Electronic Supplementary Information for

AIE-active difluoroboronated acylhydrozone dyes (BOAHY) emitting across the entire visible region and their photo-switching properties

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Contents:

1. Crystal diagrams and selected data

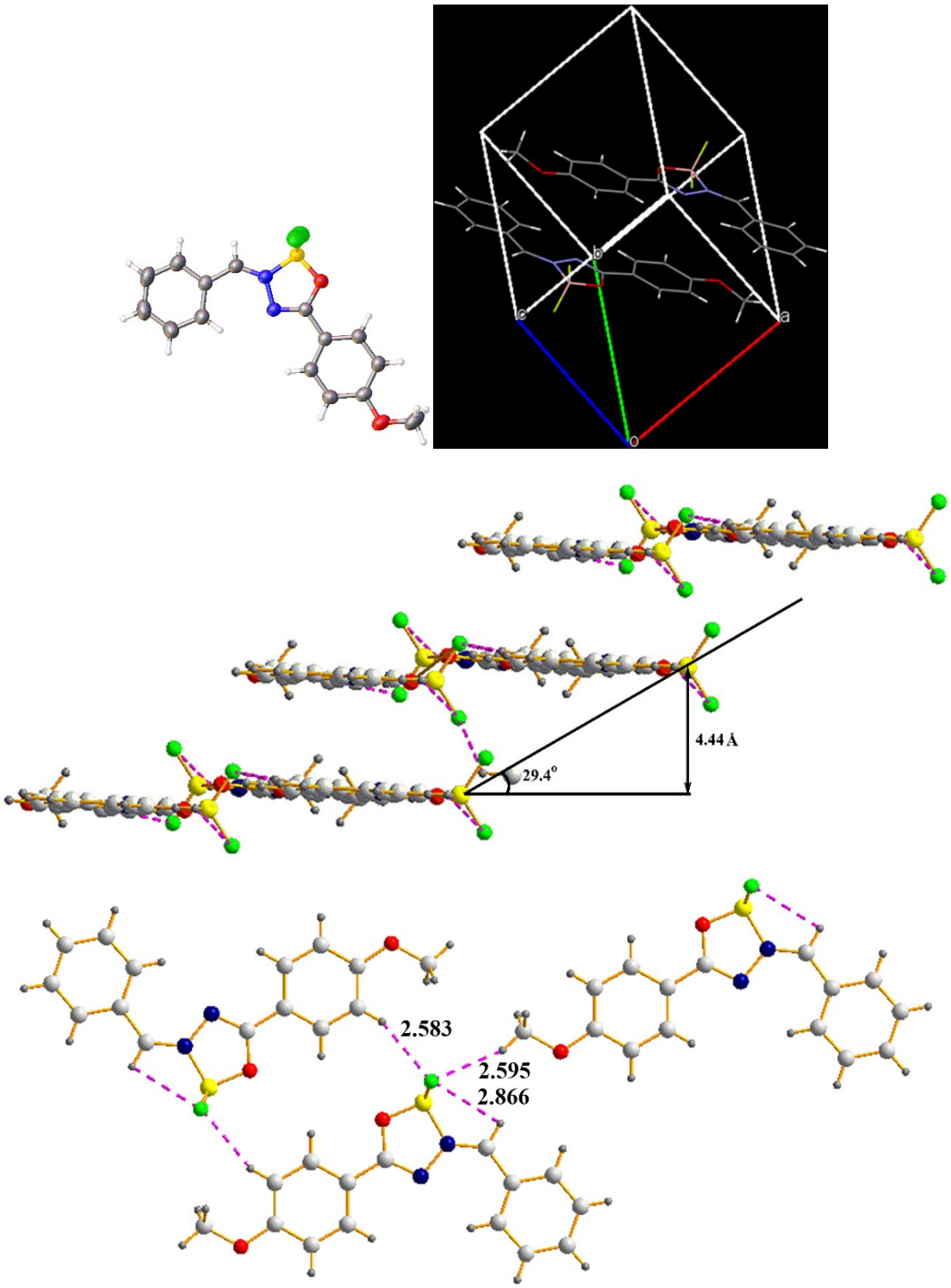


Figure S1. Crystal-packing pattern of BOAPY **1b** between the adjacent interlayered crystals from side view. Interlayer distance is 4.44 Å. Slip angle of 29.4° for coplanar inclined arrangements of its transition dipole. Intermolecular hydrogen bond lengths are 2.583 and 2.595 Å. Intramolecular hydrogen bond lengths is 2.866 Å. C, light gray; N, blue; O, red; B, yellow; F, green; H, gray.

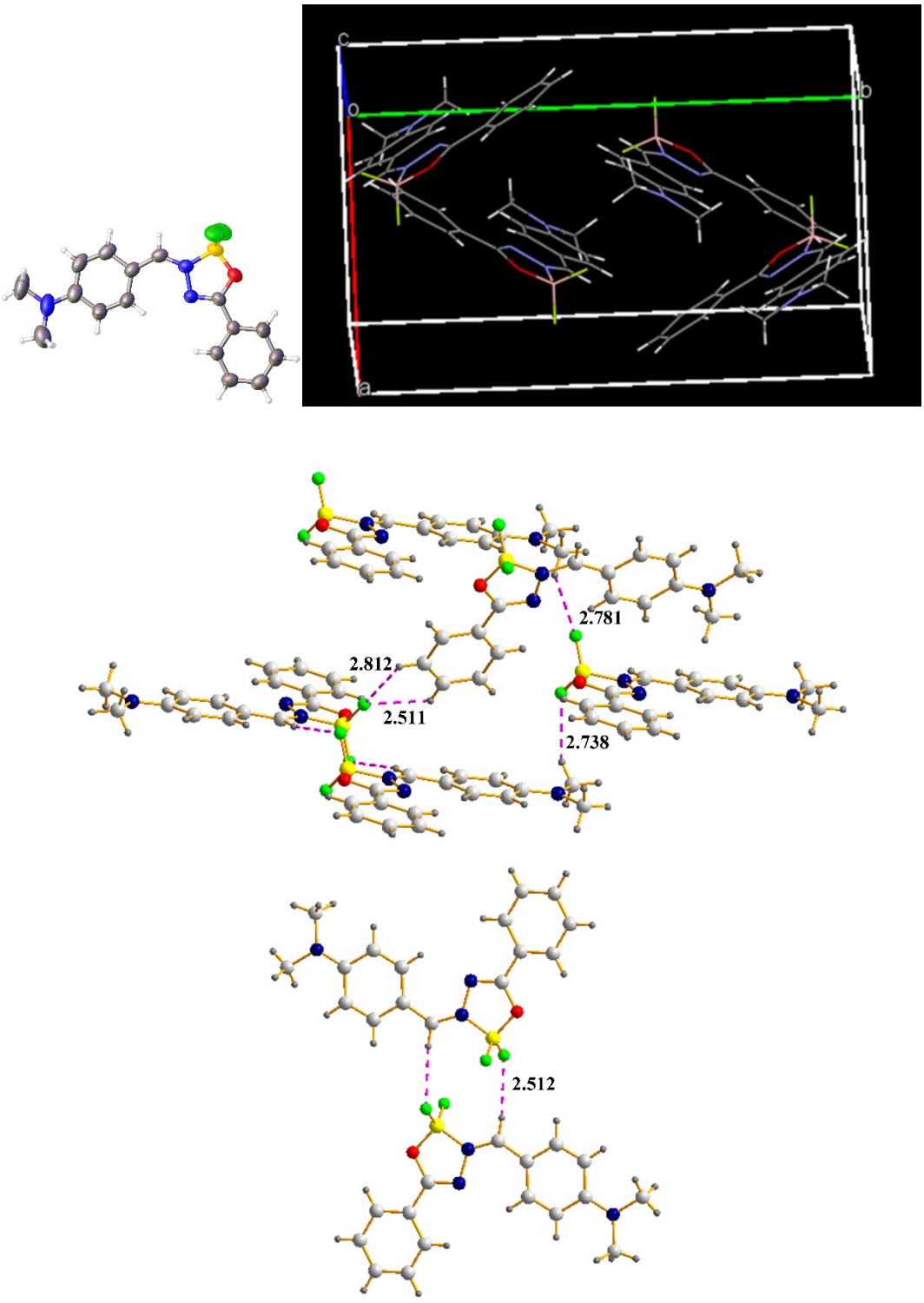


Figure S2. Crystal-packing pattern of BOAPY **2d** between the adjacent interlayered crystals from side view. Intermolecular hydrogen bond lengths are 2.781, 2.738, 2.812, 2.511 and 2.512 Å. Intramolecular hydrogen bonds were not observed. C, light gray; N, blue; O, red; B, yellow; F, green; H, gray.

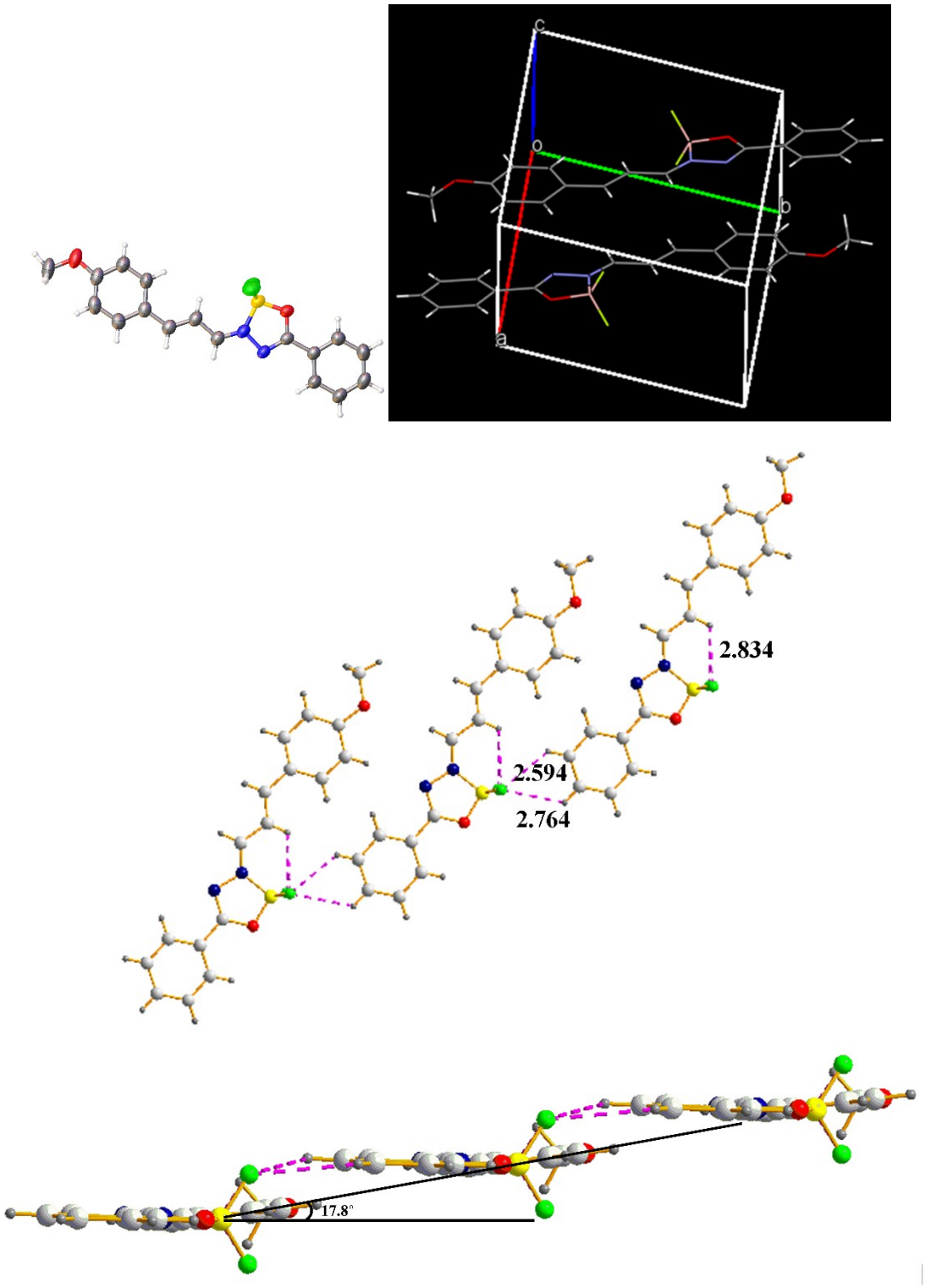


Figure S3. Crystal-packing pattern of BOAPY **2e** between the adjacent interlayered crystals. Slip angle of 17.8° for coplanar inclined arrangements of its transition dipole. Intermolecular hydrogen bond lengths are 2.594 and 2.764 Å. Intramolecular hydrogen bond length is 2.834 Å. C, light gray; N, blue; O, red; B, yellow; F, green; H, gray.

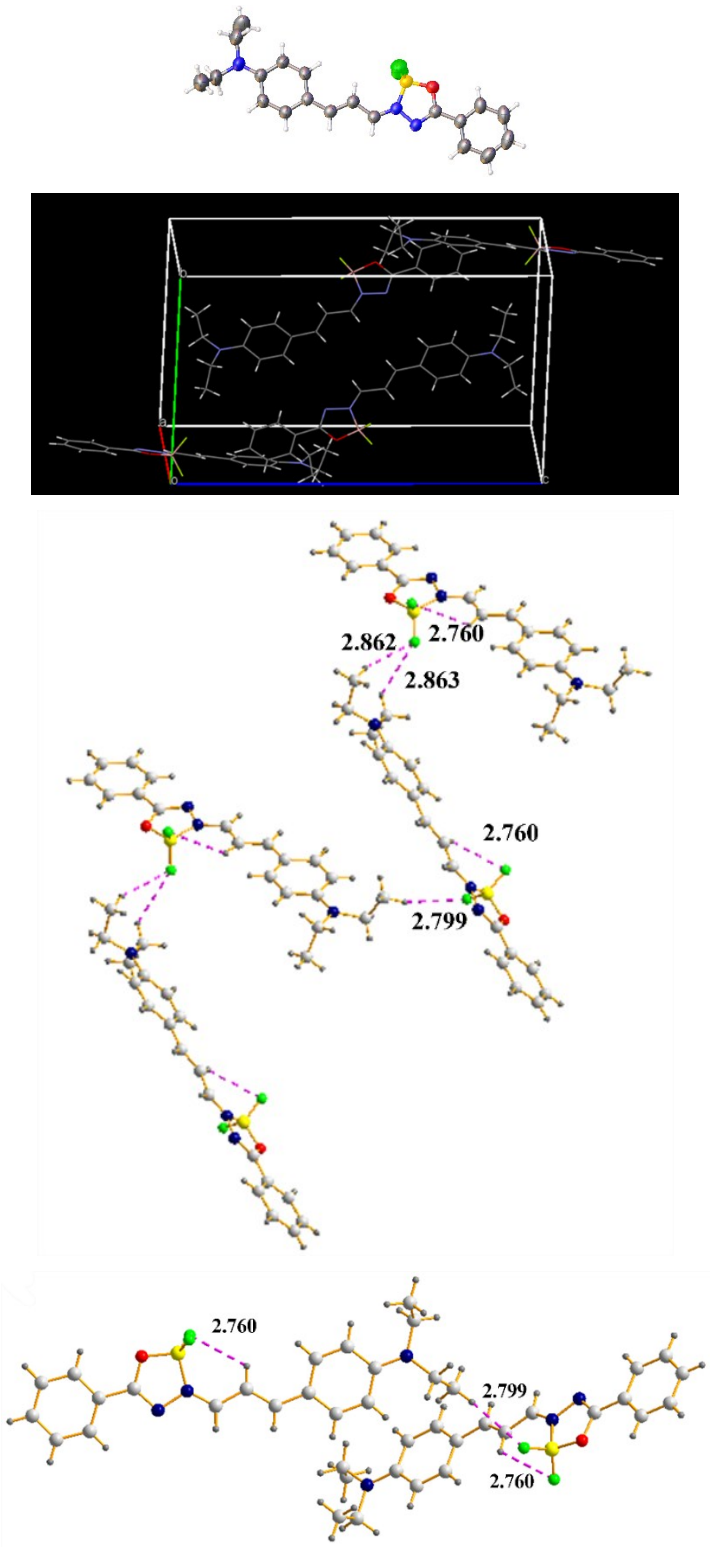


Figure S4. Crystal-packing pattern of BOAPY **2f** between the adjacent interlayered crystals. Intermolecular hydrogen bond lengths are 2.863, 2.862 and 2.799 Å. Intramolecular hydrogen bond length is 2.760 Å. C, light gray; N, blue; O, red; B, yellow; F, green; H, gray.

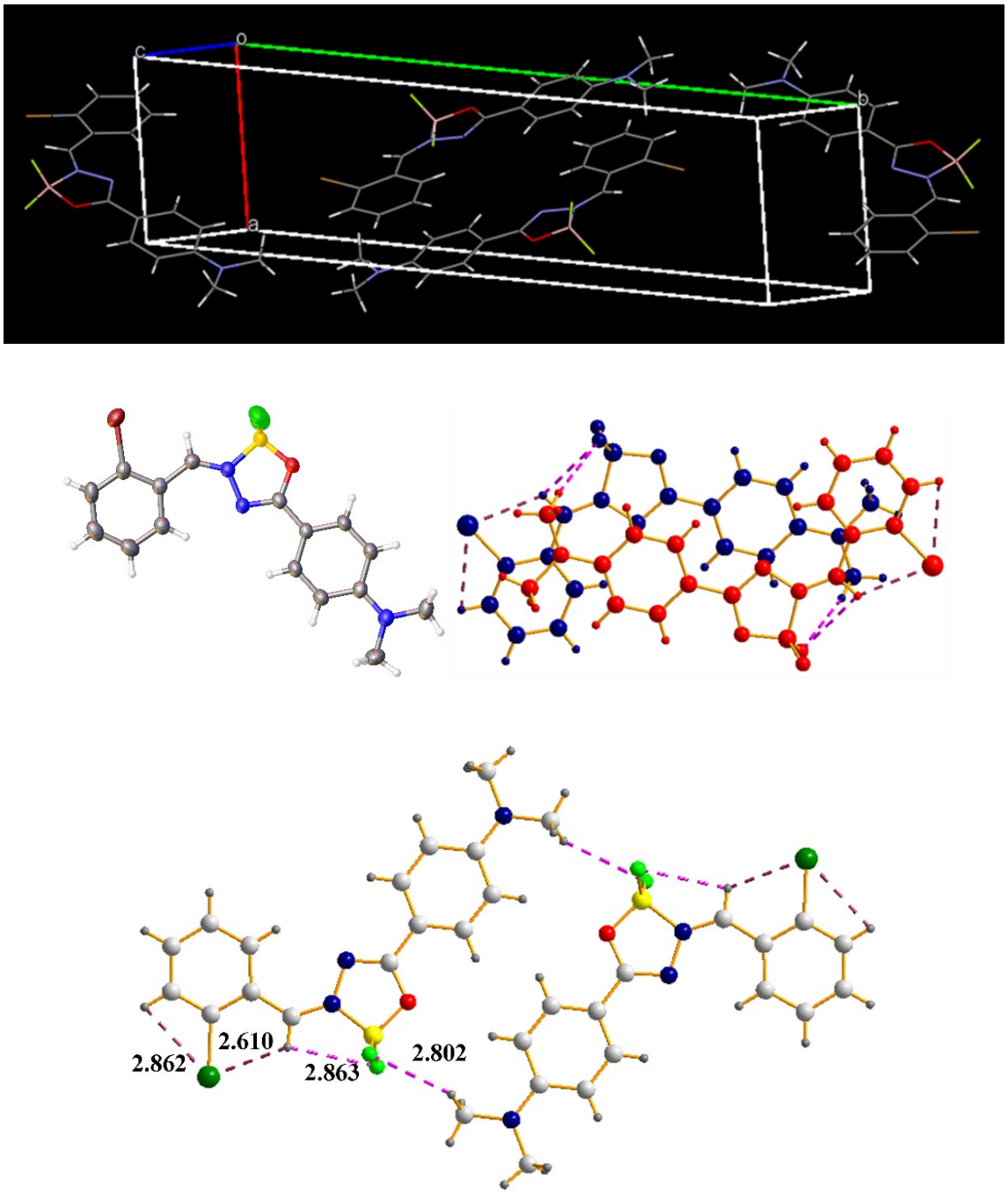
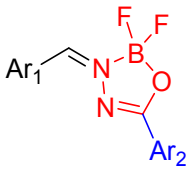


Figure S5. Crystal-packing pattern of BOAPY **2k** between the adjacent interlayered crystals. Intermolecular hydrogen bond length is 2.802 Å. Intramolecular hydrogen bond lengths are 2.863, 2.610 and 2.862 Å. C, light gray; N, blue; O, red; B, yellow; F, green; H, gray.

Table S1. Selected bond lengths [Å] and dihedral angles [deg] of **1b**, **2d-g** and **2k** obtained from crystallography.



dyes	B-N bond distances (Å)	B-O bond distances (Å)	N-N bond distances (Å)	dihedral angles of Ar_1 ring and Ar_2 ring (deg)	dihedral angles between Ar_1 and newly formed ring (deg)	dihedral angles between the newly formed ring and Ar_2 ring (deg)
1b	1.591(2)	1.466(2)	1.396(2)	1.697(3)	2.362(2)	2.362(2)
2d	1.569(3)	1.473(3)	1.402(2)	4.782(2)	5.103(2)	2.37 (7)
2e	1.592(2)	1.468(2)	1.399(2)	8.891(2)	8.018(2)	1.335(2)
2f	1.574(4)	1.466(4)	1.407(3)	2.167(3)	5.812(2)	5.711(3)
2g	1.577(2)	1.454(3)	1.436(2)	5.402(3)	3.250(3)	2.937(3)
2k	1.590(5)	1.461(5)	1.384(4)	7.341(2)	7.285(3)	4.403(3)

Table S2. Crystal data and structure refinements for **1b**, **2d** and **2e** obtained from X-ray crystallography.

Identification code	**1b**	**2d**	**2e**
CCDC no.	1873750	1873749	1541739
formula	$C_{15}H_{13}BF_2N_2O_2$	$C_{16}H_{16}BF_2N_3O$	$C_{17}H_{15}BF_2N_2O_2$
fw	302.08	315.13	328.12
crystal system	triclinic	monoclinic	triclinic
space group	*P*-1	$P2_1/n$	*P*-1
a (Å)	8.1278(7)	9.5383(5)	7.6560(9)
b (Å)	9.0511(7)	17.4670(11)	10.0738(11)
c (Å)	10.3004(8)	10.2653(6)	11.2184(12)
α (deg)	82.101(3)	90	112.3050(10)
β (deg)	84.055(3)	110.540(2)	97.3120(10)
γ (deg)	70.628(3)	90	91.8680(10)
v ($Å^3$)	706.71(10)	1601.53(16)	790.88(15)
Z	2	4	2
D_{calcd} (mg/m^3)	1.42	1.307	1.378
μ mm^{-1}	0.112	0.099	0.106
F(000)	312	656	340
2ɵ range (deg)	5.902 to 55.582	6.302 to 55.088	3.96 to 55.1
reflections collected/ unique	18925	33614	9036
R(int)	3248/0/200	3675/0/210	3535/0/219
Goodness of-fit on F^2	1.07	1.019	1.052
R_1, wR_2 [I>2σ(I)]	0.0435, 0.1087	0.0518, 0.1259	0.0390, 0.1115
R_1, wR_2 (all data)	0.0514, 0.1165	0.0915, 0.1525	0.0483, 0.1207
Largest diff. peak and hole, e. $Å^{-3}$	0.20, -0.24	0.22, -0.15	0.18, -0.15

Table S3. Crystal data and structure refinements for **2f**, **2g** and **2k** obtained from X-ray crystallography.

Identification code	**2f**	**2g**	**2k**
CCDC no.	1543020	1541741	1873751
formula	$C_{20}H_{22}BF_2N_3O$	$C_{16}H_{13}BF_2N_2O$	$C_{16}H_{15}BBrF_2N_3O$
fw	369.21	298.09	394.03
crystal system	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	6.4740(14)	14.090(4)	7.3547(5)
b (Å)	14.018(3)	9.997(3)	25.1921(15)
c (Å)	21.523(5)	20.654(6)	9.1335(5)
α (deg)	90	90	90
β (deg)	91.550(3)	100.333(8)	106.823(2)
γ (deg)	90	90	90
v (Å^3)	1952.6(7)	2862.1(14)	1619.83(17)
Z	4	8	4
D_{calcd} (mg/m^3)	1.256	1.384	1.616
μ mm^{-1}	0.091	0.104	2.567
F(000)	776	1232	792
2ɵ range (deg)	3.468 to 50.044	6.1 to 50.02	5.786 to 55.158
reflections collected/ unique	12539	42275	68284
R(int)	3417/0/246	5020/0/398	3738/0/219
Goodness of-fit on F^2	1.067	1.085	1.131
R_1, wR_2 [I>2σ(I)]	0.0591, 0.1236	0.1725, 0.3726	0.0545, 0.0956
R_1, wR_2 (all data)	0.1356, 0.1456	0.2120, 0.3908	0.0968, 0.1093
Largest diff. peak and hole, e. Å^{-3}	0.22, -0.17	0.54, -0.60	0.31, -0.64

2. Photophysical properties

Table S4. Photophysical properties of BOAHYs **1** and **2** in different organic solvents below.

dyes	solvents	λ_{abs}^{max}/nm (logε_{max})[a]	λ_{em}^{max} (nm)	Stokes Shift (cm^{-1})
1a	hexane	306 (3.32)	400	7680
	dichloromethane	302 (3.51)	397	7924
	tetrahydrofuran	310 (3.96)	400	7258
	acetonitrile	306 (3.82)	401	7742
	methanol	309 (3.86)	402	7487
1b	hexane	340 (4.35), 355 (4.46), 375 (4.33)	411	5081
	toluene	346 (4.34), 356 (4.46), 381 (4.30)	423	5261
	dichloromethane	344 (4.49), 360 (4.56), 378 (4.43)	440	6342
	acetonitrile	342 (4.36), 358 (4.44), 375 (4.28)	451	7067
	methanol	336 (4.36), 350 (4.43), 367 (4.27)	413, 444	7239
2a	hexane	330 (4.26), 345 (4.29), 363 (4.05)	393	4858
	toluene	335 (4.15), 350 (4.16), 367 (3.93)	386	3944
	dichloromethane	333 (4.16), 347 (4.18), 365 (3.92)	394	4649
	methanol	329 (3.93), 344 (4.42), 360 (4.13)	417	6414
	acetonitrile	329 (4.24), 344 (4.24), 361 (3.96)	422	6698
2b	hexane	339 (4.09), 354 (4.13), 373 (3.91)	392	3988
	toluene	347 (4.24), 361 (4.29), 379 (4.09)	387	2979
	dichloromethane	349 (4.21), 362 (4.25), 380 (4.06)	392	3143
	methanol	349 (4.21), 362 (4.26), 379 (4.06)	422	4957
	acetonitrile	346 (4.40), 360 (4.44), 378 (4.23)	417	4921
2c	hexane	342 (4.12), 358 (4.16), 377 (3.93)	412	4968
	toluene	348 (4.03), 364 (4.08), 382 (3.88)	406	4105
	dichloromethane	348 (4.09), 363 (4.13), 382 (3.92)	408	4226
	methanol	345 (4.16), 360 (4.20), 378 (sh, 3.99)	411	4655
	acetonitrile	343 (4.30), 358 (4.34), 376 (4.15)	418	5231
2d	hexane	376 (sh, 4.29), 394 (4.52), 415 (4.47)	432, 455	4618
	toluene	410 (4.61), 429 (4.59)	457, 470	3114
	dichloromethane	417 (4.62), 433 (4.62)	466, 488	3489
	methanol	425 (4.62)	487	2996
	acetonitrile	415 (4.59), 429 (sh, 4.58)	476	3088
2e	hexane	381 (4.45), 397 (4.40), 420 (4.04)	466	4787
	toluene	392 (4.58)	481	4720
	dichloromethane	394 (4.46)	487	4847
	methanol	387 (4.44)	486	5264
	acetonitrile	387 (4.50)	493	5556
2f	hexane	451 (4.20), 471 (4.14)	489, 514	2718

	toluene	478 (4.42)	533	2519
	dichloromethane	495 (4.46)	562	2408
	methanol	480 (4.53)	562	3040
	acetonitrile	488 (4.44)	571	2979
	hexane	356 (4.33), 373 (4.39), 393 (4.17)	419	4224
	toluene	361 (4.24), 378 (4.30), 397 (sh, 4.09)	452	5577
2g	dichloromethane	362 (4.28), 378 (4.34), 396 (sh, 4.15)	447	5253
	methanol	360 (4.30), 374 (4.35), 393 (sh, 4.15)	450	5556
	acetonitrile	357 (4.24), 373 (4.39), 392 (sh, 4.07)	449	5739
	hexane	399 (4.31), 422 (4.32)	443 (sh),	3371
	toluene	416 (4.32), 431 (4.33)	501	4078
2h	dichloromethane	419 (4.56)	555	5848
	methanol	420 (4.28)	578	6508
	acetonitrile	419 (4.27)	604	7310
	hexane	406 (4.52), 428 (4.52)	457, 480	3797
	toluene	428 (4.47)	526	4353
2i	dichloromethane	431 (4.62)	588	6195
	methanol	421 (4.41)	597	7003
	acetonitrile	425 (4.34)	616	7633
	hexane	420 (3.92), 439 (3.86)	477, 492	3484
	toluene	438 (4.47)	537	4209
2j	dichloromethane	442 (4.44)	589	5647
	methanol	433 (4.46)	619	6940
	acetonitrile	431 (4.36)	645, 701	7698
	hexane	414 (3.90), 431 (3.83)	521	4961
	toluene	429 (4.70)	544	4928
2k	dichloromethane	435 (4.73)	581	5777
	methanol	429 (4.66)	602	6699
	acetonitrile	430 (4.47)	634	7483
	hexane	411 (3.66), 432 (3.63)	496, 515	4913
	toluene	433 (4.05)	526	4083
2l	dichloromethane	436 (4.69)	587	5900
	methanol	431 (4.64)	602	6591
	acetonitrile	436 (4.68)	625	6936

[a]Molar absorption coefficients were obtained at the maximum of the highest peak.

Table S5. Photophyscial properties of BOAHYs **1** and **2** in dichloromethane, thin film and powder states at room temperature.

	dichloromethane		powder	thin film
	λ_{abs}^{max}/nm (lgε)	λ_{em}^{max}/nm (ϕ^a)	λ_{em}^{max}/nm (ϕ^a)	λ_{em}^{max}/nm (ϕ^a)
1a	302 (3.51)	397 (0.01)	-	-
1b	344 (4.49), 360 (4.56), 378 (4.43)	440 (0.03)	470 (0.36)	505 (0.37)
2d	417 (4.62), 434 (4.62)	466, 488 (0.06)	518, 544[b] (0.17)	573 (0.51)
2e	394 (4.46)	487 (0.05)	550 (0.05)	540 (0.11)
2f	495 (4.46)	562 (0.11)	629 (0.58)	704 (0.30)
2g	338 (4.51), 354 (4.50), 373(4.22)	409 (0.02)	425, 443, 474[b] (0.04)	425, 461 (0.10)
2h	419 (4.56)	555 (0.15)	585 (0.32)	574 (0.27)
2i	431 (4.62)	588 (0.20)	579 (0.62)	602 (0.37)
2j	442 (4.44)	589 (0.11)	583 (0.34)	603 (0.60)
2k	435 (4.73)	581 (0.16)	622 (0.18)	616 (0.25)
2l	436 (4.69)	587 (0.30)	608 (0.53)	595 (0.58)

[a]fluorescence quantum yield; [b]shoulder peak; - means not detected.

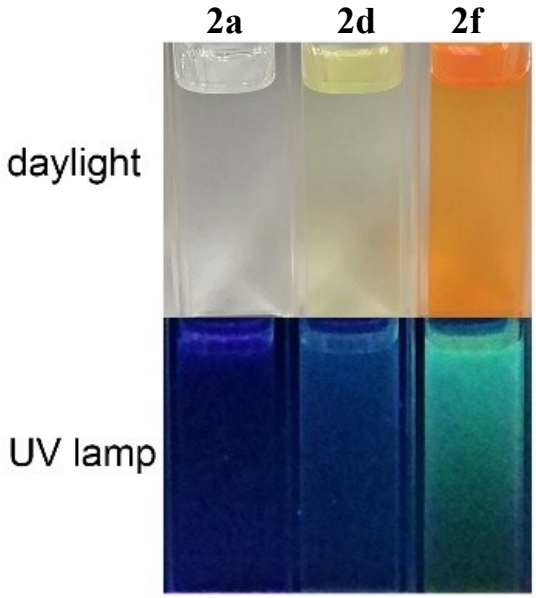


Figure S6. Photographs of **2a**, **2d** and **2f** in dichloromethane under daylight and under 365 nm hand-held UV lamp irradiation condition.

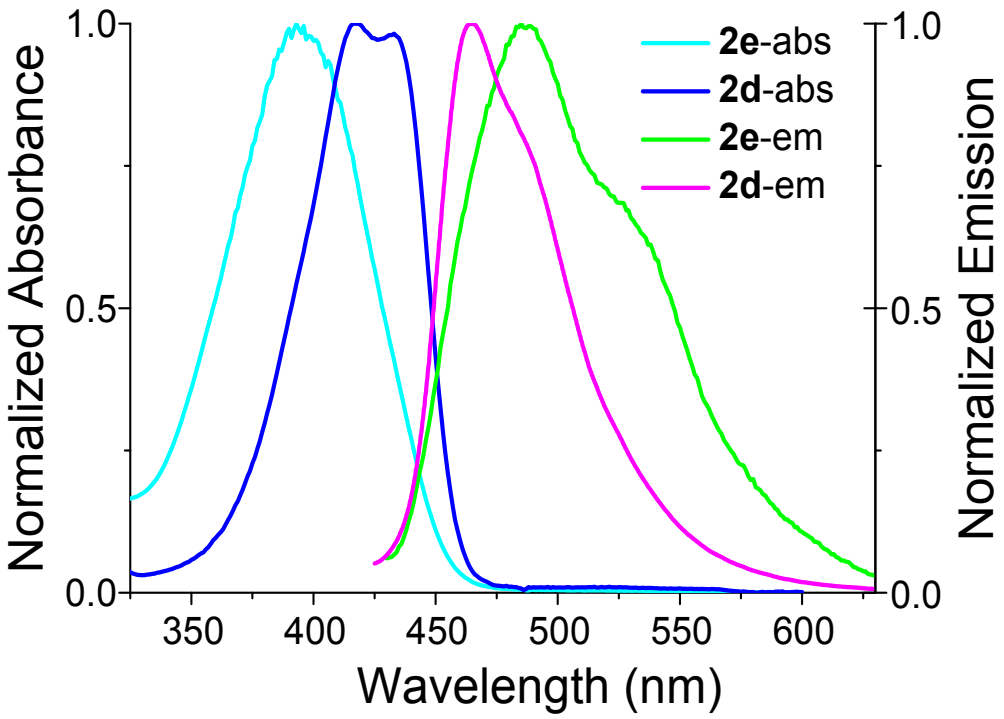


Figure S7. Normalized absorption and emission spectra of **2d** and **2e** in dichloromethane.

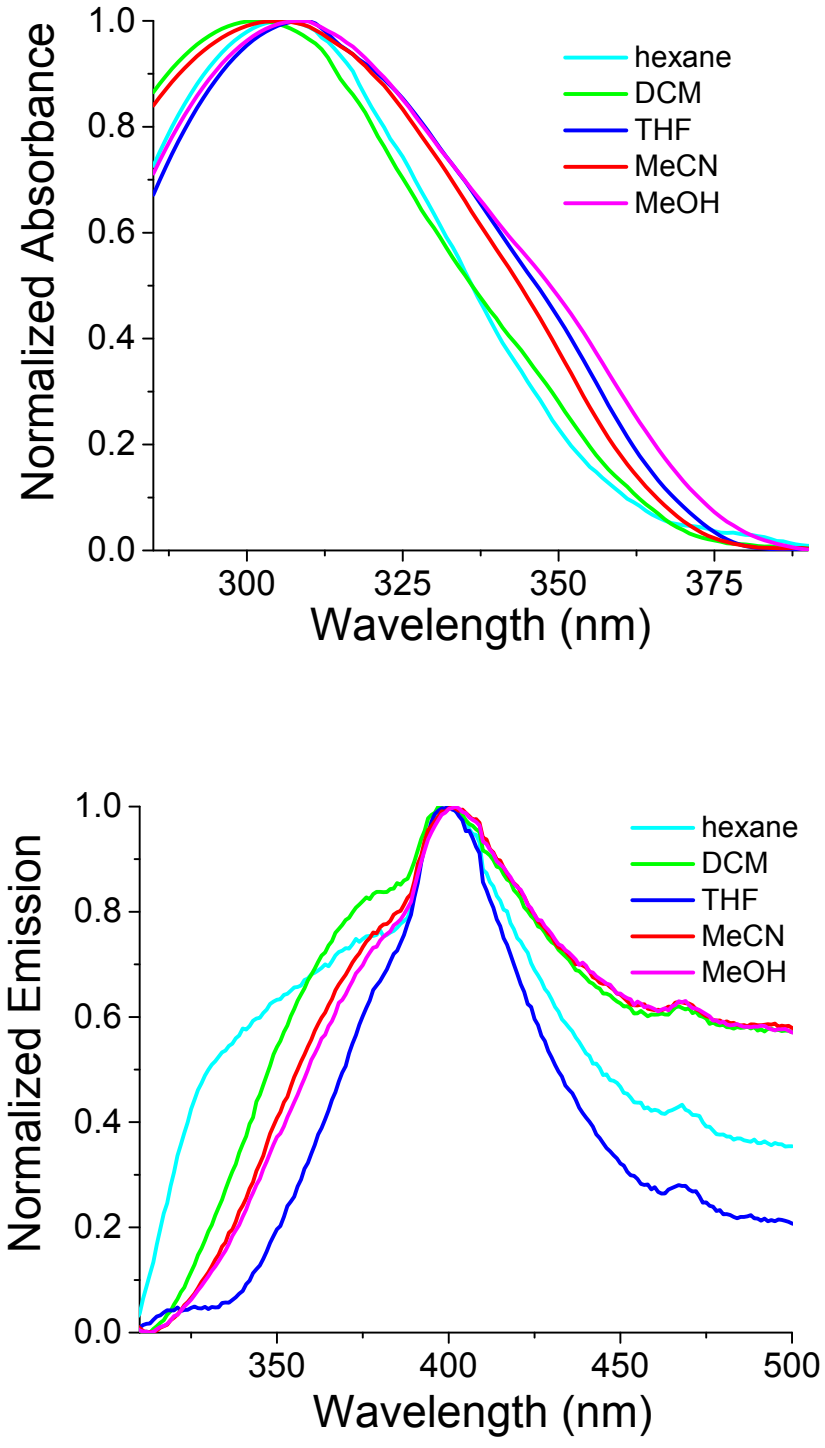


Figure S8. Normalized UV-vis (top) and fluorescence spectra (bottom) of **1a** in different solvents, excited at 270 nm.

