Electronic Supplementary Material (ESI) for Dalton Transactions.

Facial Synthesis of Highly Fluorescent BF_2 Complexes Bearing Isoindolin-1-one Ligand

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1. Crystal data for 1a and 1c

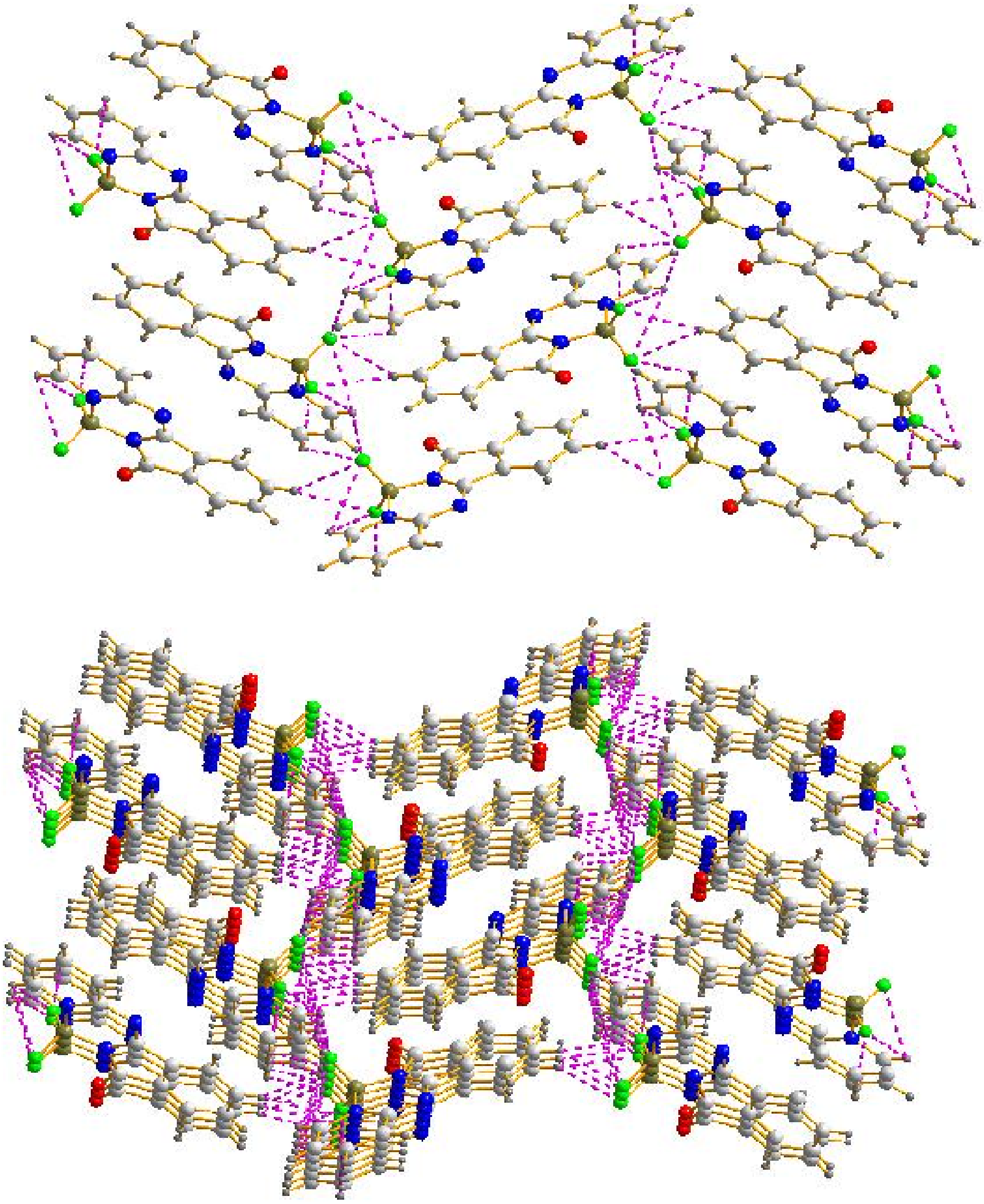


Fig. S1. Intermolecular crystal packing of **1a** through H-bonding.

