311.9	0.0011	H-13→L+1 (50), H-12→LUMO (45)
32	311.9	0.0002	H-13→LUMO (46), H-12→L+1 (50)
33	304.1	0.0057	H-16→LUMO (22), H-15→LUMO (36), H-14→L+1 (40)
34	303.8	0.0014	H-15→L+1 (52), H-14→LUMO (43)
35	302.5	0.0247	H-16→LUMO (70), H-15→LUMO (11), H-14→L+1 (13)
36	301.0	0.0348	H-16→L+1 (90)
37	285.3	0.2431	H-1→L+3 (50), HOMO→L+4 (41)
38	285.1	0.2401	H-7→L+2 (18), H-2→L+2 (59)

39	282.9	0.4341	H-1→L+4 (25), HOMO→L+3 (44), HOMO→L+5 (23)
40	280.9	0.0028	H-3→L+2 (36), H-1→L+5 (55)
41	280.1	0.0135	H-3→L+2 (62), H-1→L+5 (31)
42	279.8	0.1399	H-2→L+2 (21), H-1→L+4 (12), HOMO→L+5 (56)
43	275.9	0.0001	H-1→L+3 (44), HOMO→L+4 (50)
44	275.9	0.0006	H-1→L+4 (51), HOMO→L+3 (43)
45	273.3	0.0036	H-7→L+2 (57), H-2→L+2 (17)
46	270.1	0.112	H-17→L+1 (11), H-6→L+2 (15), H-4→L+2 (57)
47	268.9	0	H-5→L+2 (51), H-1→L+6 (29), HOMO→L+7 (11)
48	268.4	0.0026	H-5→L+2 (39), H-1→L+6 (36), HOMO→L+7 (15)
49	268.2	0.0074	H-4→L+2 (31), H-1→L+7 (14), HOMO→L+6 (40)
50	267.6	0.1496	H-17→L+1 (29), H-6→L+2 (27), H-4→L+2 (10), HOMO→L+6 (21)
51	264.8	0.0799	H-17→LUMO (94)
52	262.8	0.0012	H-1→L+6 (25), HOMO→L+7 (59)
53	262.7	0.003	H-1→L+7 (59), HOMO→L+6 (21)
54	262.1	0.0909	H-17→L+1 (48), H-6→L+2 (36)
55	254.8	0.0027	H-3→L+4 (12), H-2→L+3 (13), H-1→L+9 (16), HOMO→L+8 (20), HOMO→L+10 (15)
56	254.8	0	H-3→L+3 (14), H-2→L+4 (13), H-1→L+8 (15), H-1→L+10 (16), HOMO→L+9 (17)
57	253.6	0.0094	HOMO→L+8 (67)
58	253.5	0.0004	H-1→L+8 (56)
59	253.5	0.001	H-1→L+11 (24), HOMO→L+12 (23)
60	253.4	0.0012	H-1→L+8 (17), H-1→L+12 (21), HOMO→L+11 (21)
61	247.0	0.017	H-18→LUMO (13), H-8→L+2 (66)
62	245.0	0.0006	H-10→L+2 (94)
63	244.6	0.011	H-11→L+2 (91)
64	243.8	0.0667	H-18→LUMO (72), H-8→L+2 (12)
65	242.8	0.1485	H-18→L+1 (67), H-9→L+2 (17)
66	241.6	0.0166	H-18→L+1 (20), H-9→L+2 (69)
67	240.7	0.0023	H-3→L+3 (24), H-2→L+4 (26), H-1→L+10 (18), HOMO→L+9 (19)
68	240.7	0.0739	H-3→L+4 (21), H-2→L+3 (29), H-1→L+9 (19), HOMO→L+10 (18)
69	237.2	0.0427	H-19→LUMO (75)
70	237.0	0.0922	H-19→L+1 (63)
71	236.8	0.0023	H-1→L+11 (45), HOMO→L+12 (32)
72	236.8	0.0013	H-1→L+12 (38), HOMO→L+11 (39)
73	236.7	0.0287	H-19→L+1 (18), H-2→L+5 (26), HOMO→L+12 (15)
74	236.2	0.0234	H-5→L+4 (11), H-4→L+3 (11), H-3→L+5 (16), H-1→L+12 (16), HOMO→L+11 (10)
75	235.3	0	H-1→L+9 (32), H-1→L+10 (10), HOMO→L+10 (3)