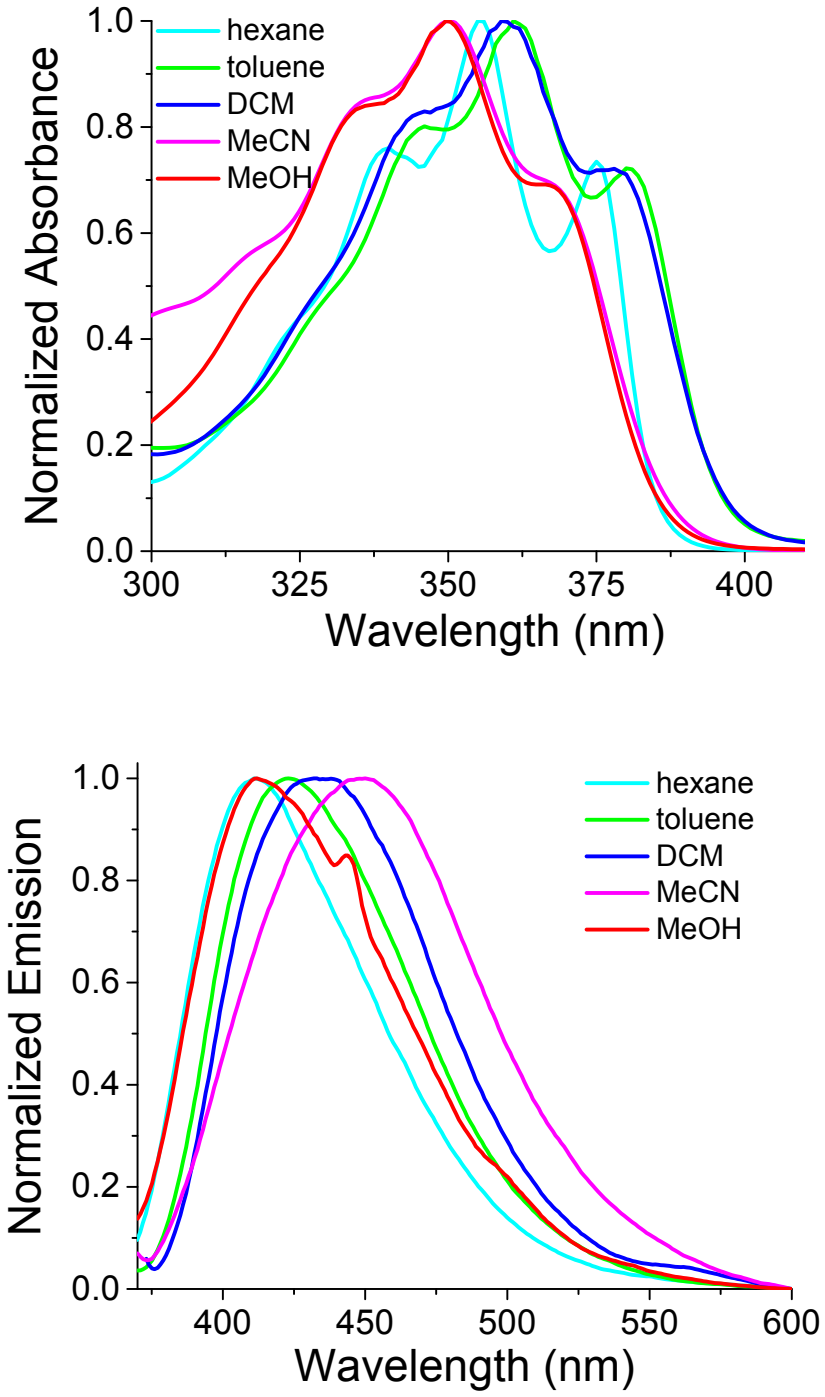


Figure S9. Normalized UV-vis (top) and fluorescence spectra (bottom) of **1b** in different solvents, excited at 360 nm.

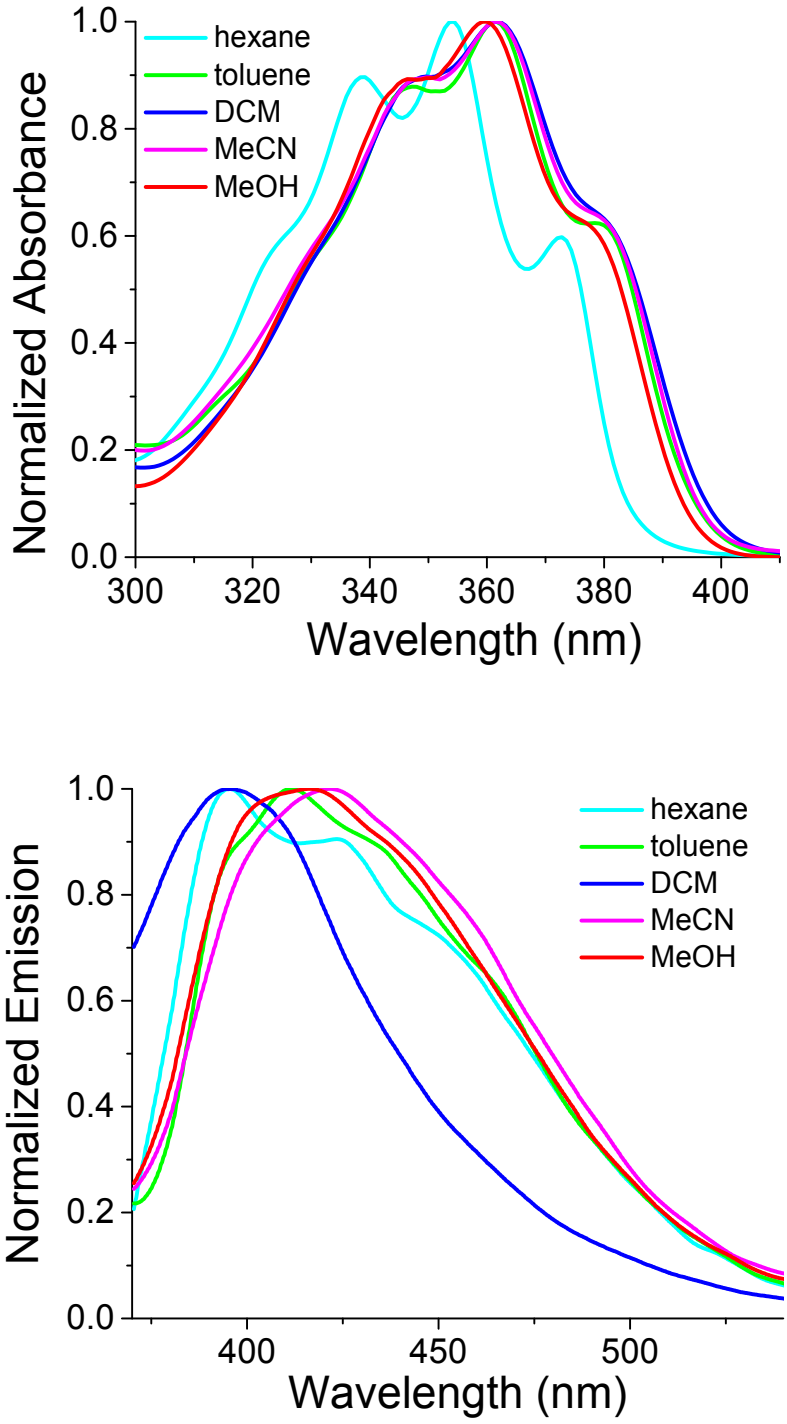


Figure S10. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2a** in different solvents, excited at 320 nm.

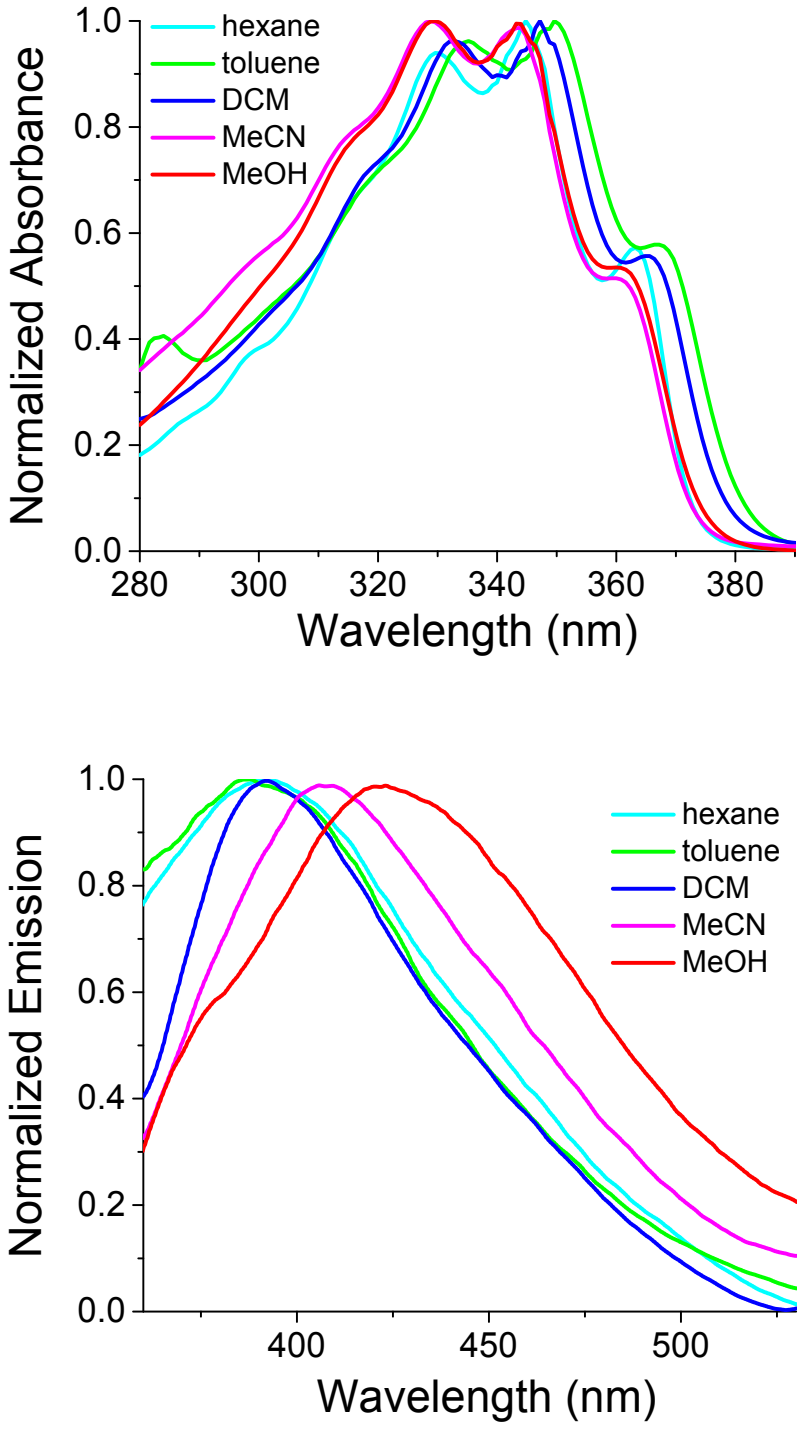


Figure S11. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2b** in different solvents, excited at 330 nm.

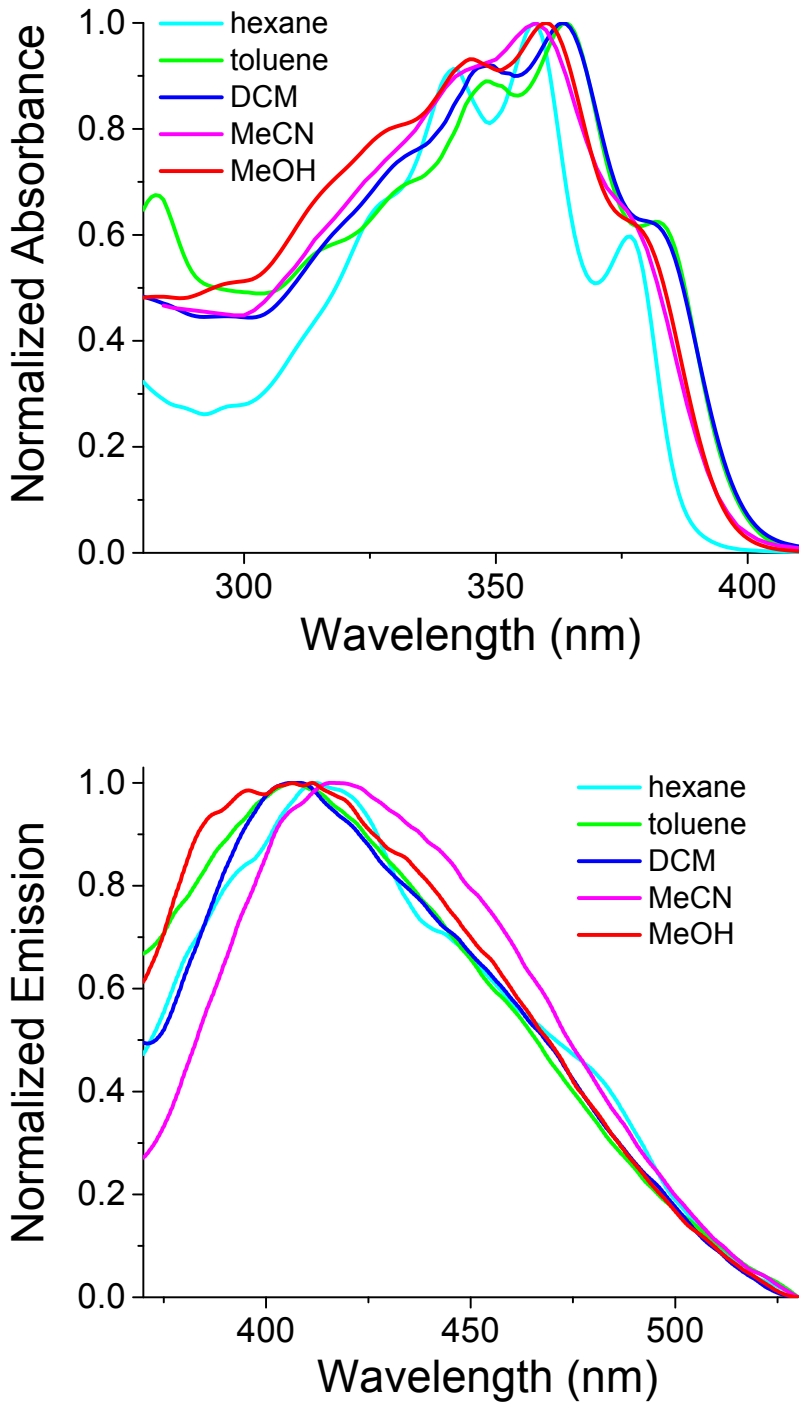


Figure S12. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2c** in different solvents, excited at 330 nm.

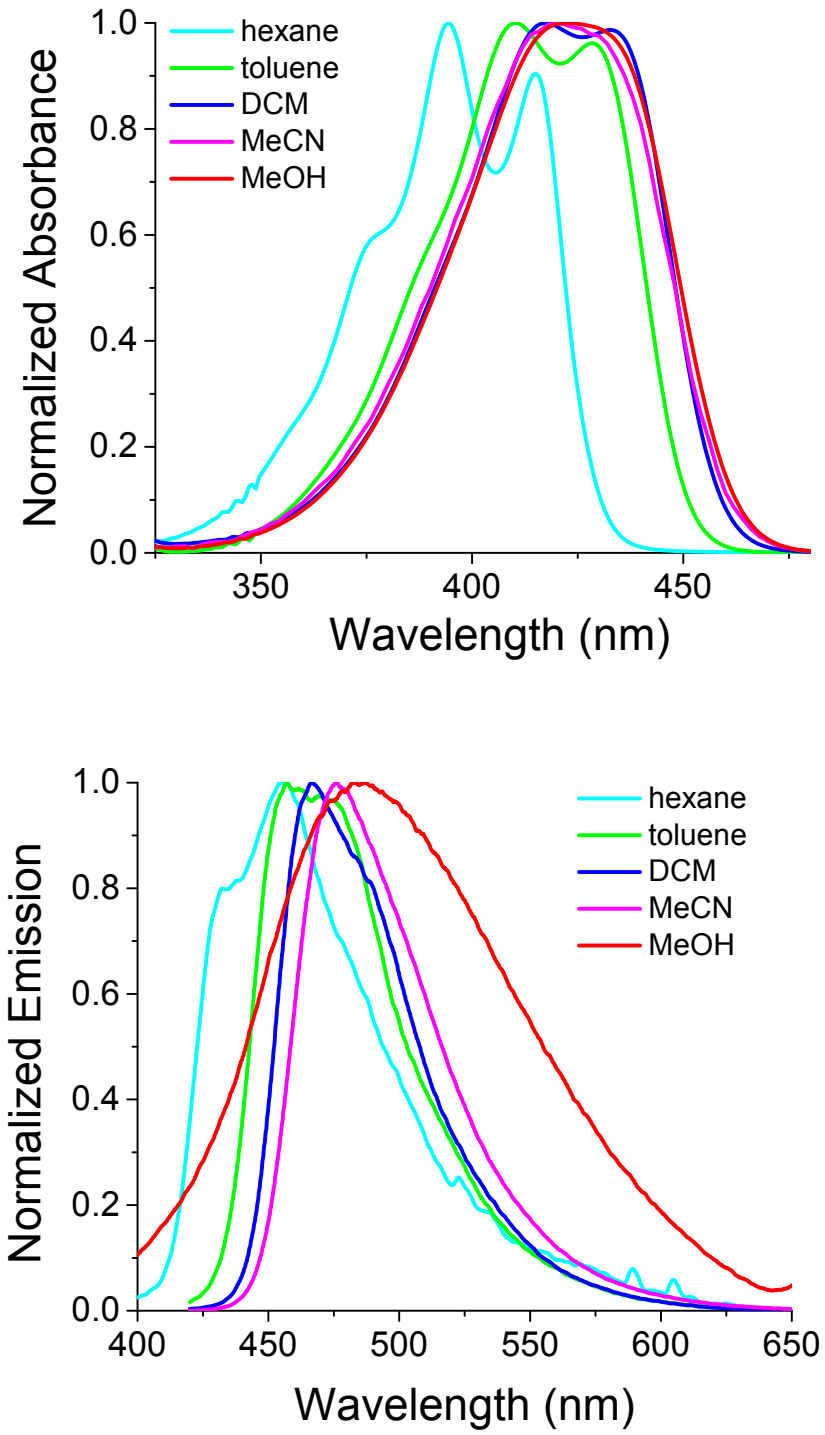


Figure S13. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2d** in different solvents, excited at 350 nm.

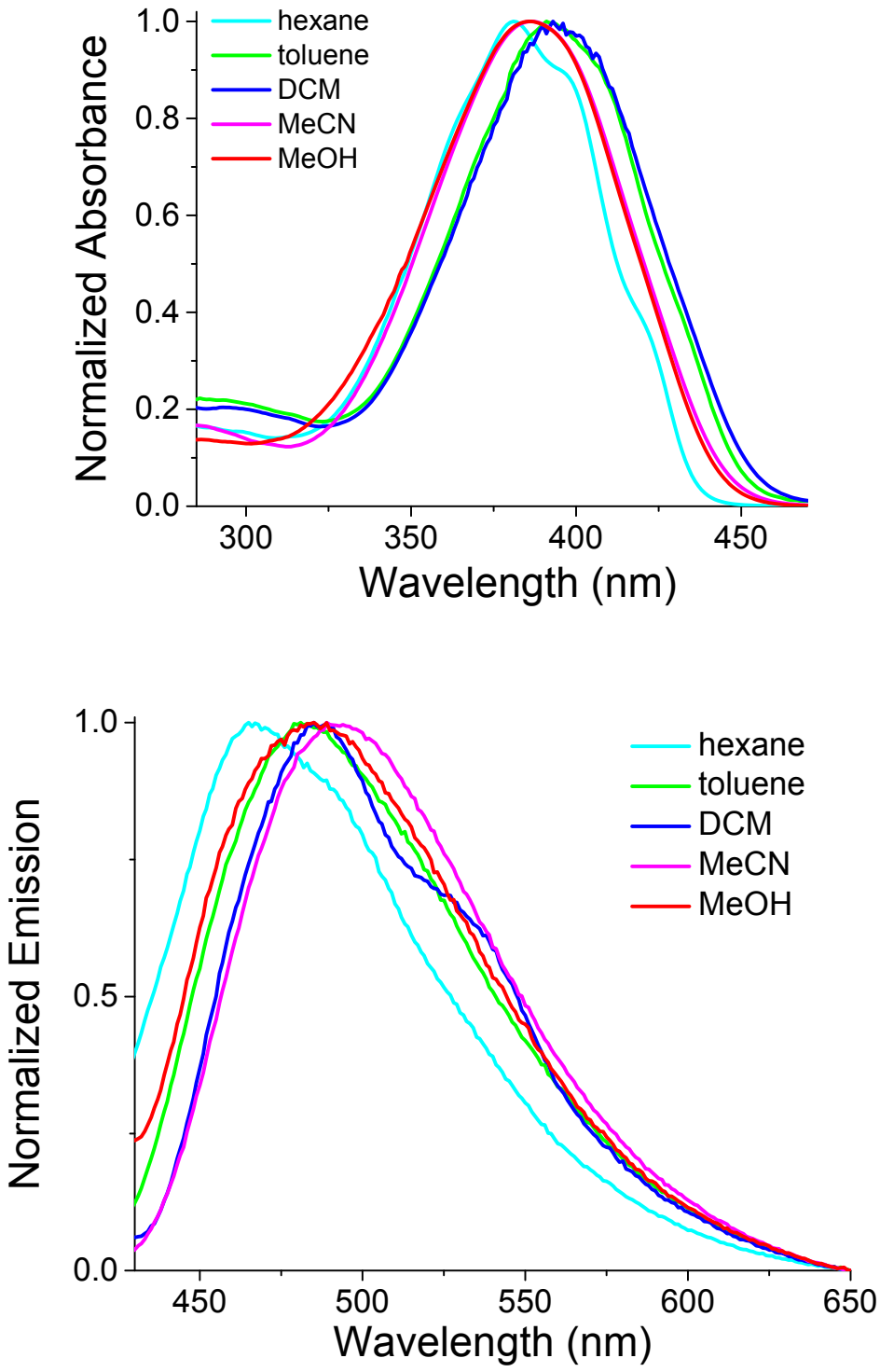


Figure S14. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2e** in different solvents, excited at 400 nm.

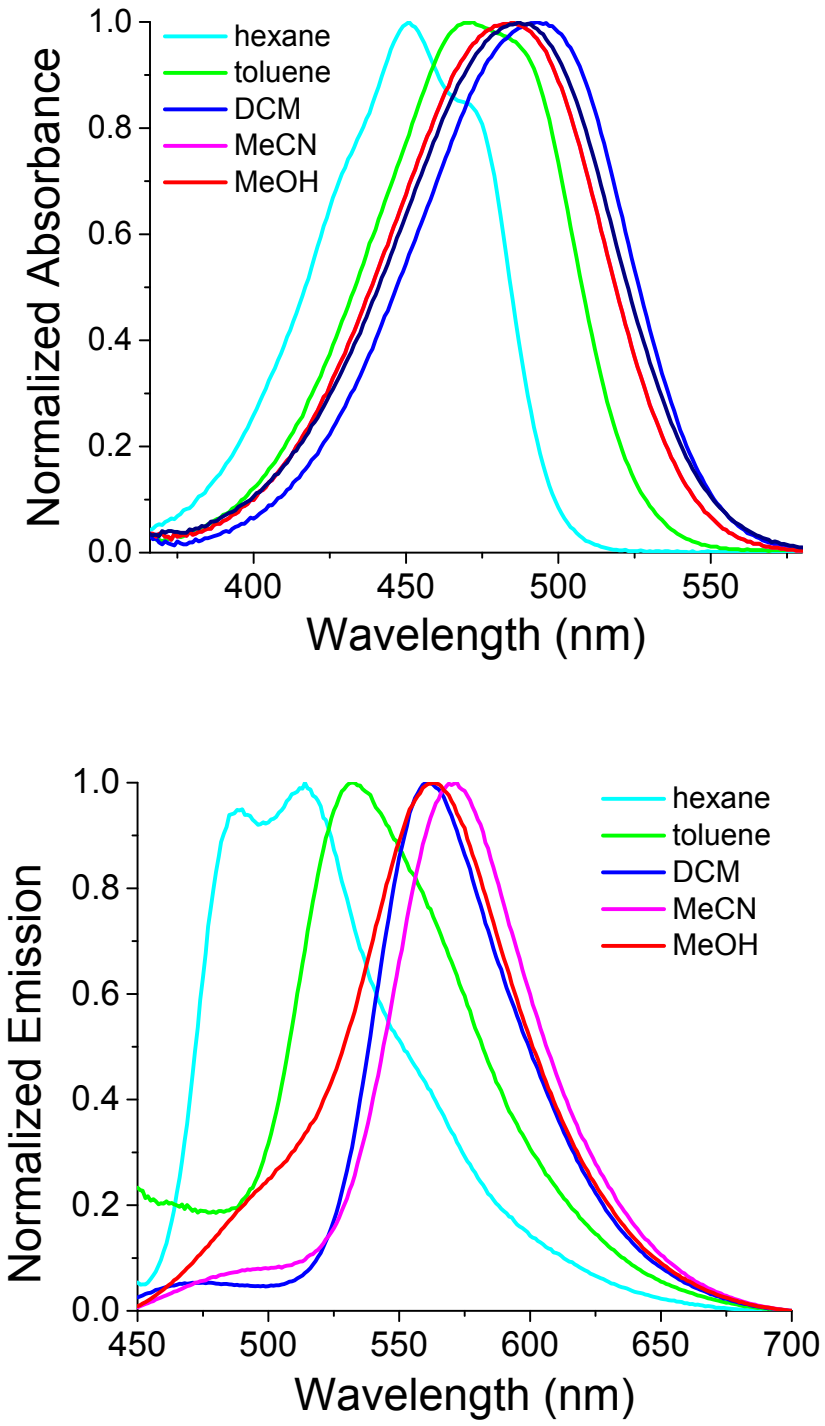


Figure S15. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2f** in different solvents, excited at 420 nm.

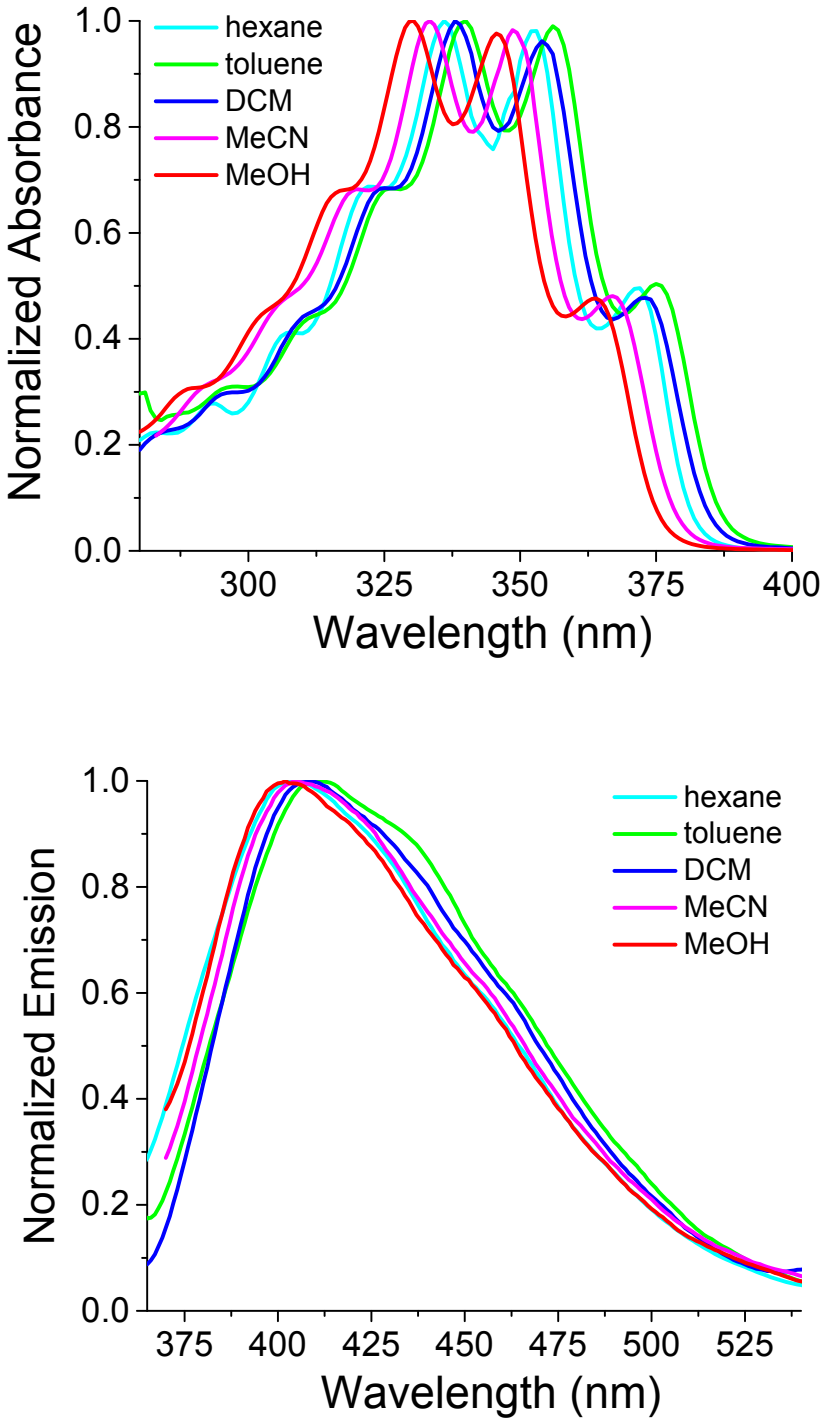


Figure S16. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2g** in different solvents, excited at 330 nm.

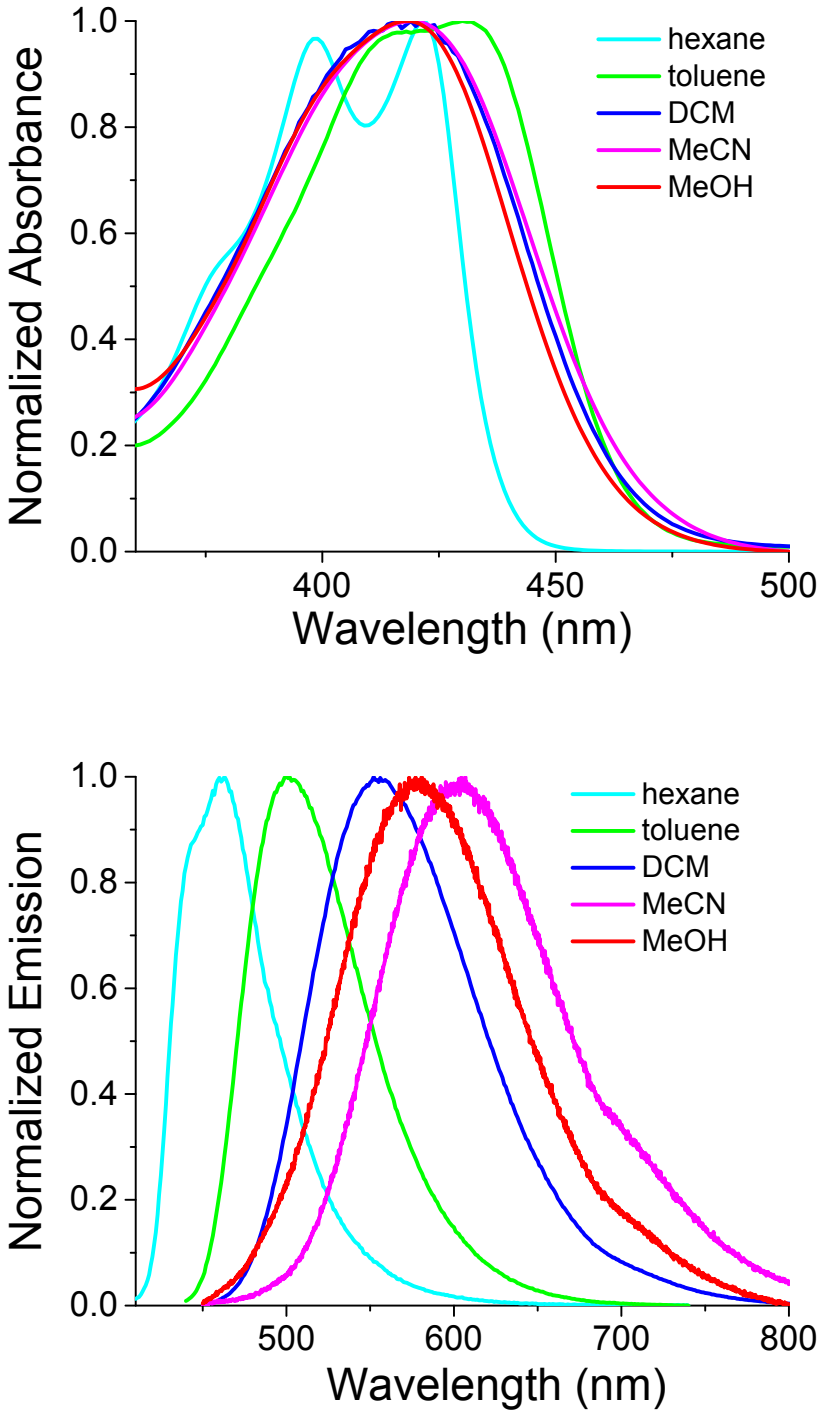


Figure S17. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2h** in hexane, toluene, dichloromethane, acetonitrile and methanol, respectively excited at 380, 420, 430, 430 and 430 nm.

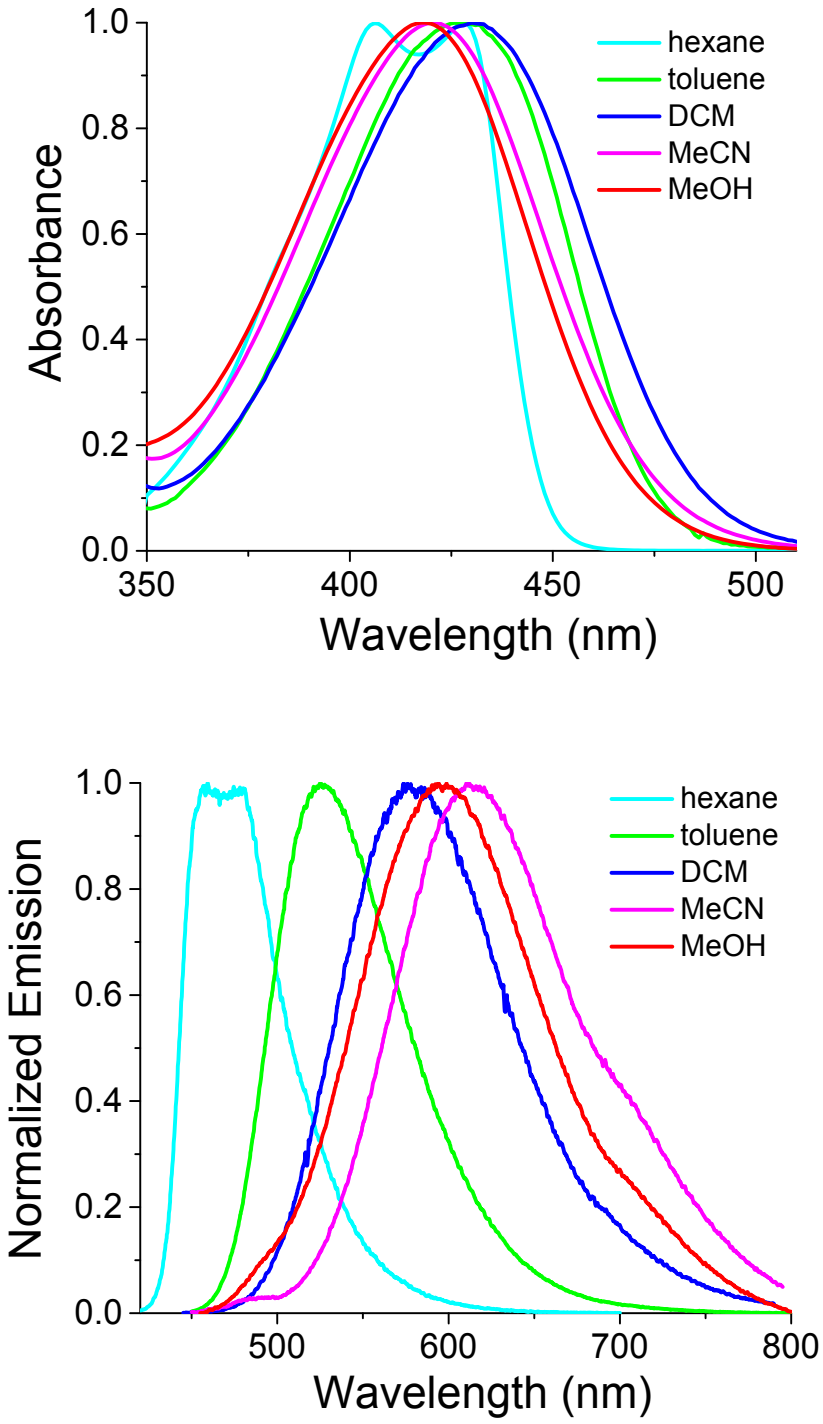


Figure S18. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2i** in hexane, toluene, dichloromethane, acetonitrile and methanol, respectively excited at 390, 430, 430, 430 and 430 nm.

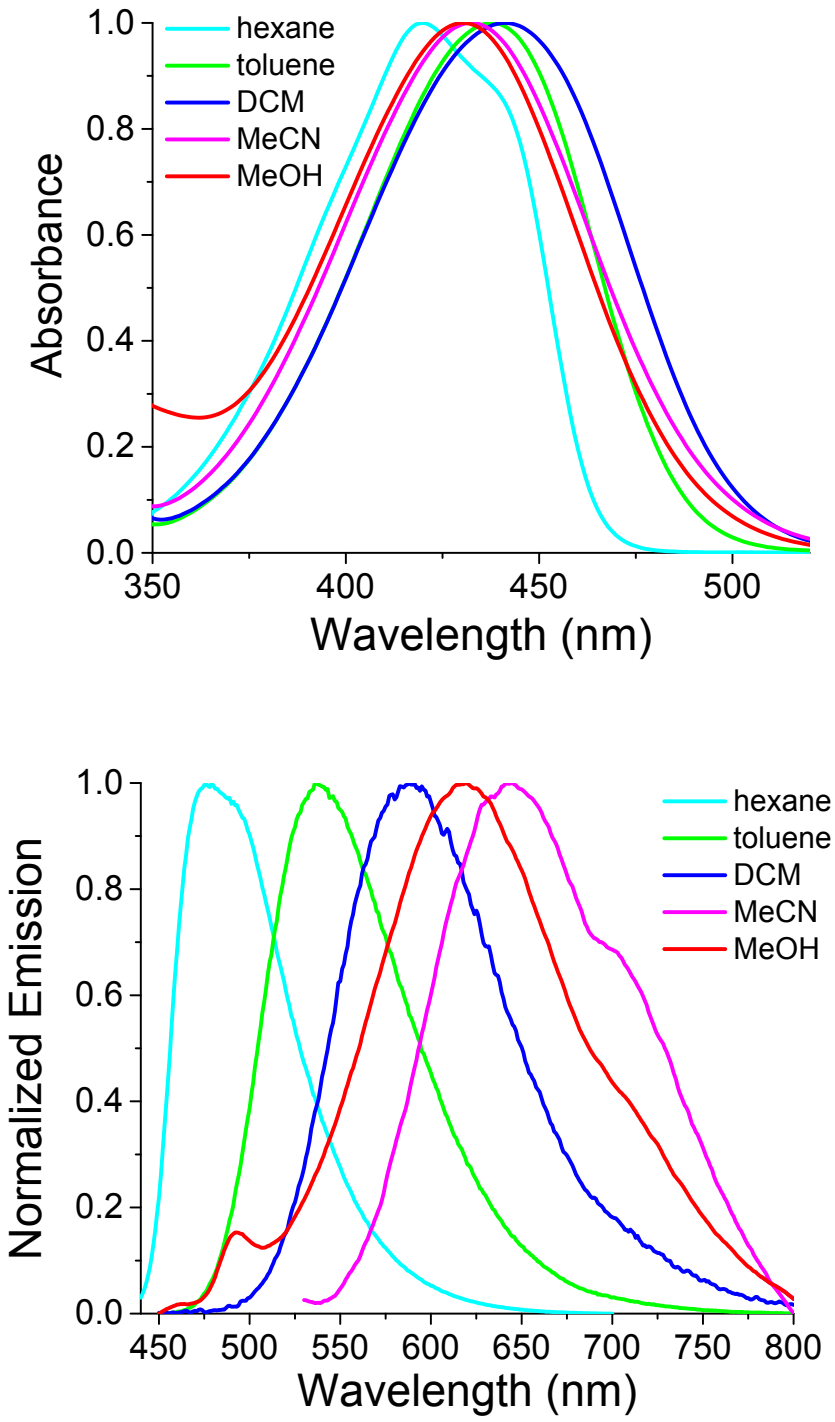


Figure S19. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2j** in hexane, toluene, dichloromethane, acetonitrile and methanol, respectively excited at 420, 430, 430, 430 and 430 nm.