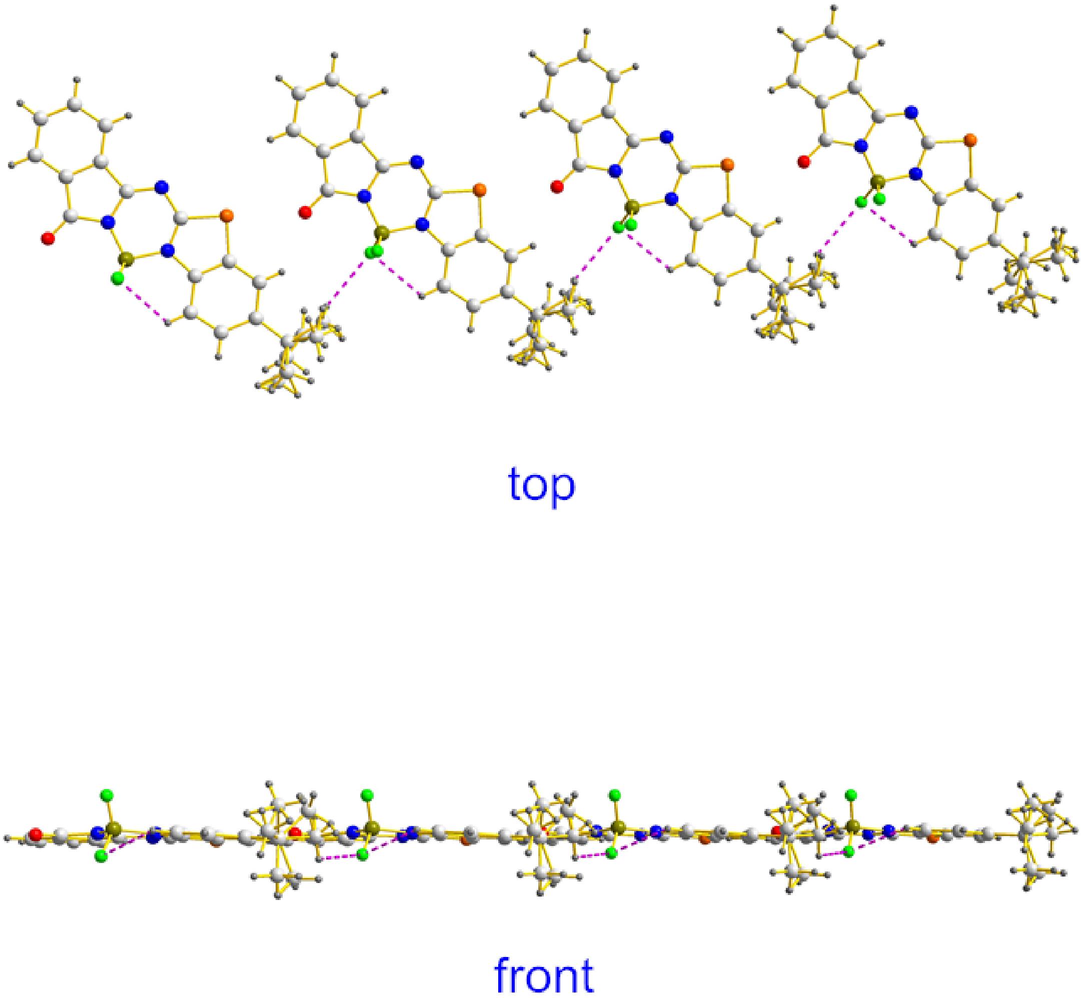
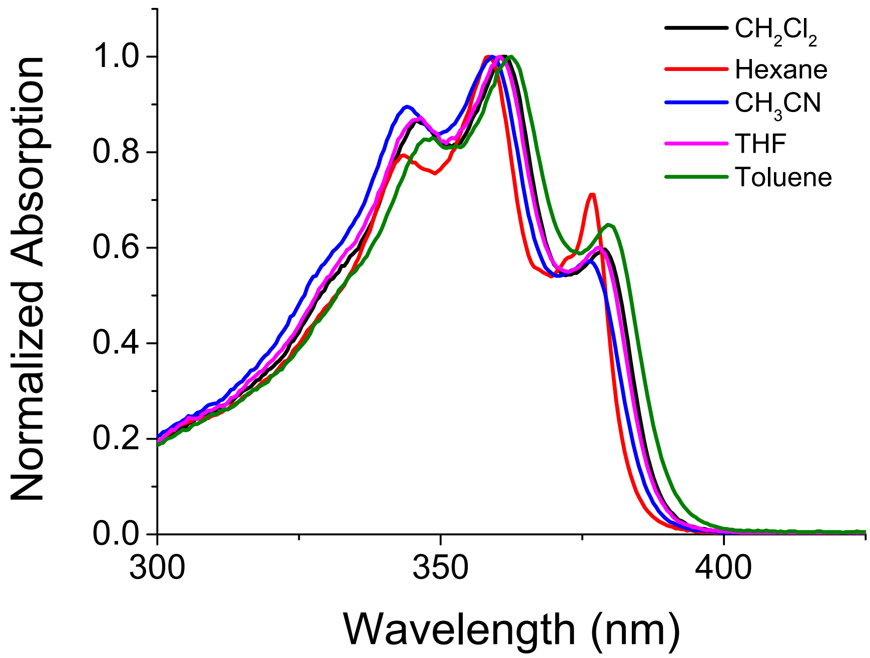