Table 7. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **DPA-OMe (8)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	574.3	0.0129	H-1→L+1 (20), HOMO→LUMO (74)
2	572.4	0.0078	H-1→LUMO (31), HOMO→L+1 (63)
3	537.7	0.018	H-2→LUMO (18), H-1→L+1 (71), HOMO→LUMO (10)
4	532.8	0.2454	H-2→L+1 (47), H-1→LUMO (44)
5	515.8	0.0274	H-2→LUMO (76), HOMO→LUMO (14)
6	503.5	0.8822	H-2→L+1 (46), H-1→LUMO (23), HOMO→L+1 (28)
7	442.9	0.0209	HOMO→L+2 (98)
8	439.2	0.0174	H-1→L+2 (99)
9	432.1	0.0517	H-4→LUMO (54), H-3→L+1 (45)
10	429.9	0.129	H-4→L+1 (39), H-3→LUMO (59)
11	411.7	0.0005	H-4→LUMO (44), H-3→L+1 (54)
12	411.6	0.0039	H-4→L+1 (59), H-3→LUMO (39)
13	405.5	0.0006	H-6→LUMO (47), H-5→L+1 (50)
14	403.8	0.1062	H-6→L+1 (33), H-5→LUMO (62)
15	388.0	0.0156	H-6→LUMO (43), H-5→L+1 (38), H-2→L+2 (16)
16	387.5	0.0022	H-6→L+1 (64), H-5→LUMO (34)
17	387.3	0.1153	H-2→L+2 (80)
18	355.1	0.0007	H-11→L+1 (12), H-10→LUMO (44), H-9→L+1 (41)
19	355.0	0.0673	H-11→LUMO (11), H-10→L+1 (33), H-9→LUMO (53)
20	349.0	0.0234	H-8→L+1 (21), H-7→LUMO (69)
21	344.2	0.195	H-8→LUMO (31), H-7→L+1 (58)
22	342.8	0.0141	H-11→LUMO (39), H-10→L+1 (14), H-9→LUMO (34)
23	341.3	0.0241	H-11→L+1 (29), H-10→LUMO (14), H-9→L+1 (47)
24	336.8	0	H-8→LUMO (54), H-7→L+1 (36)
25	336.3	0	H-8→L+1 (66), H-7→LUMO (26)
26	334.5	0.0018	H-3→L+2 (99)
27	334.4	0	H-4→L+2 (98)
28	331.2	0	H-11→LUMO (41), H-10→L+1 (43)
29	330.8	0.0006	H-11→L+1 (54), H-10→LUMO (34)
30	330.2	0.007	H-14→LUMO (18), H-13→L+1 (42), H-12→LUMO (31)
31	329.1	0.1027	H-14→L+1 (12), H-13→LUMO (48), H-12→L+1 (29)
32	321.0	0.0009	H-5→L+2 (67)
33	318.6	0.0078	H-9→L+2 (18), H-5→L+2 (29), H-2→L+3 (14), HOMO→L+3 (14)
34	318.2	0	H-6→L+2 (95)
35	316.4	0.0084	H-15→LUMO (37), H-14→L+1 (32), H-12→L+1 (19)
36	316.0	0.0717	H-15→L+1 (13), H-14→LUMO (33), H-12→LUMO (28)
37	313.0	0.0002	H-13→LUMO (42), H-12→L+1 (42)
38	313.0	0.0242	H-16→LUMO (10), H-14→LUMO (14), H-13→L+1 (50), H-12→LUMO (19)
39	312.5	0.0318	H-16→LUMO (53), H-15→L+1 (26)

40	311.4	0.0213	H-16→L+1 (55), H-15→LUMO (21), H-14→L+1 (20)
41	305.9	0.0028	H-16→LUMO (22), H-15→L+1 (47), H-14→LUMO (22)
42	305.6	0.0055	H-16→L+1 (36), H-15→LUMO (31), H-14→L+1 (24)
43	298.0	0.0944	H-1→L+3 (99)
44	297.4	0.0719	H-2→L+3 (16), HOMO→L+3 (71)
45	288.0	0.0087	H-7→L+2 (72)
46	285.4	0.0129	H-11→L+2 (49), H-9→L+2 (35)
47	285.3	0.0037	H-10→L+2 (88)
48	282.7	0.0738	H-1→L+4 (48), HOMO→L+5 (31)
49	282.7	0.0669	H-8→L+2 (77), HOMO→L+4 (10)
50	281.0	0.4438	H-8→L+2 (14), HOMO→L+4 (74)
51	277.9	0.0037	H-1→L+4 (18), HOMO→L+5 (37), HOMO→L+6 (29)
52	276.4	0.0922	H-1→L+5 (81), HOMO→L+4 (11)
53	276.2	0.0035	H-1→L+4 (24), HOMO→L+5 (21), HOMO→L+6 (31)
54	272.6	0.0189	H-1→L+6 (79)
55	271.8	0.0115	H-15→L+2 (11), H-13→L+2 (87)
56	271.6	0.0052	H-14→L+2 (32), H-12→L+2 (66)
57	270.2	0.0005	H-16→L+2 (25), H-2→L+6 (11), HOMO→L+6 (25)
58	268.5	0.0032	H-1→L+8 (38), HOMO→L+7 (54)
59	267.6	0.0059	H-16→L+2 (10), H-1→L+7 (19), HOMO→L+8 (52)
60	264.1	0.0007	H-1→L+8 (53), HOMO→L+7 (33)
61	264.1	0.0001	H-1→L+7 (65), HOMO→L+8 (19)
62	262.8	0.0403	H-16→L+2 (17), H-14→L+2 (37), H-12→L+2 (19), H-11→L+2 (11)
63	262.3	0	H-15→L+2 (85)
64	260.2	0.335	H-17→L+1 (28), H-2→L+5 (11), H-2→L+6 (17)
65	260.1	0.024	H-2→L+4 (93)
66	259.2	0.0859	H-2→L+3 (12), H-2→L+5 (68)
67	256.2	0.08	H-17→LUMO (83)
68	255.9	0.0224	H-17→L+1 (38), H-16→L+2 (10), H-2→L+6 (23)
69	254.1	0.0006	H-4→L+5 (11), H-3→L+4 (16), H-1→L+9 (19), HOMO→L+11 (17)
70	254.0	0.0064	H-4→L+4 (14), H-3→L+5 (11), H-1→L+11 (14), HOMO→L+9 (19)
71	253.0	0.0065	H-18→LUMO (10), H-1→L+10 (20), HOMO→L+12 (19)
72	252.9	0.003	H-18→L+1 (10), H-1→L+12 (17), HOMO→L+10 (22)
73	249.7	0.4864	H-18→LUMO (34), H-2→L+6 (21)
74	247.8	0.0734	H-2→L+6 (15), H-2→L+8 (72)
75	247.5	0.0128	H-2→L+7 (93)