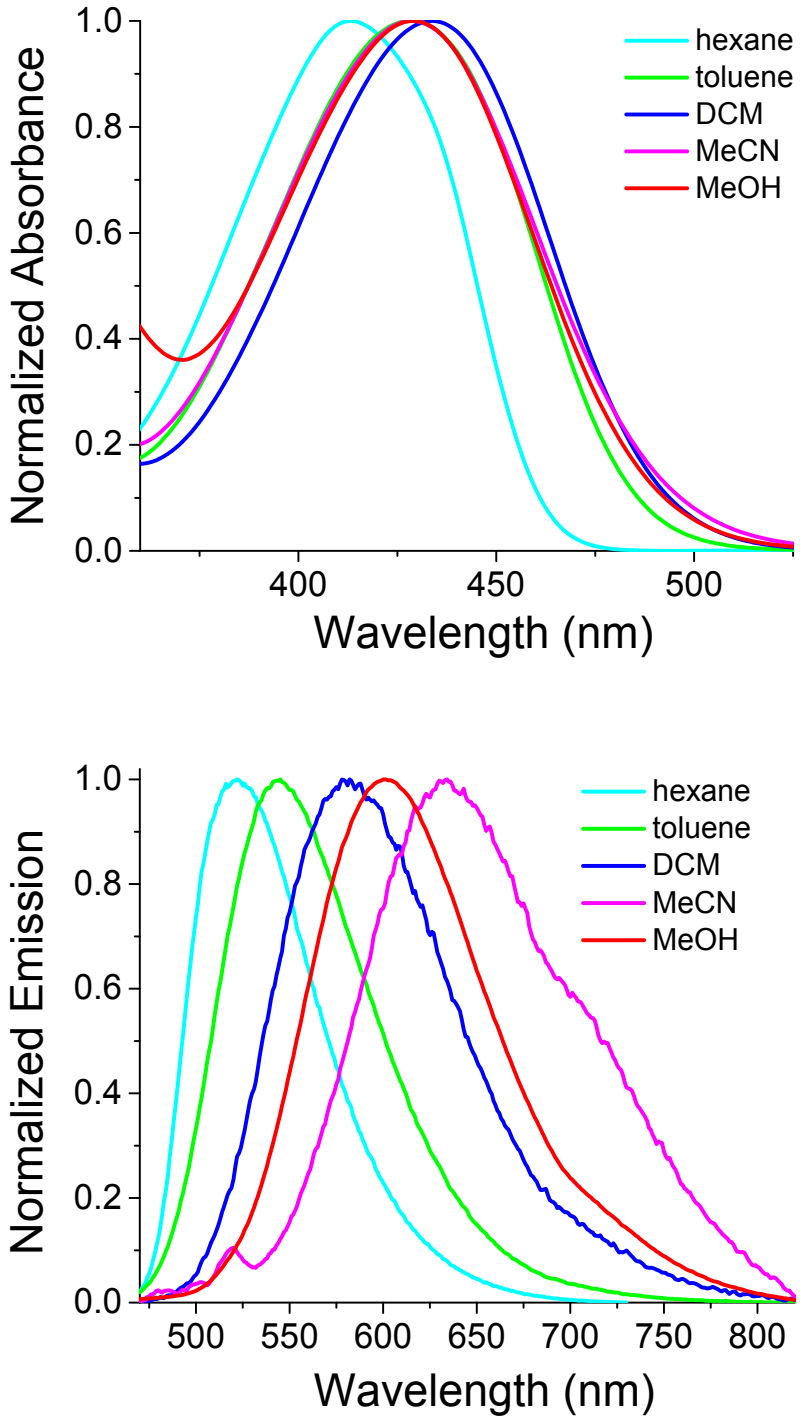


Figure S20. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2k** in hexane, toluene, dichloromethane, acetonitrile and methanol, excited at 430 nm.

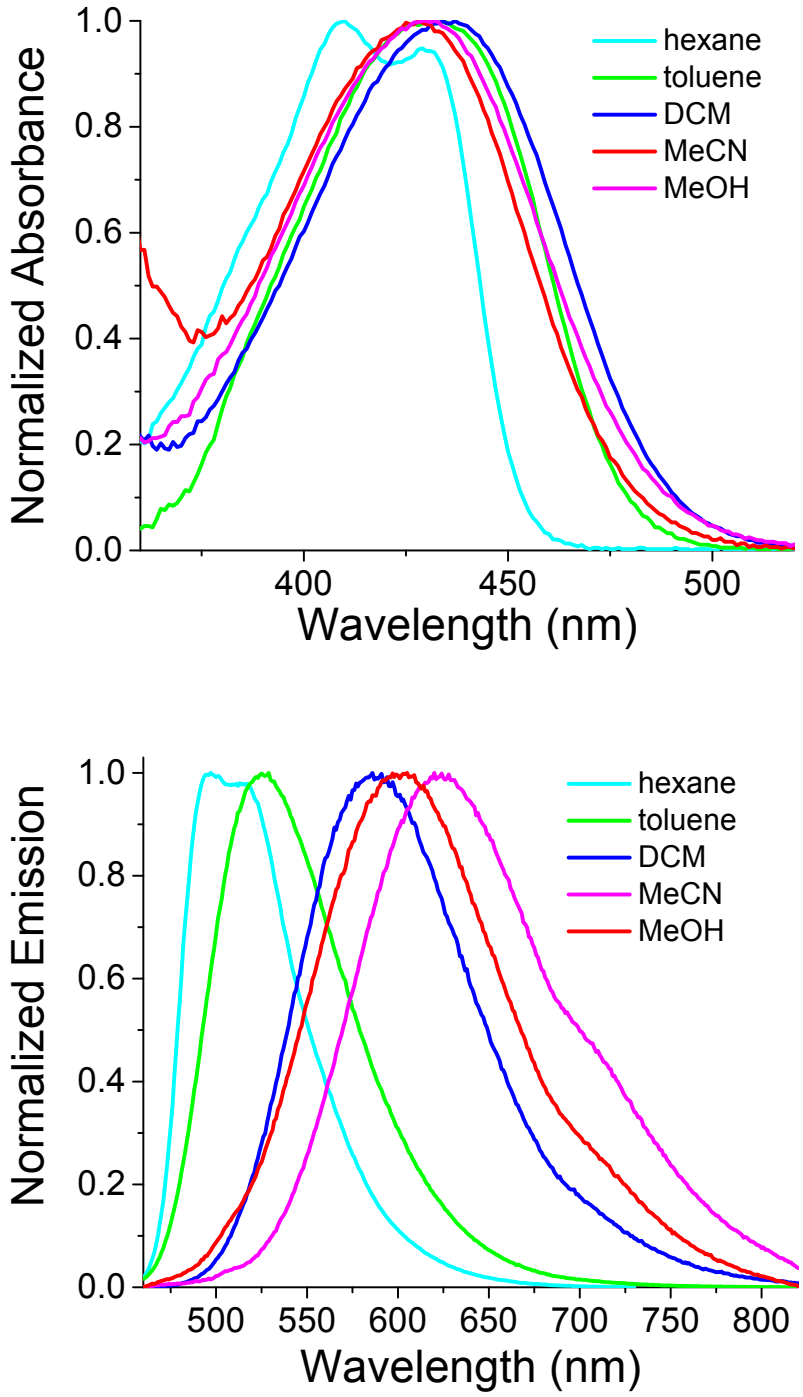


Figure S21. Normalized UV-vis (top) and fluorescence spectra (bottom) of **2l** in hexane, toluene, dichloromethane, acetonitrile and methanol, excited at 450 nm.

3. Solid-state emission properties

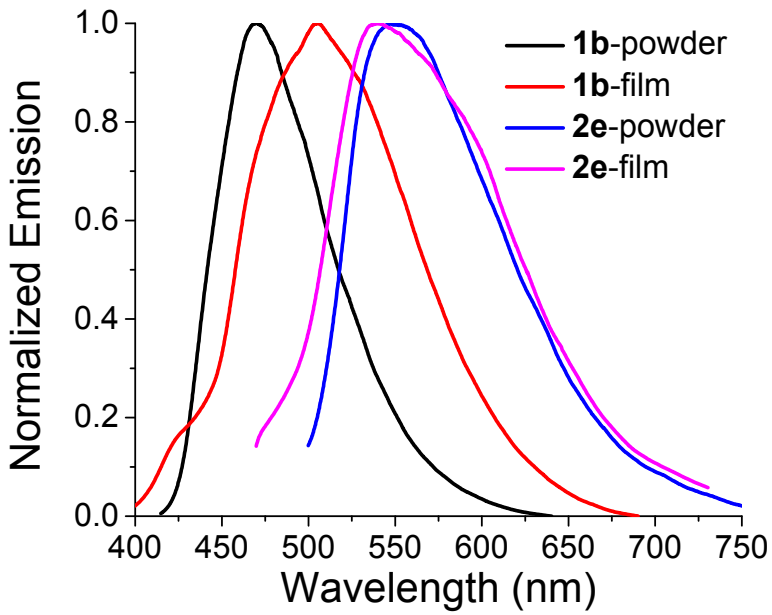


Figure S22. Normalized emission spectra of **1b** (excited at 380 nm) and **2e** (excited at 480 nm) in the powder state and the thin film state.

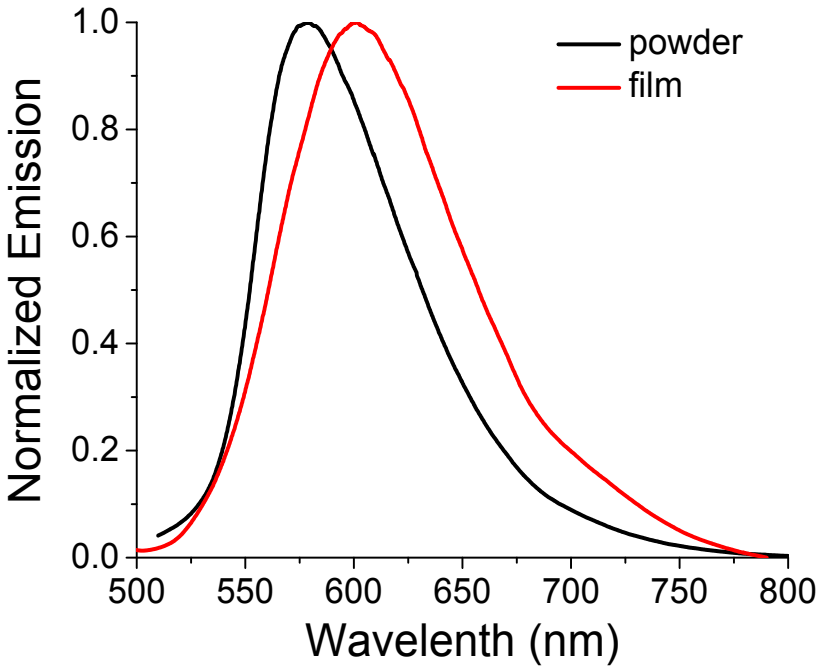


Figure S23. Normalized emission spectra of **2i** in the powder state and the thin film state, excited at 480 nm.

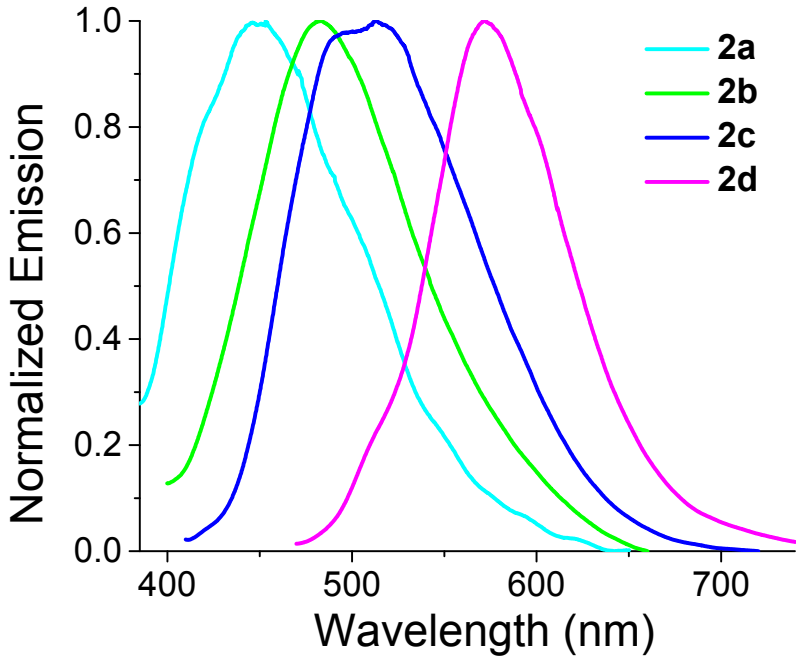


Figure S24. Normalized emission spectra of **2a-d** in the thin film state.

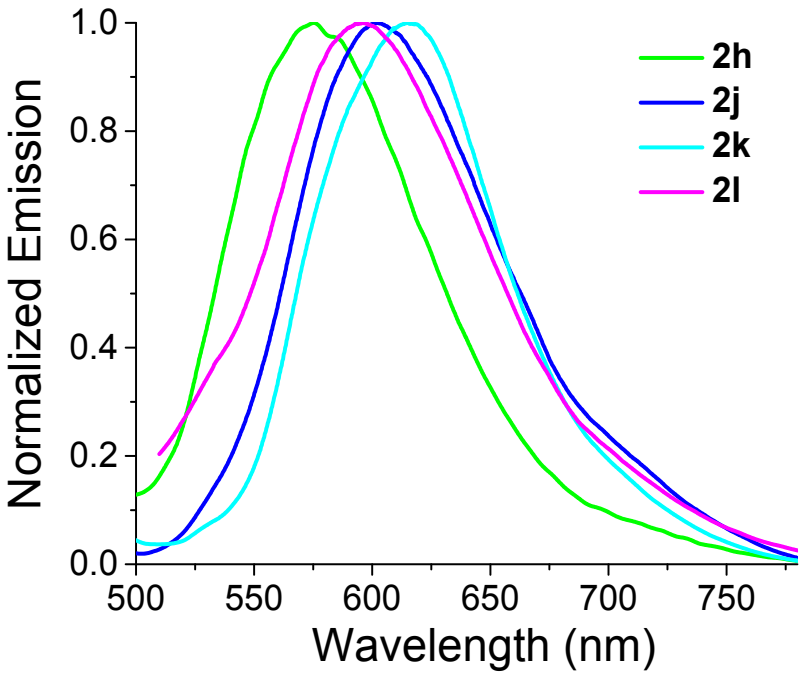


Figure S25. Normalized emission spectra of **2h** and **2j-l** in their thin film state, excited at 480 nm.

4. Aggregation-induced emission properties

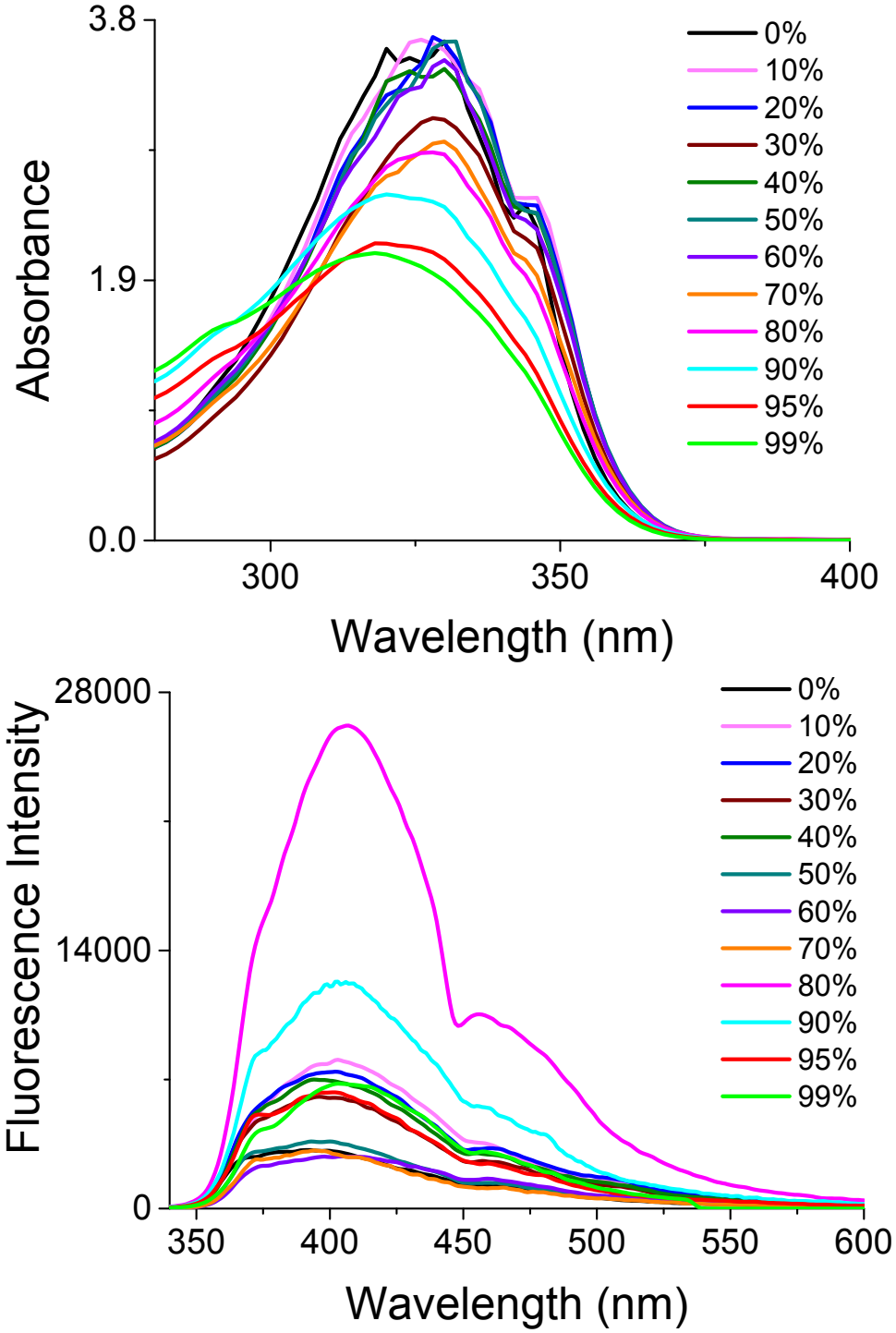


Figure S26. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **1a** (1.2 x 10^{-4} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 330 nm.

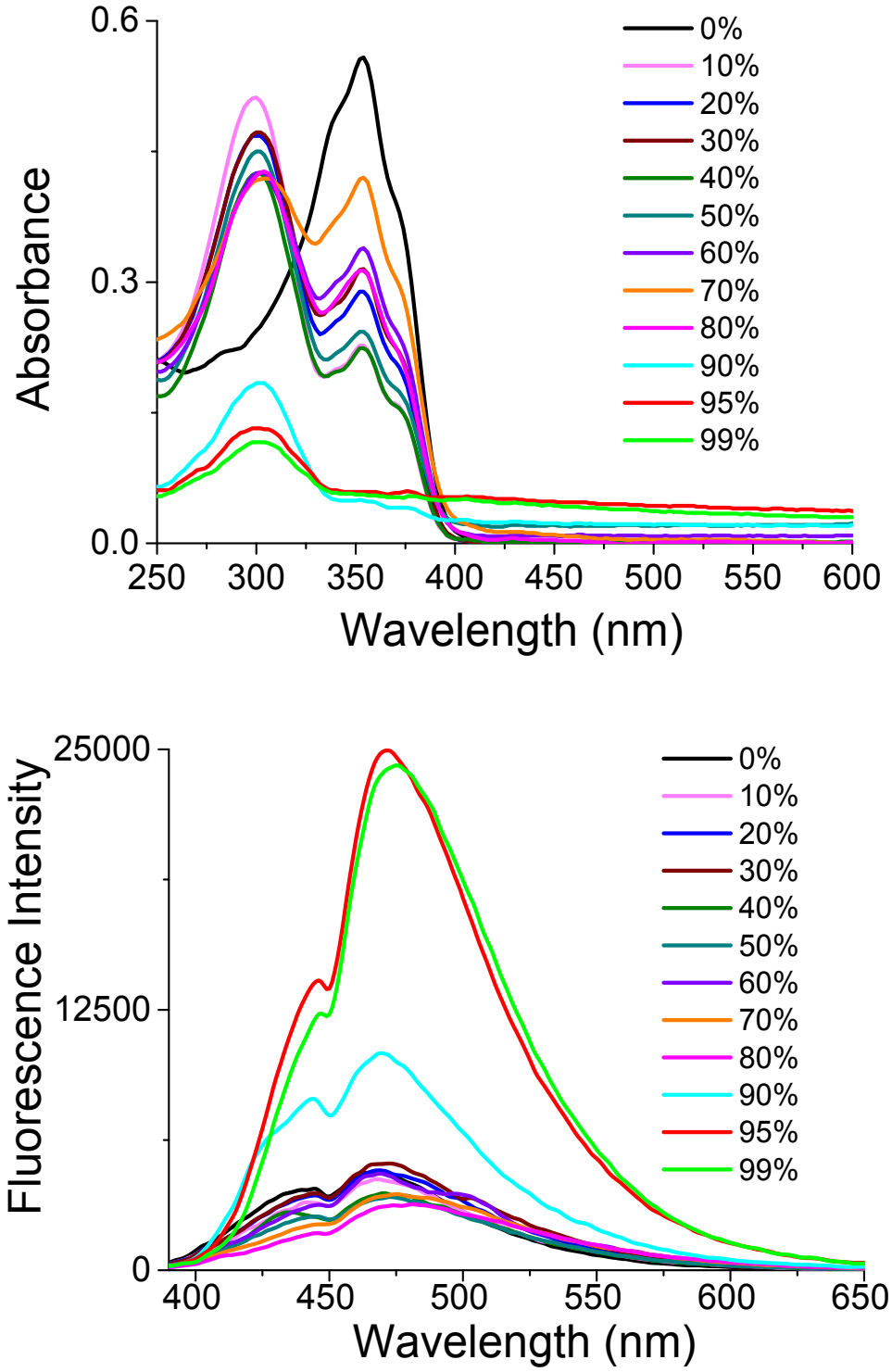


Figure S27. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **1b** (2.1 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 370 nm.

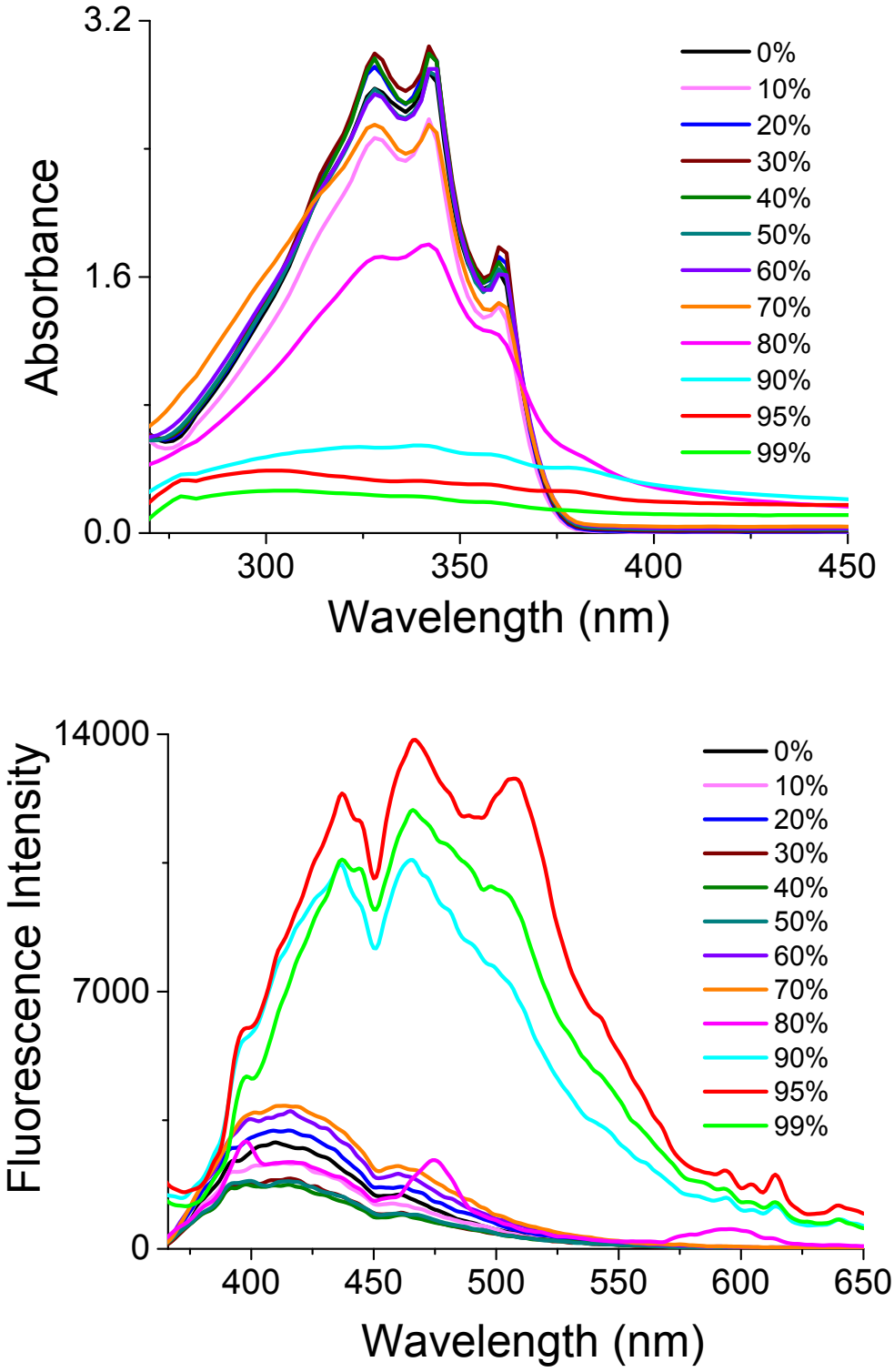


Figure S28. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2a** (1.1 x 10^{-4} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 350 nm.

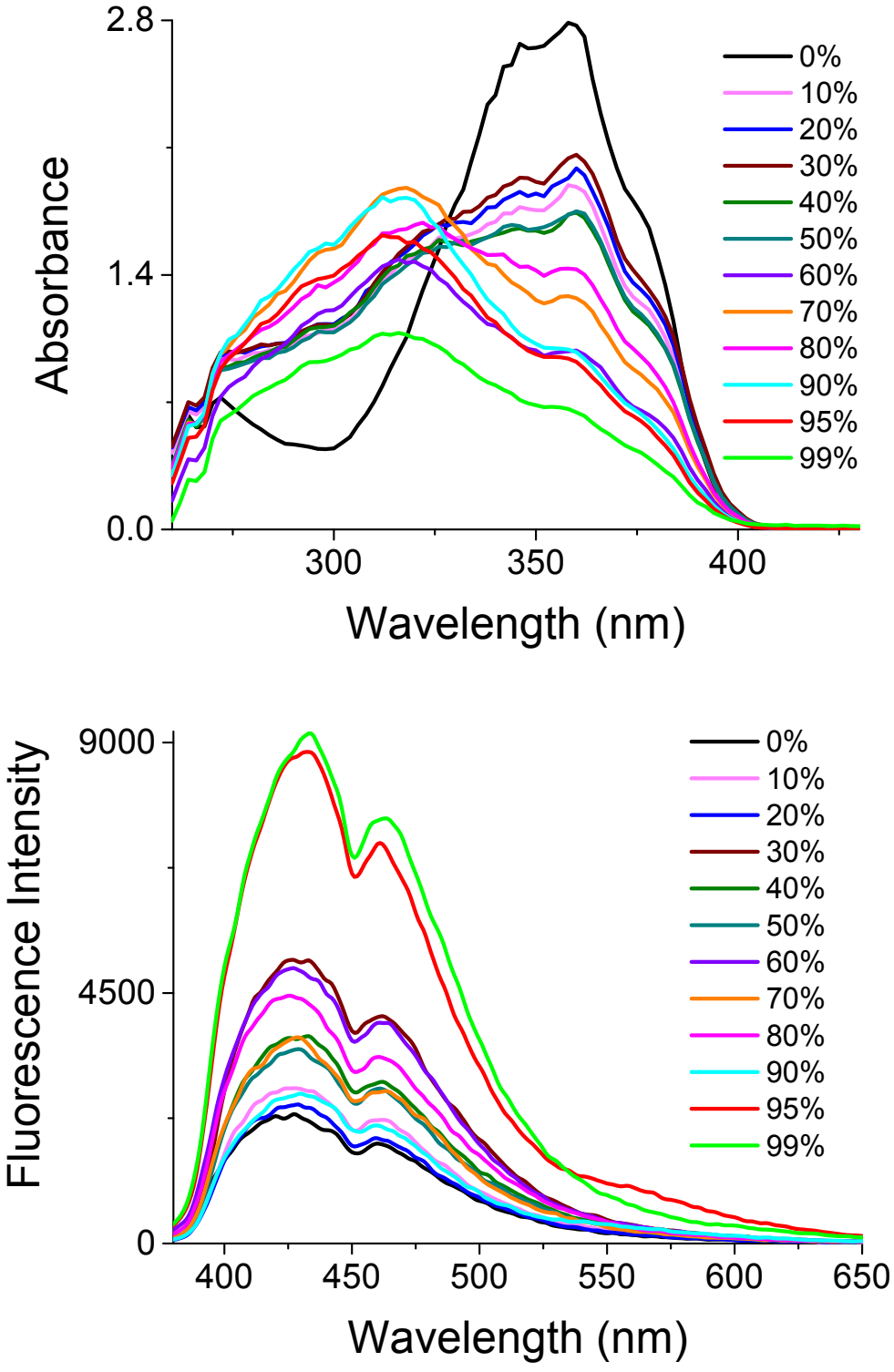


Figure S29. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2b** (1.0×10^{-4} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 350 nm.

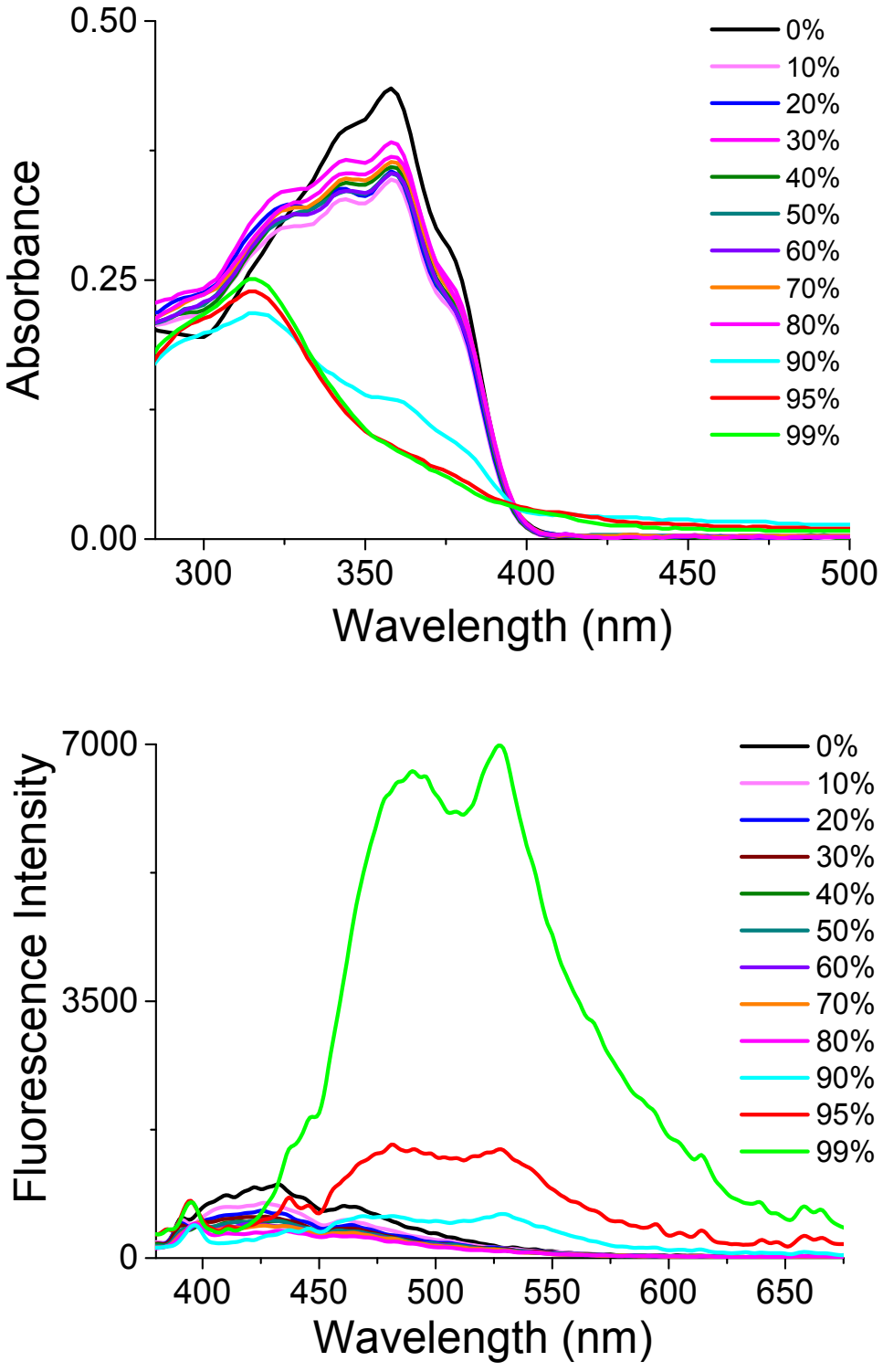


Figure S30. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2c** (2.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 350 nm.

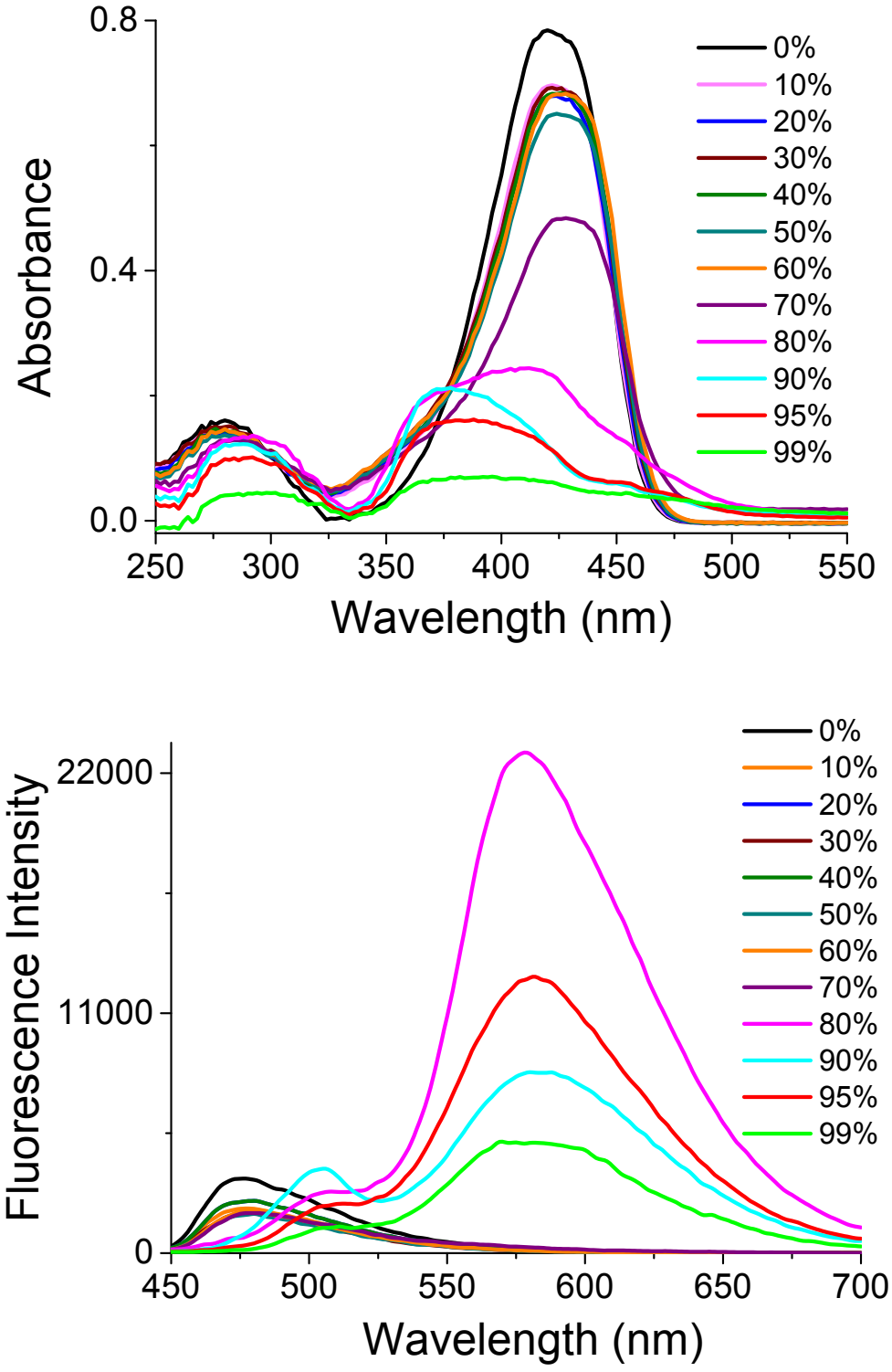


Figure S31. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2d** (2.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 420 nm.