Fig. S2. Intermolecular crystal packing of **1c** through H-bonding.

2. Table S1. Selected bond lengths (Å) for crystals 1a and 1c

compound	Bond	Bond lengths
1a	N(1)-C(1)	1.407(17)
	N(1)-C(8)	1.371(17)
	N(2)-C(8)	1.289(16)
	N(2)-C(9)	1.385(15)
	N(3)-C(9)	1.356(17)
	C(1)-O(1)	1.207(18)
	B(1)-N(1)	1.518(17)
	B(1)-N(3)	1.589(19)
	F(1)-H(1)	2.825(9)
1c	N(1)-C(1)	1.400(37)
	N(1)-C(8)	1.351(52)
	N(2)-C(8)	1.304(38)
	N(2)-C(9)	1.356(41)
	N(3)-C(9)	1.319(44)
	C(1)-O(1)	1.204(57)
	B(1)-N(1)	1.546(5)
	B(1)-N(3)	1.579(45)
	C(9)-S(1)	1.718(30)
	F(1)-H(1)	2.646(21)

3. UV-Vis and fluorescence spectra



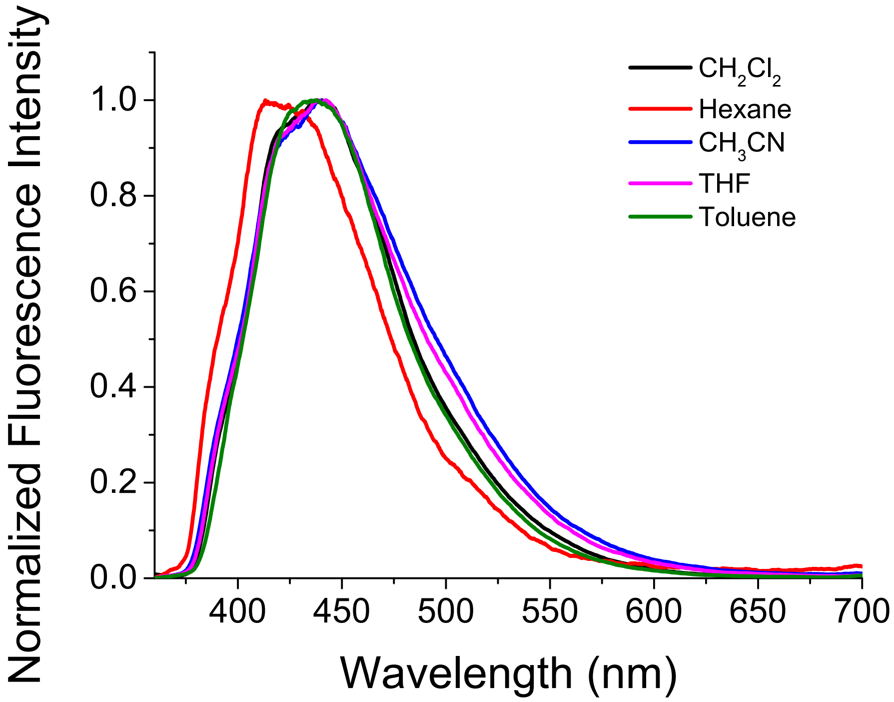


Fig. S3. Absorption (top) and emission (bottom) spectra of **1a** recorded in different solvents.