Table 8. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **DPO-O (9)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	597.5	0.0001	H-1→L+1 (38), HOMO→LUMO (62)
2	597.2	0.0018	H-1→LUMO (55), HOMO→L+1 (45)
3	571.3	0.0066	H-1→L+1 (62), HOMO→LUMO (37)
4	559.1	0.7257	H-1→LUMO (45), HOMO→L+1 (54)
5	472.6	0.0656	H-3→LUMO (44), H-2→L+1 (55)
6	467.3	0.2492	H-3→L+1 (36), H-2→LUMO (62)
7	444.7	0.0032	H-3→LUMO (55), H-2→L+1 (43)
8	444.4	0	H-3→L+1 (61), H-2→LUMO (37)
9	404.9	0.0337	H-6→L+1 (10), H-5→L+1 (49), H-4→LUMO (37)
10	403.9	0.0379	H-5→LUMO (53), H-4→L+1 (43)
11	401.6	0.1527	H-6→L+1 (69), H-4→LUMO (19)
12	398.7	0.1502	H-6→LUMO (82), H-5→LUMO (10)
13	396.0	0.0055	H-7→LUMO (78)
14	395.3	0.0834	H-7→L+1 (85)
15	380.9	0.0007	H-7→LUMO (10), H-6→L+1 (14), H-5→L+1 (40), H-4→LUMO (36)
16	380.9	0	H-7→L+1 (12), H-6→LUMO (12), H-5→LUMO (33), H-4→L+1 (43)
17	358.8	0.0269	H-8→LUMO (87)
18	356.4	0.0109	H-8→L+1 (25), HOMO→L+2 (70)
19	355.6	0.016	H-1→L+2 (97)
20	355.5	0.0626	H-8→L+1 (58), HOMO→L+2 (28)
21	346.9	0.0017	H-11→LUMO (50), H-10→L+1 (46)
22	346.7	0.0268	H-11→L+1 (45), H-10→LUMO (52)
23	339.9	0.0197	H-13→L+1 (26), H-12→LUMO (26), H-9→L+1 (38)
24	339.7	0.0277	H-13→LUMO (15), H-12→L+1 (11), H-9→LUMO (58), H-8→L+1 (11)
25	335.0	0.0735	H-13→LUMO (31), H-12→L+1 (29), H-9→LUMO (27)
26	334.9	0.008	H-13→L+1 (17), H-12→LUMO (23), H-9→L+1 (49)
27	323.7	0.0002	H-11→LUMO (41), H-10→L+1 (46)
28	323.7	0.0001	H-11→L+1 (45), H-10→LUMO (41)
29	313.2	0	H-13→L+1 (44), H-12→LUMO (42)
30	313.1	0.0001	H-13→LUMO (40), H-12→L+1 (47)
31	306.1	0.2006	H-14→LUMO (20), H-1→L+4 (30), HOMO→L+3 (37)
32	301.4	0.5938	H-16→L+1 (13), H-15→LUMO (19), H-14→L+1 (14), H-1→L+3 (19), HOMO→L+4 (16)
33	300.9	0.0083	H-16→LUMO (42), H-15→L+1 (34)
34	300.8	0.4839	H-16→L+1 (22), H-15→LUMO (23), H-14→L+1 (12), H-1→L+3 (13), HOMO→L+4 (12)
35	297.6	0.0011	H-1→L+4 (35), HOMO→L+3 (56)
36	297.5	0.0019	H-1→L+3 (46), HOMO→L+4 (53)
37	296.7	0.1778	H-14→L+1 (46), H-2→L+2 (35)

38	296.5	0.0153	H-14→LUMO (63), H-1→L+4 (28)
39	291.3	0.0786	H-14→L+1 (23), H-2→L+2 (54)
40	289.6	0.009	H-3→L+2 (94)
41	287.8	0.0001	H-16→L+1 (53), H-15→LUMO (45)
42	287.8	0.0001	H-16→LUMO (45), H-15→L+1 (52)
43	285.8	0.0202	HOMO→L+5 (79)
44	285.4	0.0012	H-1→L+5 (76)
45	276.4	0.0005	HOMO→L+6 (76)
46	276.1	0.0183	H-1→L+6 (75)
47	273.3	0.005	H-6→L+2 (50), H-5→L+2 (17)
48	272.4	0.1015	H-3→L+4 (34), H-2→L+3 (39)
49	272.3	0.0107	H-3→L+3 (30), H-2→L+4 (31)
50	271.5	0.0011	H-1→L+6 (10), HOMO→L+7 (71)
51	271.2	0.0001	H-1→L+7 (68)
52	267.1	0.2147	H-17→L+1 (49), H-7→L+2 (30), H-4→L+2 (10)
53	264.0	0.0354	H-17→LUMO (90)
54	262.5	0.0129	H-17→L+1 (10), H-4→L+2 (75)
55	262.2	0.0072	H-6→L+2 (24), H-5→L+2 (71)
56	260.7	0.037	H-7→L+2 (15), H-4→L+2 (10), H-1→L+10 (17), HOMO→L+9 (13)
57	260.2	0.0317	H-2→L+6 (10), H-1→L+9 (18), HOMO→L+10 (23)
58	259.8	0.0742	H-17→L+1 (32), H-7→L+2 (33)
59	258.4	0	HOMO→L+8 (88)
60	258.2	0.0074	H-1→L+8 (88)
61	254.8	0.0027	H-3→L+4 (47), H-2→L+3 (49)
62	254.8	0.0002	H-3→L+3 (47), H-2→L+4 (50)
63	254.3	0	H-19→L+1 (46), H-18→LUMO (49)
64	254.3	0.004	H-19→LUMO (49), H-18→L+1 (45)
65	251.3	0.0015	H-8→L+2 (76), H-7→L+2 (10)
66	248.4	0.0023	H-22→LUMO (20), H-21→L+1 (24), H-2→L+5 (18)
67	248.4	0	H-22→L+1 (20), H-21→LUMO (27), H-3→L+5 (14), H-2→L+6 (10)
68	247.8	0.0154	H-1→L+11 (31), HOMO→L+12 (35)
69	247.7	0.3337	H-1→L+12 (32), HOMO→L+11 (33)
70	245.7	0.0069	H-22→LUMO (13), H-21→L+1 (16), H-2→L+5 (34)
71	245.4	0.0334	H-22→L+1 (13), H-21→LUMO (16), H-3→L+5 (28), H-2→L+6 (16)
72	242.9	0.0504	H-9→L+2 (54)
73	241.8	0.0145	H-5→L+3 (27), H-4→L+4 (28), H-1→L+10 (10), HOMO→L+9 (14)
74	241.8	0	H-5→L+4 (22), H-4→L+3 (26), H-1→L+9 (10), HOMO→L+10 (20)
75	241.4	0.1024	H-3→L+6 (30), H-2→L+5 (22), H-2→L+7 (18)