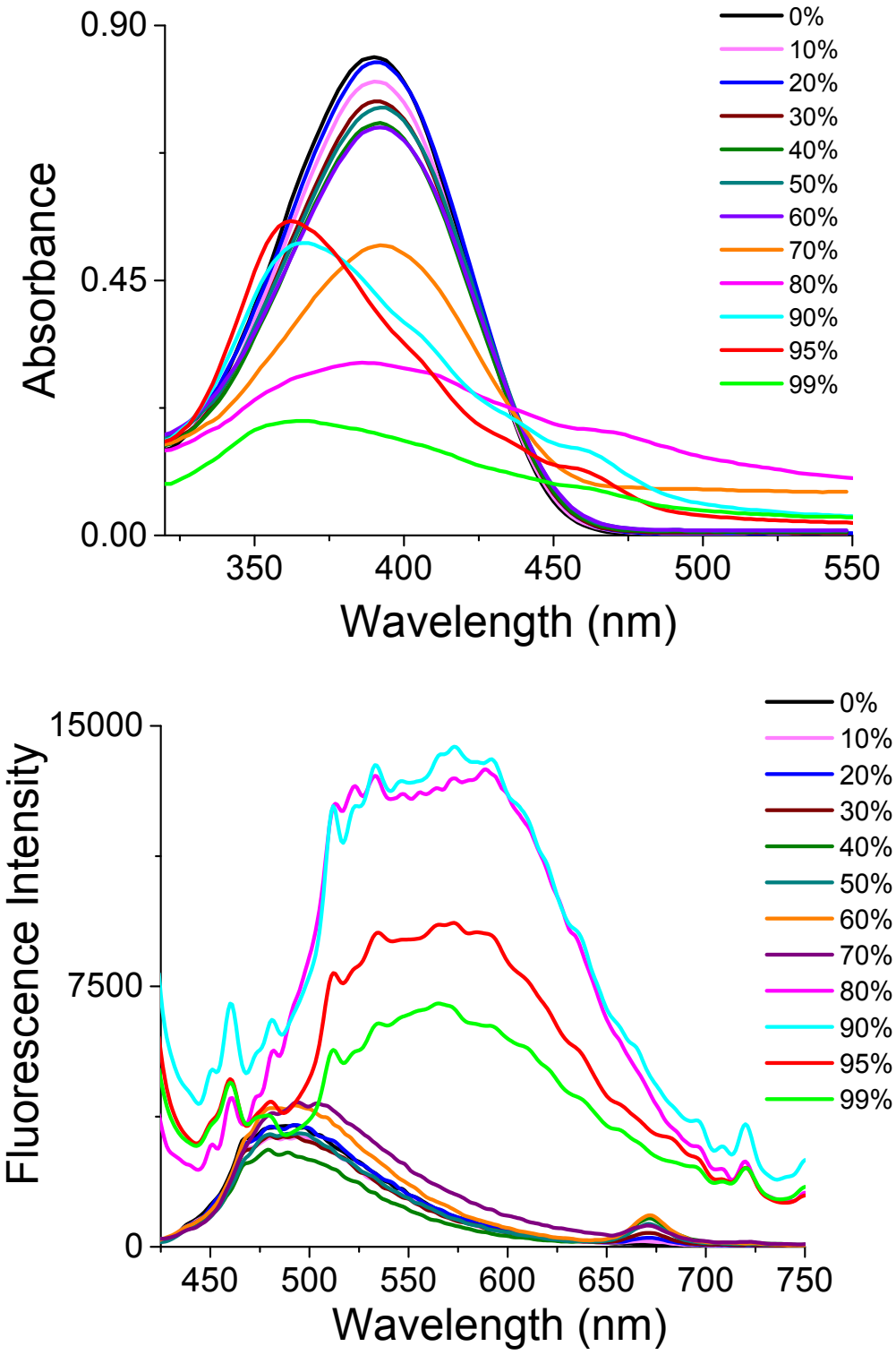


Figure S32. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2e** (2.7 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 410 nm.

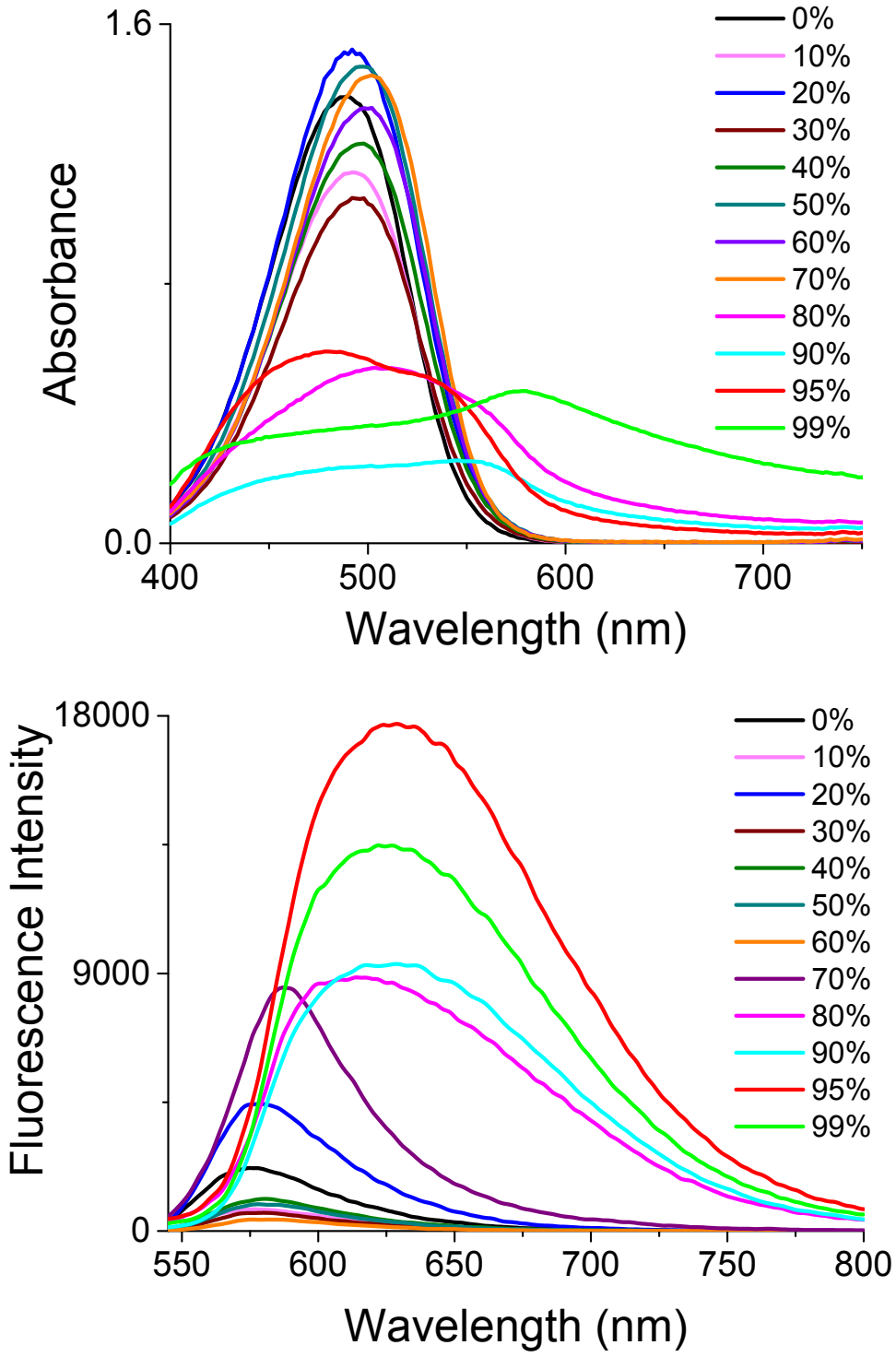


Figure S33. UV-vis (top) and fluorescence (bottom) spectra of BOAHY **2f** (5 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 510 nm.

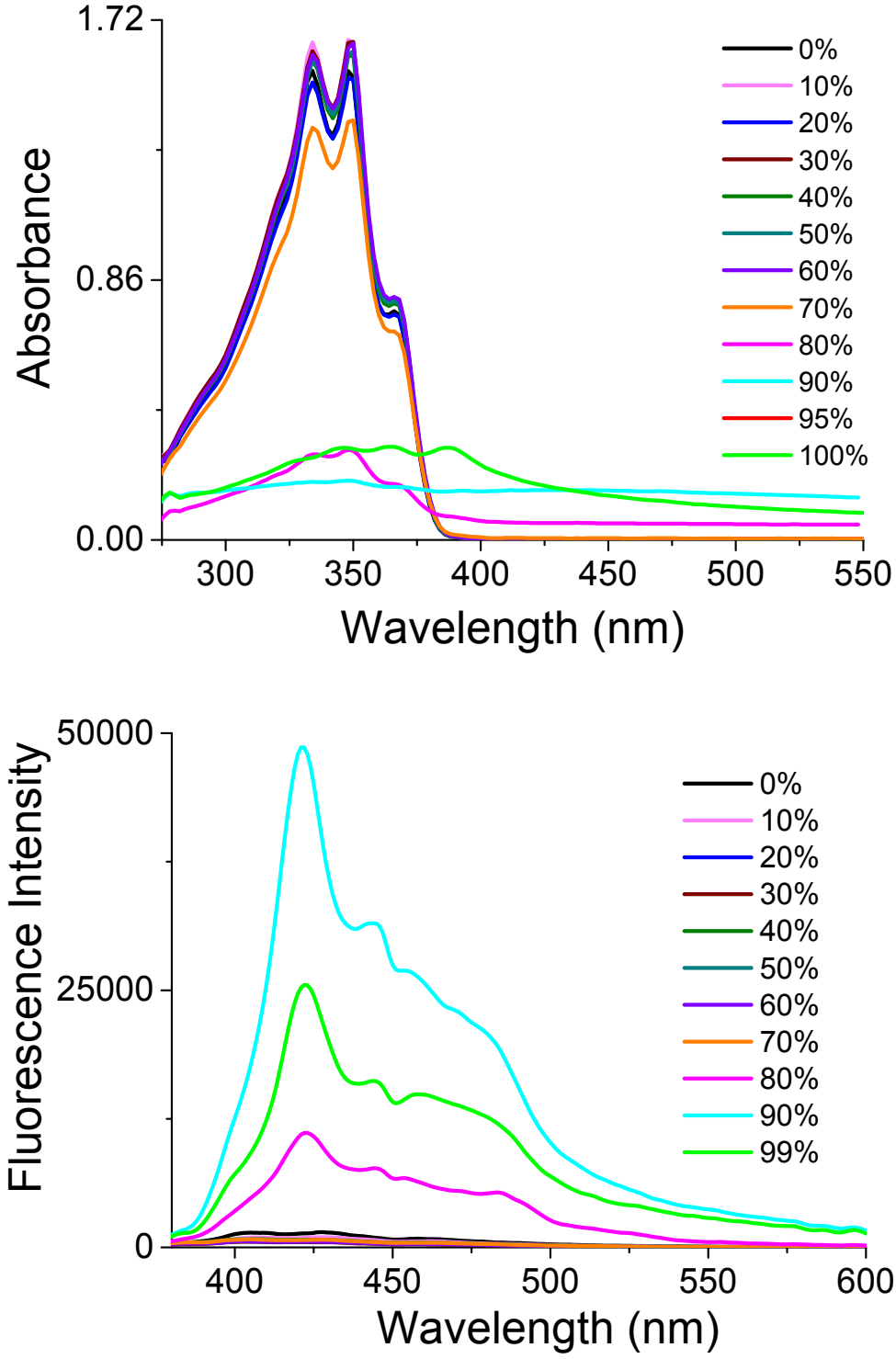


Figure S34. UV-vis (top) and fluorescence (bottom) spectra of **2g** (4.1 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 340 nm.

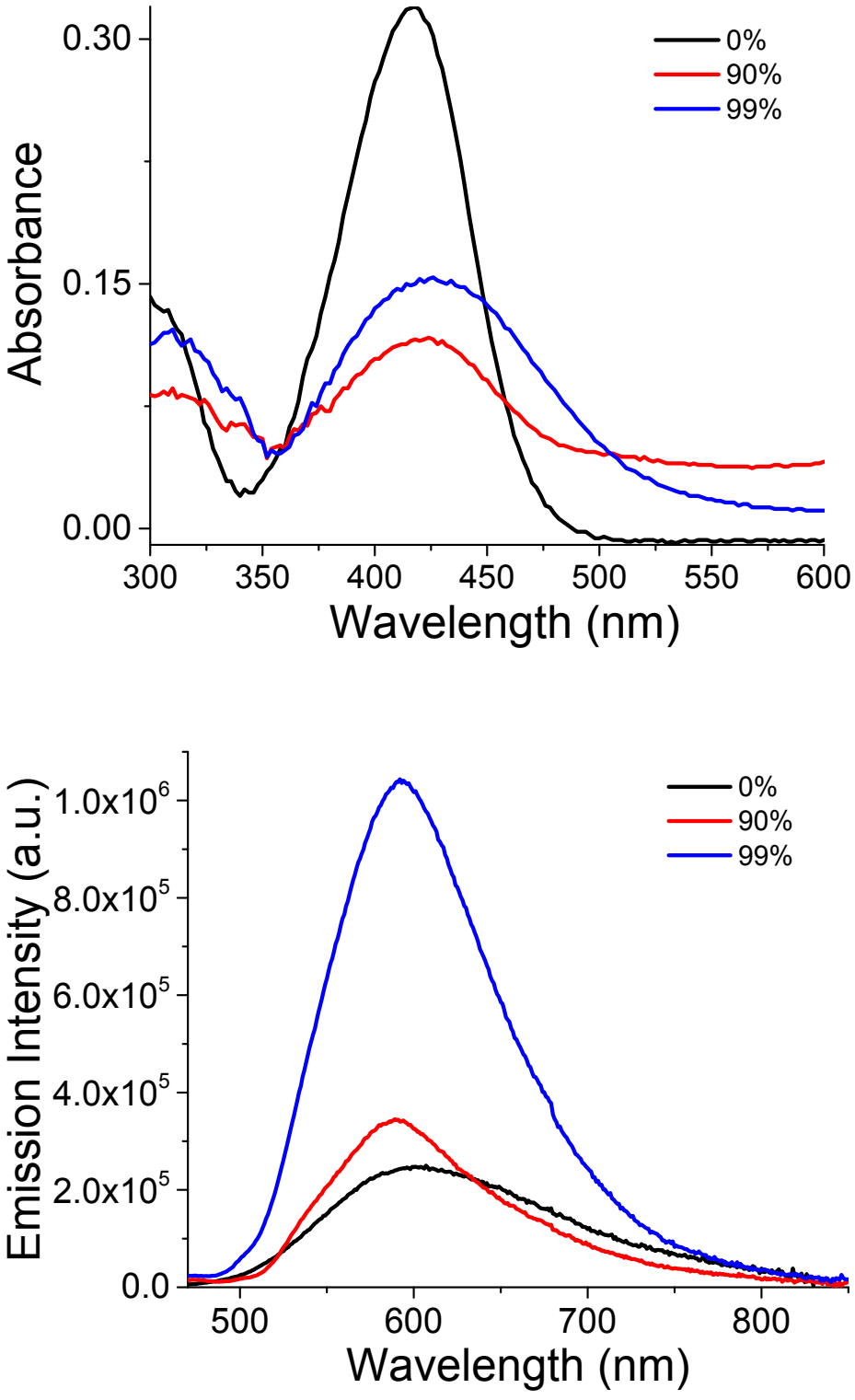


Figure S35. UV-vis (top) and fluorescence (bottom) spectra of **2h** (1.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 440 nm.

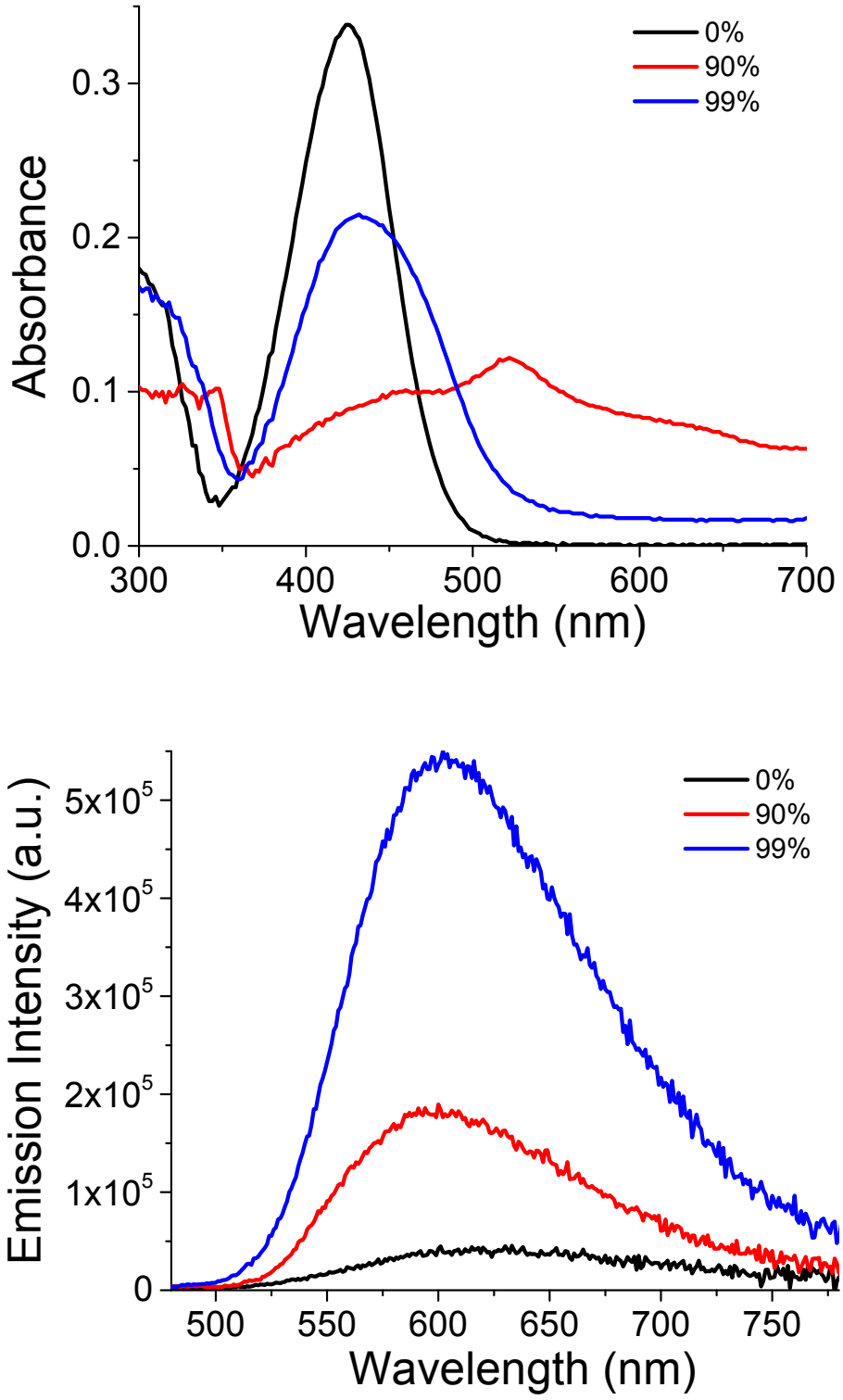


Figure S36. UV-vis (top) and fluorescence (bottom) spectra of **2i** (1.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 440 nm.

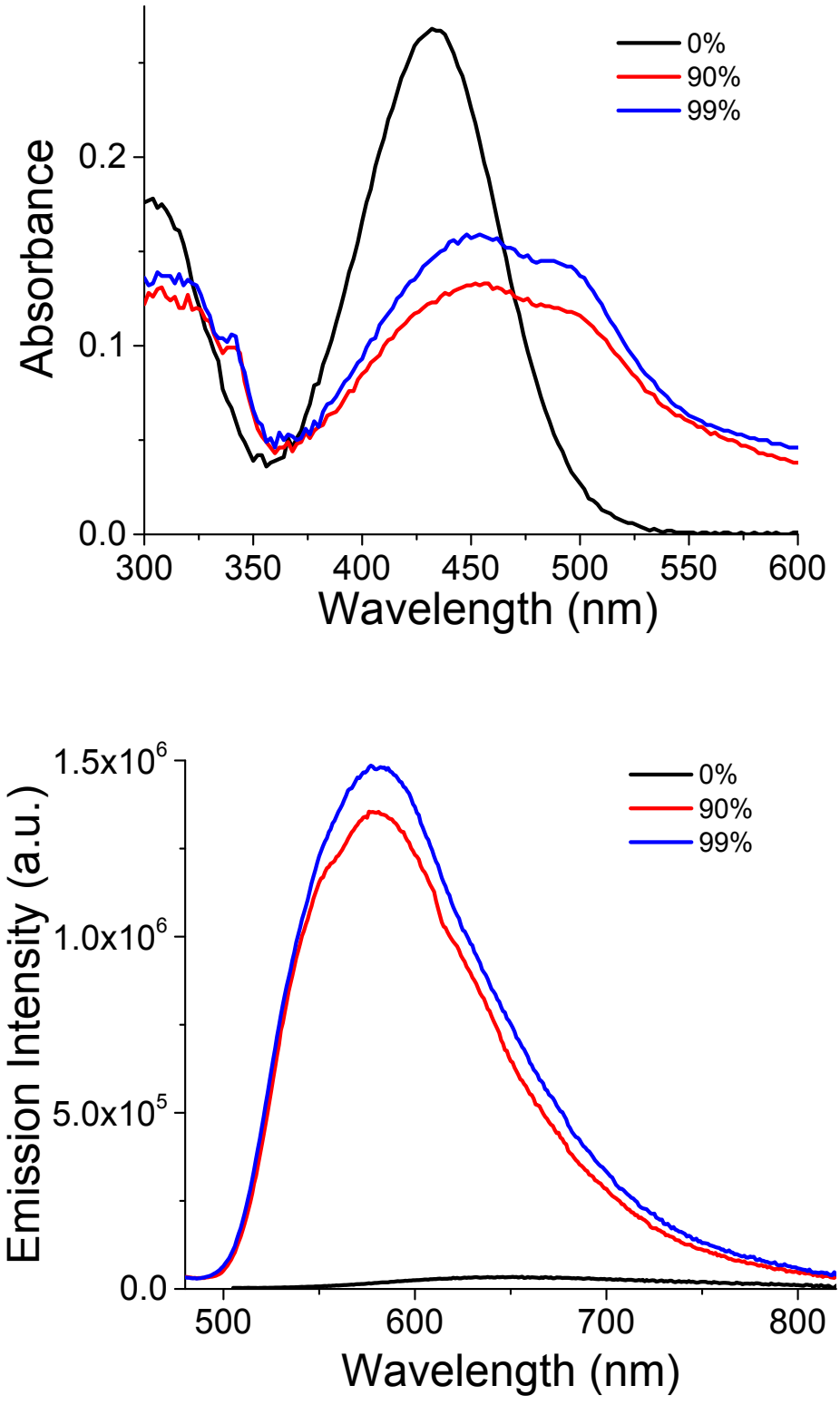


Figure S37. UV-vis (top) and fluorescence (bottom) spectra of **2j** (1.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 450 nm.

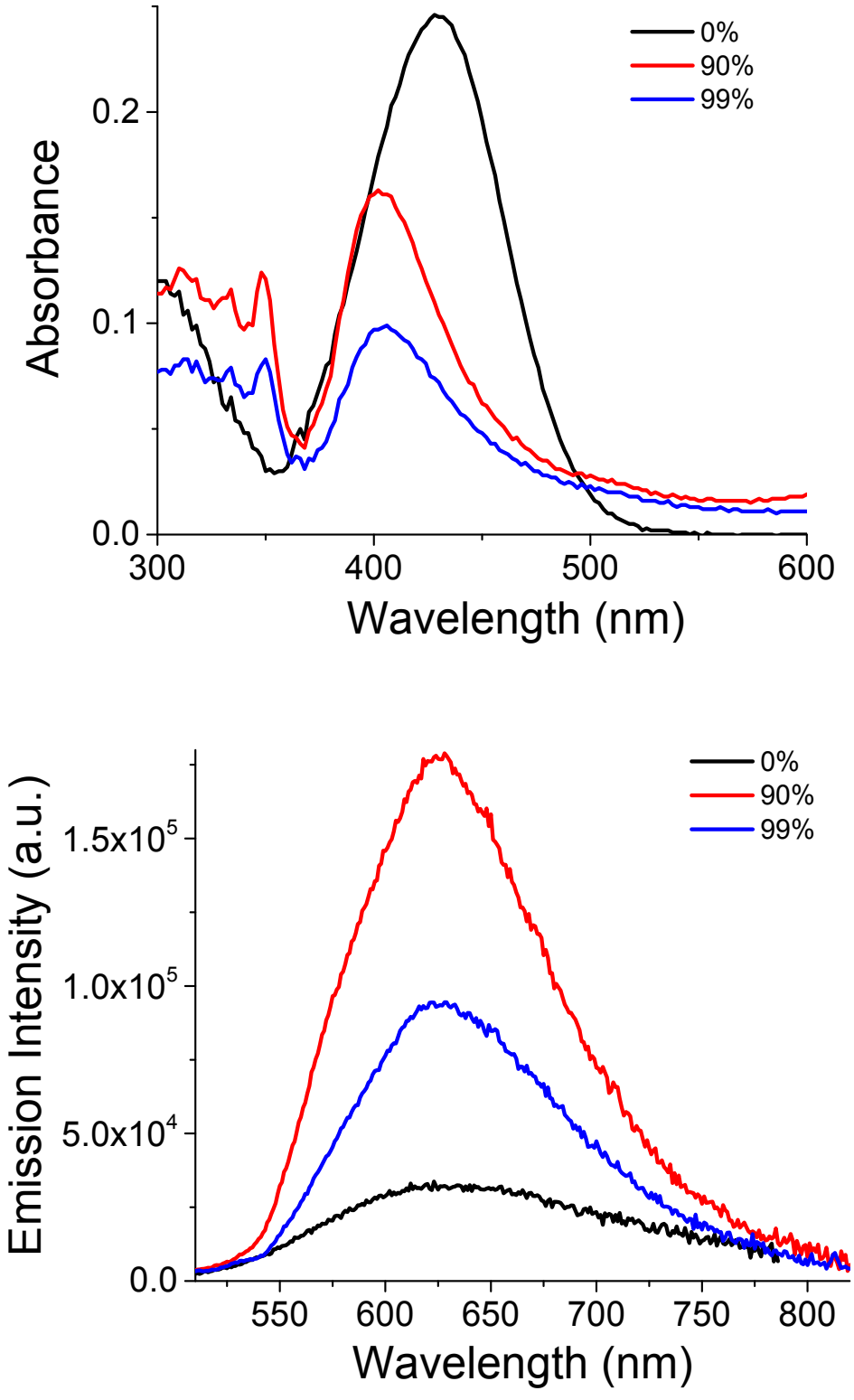


Figure S38. UV-vis (top) and fluorescence (bottom) spectra of **2k** (1.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 480 nm.

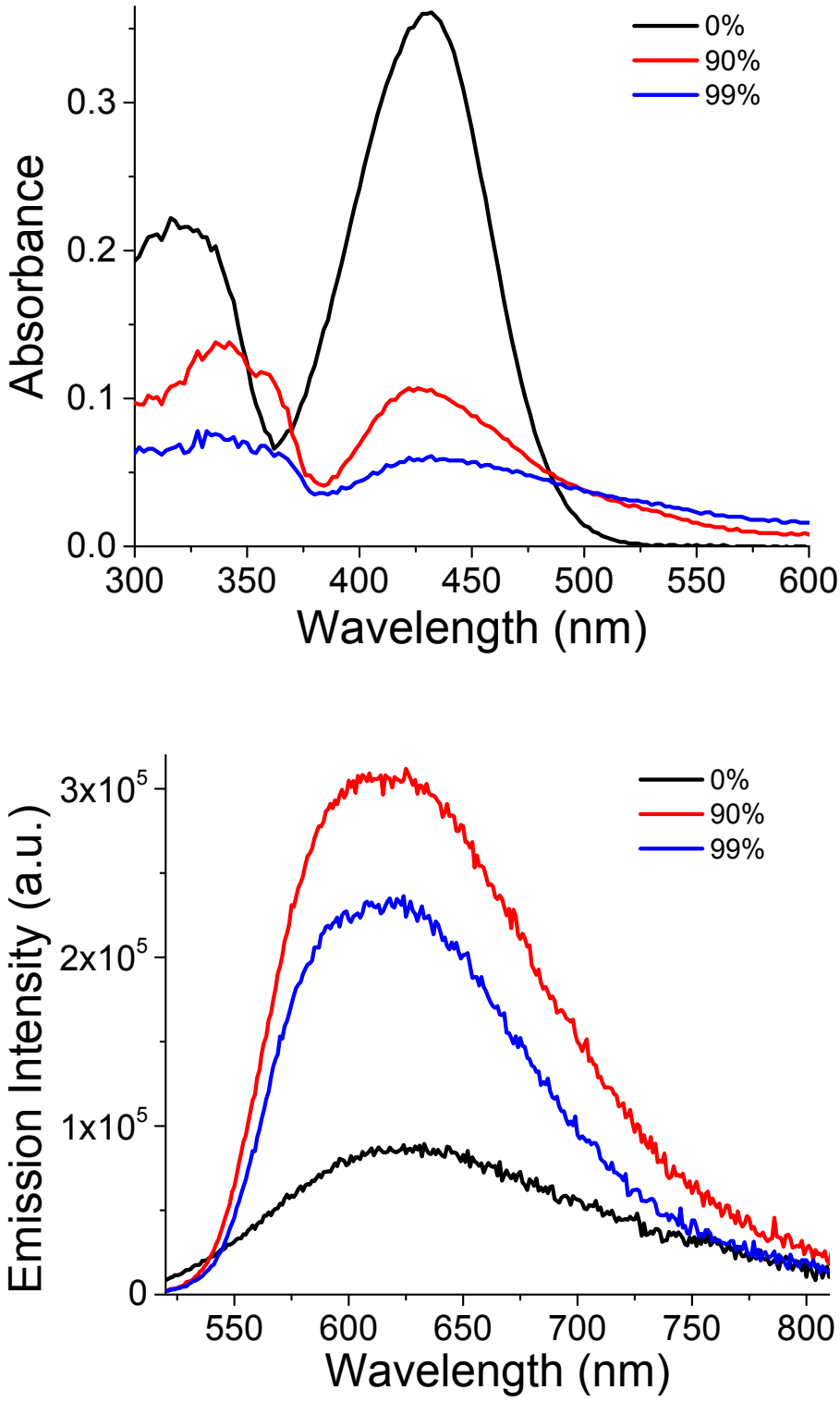


Figure S39. UV-vis (top) and fluorescence (bottom) spectra of **2l** (1.0 x 10^{-5} mol/L) in acetonitrile/water with different water fractions (f_w), excited at 480 nm.

5. Viscosity sensitivity studies

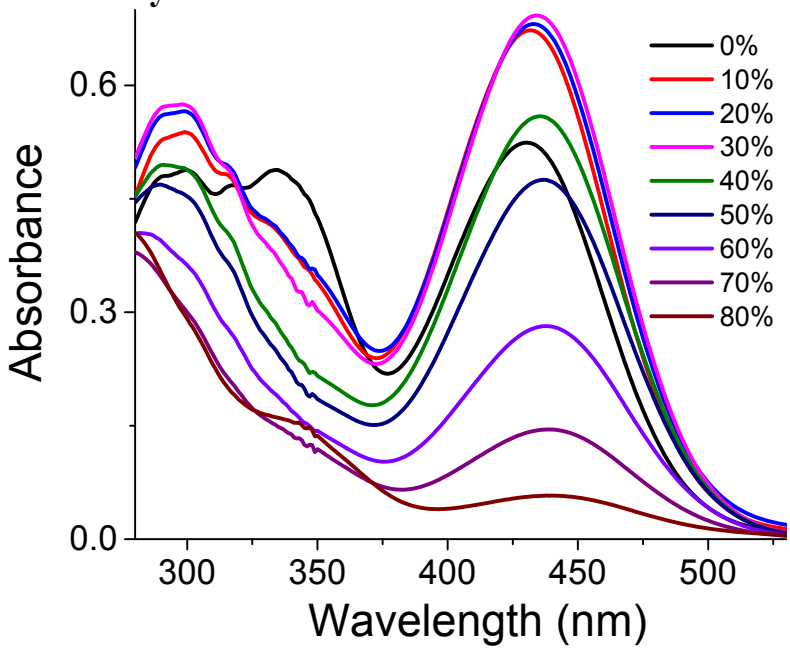


Figure S40. Absorbance spectra of **2j** in glycerol/methanol systems with different viscosities.

6. *Z*/*E* photoisomerization studies

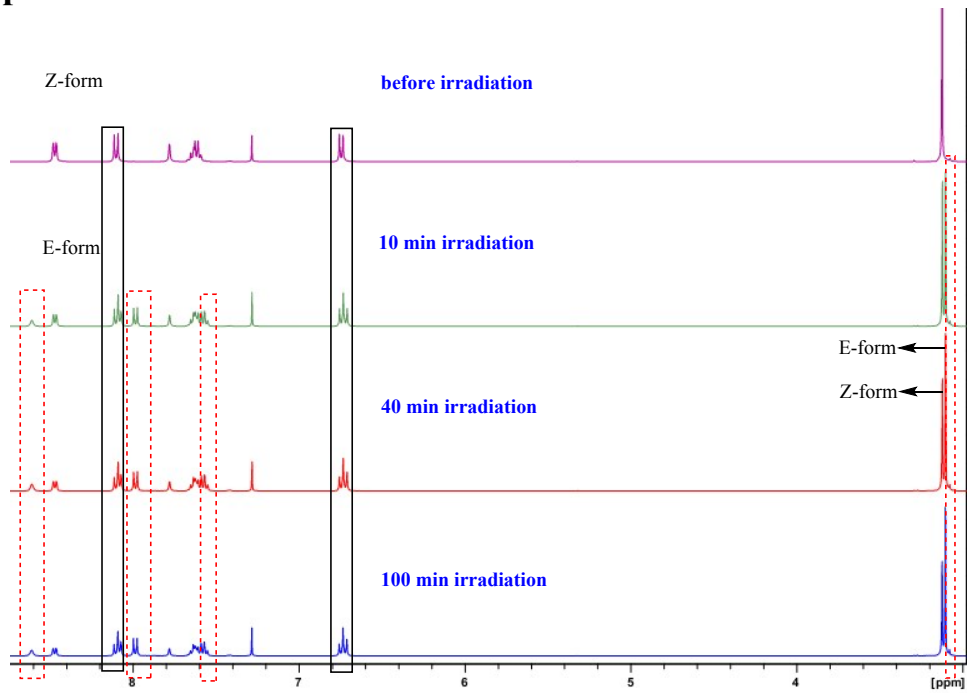


Figure 41. *Z*/*E* photoisomerization process was monitored *via* ^{1}H NMR spectroscopy. Pure *Z*-form isomer of **2h** (before irradiation, upper spectra) in chloroform-*d* (20 mM) was irradiated by a 3 W 365 nm UV lamp for 10, 40 and 100 min (lower spectra).

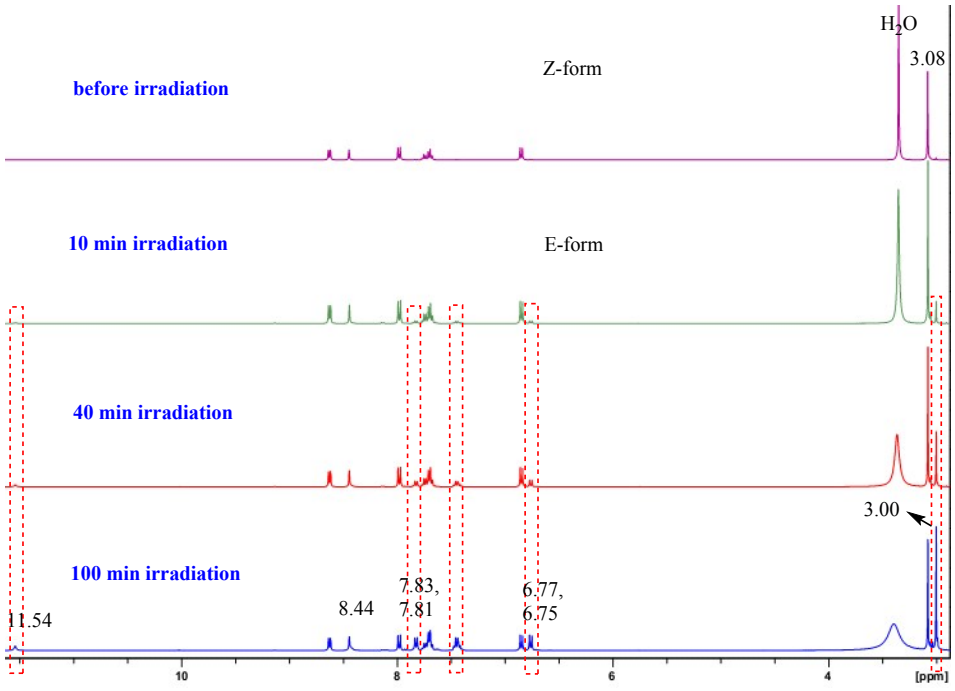


Figure S42. *Z*/*E* isomerization changes *via* ^{1}H NMR spectroscopy by irradiating its *Z*-form of **2h** in DMSO-d_6 (20 mM) with a 365 nm LED lamp for 10, 40 and 100 min.

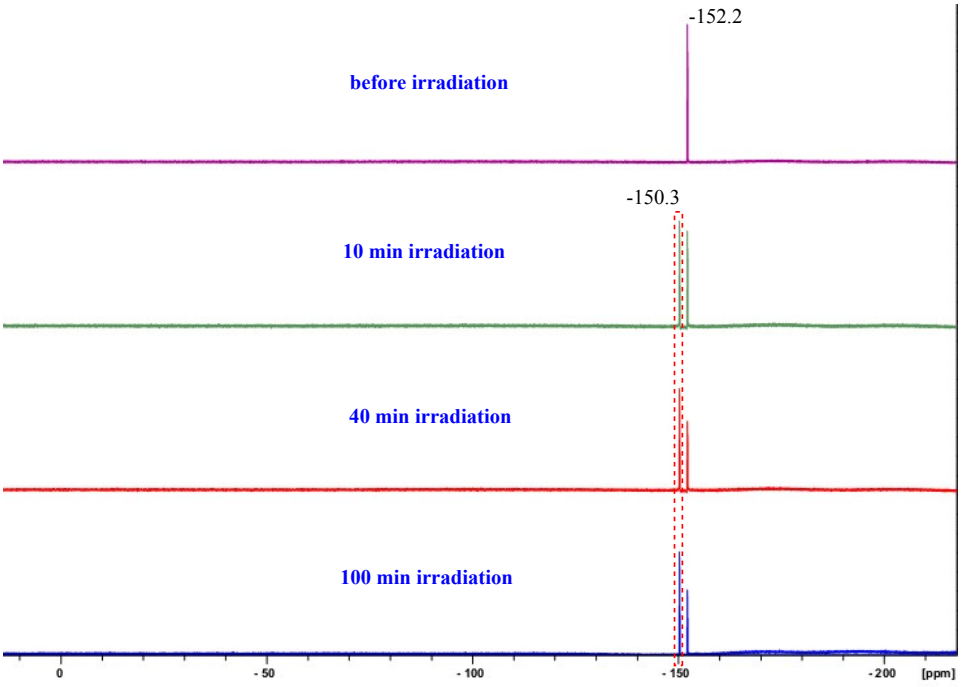


Figure S43. *Z*/*E* photoisomerization process was monitored *via* ^{19}F NMR spectroscopy. Pure *Z*-form isomer of **2h** (before irradiation, upper spectra) in chloroform-*d* (20 mM) was irradiated by a 3 W 365 nm UV lamp for 10, 40 and 100 min (lower spectra).

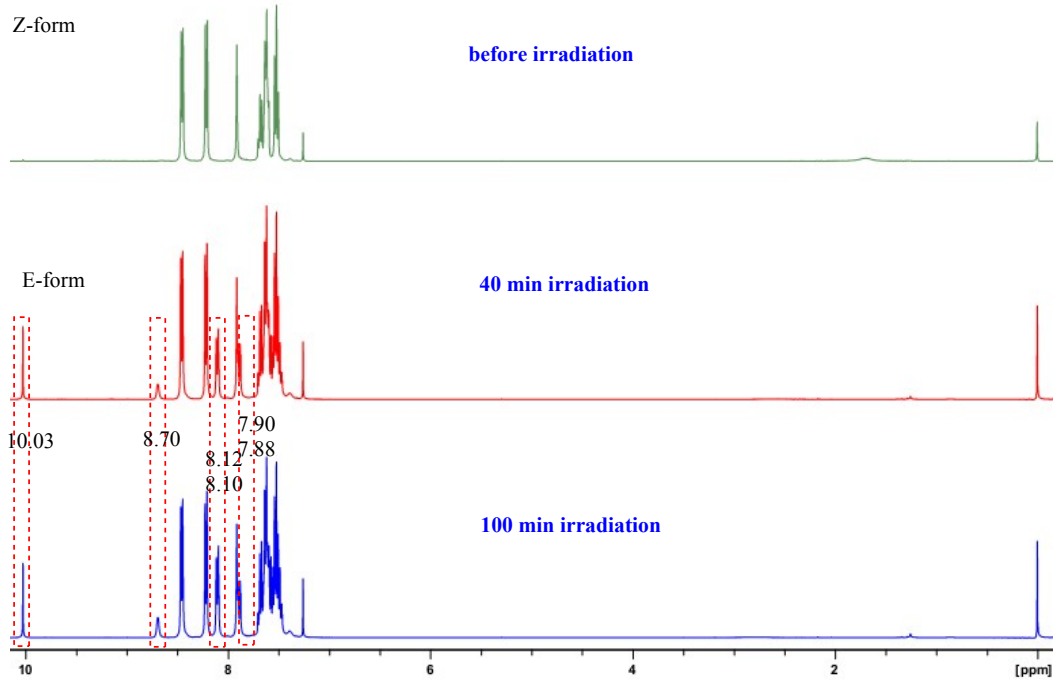


Figure S44. *Z*/*E* isomerization changes *via* ^{1}H NMR spectroscopy by irradiating its Z form of **2a** in chloroform-*d* (20 mM) with a 365 nm LED lamp for 10, 20 and 100 min.