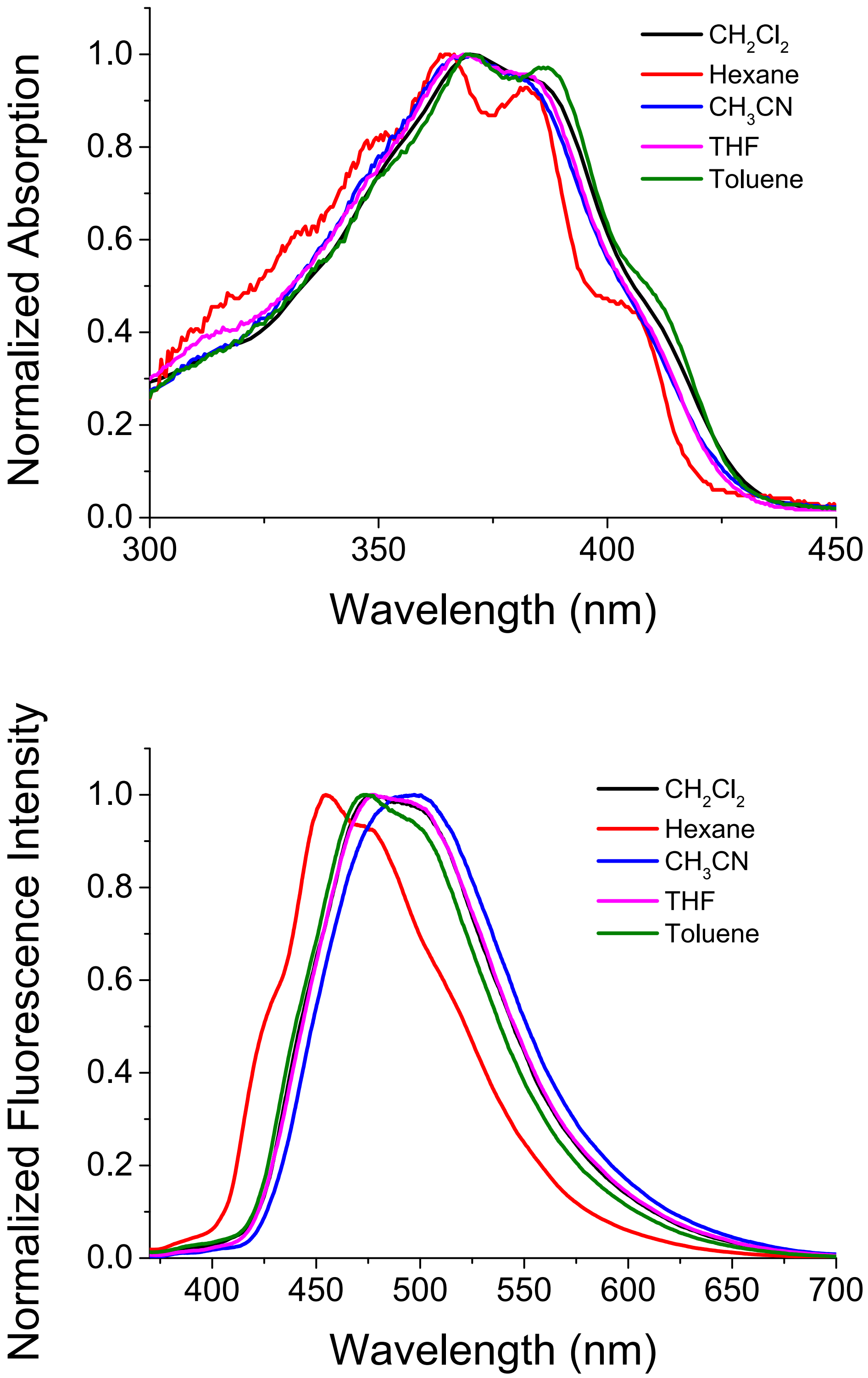


Fig. S4. Absorption (top) and emission (bottom) spectra of **1b** recorded in different solvents.