Table 9. Computed oscillator strengths (F), positions of the first electronic transitions and major contributions of **DPA-O (10)**.

Transition No.	Wavelength (nm)	Osc. Strength	Major contributors (%)
1	608.8	0.0137	H-1→L+1 (20), HOMO→LUMO (79)
2	605.8	0.0038	H-1→LUMO (48), HOMO→L+1 (51)
3	572.3	0.0057	H-1→L+1 (79), HOMO→LUMO (19)
4	561.6	0.478	H-2→L+1 (16), H-1→LUMO (46), HOMO→L+1 (37)
5	532.9	0.1779	H-2→LUMO (97)
6	530.6	0.2299	H-2→L+1 (82), HOMO→L+1 (12)
7	463.2	0.0117	H-4→L+1 (23), H-3→LUMO (76)
8	458.7	0.1315	H-4→LUMO (49), H-3→L+1 (47)
9	450.4	0.0064	HOMO→L+2 (97)
10	447.2	0.0328	H-1→L+2 (99)
11	440.1	0.0129	H-4→LUMO (49), H-3→L+1 (50)
12	438.5	0.0004	H-4→L+1 (76), H-3→LUMO (23)
13	400.6	0.0031	H-6→LUMO (60), H-5→L+1 (37)
14	399.7	0.1188	H-6→L+1 (35), H-5→LUMO (62)
15	389.8	0.1068	H-2→L+2 (95)
16	382.7	0.0006	H-6→LUMO (38), H-5→L+1 (61)
17	382.6	0.0027	H-6→L+1 (63), H-5→LUMO (36)
18	366.3	0.0418	H-7→LUMO (88)
19	358.9	0.1823	H-7→L+1 (82)
20	348.6	0.0055	H-9→LUMO (21), H-3→L+2 (68)
21	348.2	0.0059	H-9→LUMO (59), H-3→L+2 (26)
22	348.0	0.0007	H-8→LUMO (79), H-7→L+1 (13)
23	345.2	0.0003	H-8→L+1 (77)
24	345.1	0	H-11→LUMO (38), H-10→L+1 (25), H-9→L+1 (31)
25	342.7	0.0011	H-4→L+2 (91)
26	342.5	0.0218	H-11→L+1 (32), H-10→LUMO (52), H-9→LUMO (10)
27	339.4	0.0159	H-11→LUMO (14), H-10→L+1 (14), H-9→L+1 (67)
28	334.4	0.0141	H-13→LUMO (50), H-12→L+1 (35)
29	333.5	0.0744	H-13→L+1 (32), H-12→LUMO (50)
30	322.6	0.0001	H-11→LUMO (38), H-10→L+1 (51)
31	322.6	0.0002	H-11→L+1 (53), H-10→LUMO (36)
32	318.3	0.0596	H-9→L+2 (21), HOMO→L+3 (46)
33	314.7	0.0032	H-13→LUMO (37), H-12→L+1 (45)
34	314.3	0.001	H-13→L+1 (53), H-12→LUMO (36)
35	311.6	0.0518	H-14→LUMO (31), H-9→L+2 (13), H-1→L+4 (11), HOMO→L+3 (13)
36	308.8	0.0132	H-6→L+2 (95)
37	308.8	0.0031	H-5→L+2 (89)
38	308.2	0.2683	H-1→L+3 (82)
39	305.5	0.3524	H-14→L+1 (61), HOMO→L+4 (26)
40	305.0	0.0037	H-14→LUMO (25), H-2→L+3 (11), HOMO→L+3 (35)