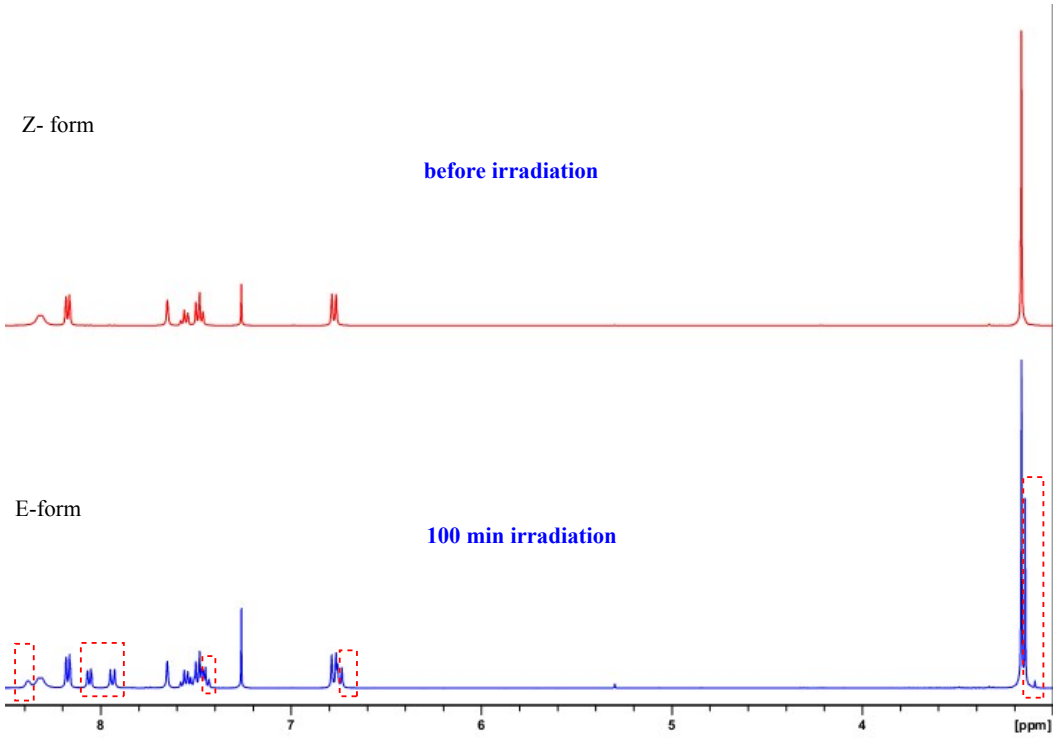


Figure S45. *Z*/*E* isomerization changes *via* ^{1}H NMR spectroscopy before and after irradiating its *Z*-form of **2d** in chloroform-*d* (20 mM) with a 365 nm LED lamp for 100 min.

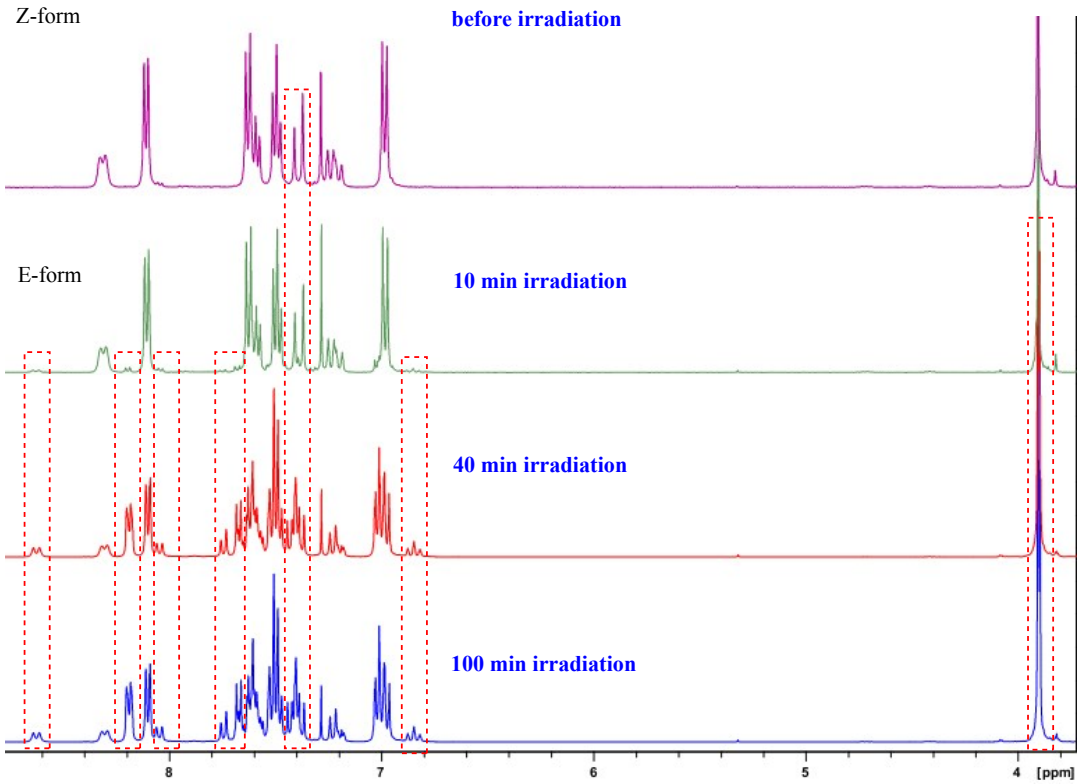


Figure S46. *Z*/*E* isomerization changes *via* ^{1}H NMR spectroscopy before and after irradiating its *Z*-form of **2e** in chloroform-*d* (20 mM) with a 365 nm LED lamp for 10, 40 and 100 min.

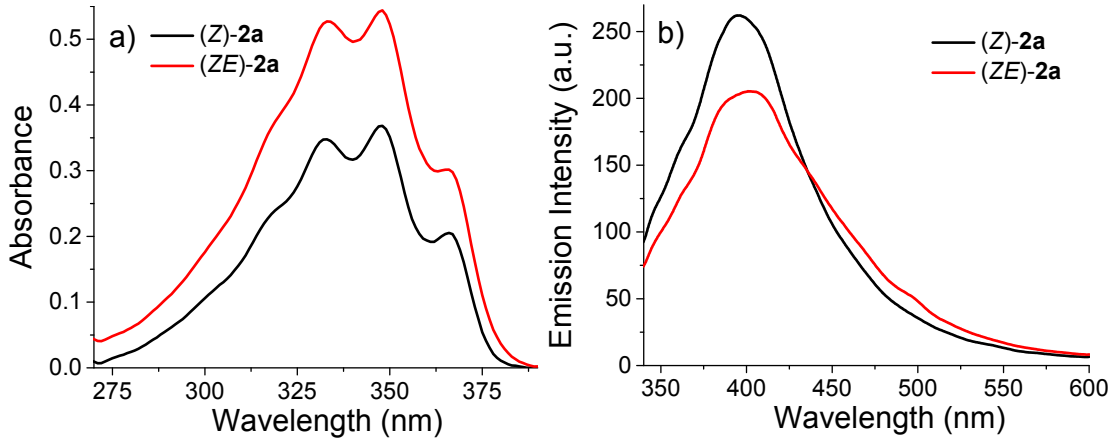
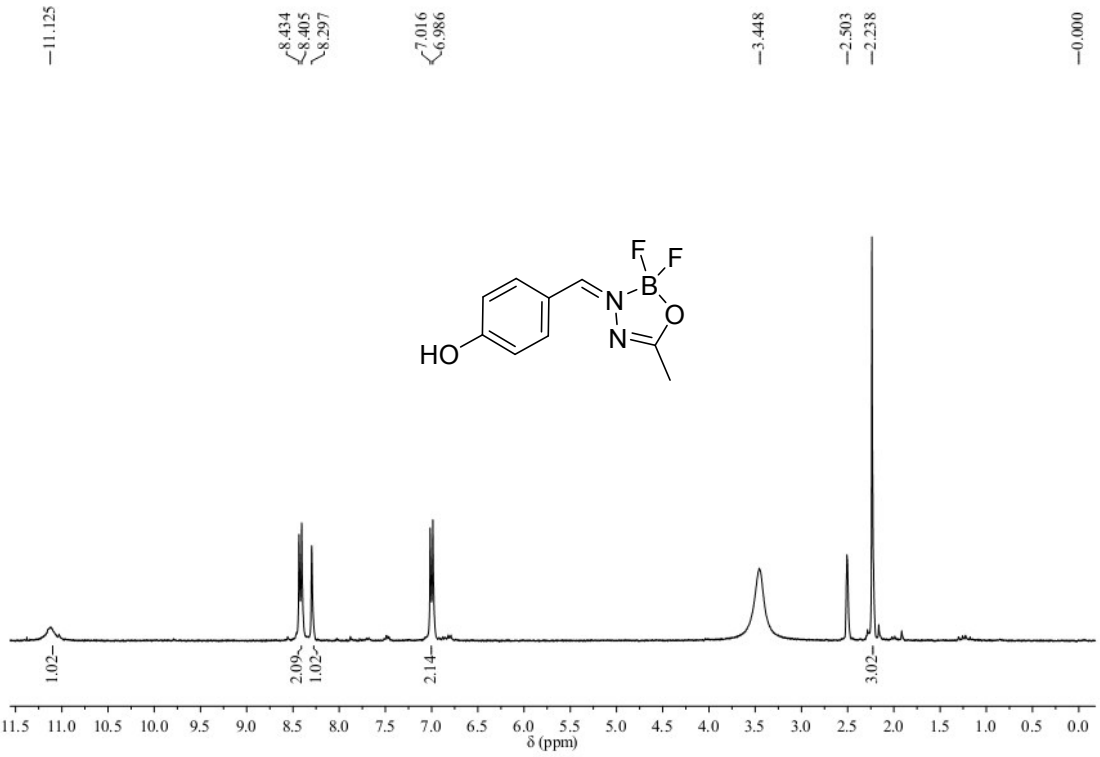
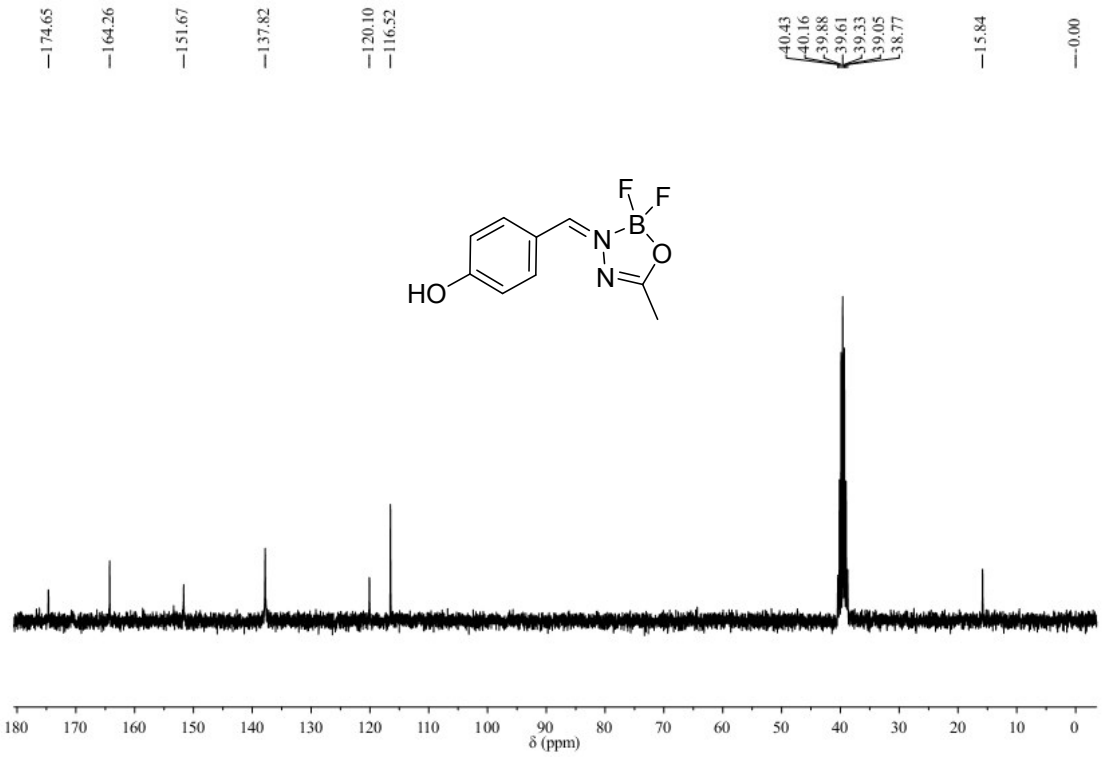


Figure S47. Absorption (a) and emission (b) spectra of (*Z*)-**2a** (a) before photoirradiation and upon irradiation with a 365 nm LED lamp for 100 min in dichloromethane, excited at 320 nm.

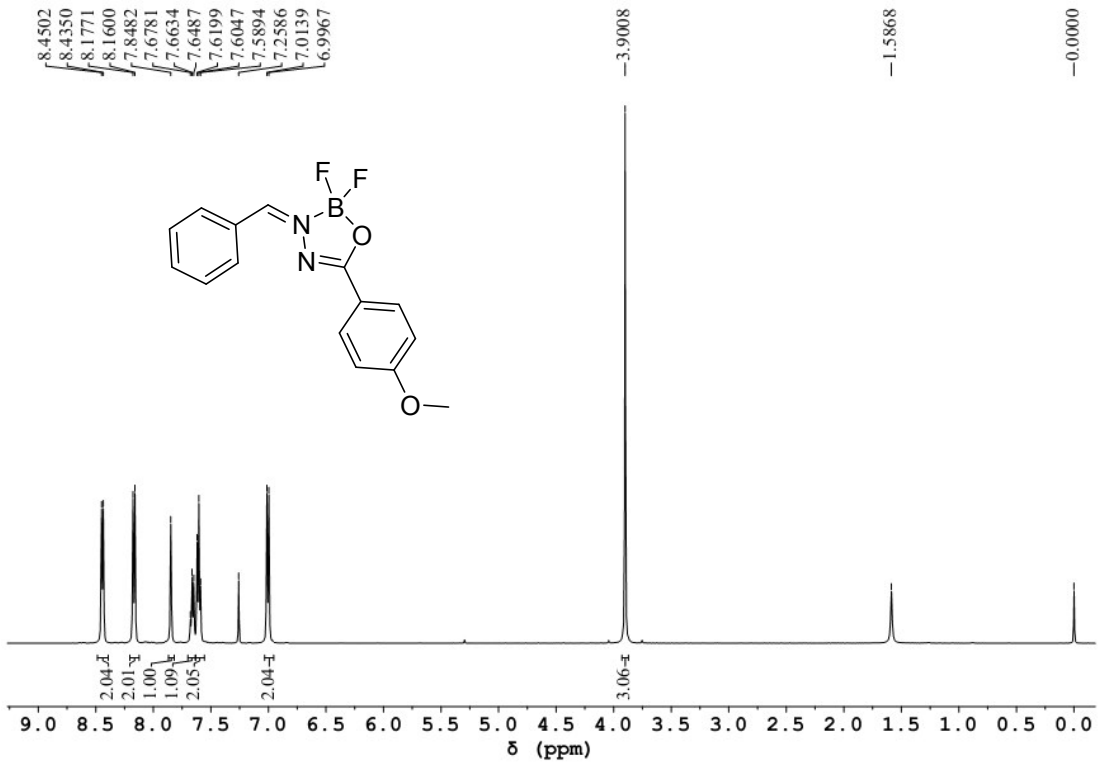
7. NMR spectra for BOAHYs



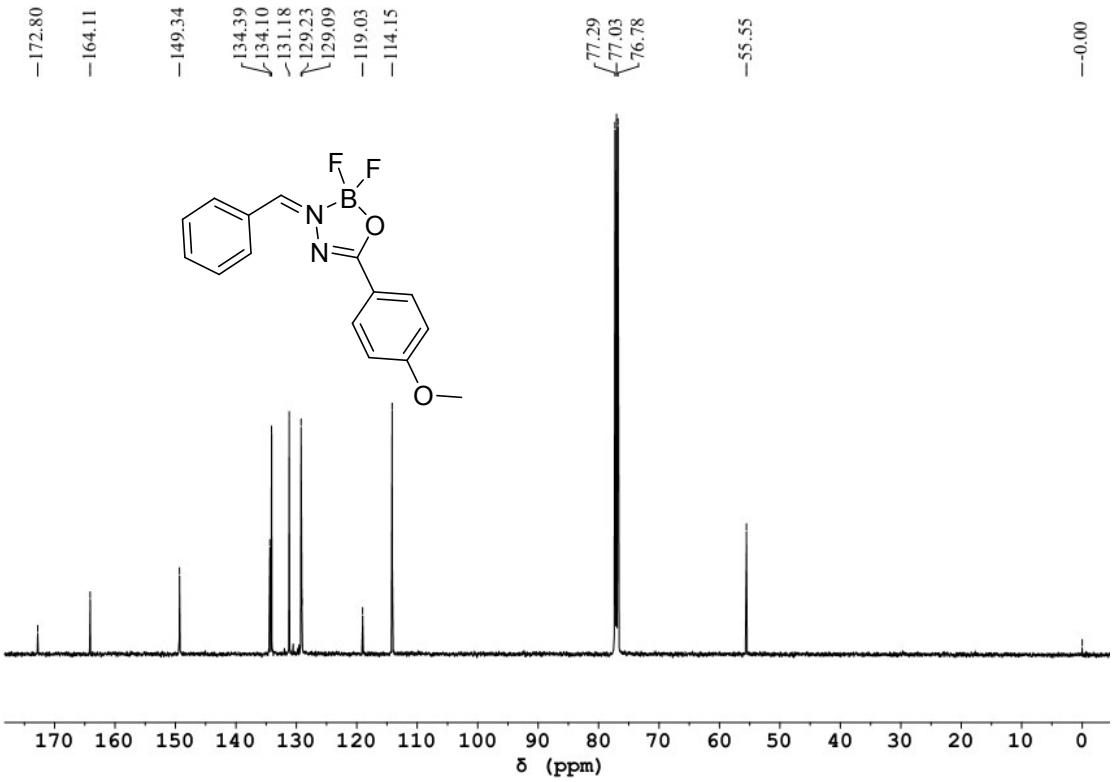
^{1}H NMR spectrum of BOAHY **1a** in DMSO-d_6



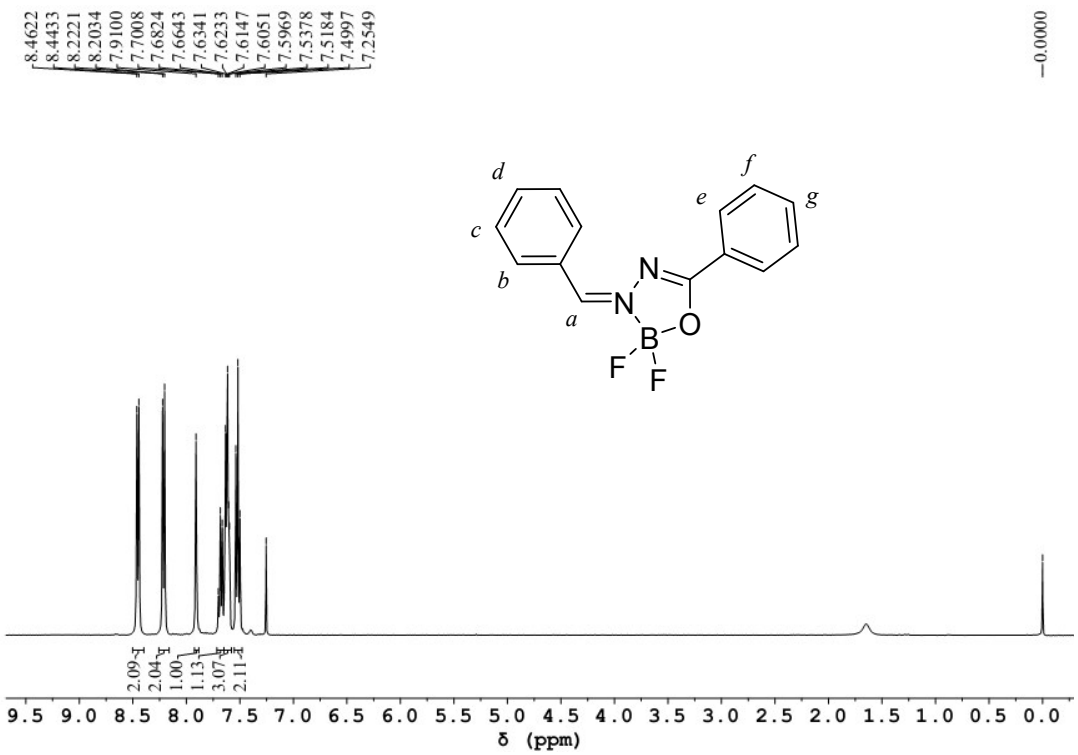
^{13}C NMR spectrum of BOAHY **1a** in DMSO-d_6



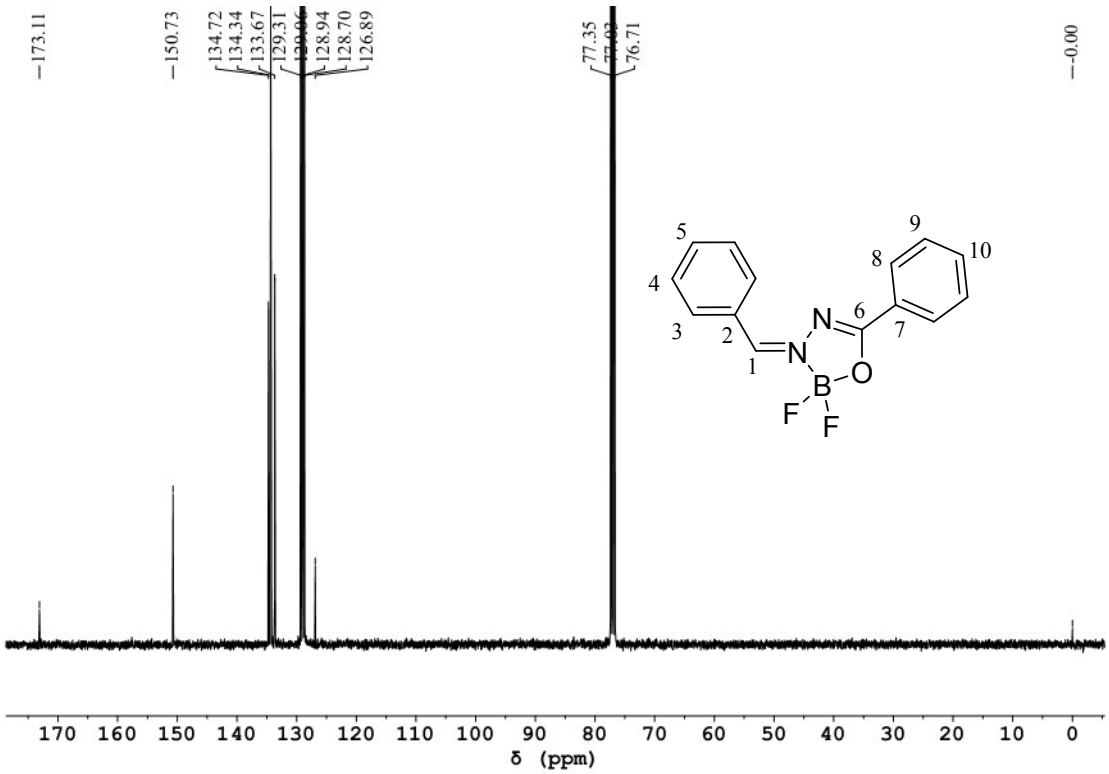
^{1}H NMR spectrum of BOAHY **1b** in $CDCl_3$



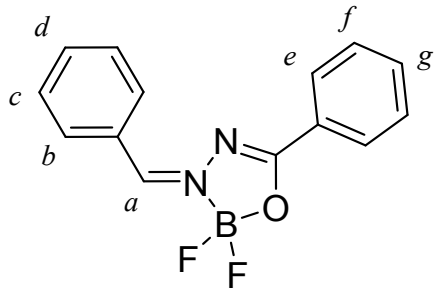
^{13}C NMR spectrum of BOAHY **1b** in $CDCl_3$



^{1}H NMR spectrum of BOAHY **2a** in $CDCl_3$



^{13}C NMR spectrum of BOAHY **2a** in $CDCl_3$



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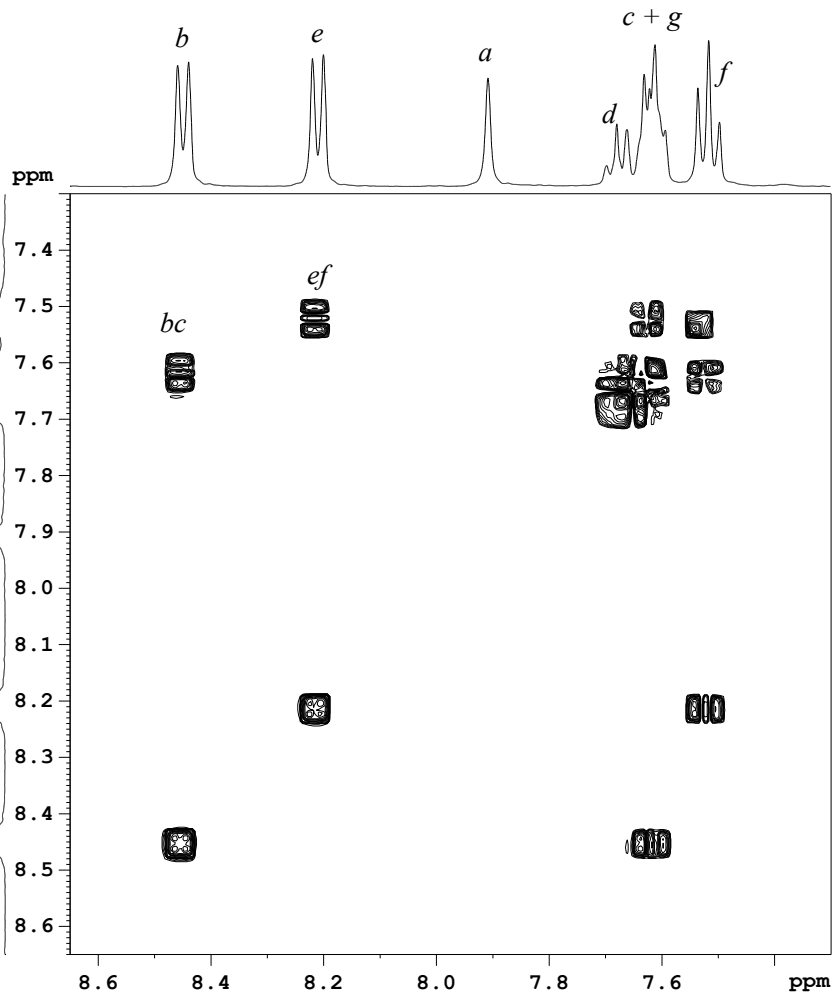

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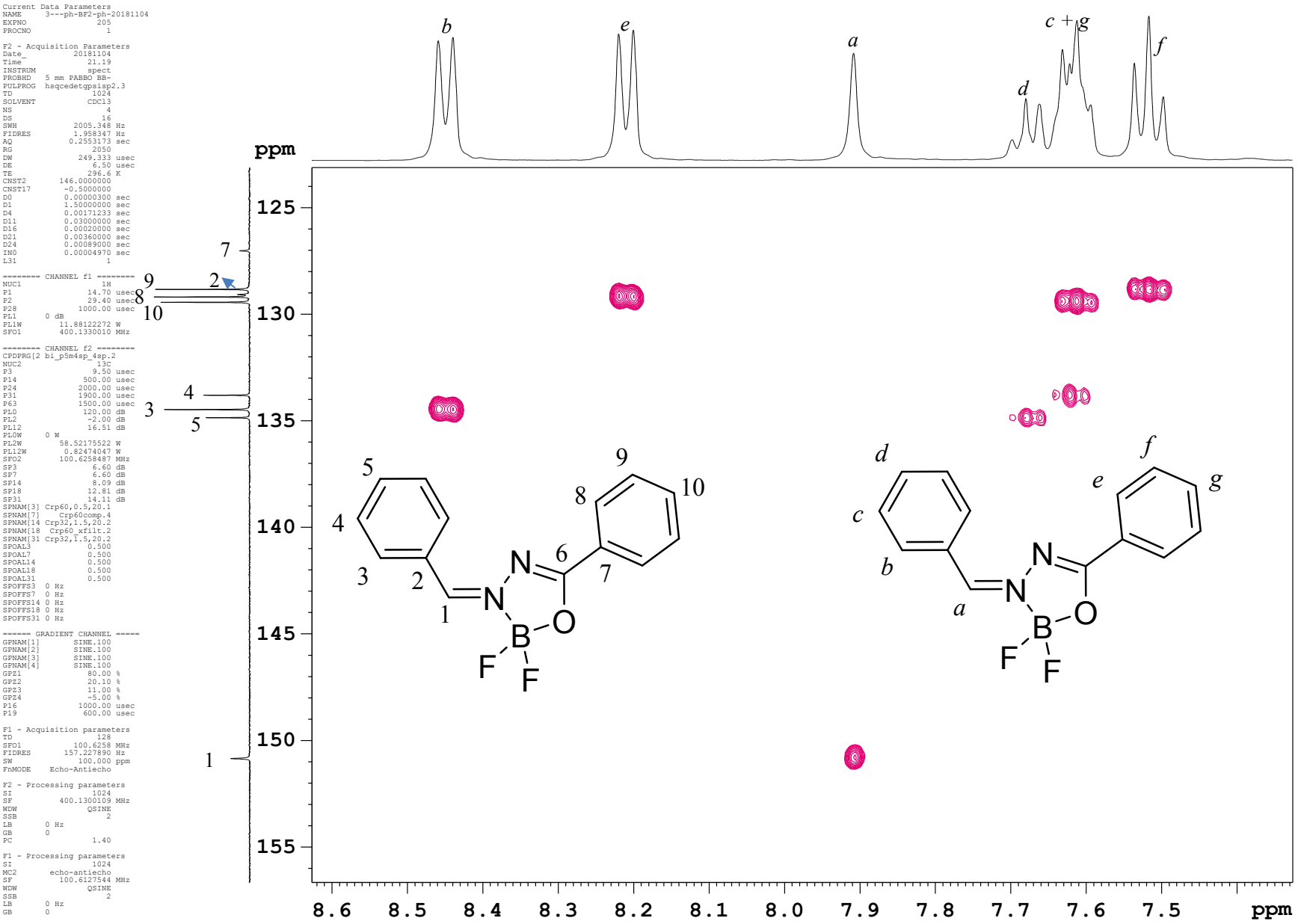


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SPOFFS18  0 Hz
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GPZ4                -5.00 %
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P19               600.00 usec

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FnMODE    Echo-Antiecho

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SSB                     2
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GB        0
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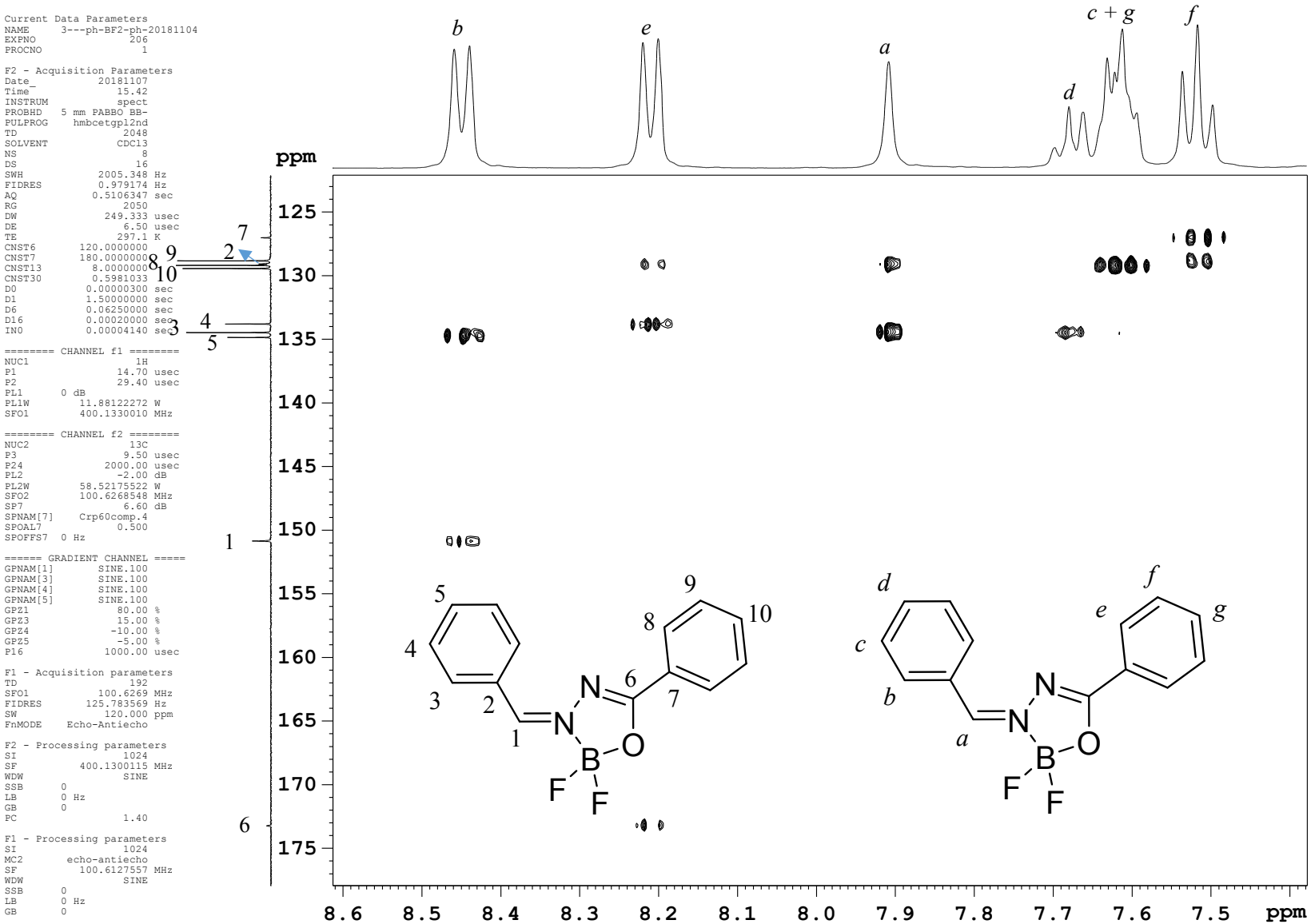
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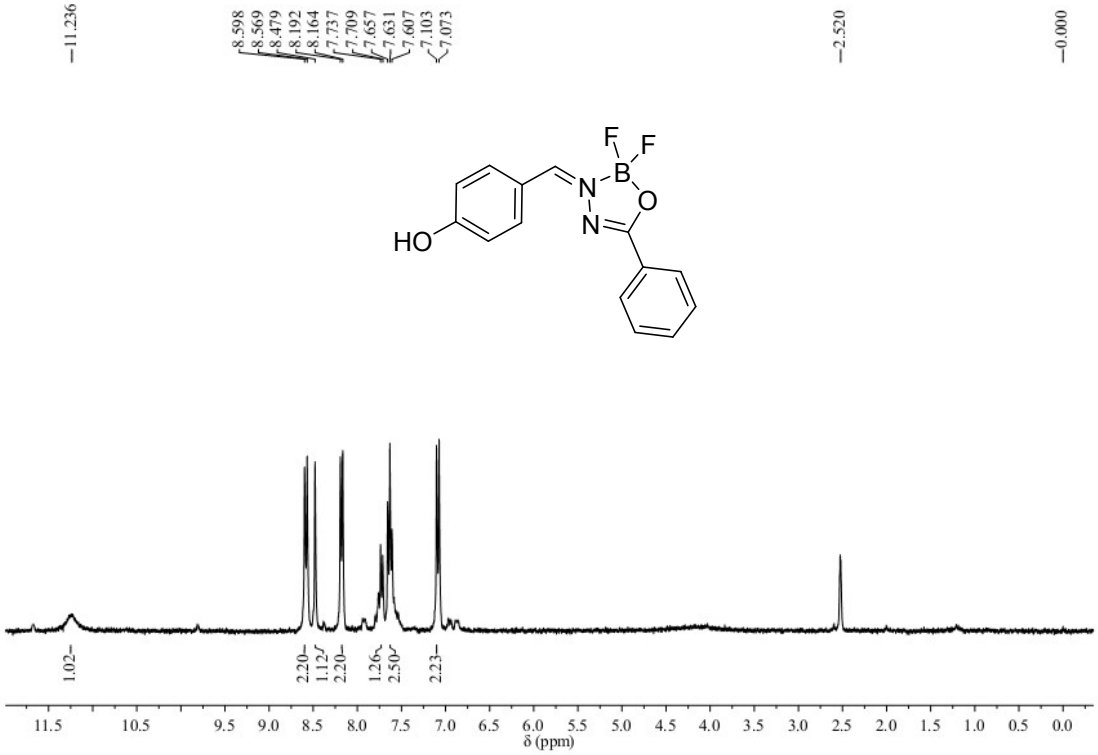
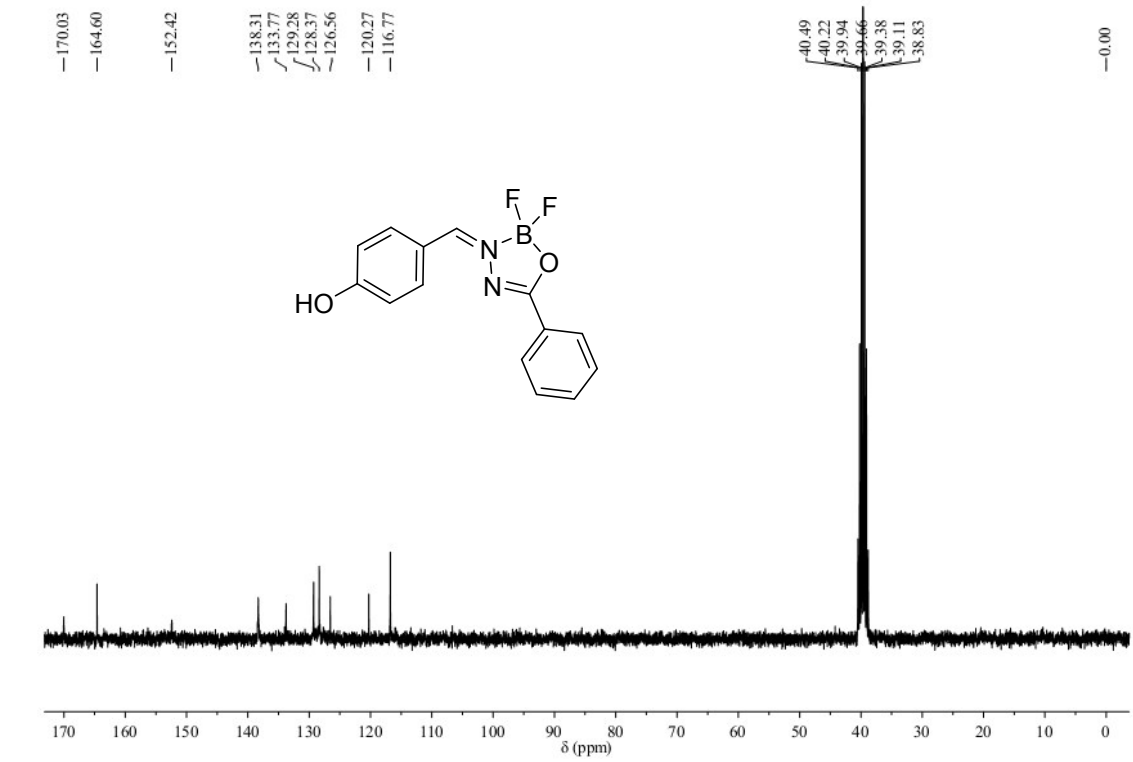
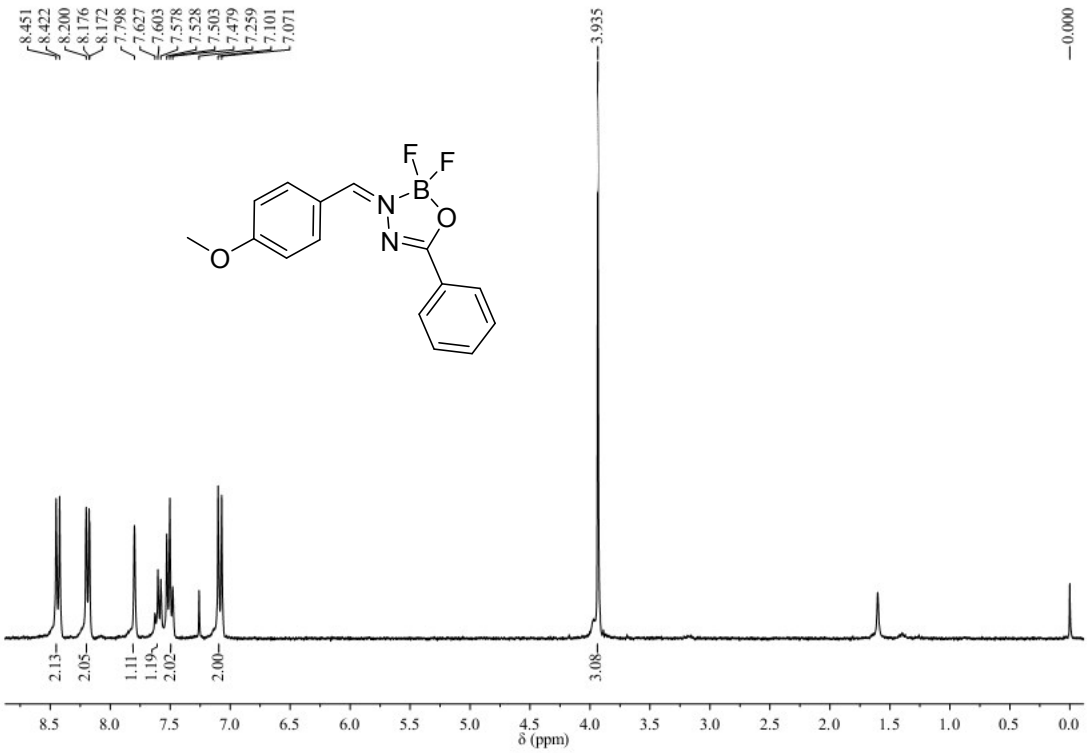