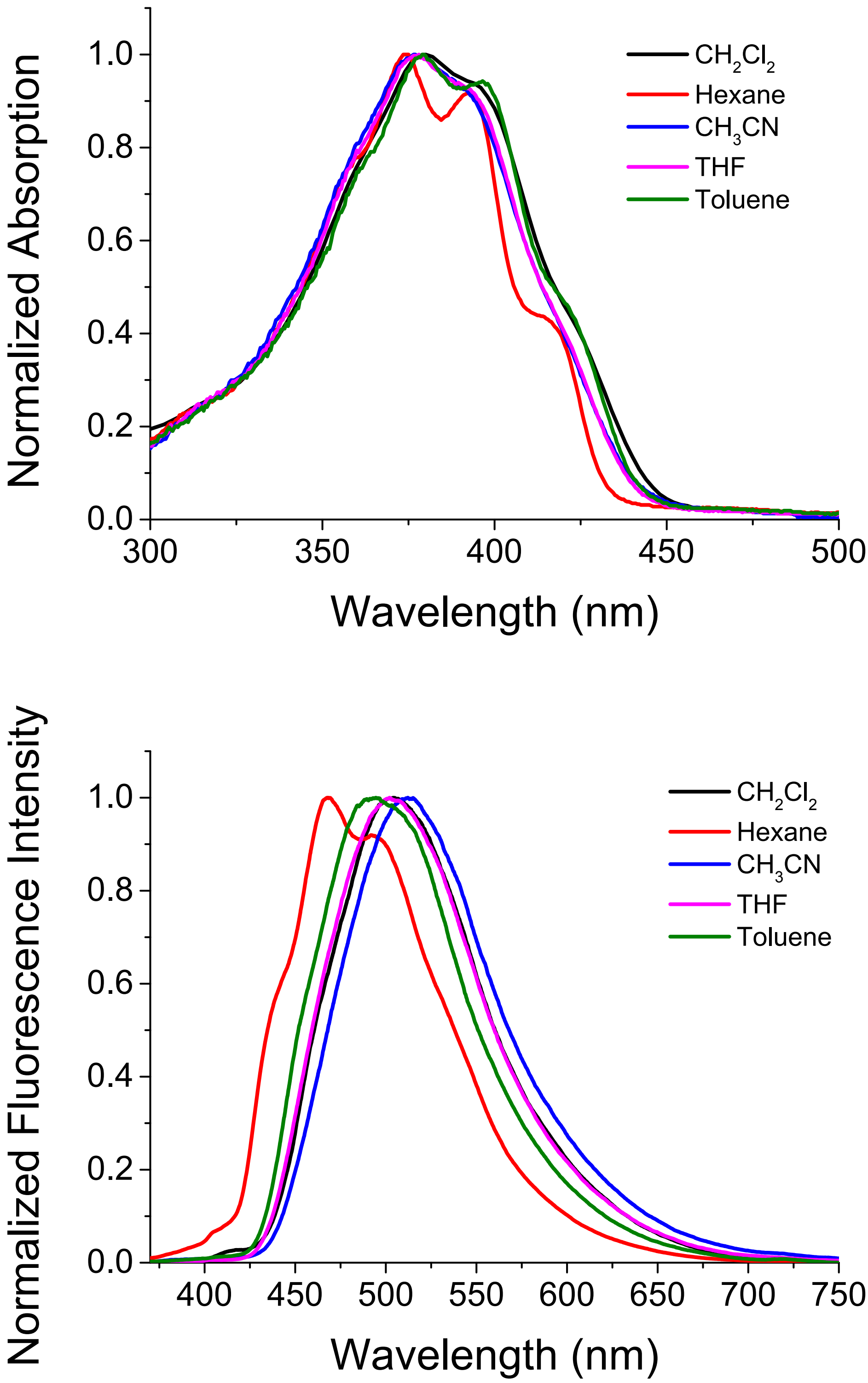
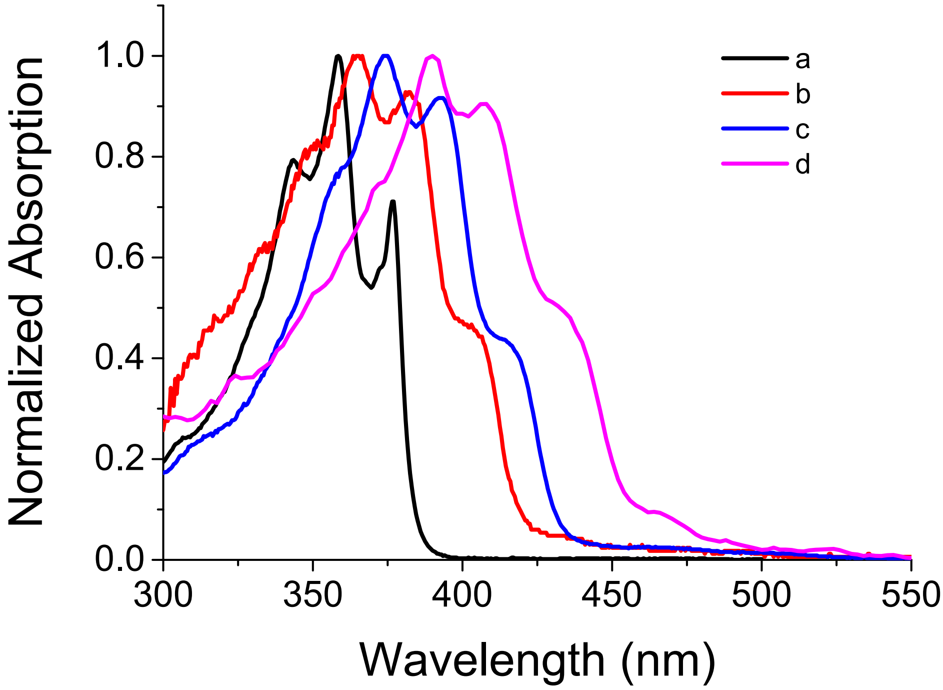