41	301.1	0.0281	H-14→LUMO (22), H-1→L+4 (63)
42	300.5	0.0703	H-1→L+5 (36), HOMO→L+4 (54)
43	299.8	0.0145	H-16→L+1 (14), H-15→LUMO (25), HOMO→L+5 (33)
44	299.4	0.0001	H-16→LUMO (45), H-15→L+1 (31), HOMO→L+7 (10)
45	298.5	0.0029	H-16→L+1 (13), H-15→LUMO (21), HOMO→L+5 (42)
46	294.7	0.5997	H-14→L+1 (23), H-1→L+5 (47), HOMO→L+4 (12)
47	294.5	0.0045	H-7→L+2 (79)
48	288.5	0.0002	H-16→LUMO (44), H-15→L+1 (54)
49	288.4	0.0003	H-16→L+1 (55), H-15→LUMO (43)
50	283.7	0.0093	H-8→L+2 (97)
51	281.9	0.0071	H-2→L+3 (15), H-2→L+5 (11), HOMO→L+6 (57)
52	280.9	0.0121	H-2→L+4 (49), H-1→L+6 (27), HOMO→L+7 (12)
53	279.9	0.0247	H-2→L+3 (27), H-2→L+5 (31), HOMO→L+6 (18)
54	279.0	0.0118	H-2→L+4 (32), H-1→L+6 (52)
55	277.3	0.0001	HOMO→L+7 (71)
56	275.6	0.0364	H-1→L+7 (79)
57	273.4	0.0027	H-10→L+2 (82)
58	273.3	0.0302	HOMO→L+8 (68)
59	272.8	0.0081	H-11→L+2 (89)
60	271.7	0.0002	H-1→L+8 (82)
61	270.4	0	H-4→L+4 (23), H-3→L+3 (35), H-3→L+5 (11)
62	270.0	0.0759	H-4→L+3 (22), H-3→L+4 (38)
63	268.3	0.0373	H-13→L+2 (77)
64	267.9	0.035	H-12→L+2 (93)
65	265.8	0.0119	H-14→L+2 (20), H-13→L+2 (16), H-2→L+6 (35), H-2→L+8 (15)
66	261.8	0.0002	H-2→L+7 (25), H-1→L+11 (14)
67	261.4	0.028	H-1→L+10 (10), HOMO→L+11 (15)
68	258.8	0.2605	H-17→L+1 (15), H-4→L+3 (32), H-3→L+4 (15)
69	258.0	0.0016	H-4→L+4 (30), H-3→L+3 (52)
70	256.3	0.2567	H-17→L+1 (25), H-4→L+3 (25), H-3→L+4 (22)
71	256.2	0.0656	H-2→L+7 (59)
72	255.9	0.0147	H-14→L+2 (28), H-2→L+6 (41)
73	254.2	0.062	H-17→LUMO (88)
74	253.8	0.0078	H-14→L+2 (25), H-2→L+8 (52)
75	253.7	0.0024	H-4→L+4 (21), H-3→L+5 (73)

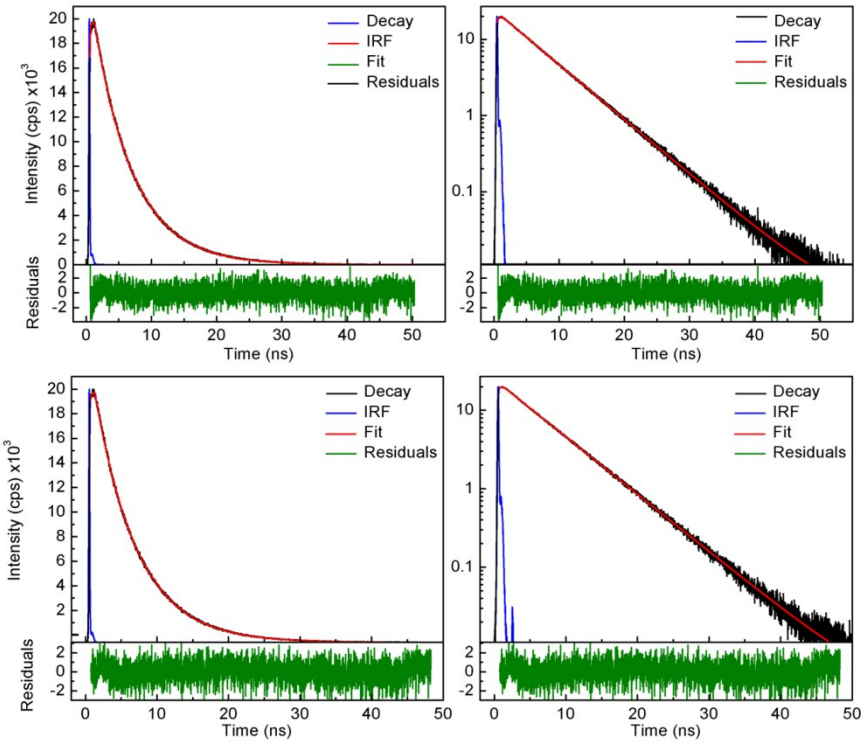

Figure S34. Fluorescence decay trace for **BOD-OMe (3)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

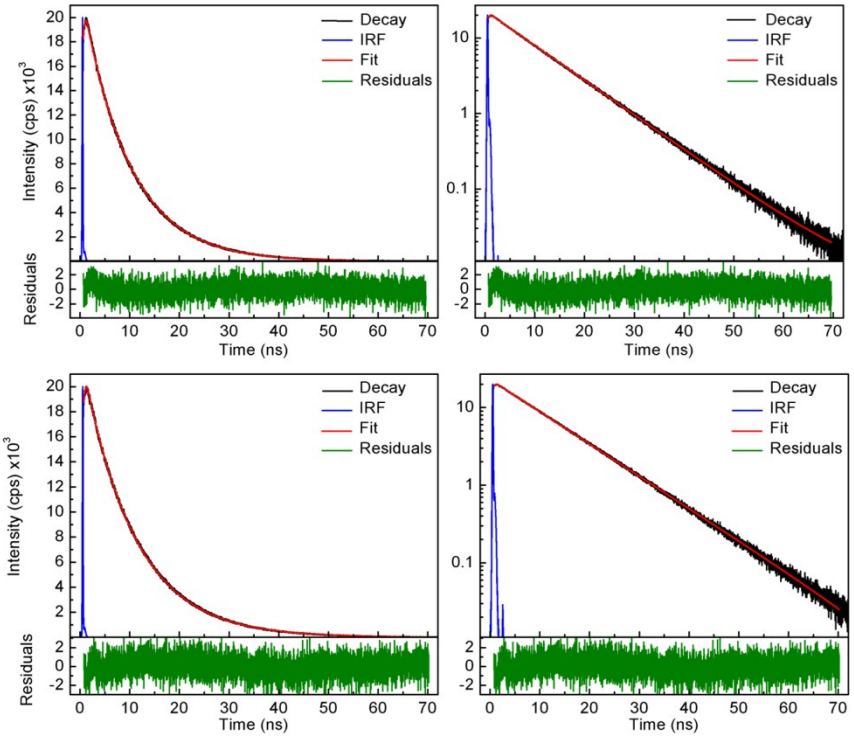

Figure S35. Fluorescence decay trace for **BOD-O (4)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