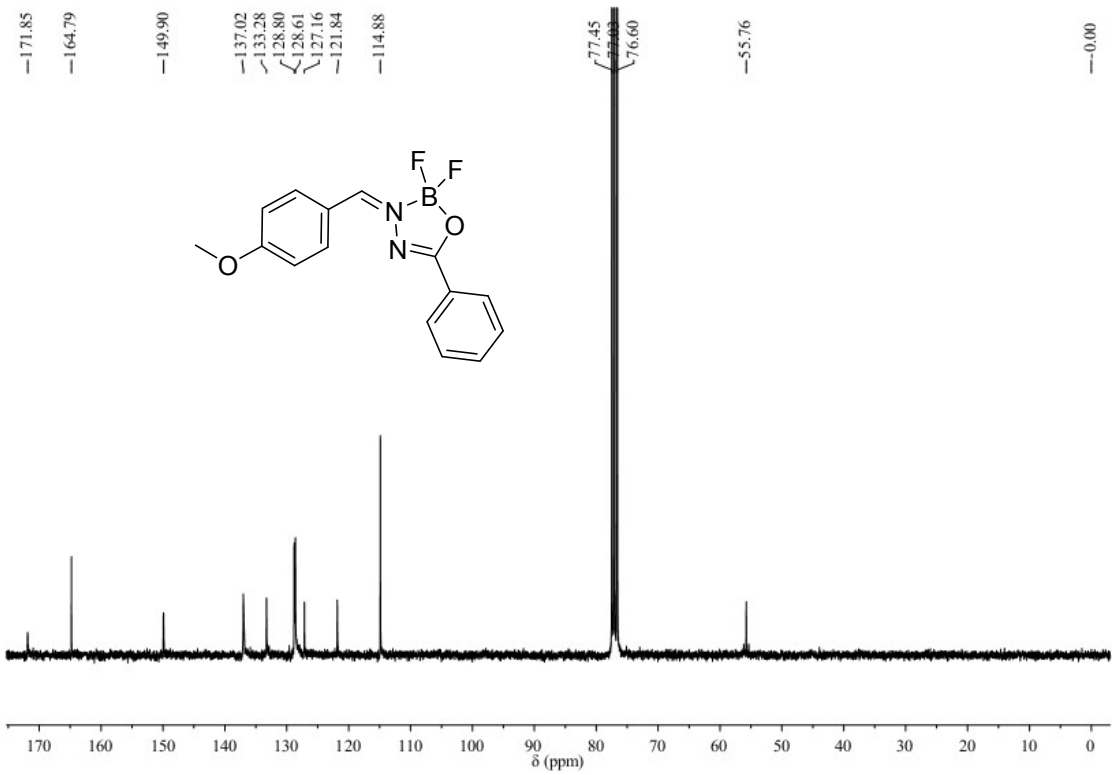
^{1}H NMR spectrum of BOAHY **2b** in DMSO-d_6



^{13}C NMR spectrum of BOAHY **2b** in DMSO-d_6



^{1}H NMR spectrum of BOAHY **2c** in $CDCl_3$



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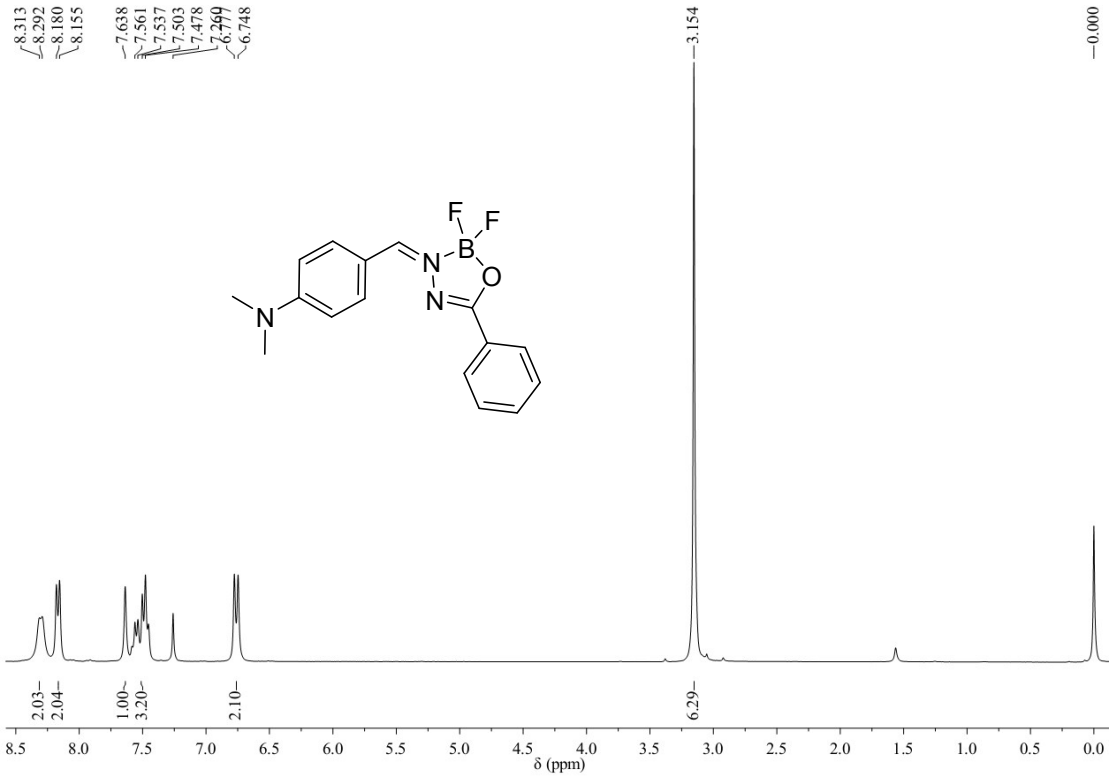

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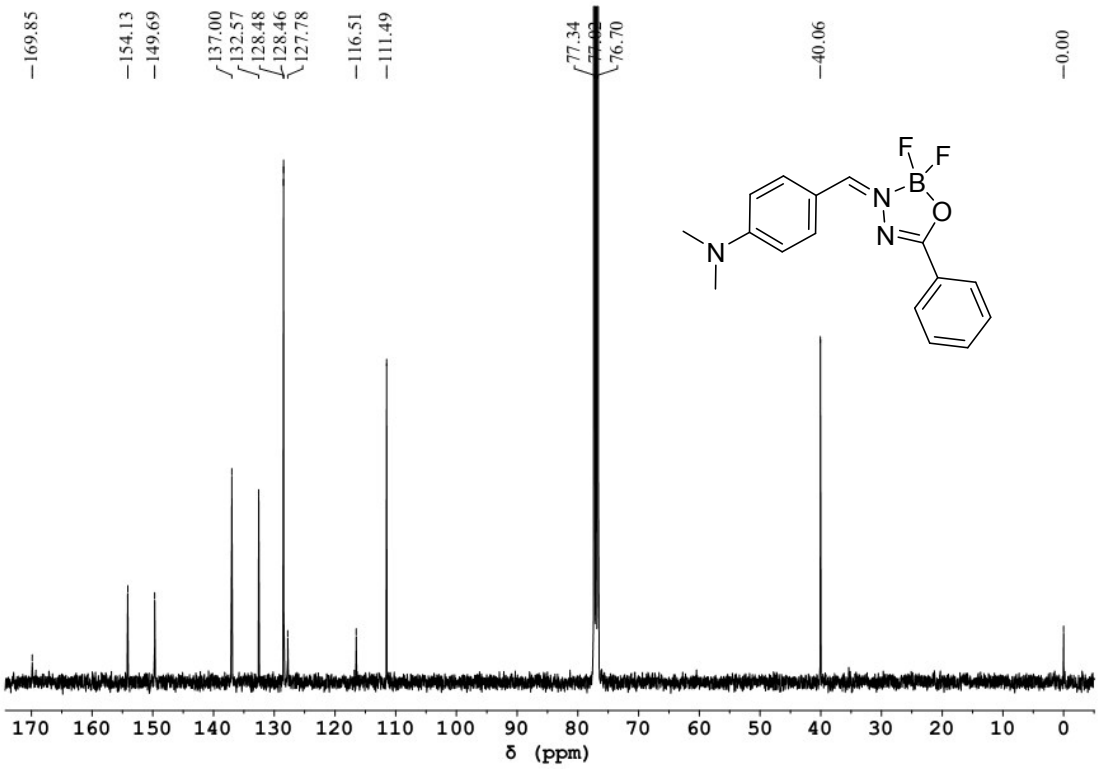

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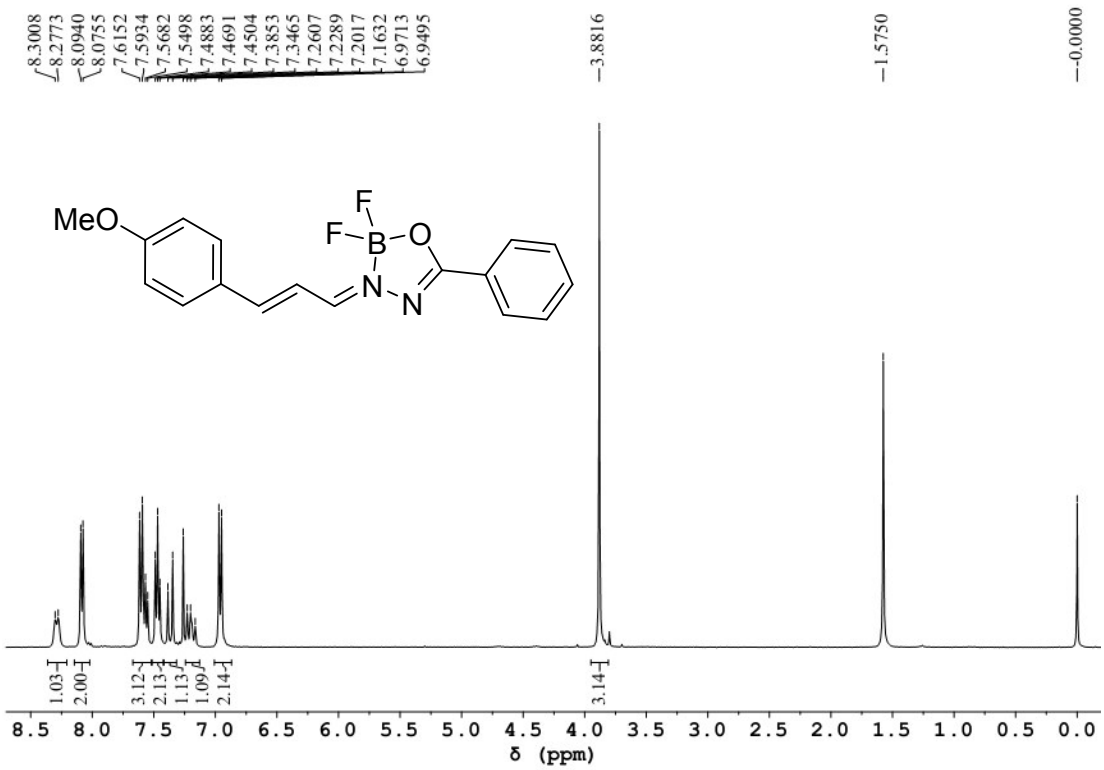

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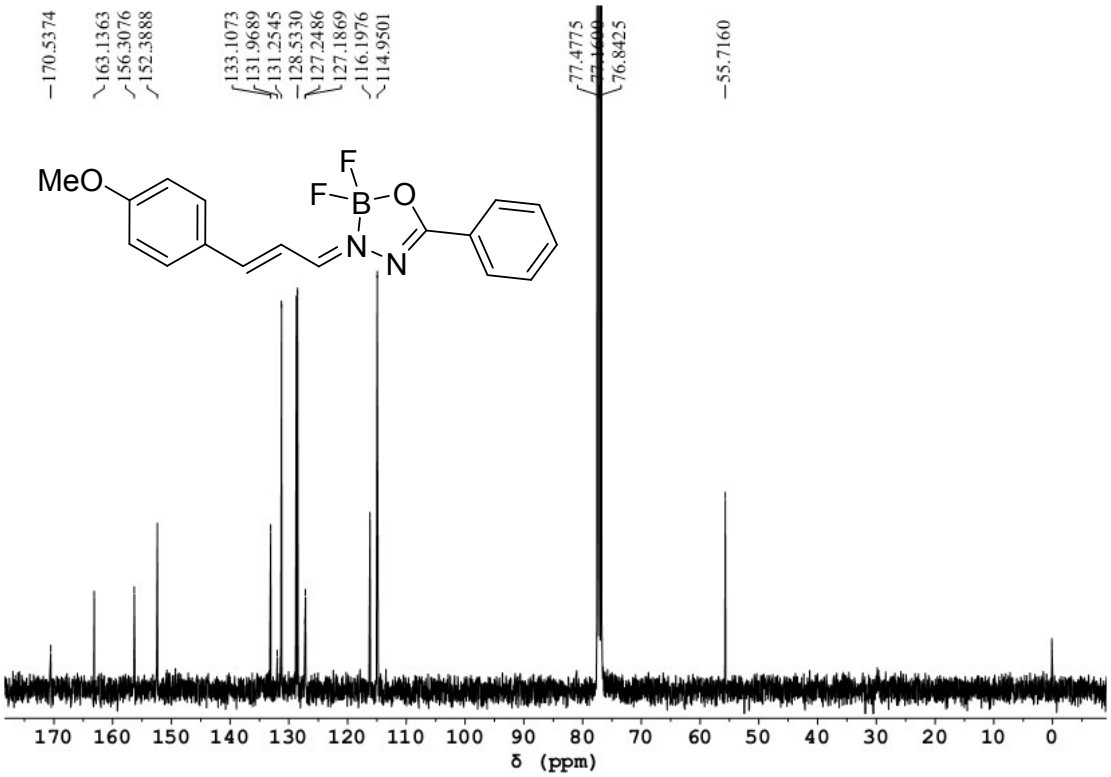
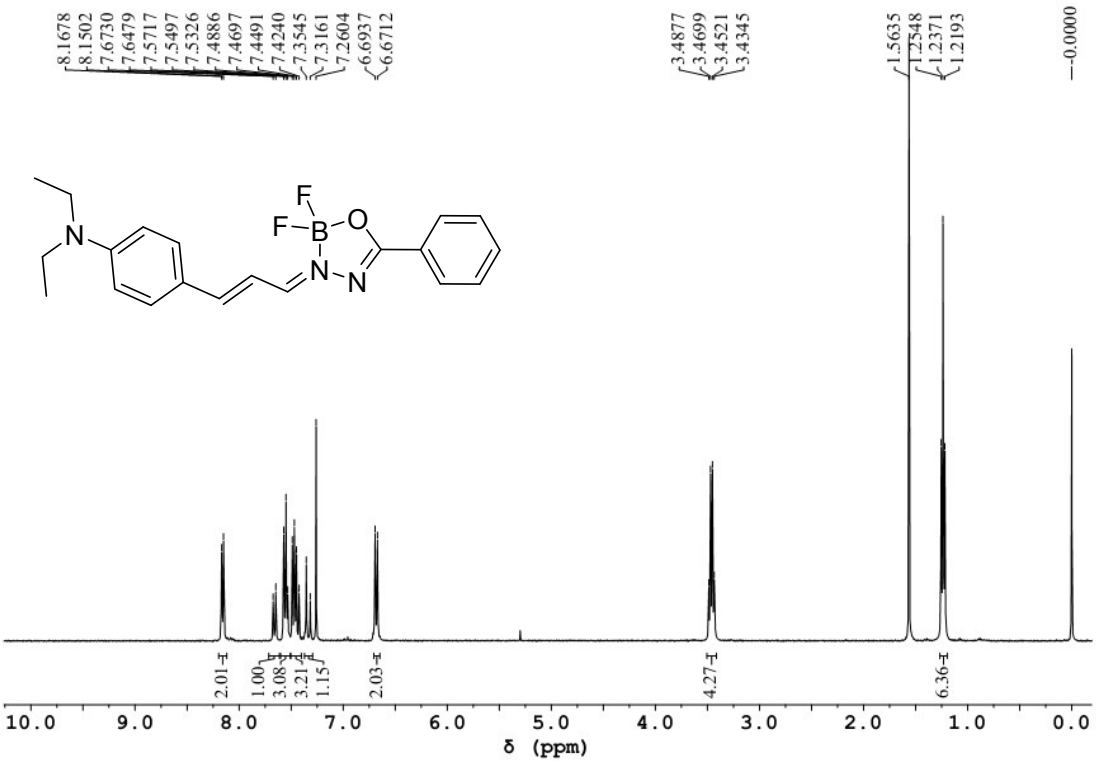
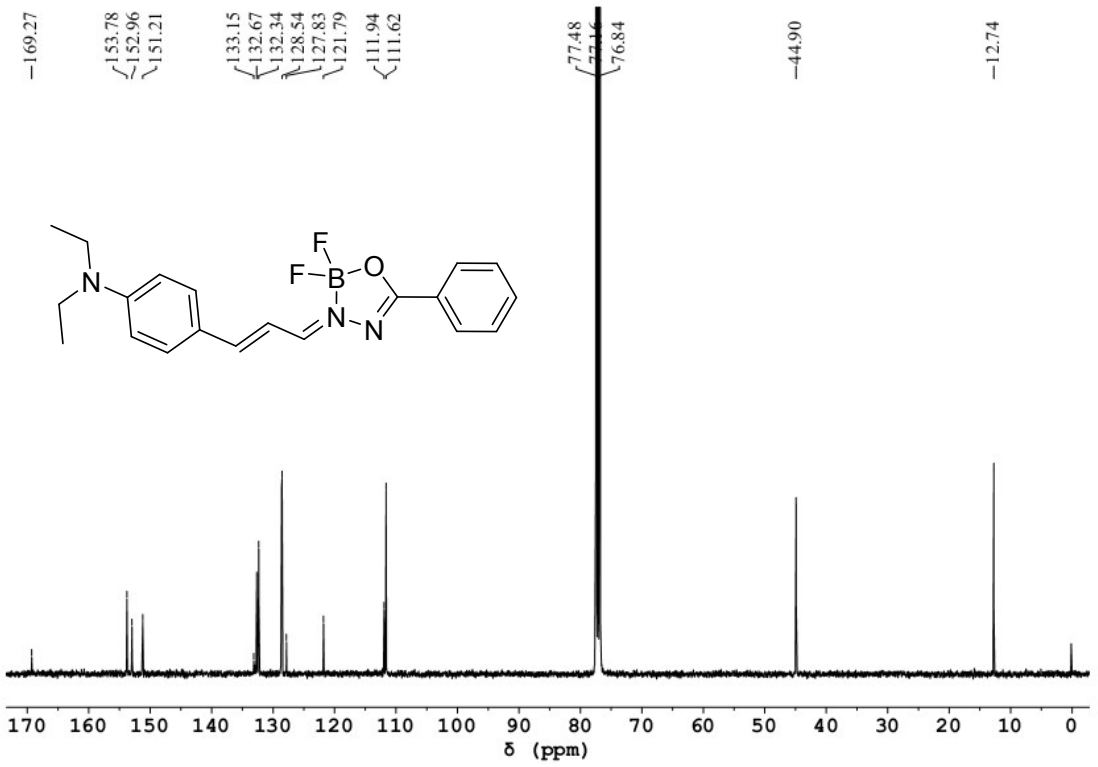


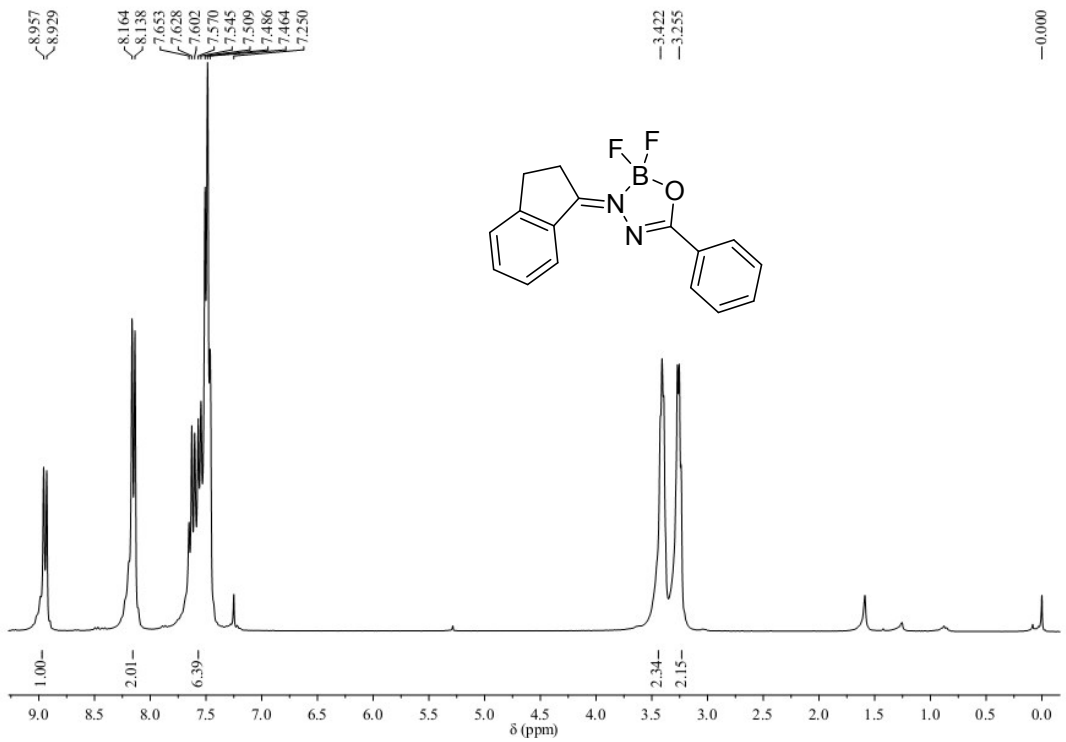
^{13}C NMR spectrum of BOAHY **2e** in $CDCl_3$



^{1}H NMR spectrum of BOAHY **2f** in $CDCl_3$



^{13}C NMR spectrum of BOAHY **2f** in $CDCl_3$



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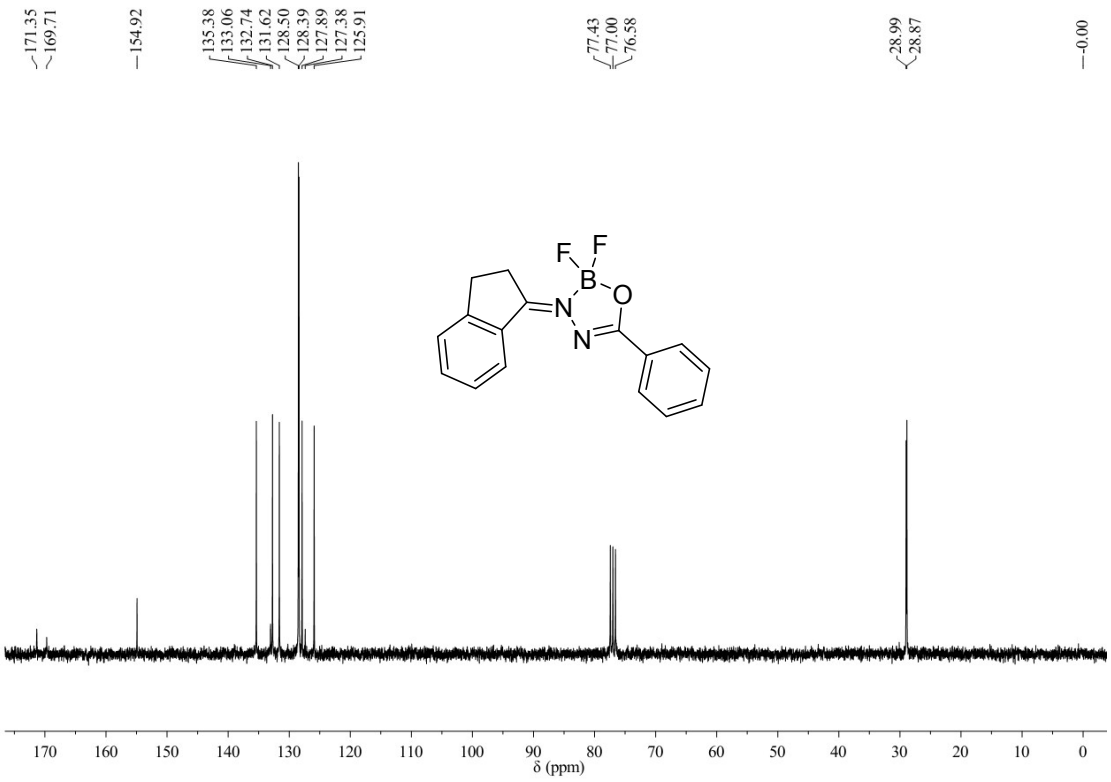

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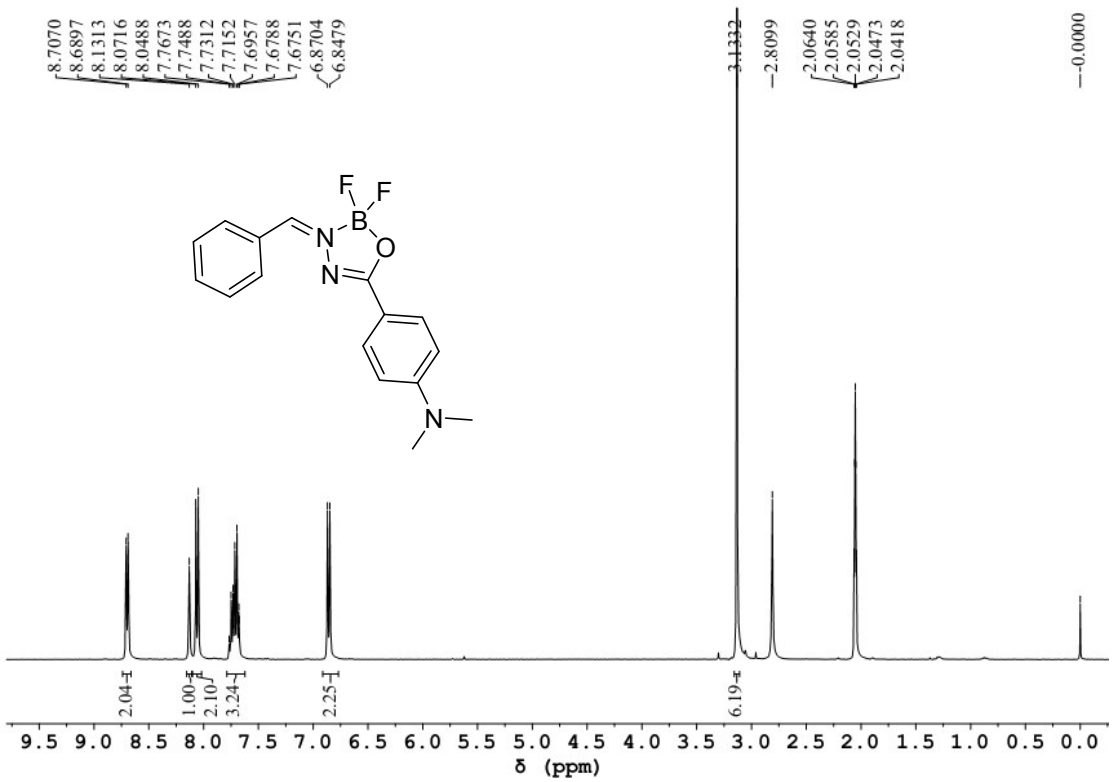
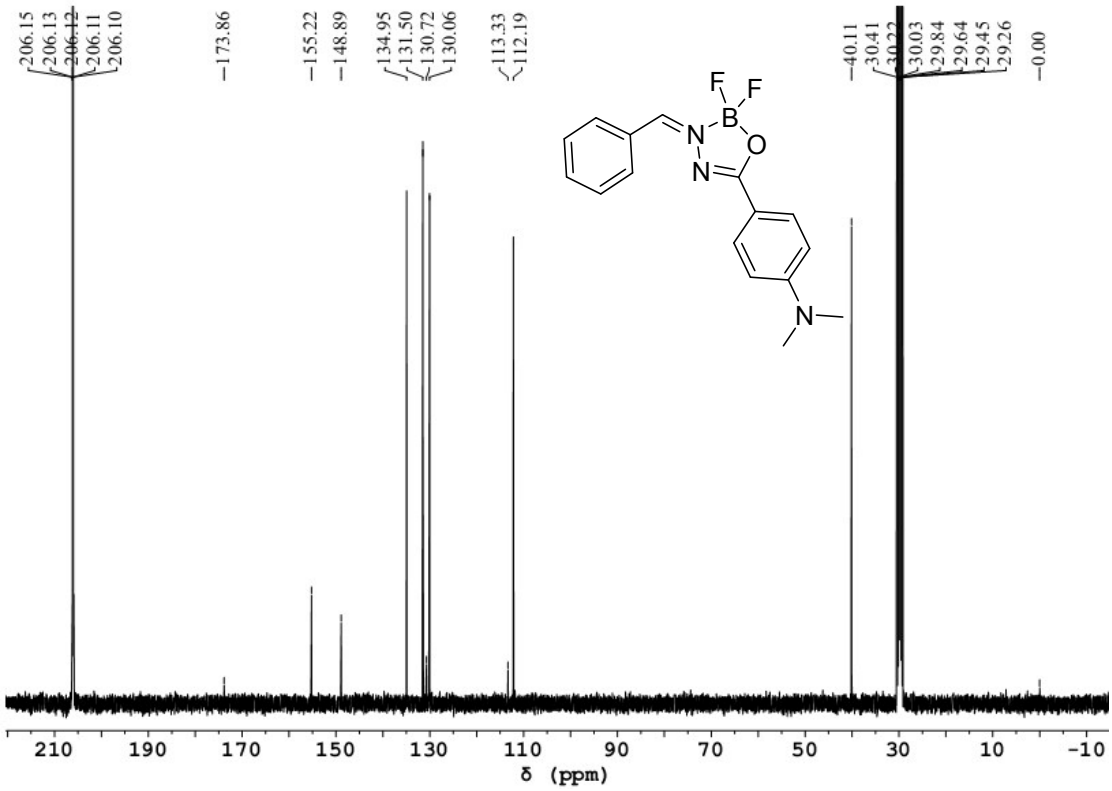


^{1}H NMR spectrum of BOAHY **2h** in acetone-d_6



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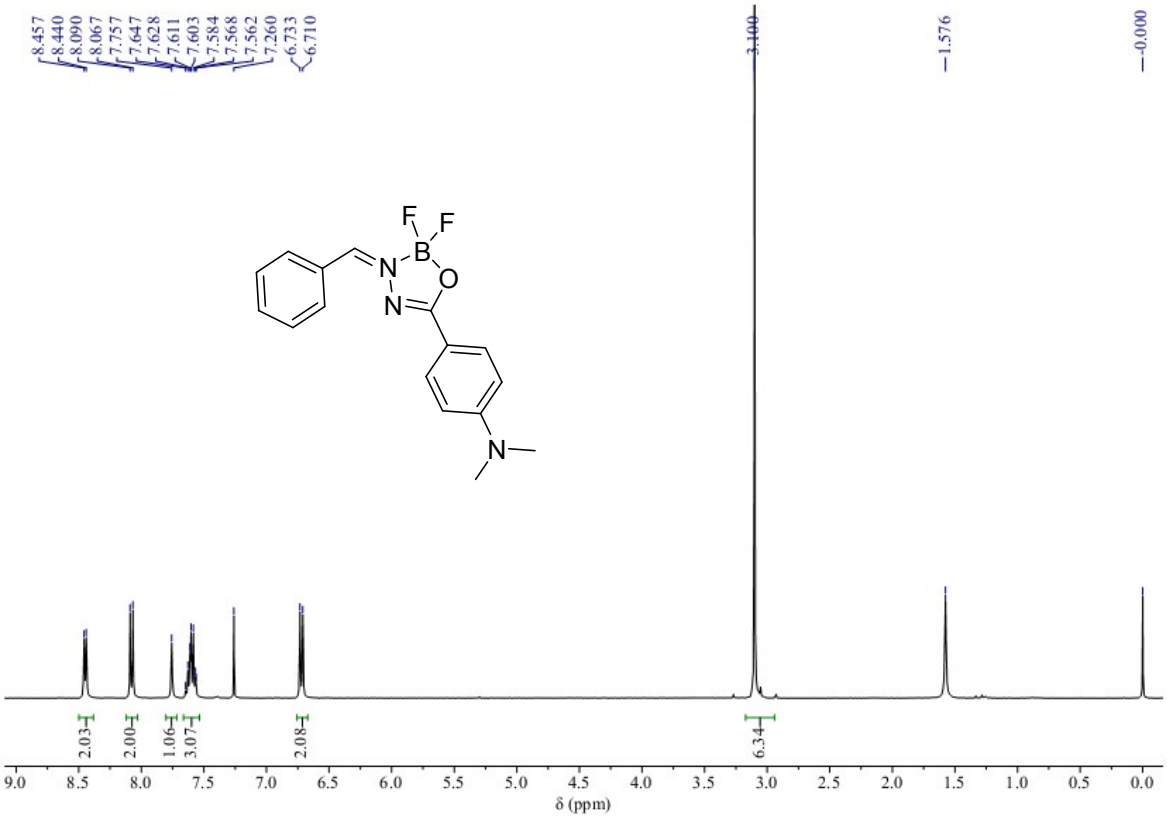

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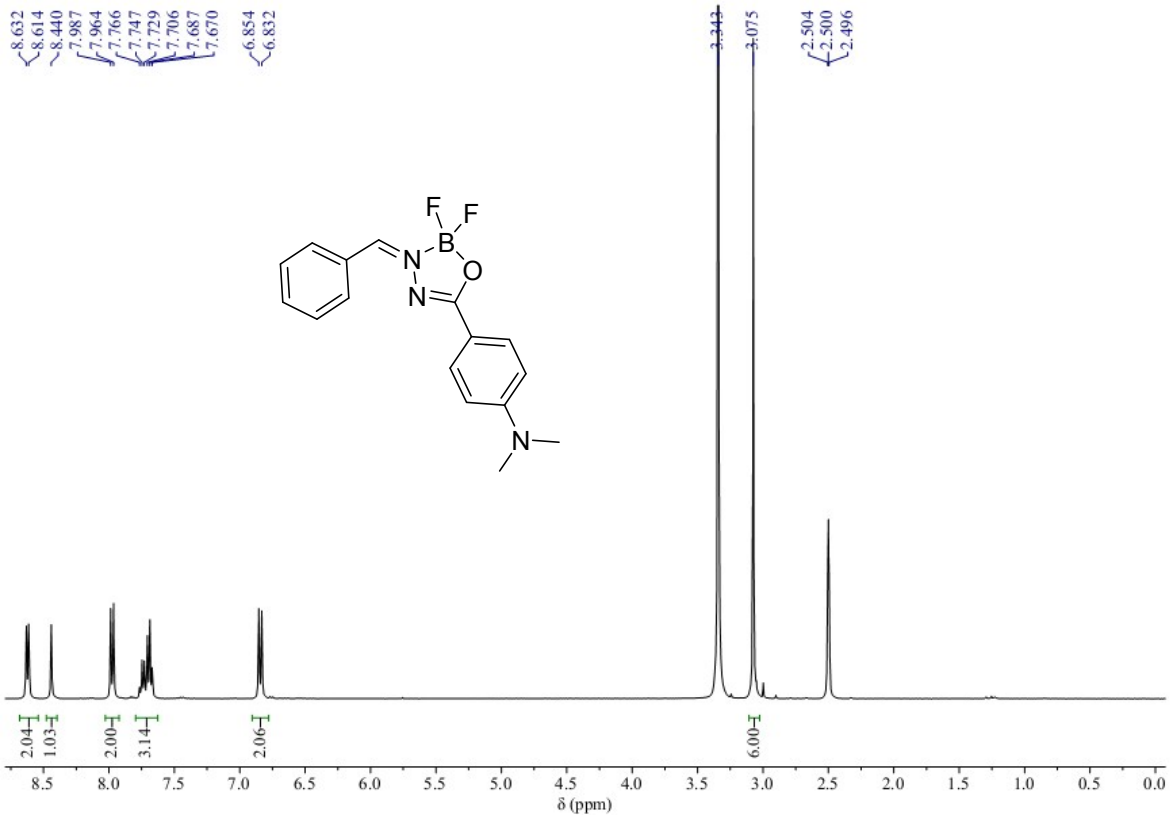