Fig. S5. Absorption (top) and emission (bottom) spectra of **1c** recorded in different solvents.



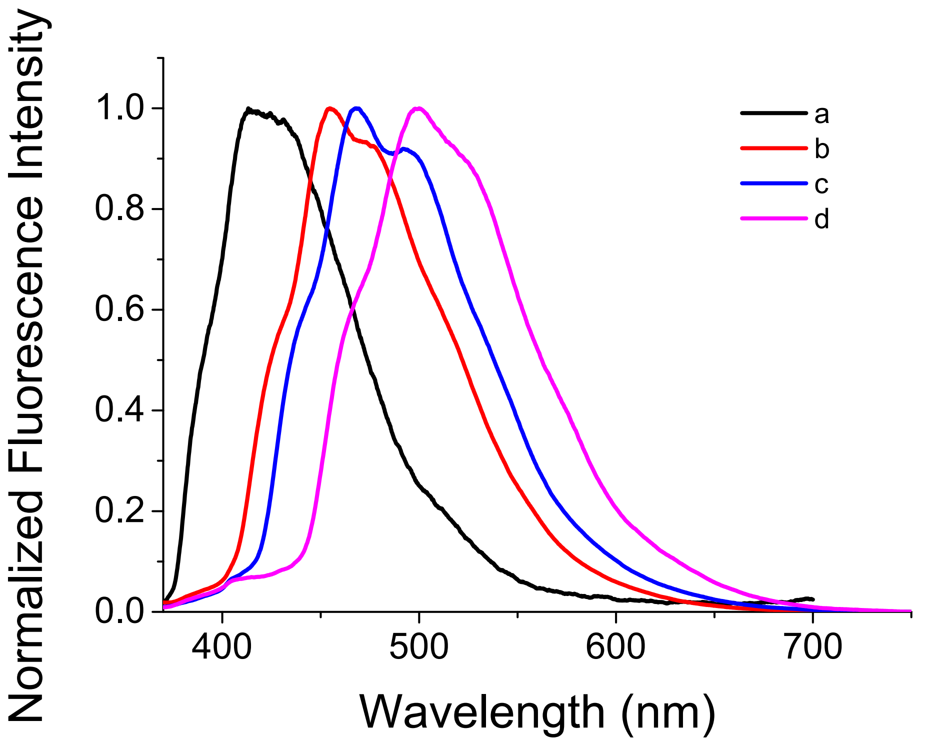


Fig. S6. Absorption (top) and emission (bottom) spectra of **1a** (black), **1b** (red), **1c** (blue) and **1d** (magenta) in hexane.