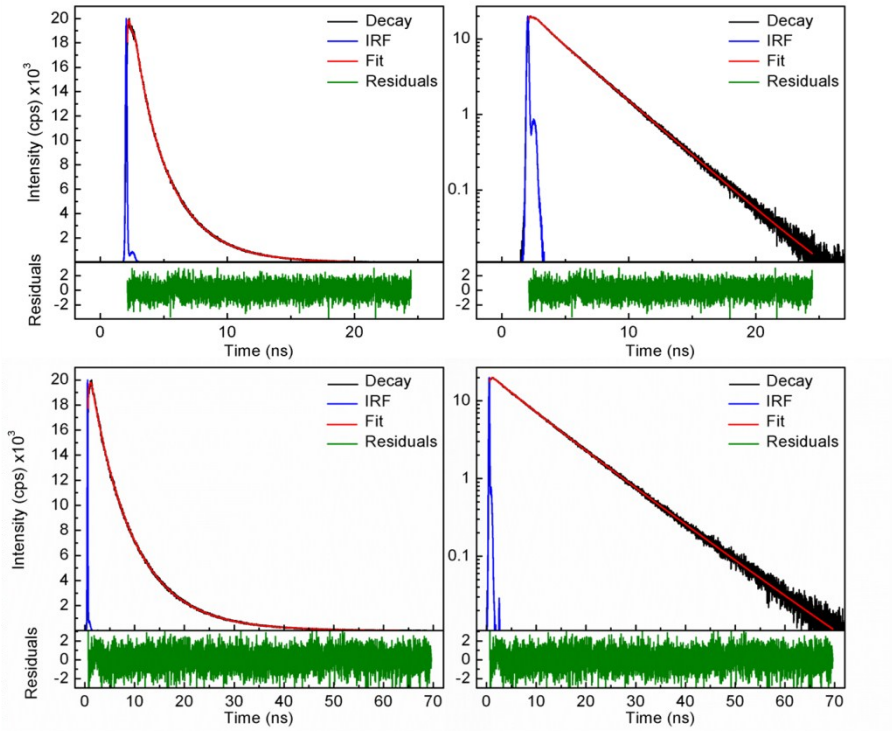

Figure S36. Fluorescence decay trace for **DPO-OMe (7)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

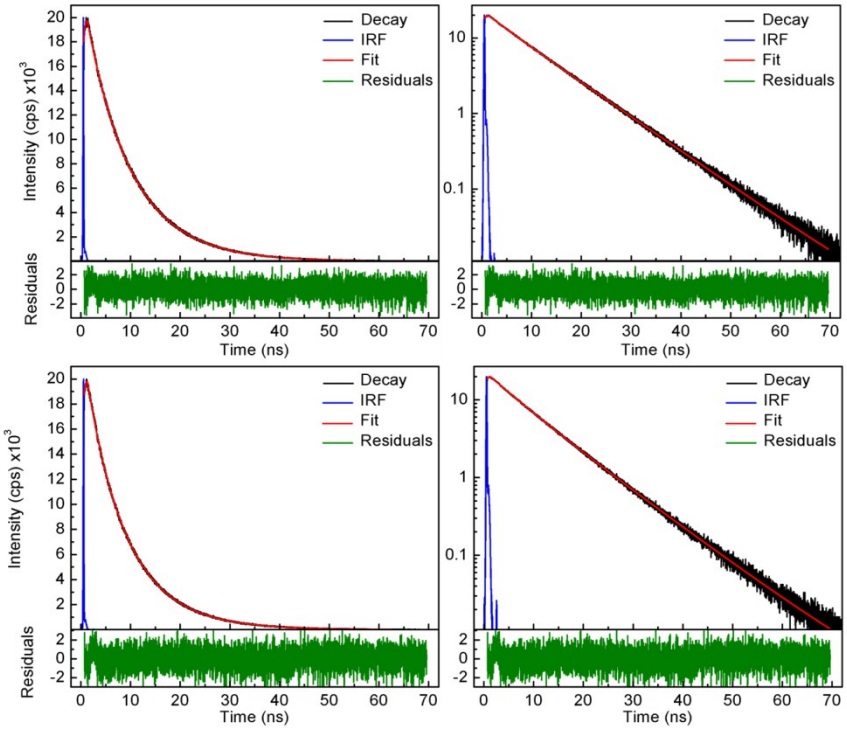

Figure S37. Fluorescence decay trace for **DPA-OMe (8)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