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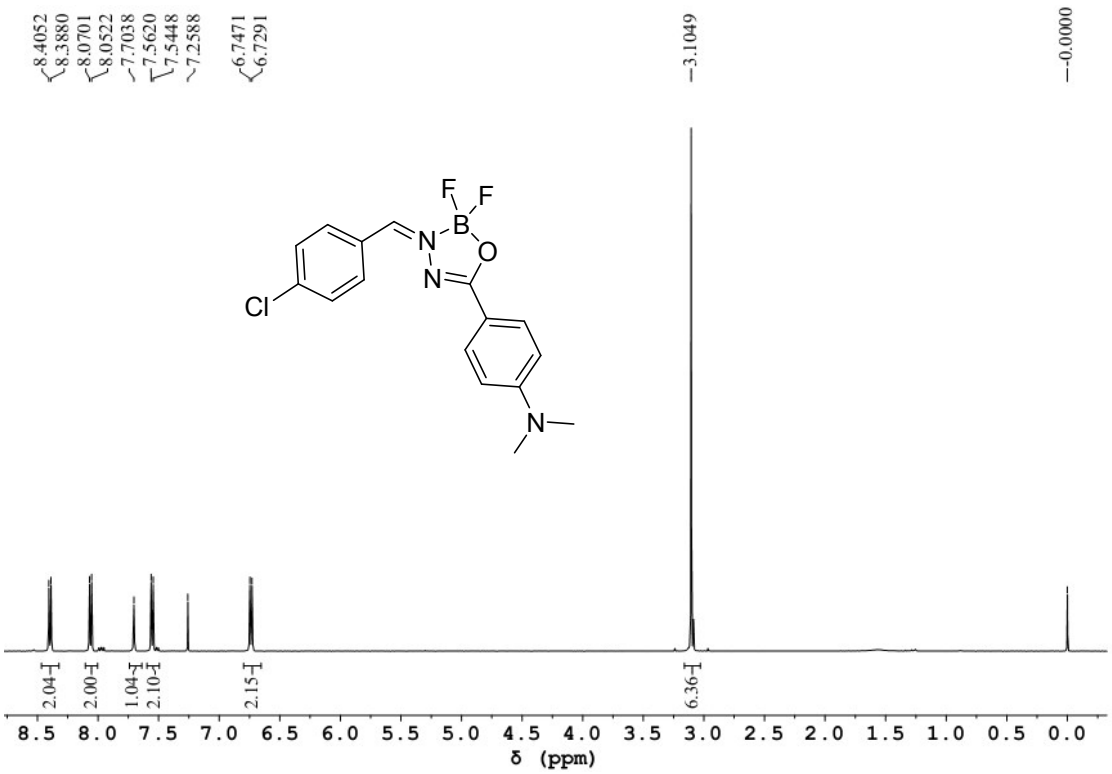
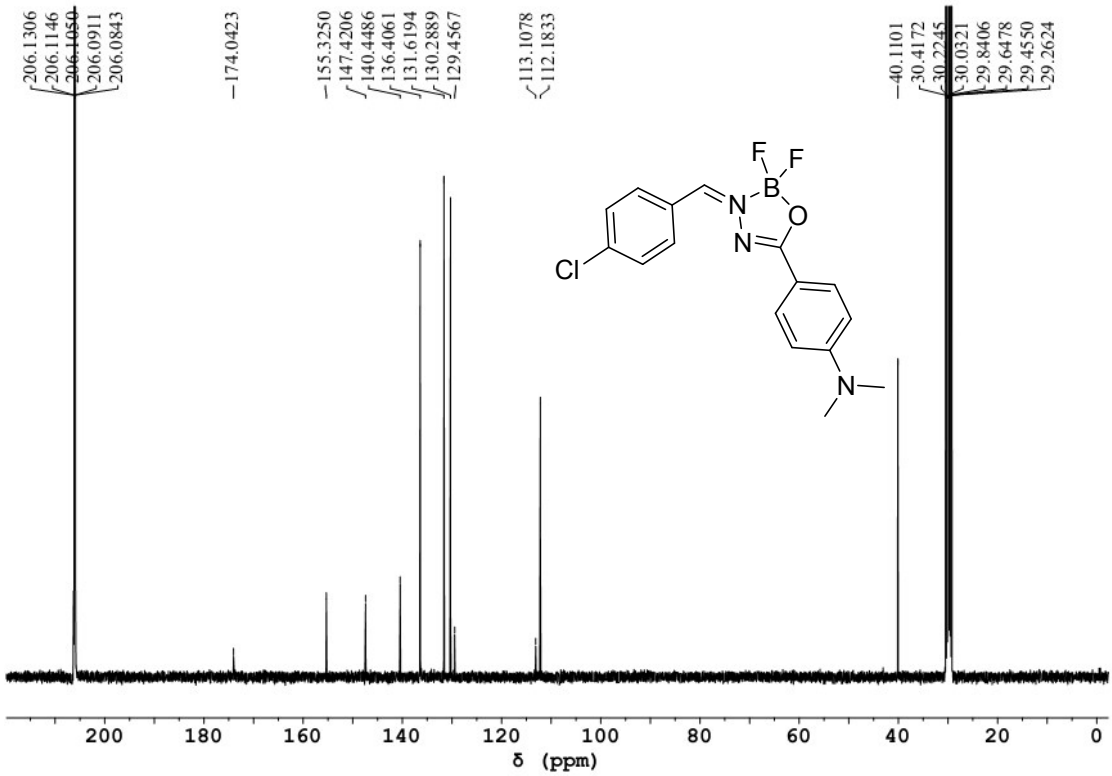


^{1}H NMR spectrum of BOAHY **2i** in $CDCl_3$



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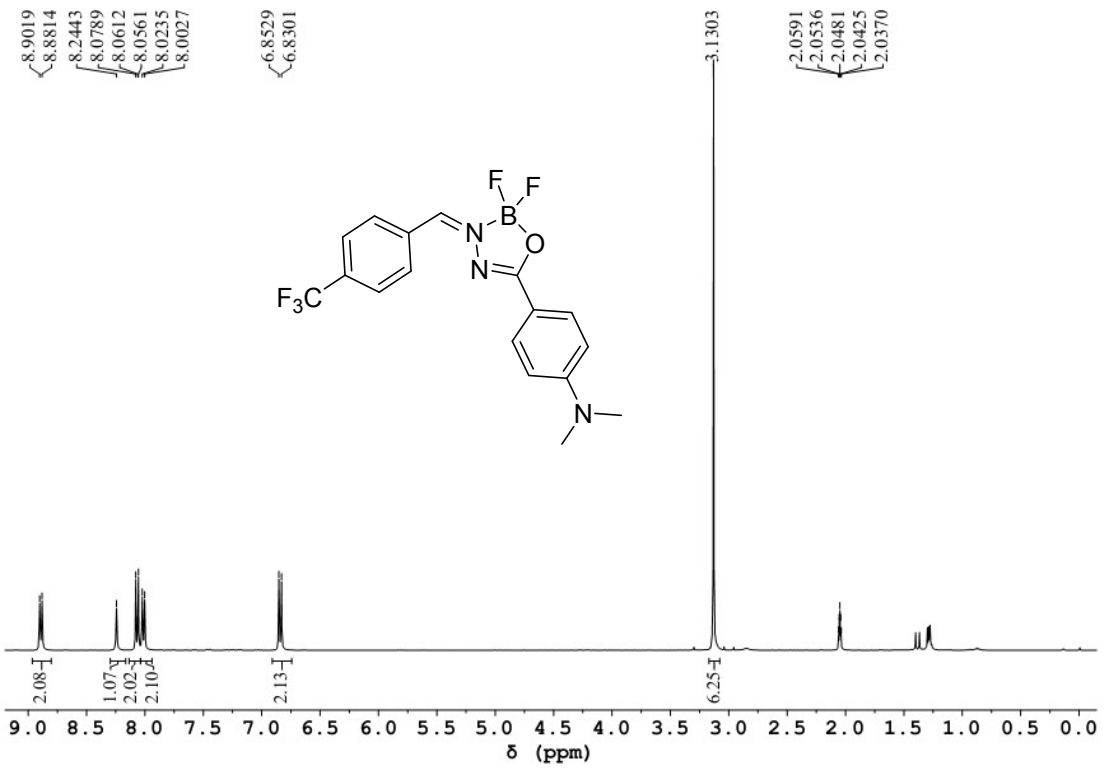
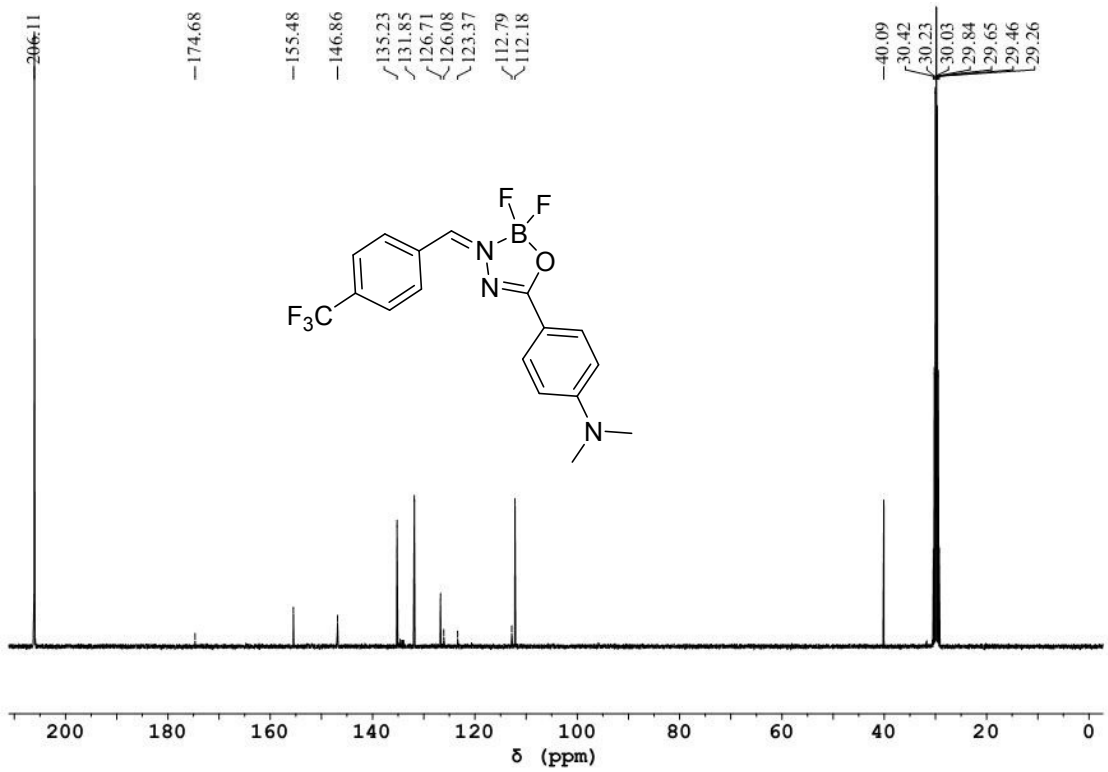


^{1}H NMR spectrum of BOAHY **2j** in $CDCl_3$



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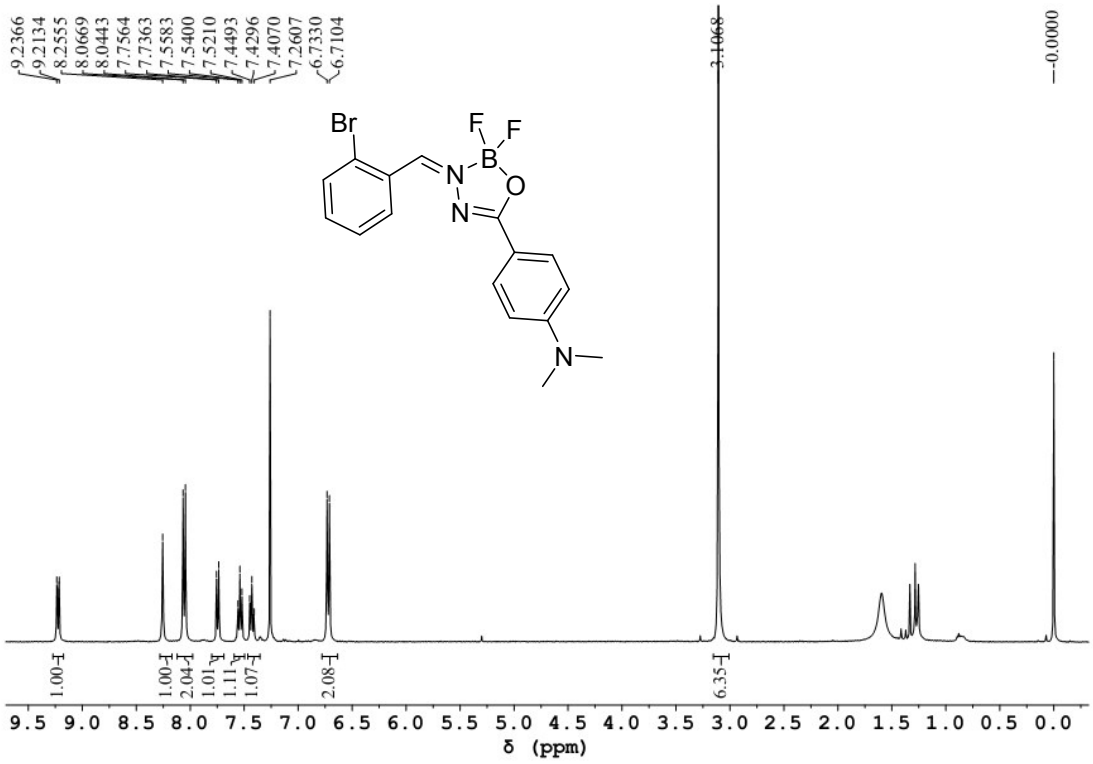
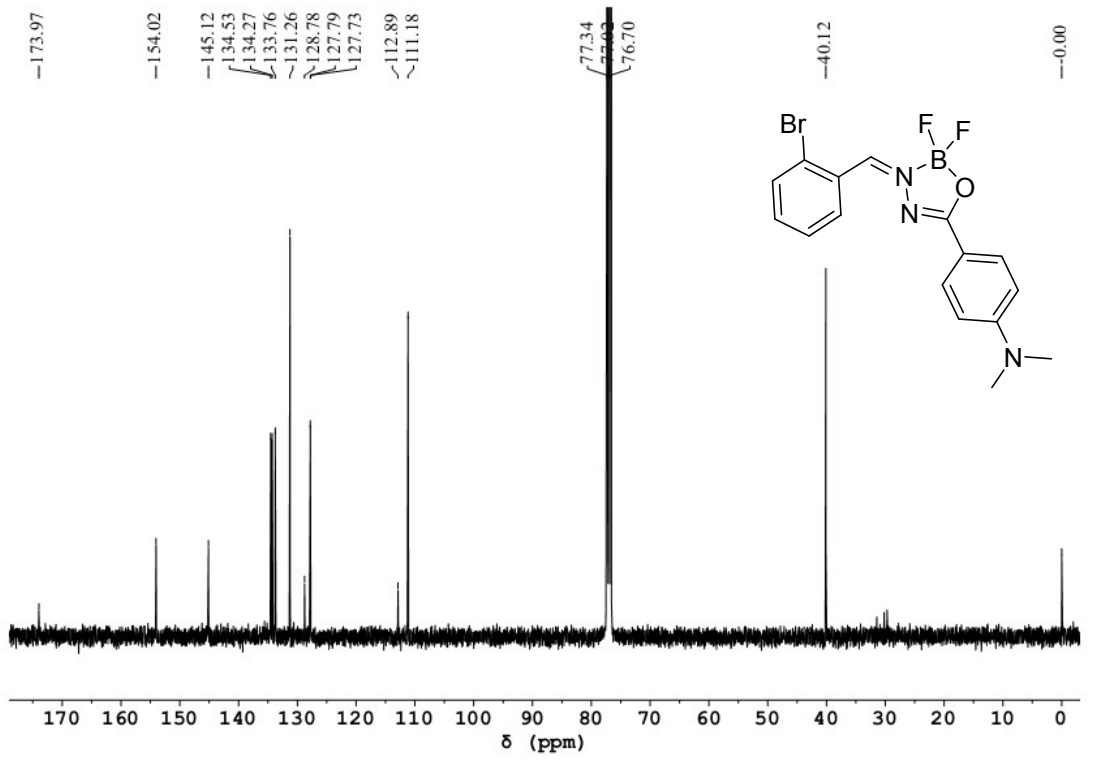
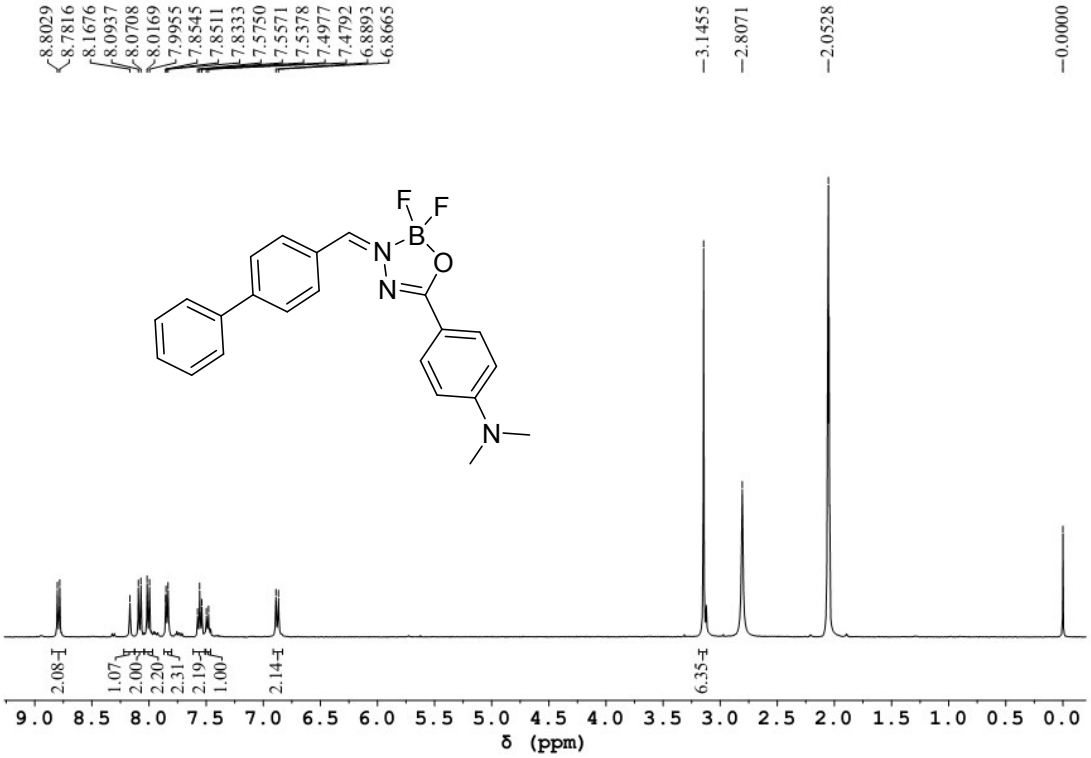


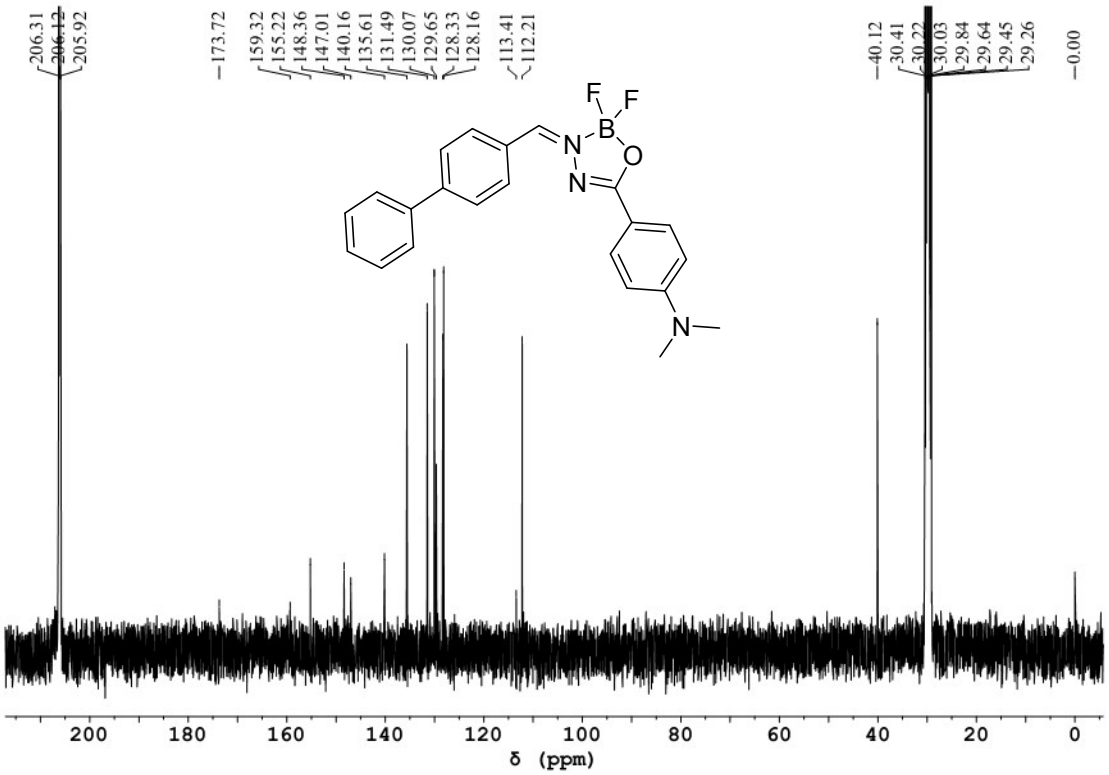
^{1}H NMR spectrum of BOAHY **2k** in $CDCl_3$



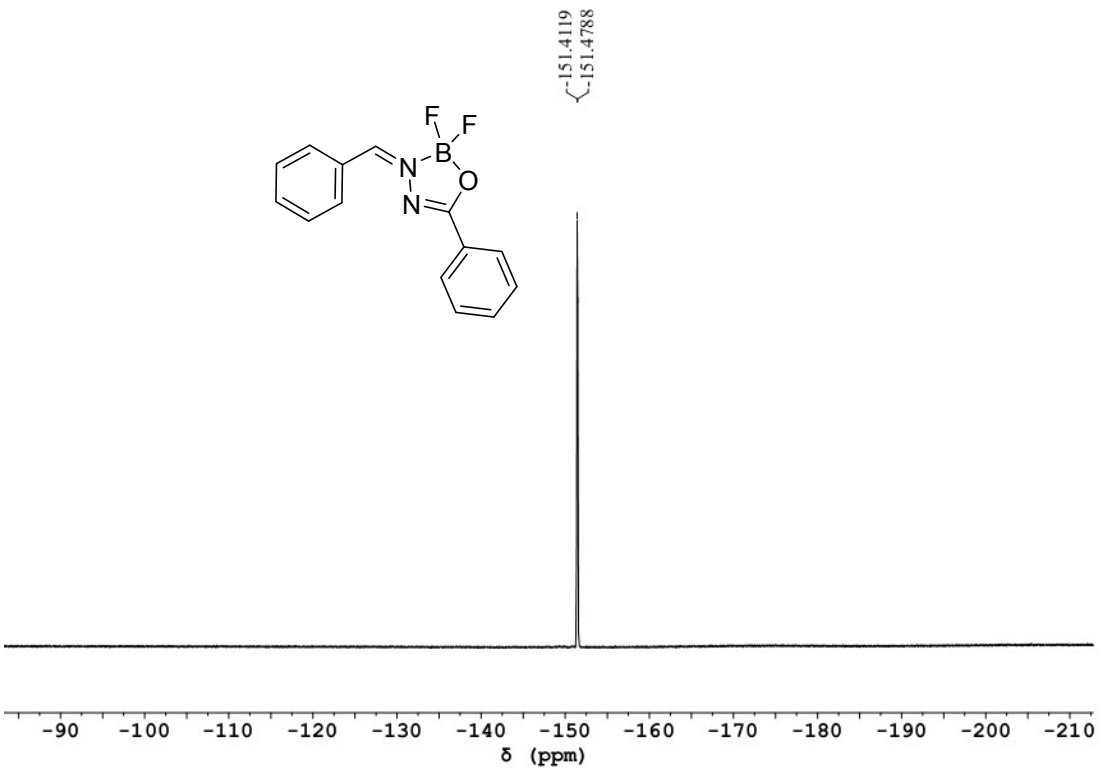
^{19}C NMR spectrum of BOAHY **2k** in $CDCl_3$



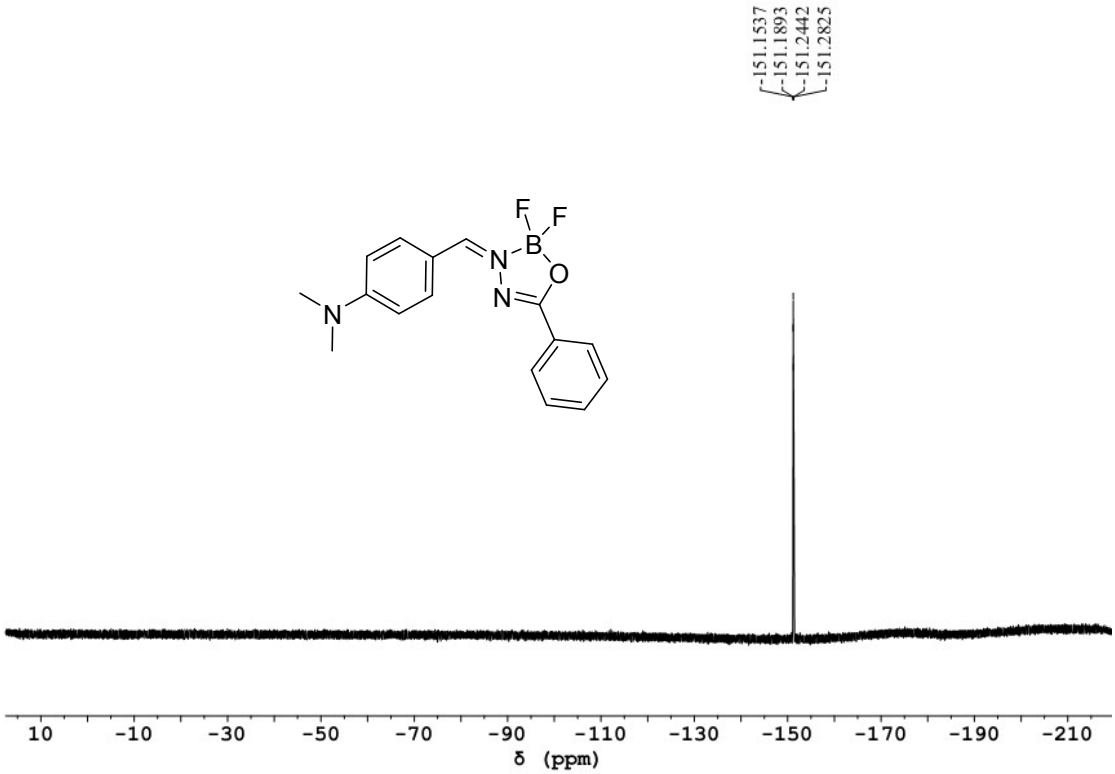
^{1}H NMR spectrum of BOAHY **2l** in acetone-d_6



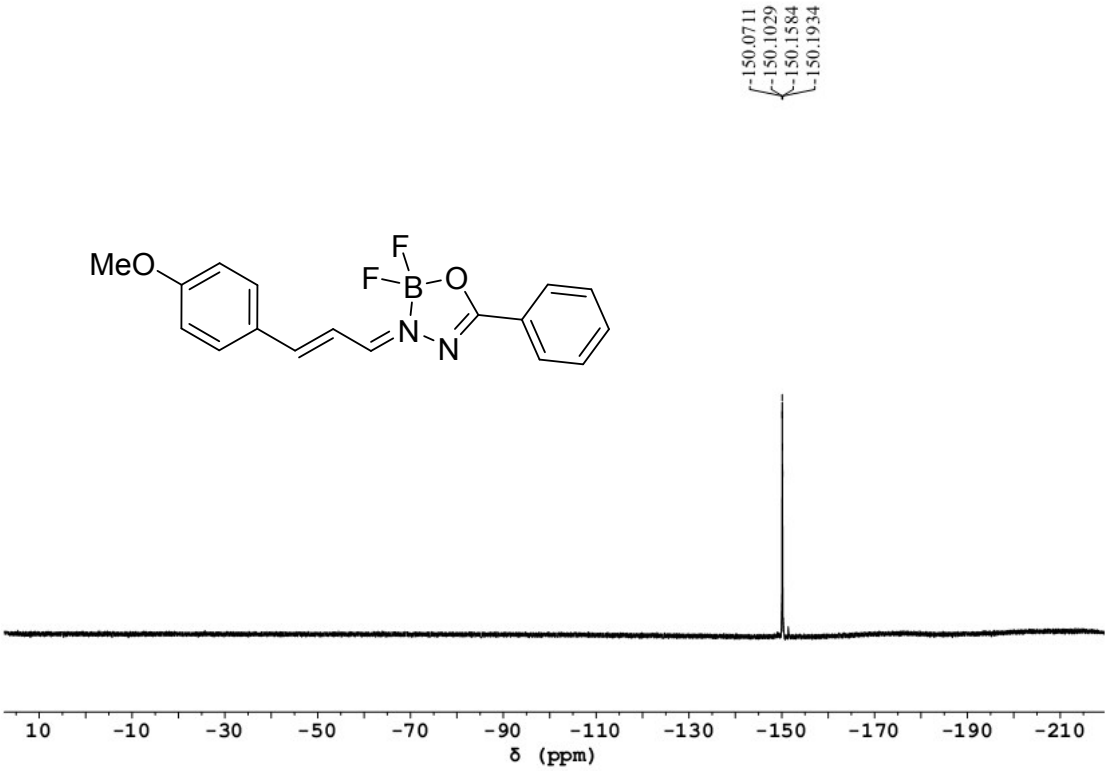
^{13}C NMR spectrum of BOAHY **2l** in acetone-d_6



^{19}F NMR spectrum of BOAHY **2a** in $CDCl_3$



^{19}F NMR spectrum of BOAHY **2d** in $CDCl_3$



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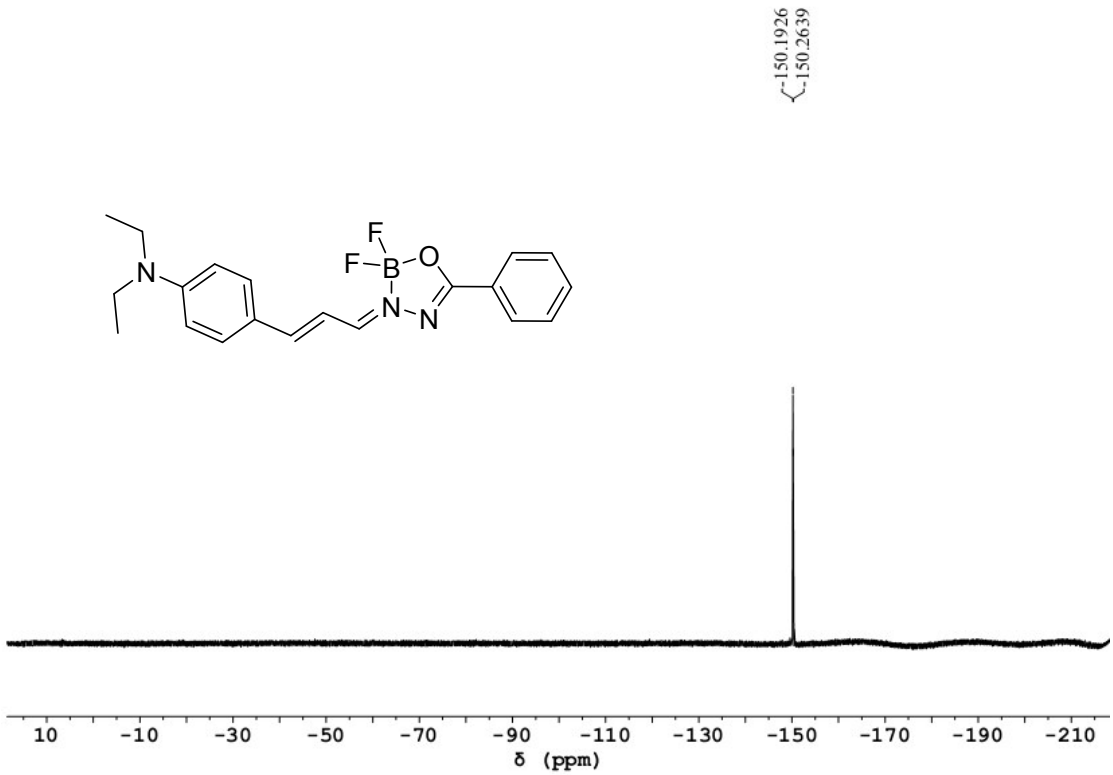
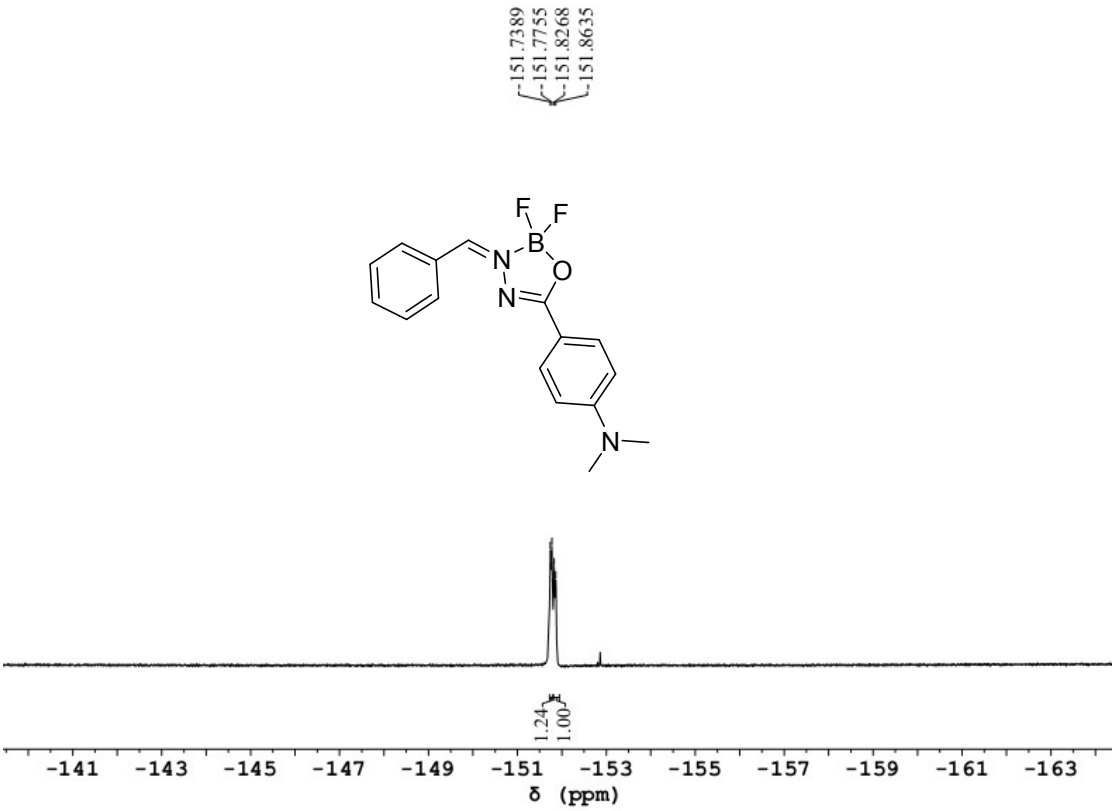
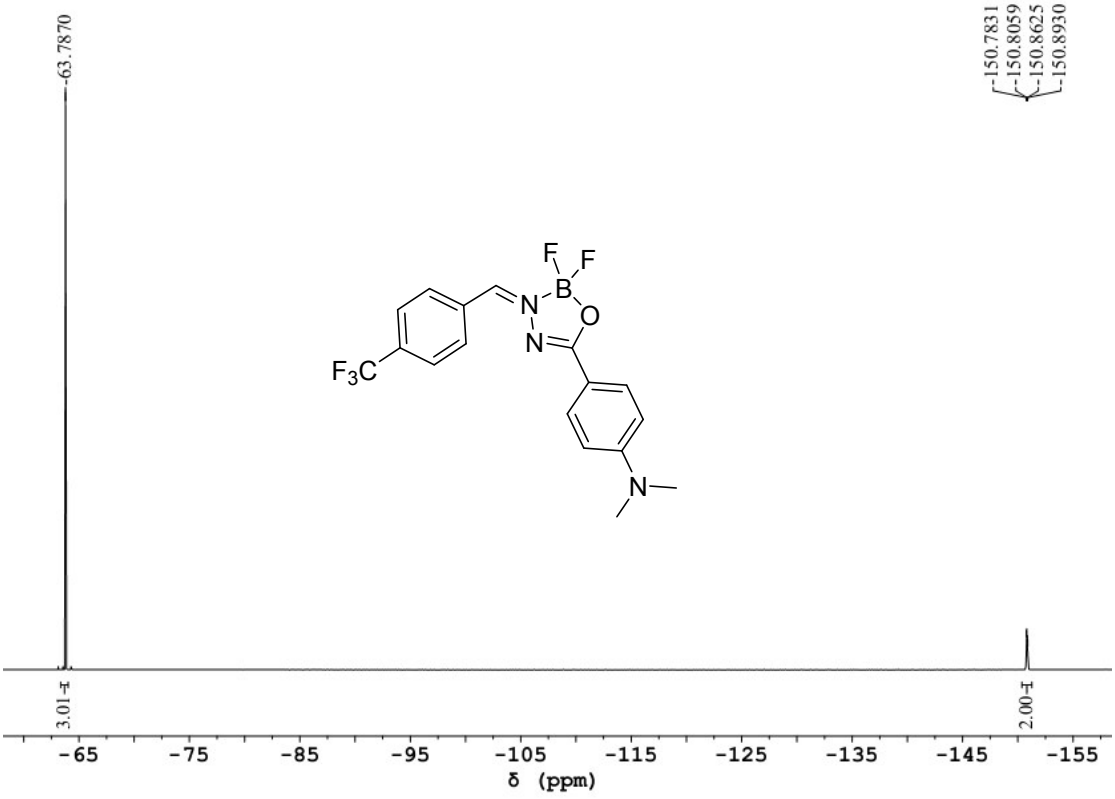


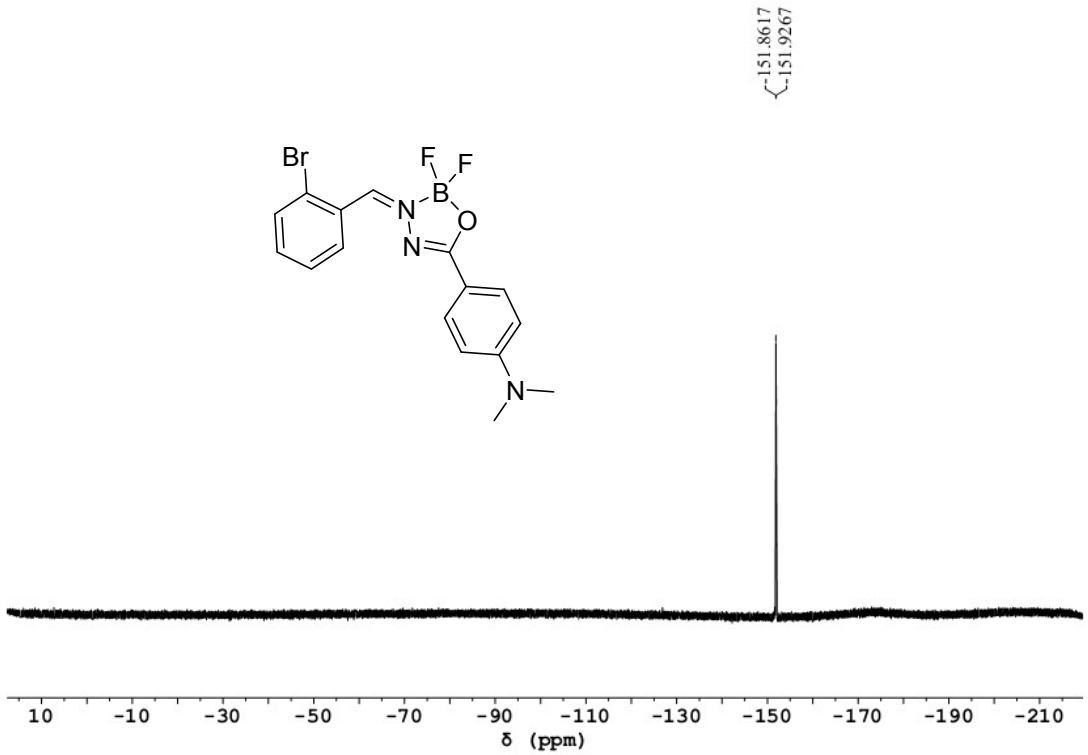
^{19}F NMR spectrum of BOAHY **2f** in $CDCl_3$