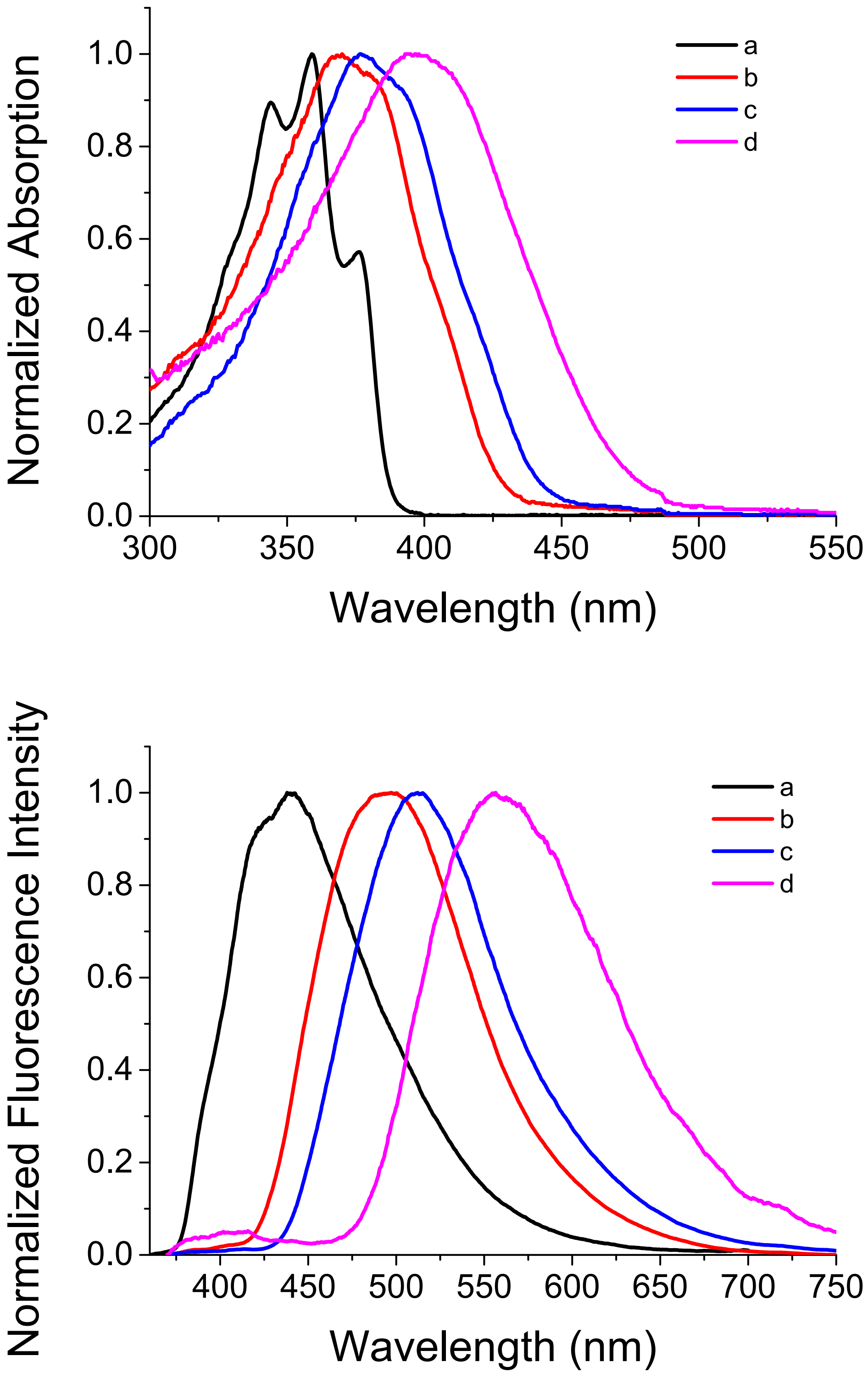


Fig. S7. Absorption (top) and emission (bottom) spectra of **1a** (black), **1b** (red), **1c** (blue) and **1d** (magenta) in acetonitrile.