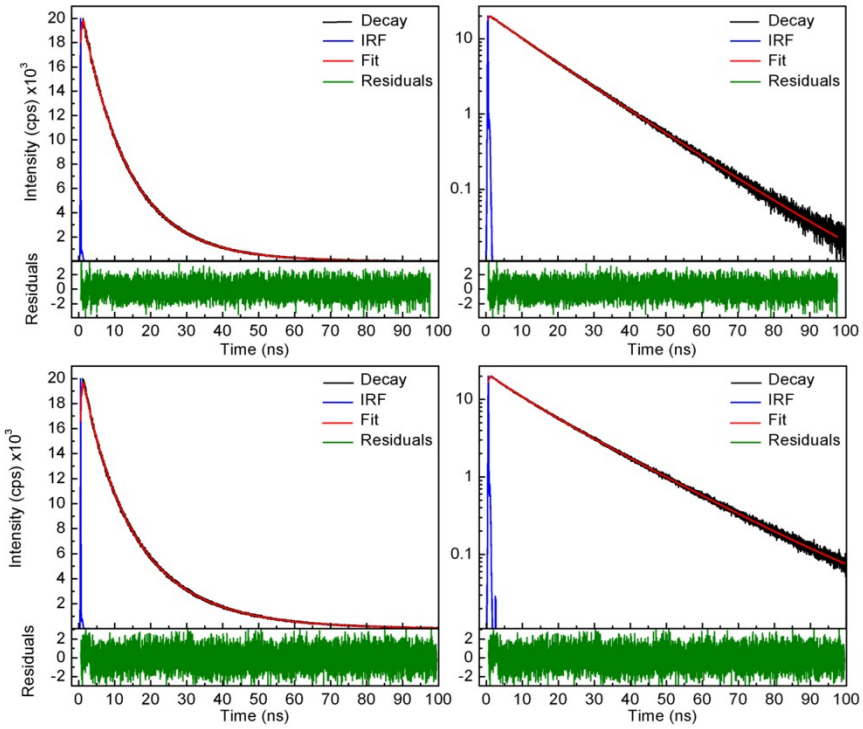

Figure S38. Fluorescence decay trace for **DPO-O (9)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

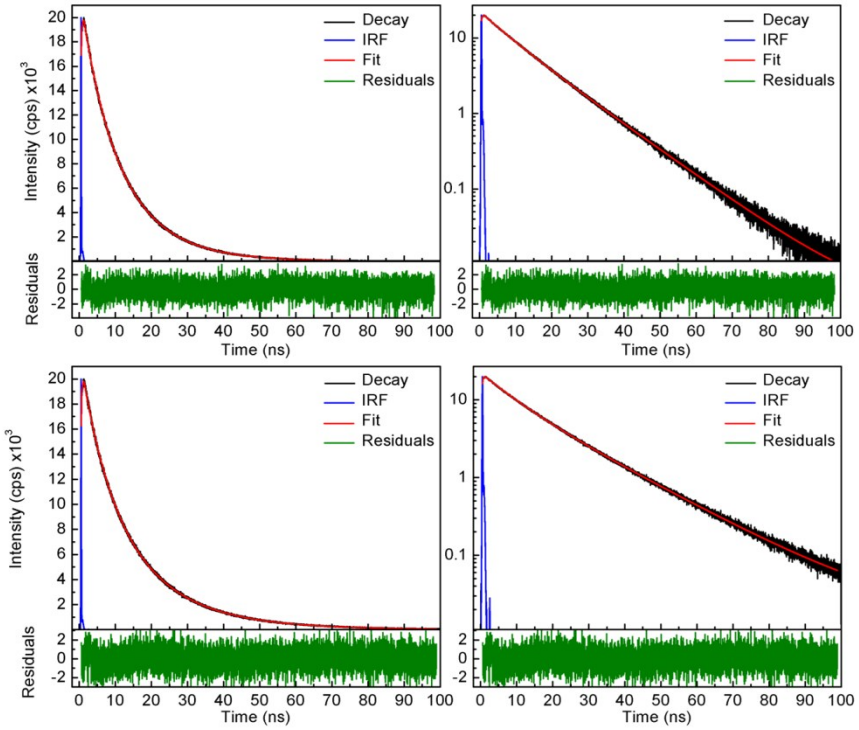

Figure S39. Fluorescence decay trace for **DPA-O (10)** at 298 (top) and 77 K (bottom). Decay traces are shown in both a liner and logarithmic scale.

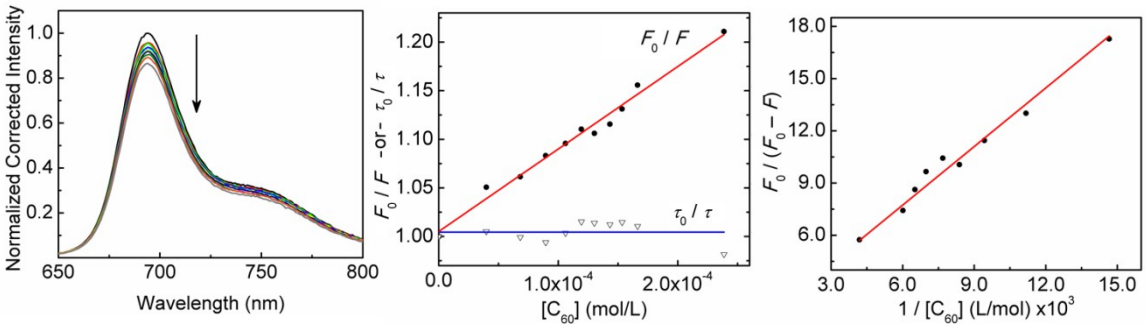

Figure S40. Left: evolution of fluorescence spectra of **BOD-O (4)** in 1,2-dichlorobenzene upon addition of C_{60}. Middle: Stern-Volmer analysis of fluorescence quenching of **BOD-O (4)** by C_{60} in 1,2-dichlorobenzene. Right: Modified Stern-Volmer analysis. See SI for the five other compounds. The C_{60} concentration was increased from 0 to 5.5 equivalents.

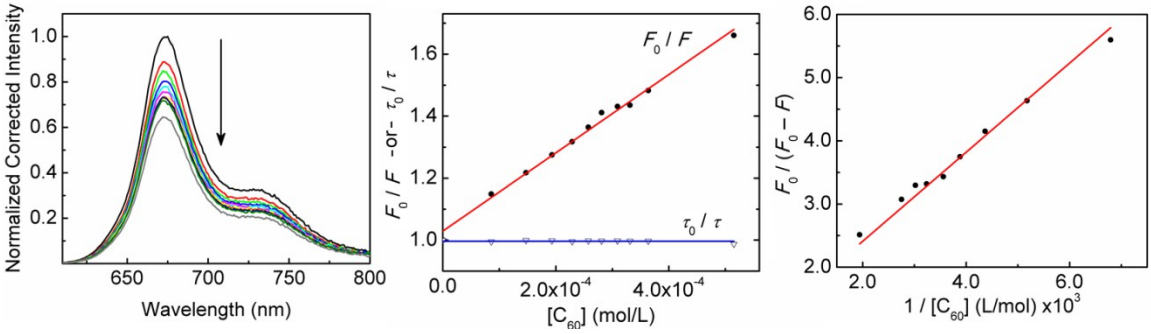

Figure S41. Left: evolution of fluorescence spectra of **DPO-OMe (7)** in 1,2-dichlorobenzene upon addition of C_{60}. Middle: Stern-Volmer analysis of fluorescence quenching of **DPO-OMe (7)** by C_{60} in 1,2-dichlorobenzene. Right: Modified Stern-Volmer analysis. See SI for the five other compounds. The C_{60} concentration was increased from 0 to 26.4 equivalents.