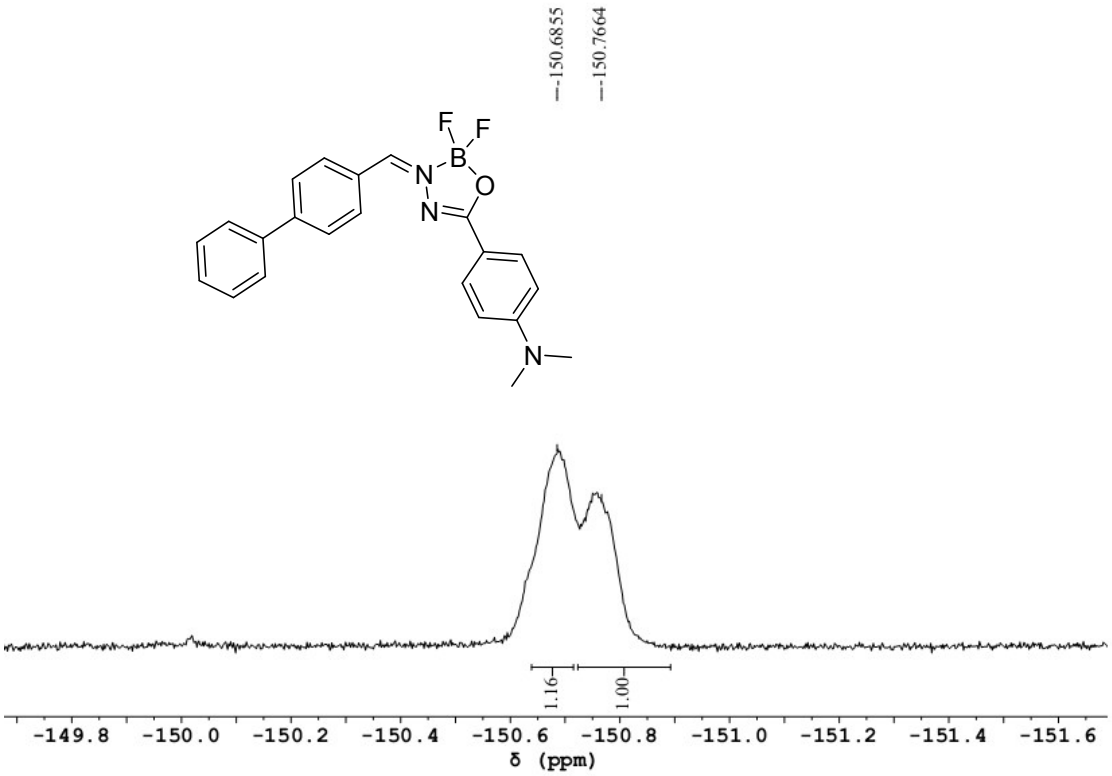
^{19}F NMR spectrum of BOAHY **2h** in acetone-d_6



^{19}F NMR spectrum of BOAHY **2j** in $CDCl_3$



^{19}F NMR spectrum of BOAHY **2k** in $CDCl_3$



^{19}F NMR spectrum of BOAHY **2l** in acetone-d_6

8. HRMS for BOAHYs

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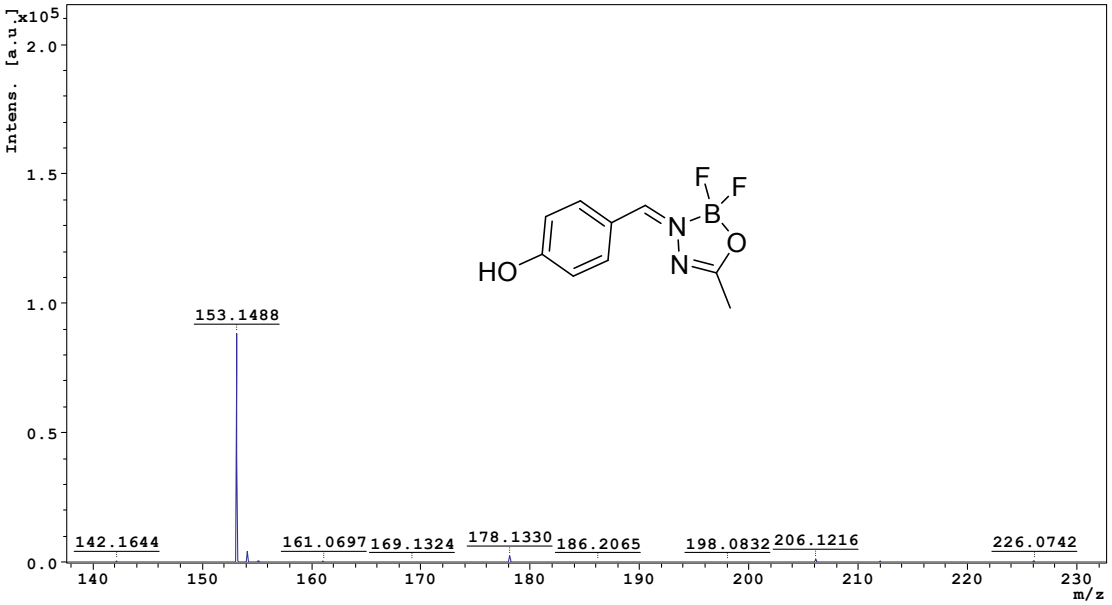

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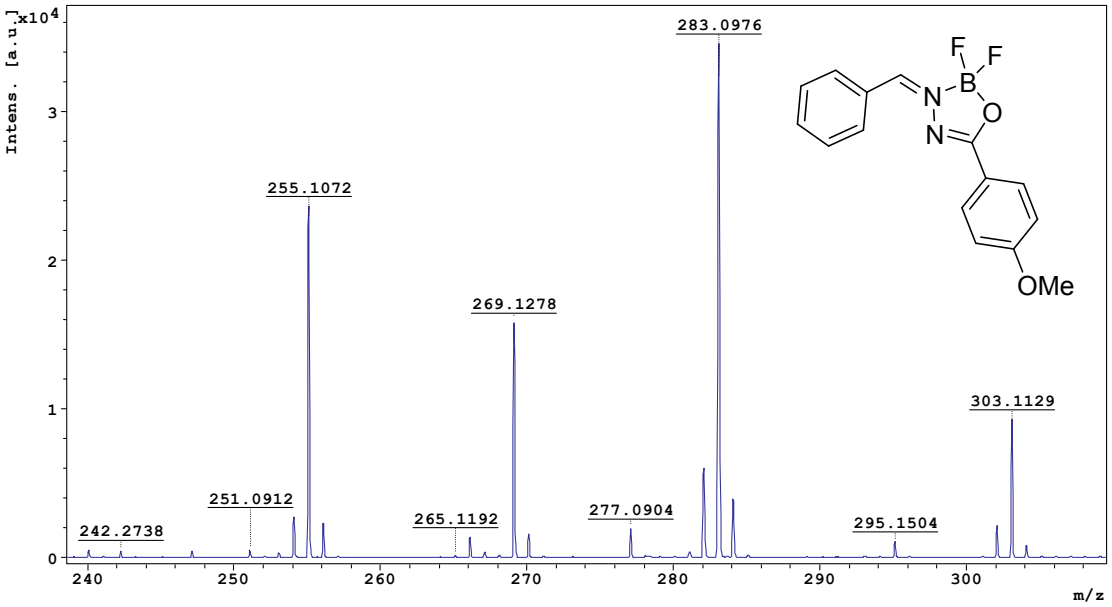

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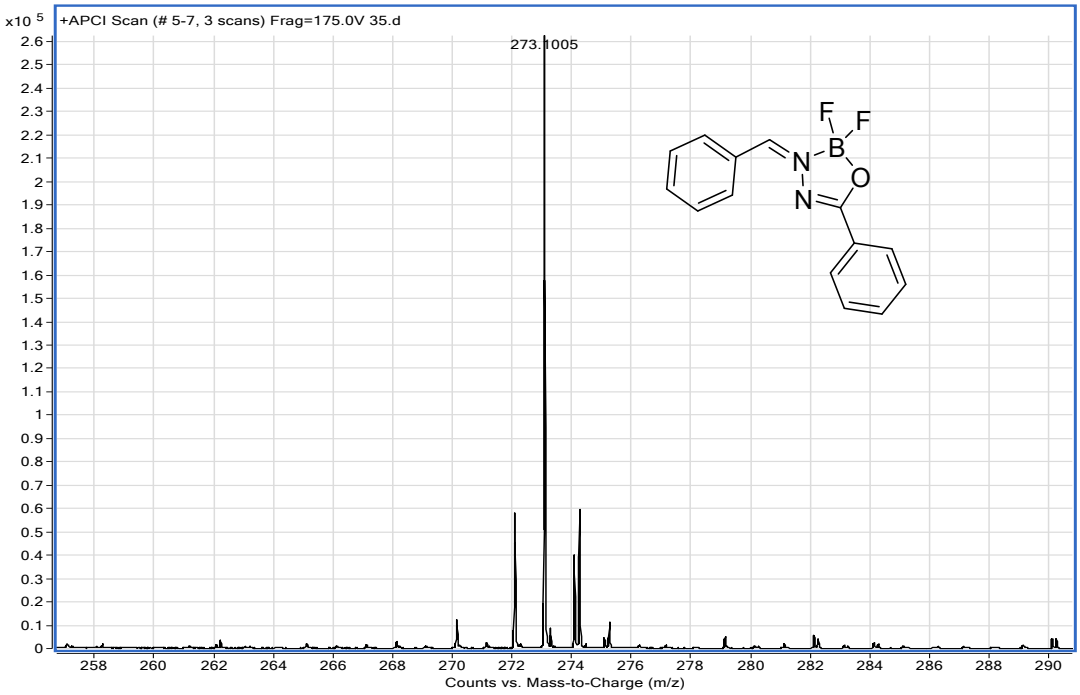

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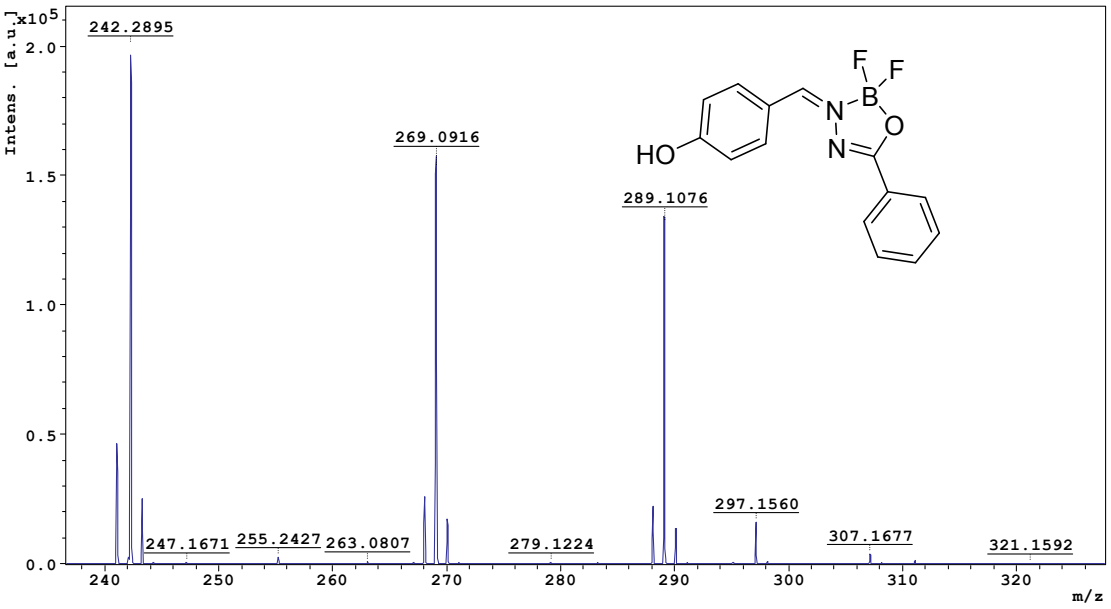

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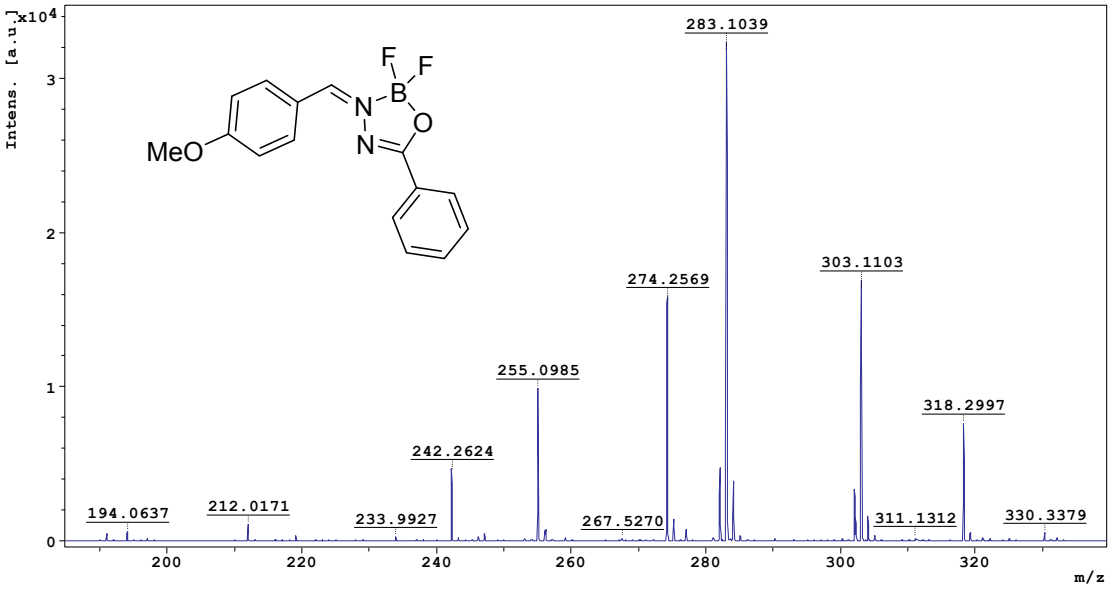

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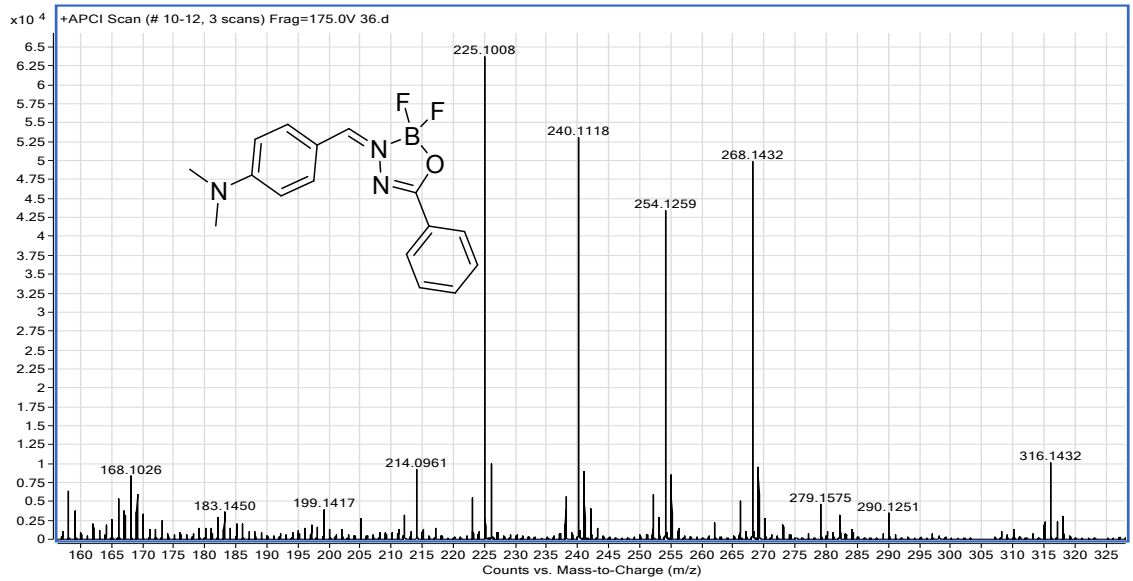
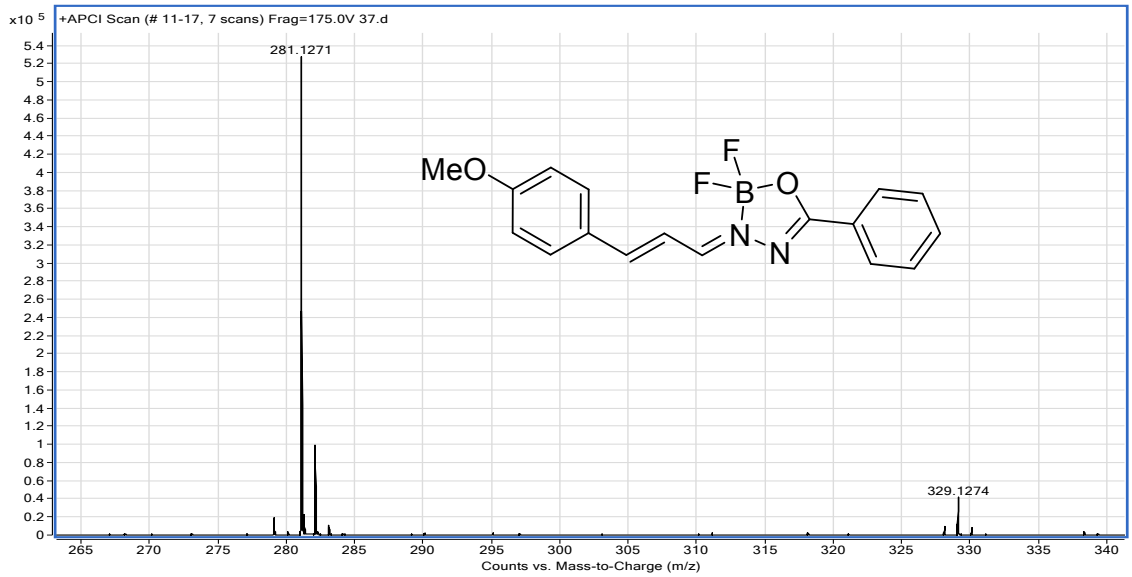


HRMS for BOAHY **2e**



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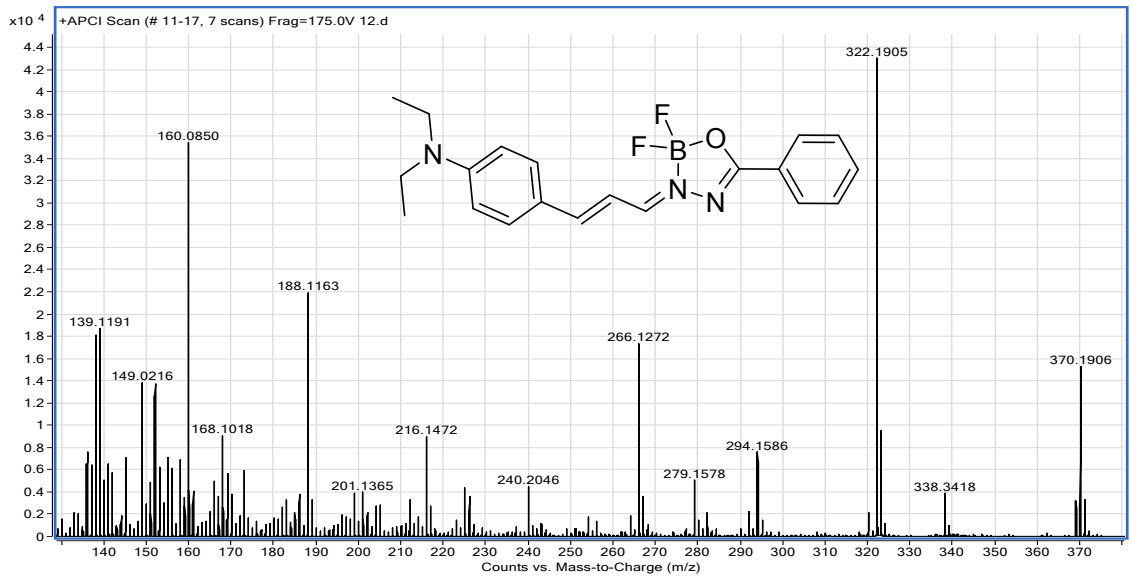

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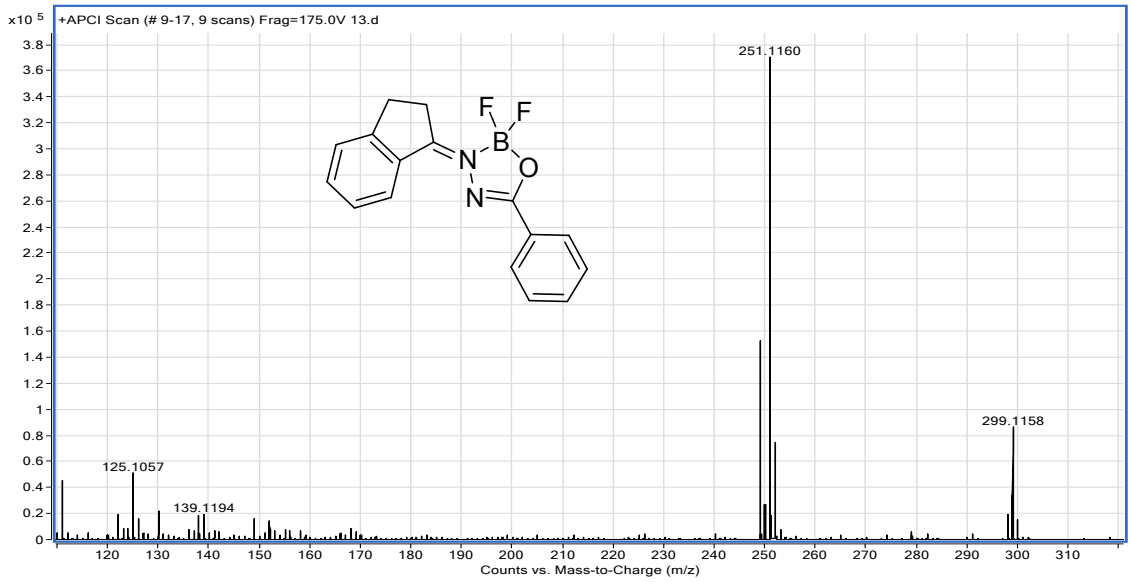

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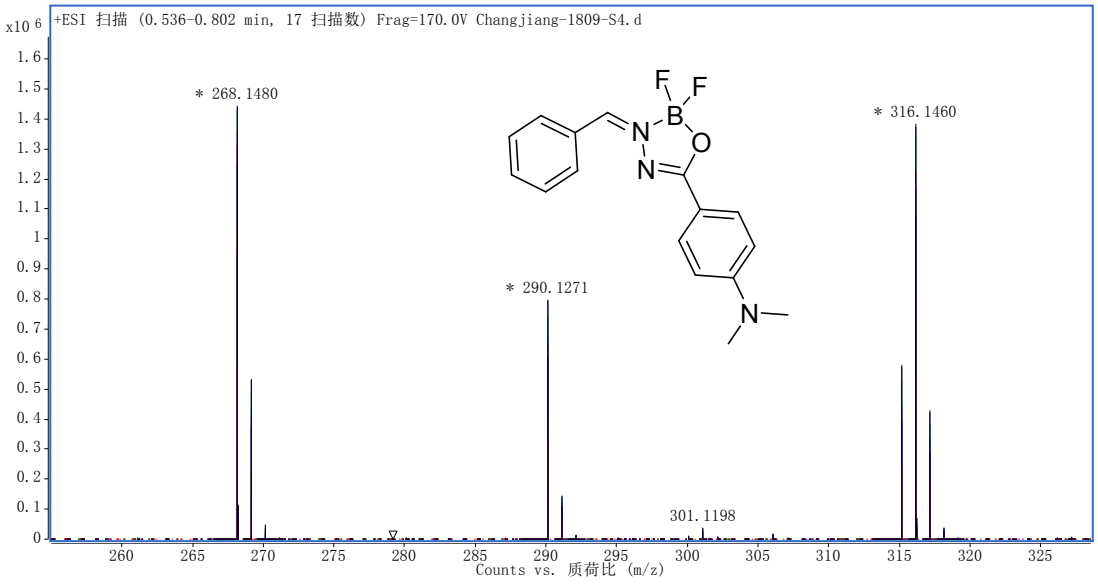
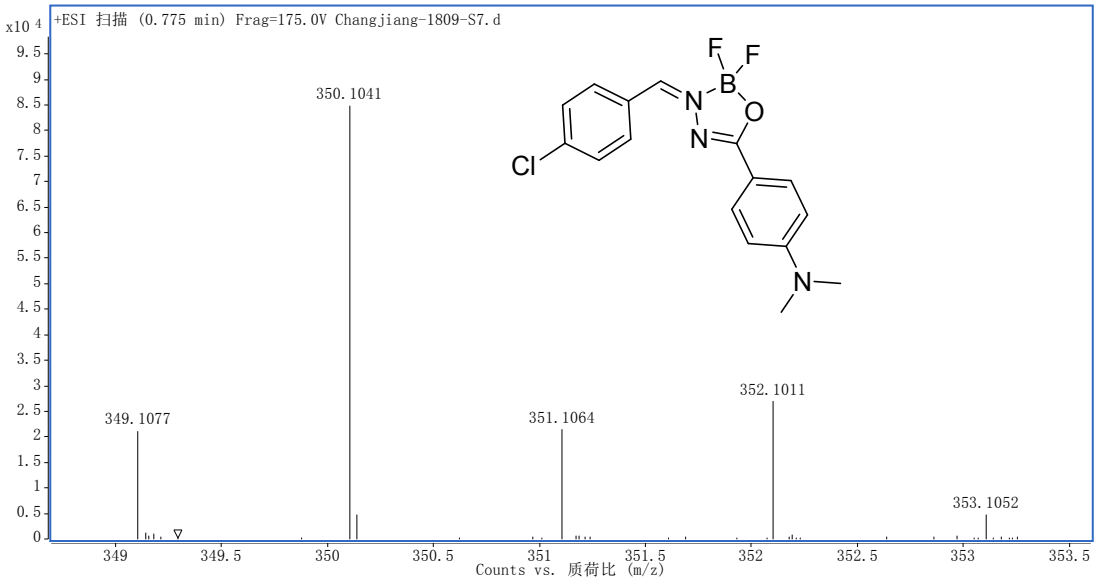


HRMS for BOAHY **2i**



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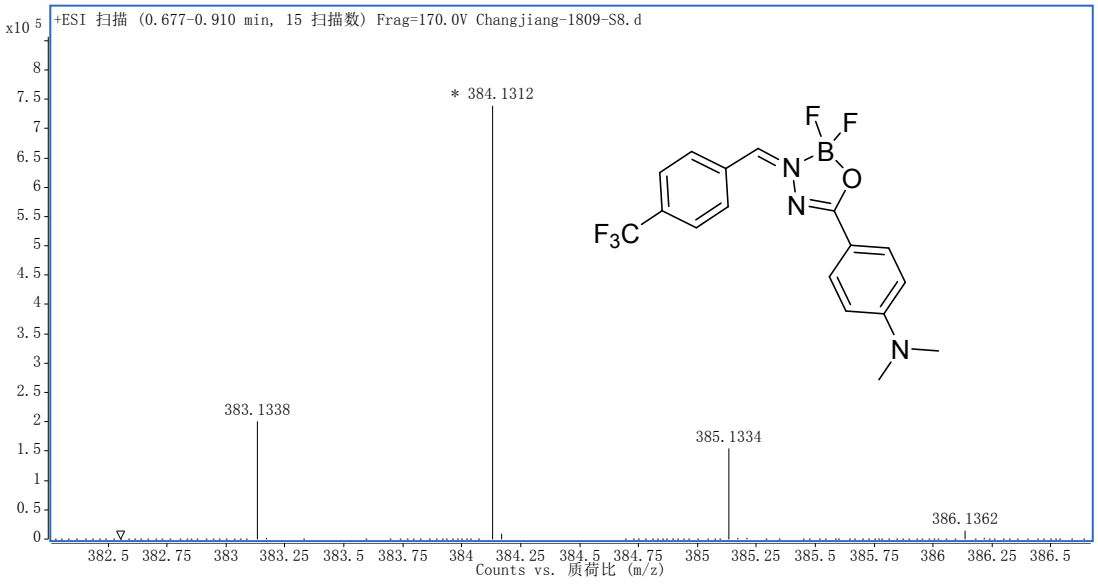

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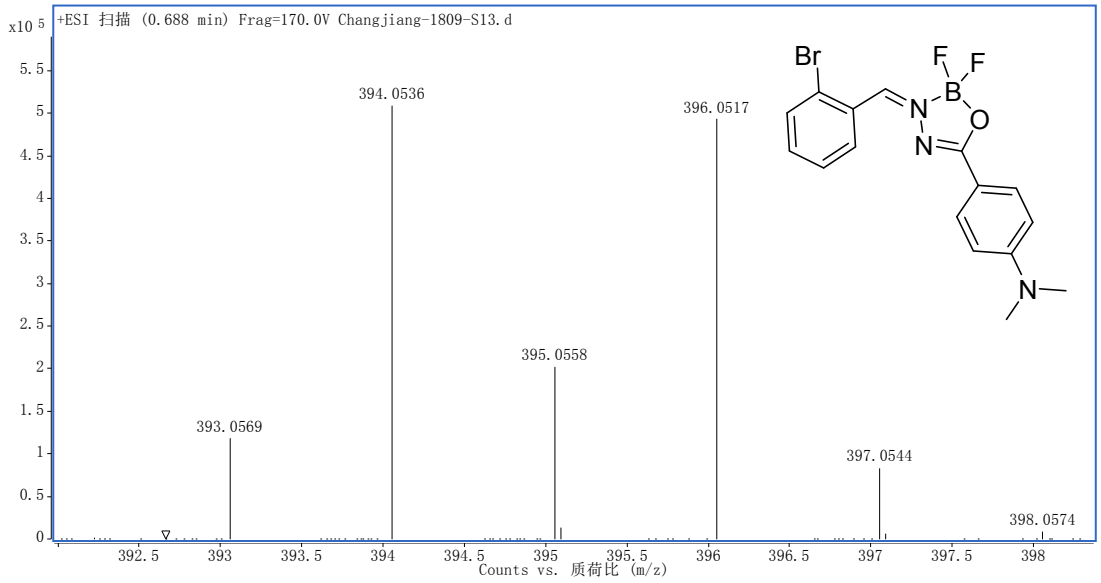

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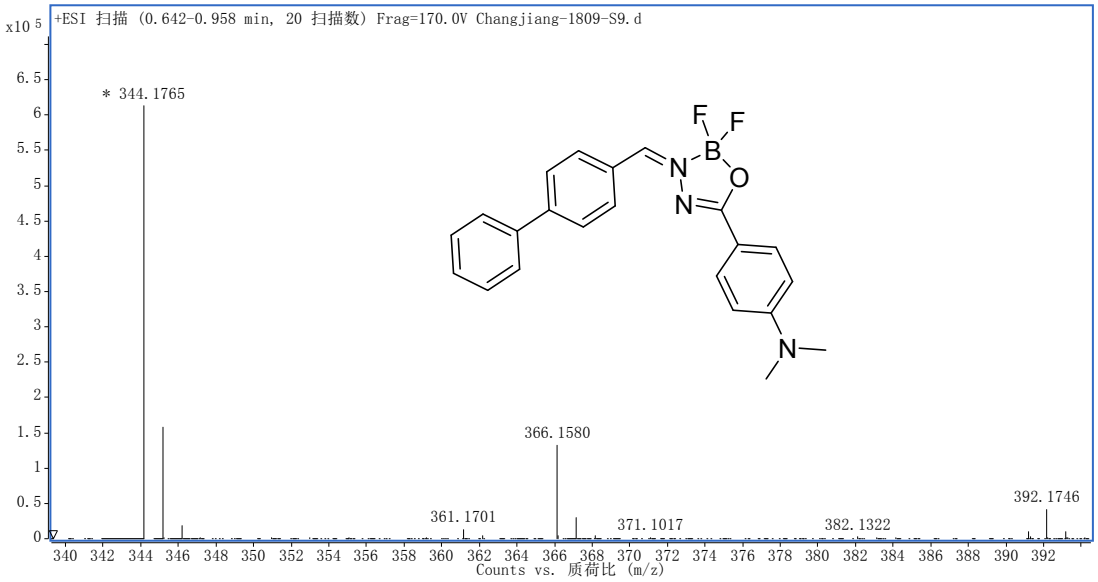

9. DFT calculations

The ground state geometries of BOAHYs **2d**, **2h** and **2k** were optimized by using DFT method at B3LYP/6-31G (d) level. The same method was used for vibrational analysis to verify that the optimized structures correspond to local minima on the energy surface. The DFT of all the molecules in dichloromethane were done using the Self-Consistent Reaction Field (SCRF) method and the Polarizable Continuum Model (PCM). All of the calculations were carried out in dichloromethane by the methods implemented in Gaussian 09 package.

DFT optimized coordinates

BOAHY **2d**

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F	6.16780000	6.29740000	2.00190000
O	4.42220000	6.39510000	3.58170000
N	5.09690000	4.30440000	2.89270000
N	4.70820000	4.23790000	4.22430000
C	5.52270000	3.29130000	2.21560000
H	5.75680000	3.48470000	1.32560000
C	5.69930000	1.90600000	2.60010000
C	6.19190000	1.05920000	1.59910000
C	6.39740000	-0.28360000	1.85460000
C	6.10290000	-0.80000000	3.09810000
C	5.61140000	0.03080000	4.09370000
C	5.41400000	1.37580000	3.85820000
H	5.08900000	1.93210000	4.54250000
C	4.33900000	5.45880000	4.52390000
C	3.82530000	5.83370000	5.82000000
C	3.37340000	7.13610000	6.04600000
H	3.41590000	7.76270000	5.34670000
C	2.86930000	7.52490000	7.26220000
H	2.56910000	8.40840000	7.37960000
C	2.79600000	6.61780000	8.33690000
C	3.26050000	5.29810000	8.10510000
H	3.22930000	4.66780000	8.80210000
C	3.75430000	4.92620000	6.88120000
H	4.05090000	4.04380000	6.75330000
B	4.95440000	5.79340000	2.36170000
H	6.78470643	-0.92151146	1.08781274
H	5.38243842	-0.37628241	5.05638401
H	2.40602091	6.91209714	9.28884826
H	6.41079599	1.45473210	0.62928615

N	6.30961194	-2.23001892	3.36868464
C	7.72878631	-2.56409344	3.18096592
H	7.92828148	-3.52526070	3.60671136
H	7.95545104	-2.58311507	2.13542238
H	8.33563045	-1.82707430	3.66412528
C	5.49197780	-3.02708207	2.44290672
H	5.50554197	-4.05269097	2.74760722
H	4.48516811	-2.66499002	2.45402409
H	5.89007493	-2.94374017	1.45322354

BOAHY **2h**

F	4.06260000	5.85440000	1.31310000
F	6.16780000	6.29740000	2.00190000
O	4.42220000	6.39510000	3.58170000
N	5.09690000	4.30440000	2.89270000
N	4.70820000	4.23790000	4.22430000
N	2.29890000	7.00210000	9.54810000
C	5.52270000	3.29130000	2.21560000
H	5.75680000	3.48470000	1.32560000
C	5.69930000	1.90600000	2.60010000
C	6.19190000	1.05920000	1.59910000
H	6.38420000	1.40690000	0.74720000
C	6.39740000	-0.28360000	1.85460000
H	6.73740000	-0.84370000	1.18070000
C	6.10290000	-0.80000000	3.09810000
H	6.23500000	-1.71480000	3.27170000
C	5.61140000	0.03080000	4.09370000
H	5.41030000	-0.32710000	4.93950000
C	5.41400000	1.37580000	3.85820000
H	5.08900000	1.93210000	4.54250000
C	4.33900000	5.45880000	4.52390000
C	3.82530000	5.83370000	5.82000000
C	3.37340000	7.13610000	6.04600000
H	3.41590000	7.76270000	5.34670000
C	2.86930000	7.52490000	7.26220000
H	2.56910000	8.40840000	7.37960000
C	2.79600000	6.61780000	8.33690000
C	3.26050000	5.29810000	8.10510000
H	3.22930000	4.66780000	8.80210000
C	3.75430000	4.92620000	6.88120000
H	4.05090000	4.04380000	6.75330000
C	1.97450000	8.39580000	9.80030000
H	2.77660000	8.93500000	9.71580000
H	1.61690000	8.48710000	10.69690000

H	1.31370000	8.69510000	9.15680000
C	2.36350000	6.11050000	10.68320000
H	1.94440000	5.26610000	10.45500000
H	1.89910000	6.51010000	11.43490000
H	3.29160000	5.95690000	10.92160000
B	4.95440000	5.79340000	2.36170000

BOAHY **2k**

F	4.06260000	5.85440000	1.31310000
F	6.16780000	6.29740000	2.00190000
O	4.42220000	6.39510000	3.58170000
N	5.09690000	4.30440000	2.89270000
N	4.70820000	4.23790000	4.22430000
N	2.29890000	7.00210000	9.54810000
C	5.52270000	3.29130000	2.21560000
H	5.75680000	3.48470000	1.32560000
C	5.69930000	1.90600000	2.60010000
C	6.19190000	1.05920000	1.59910000
H	6.38420000	1.40690000	0.74720000
C	6.39740000	-0.28360000	1.85460000
H	6.73740000	-0.84370000	1.18070000
C	6.10290000	-0.80000000	3.09810000
H	6.23500000	-1.71480000	3.27170000
C	5.61140000	0.03080000	4.09370000
H	5.41030000	-0.32710000	4.93950000
C	5.41400000	1.37580000	3.85820000
H	5.08900000	1.93210000	4.54250000
C	4.33900000	5.45880000	4.52390000
C	3.82530000	5.83370000	5.82000000
C	3.37340000	7.13610000	6.04600000
H	3.41590000	7.76270000	5.34670000
C	2.86930000	7.52490000	7.26220000
H	2.56910000	8.40840000	7.37960000
C	2.79600000	6.61780000	8.33690000
C	3.26050000	5.29810000	8.10510000
H	3.22930000	4.66780000	8.80210000
C	3.75430000	4.92620000	6.88120000
H	4.05090000	4.04380000	6.75330000
C	1.97450000	8.39580000	9.80030000
H	2.77660000	8.93500000	9.71580000
H	1.61690000	8.48710000	10.69690000
H	1.31370000	8.69510000	9.15680000
C	2.36350000	6.11050000	10.68320000
H	1.94440000	5.26610000	10.45500000

H	1.89910000	6.51010000	11.43490000
H	3.29160000	5.95690000	10.92160000
B	4.95440000	5.79340000	2.36170000