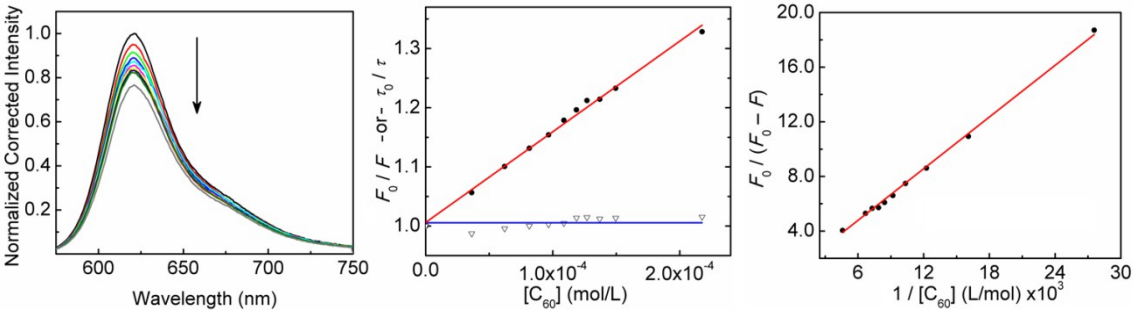

Figure S42. Left: evolution of fluorescence spectra of **DPA-OMe (8)** in 1,2-dichlorobenzene upon addition of C_{60}. Middle: Stern-Volmer analysis of fluorescence quenching of **DPA-OMe (8)** by C_{60} in 1,2-dichlorobenzene. Right: Modified Stern-Volmer analysis. See SI for the five other compounds. The C_{60} concentration was increased from 0 to 15.0 equivalents.

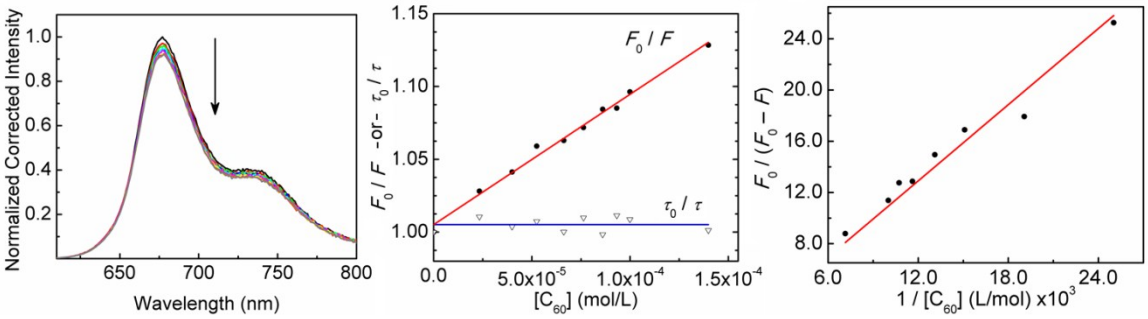

Figure S43. Left: evolution of fluorescence spectra of **DPO-O (9)** in 1,2-dichlorobenzene upon addition of C_{60}. Middle: Stern-Volmer analysis of fluorescence quenching of **DPO-O (9)** by C_{60} in 1,2-dichlorobenzene. Right: Modified Stern-Volmer analysis. See SI for the five other compounds. The C_{60} concentration was increased from 0 to 10.0 equivalents.

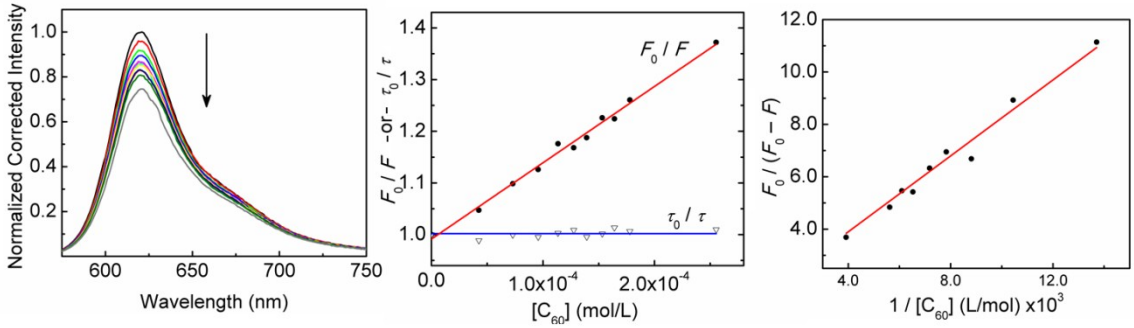

Figure S44. Left: evolution of fluorescence spectra of **DPA-O (10)** in 1,2-dichlorobenzene upon addition of C_{60}. Middle: Stern-Volmer analysis of fluorescence quenching of **DPA-O (10)** by C_{60} in 1,2-dichlorobenzene. Right: Modified Stern-Volmer analysis. See SI for the five other compounds. The C_{60} concentration was increased from 0 to 15.3 equivalents.