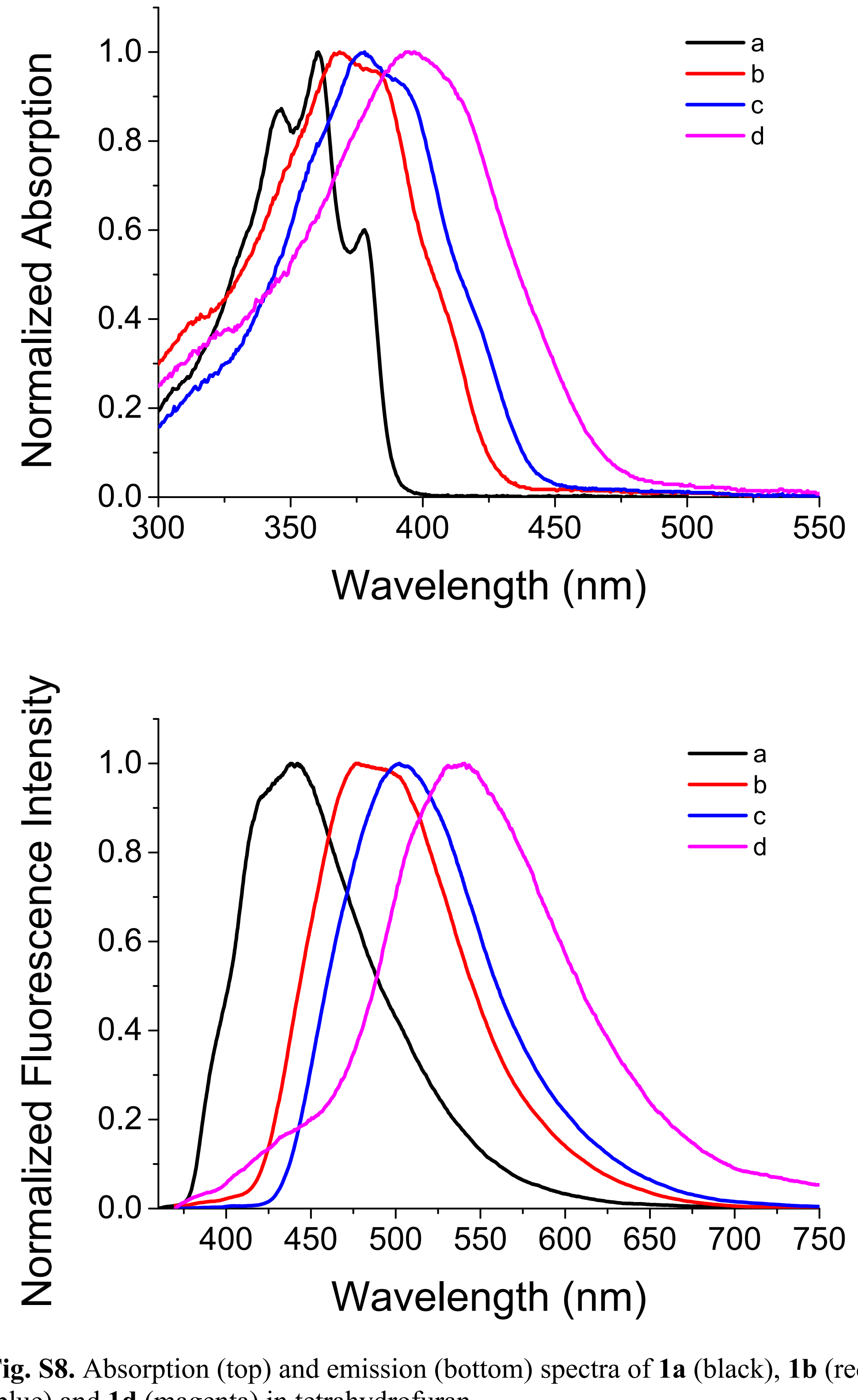
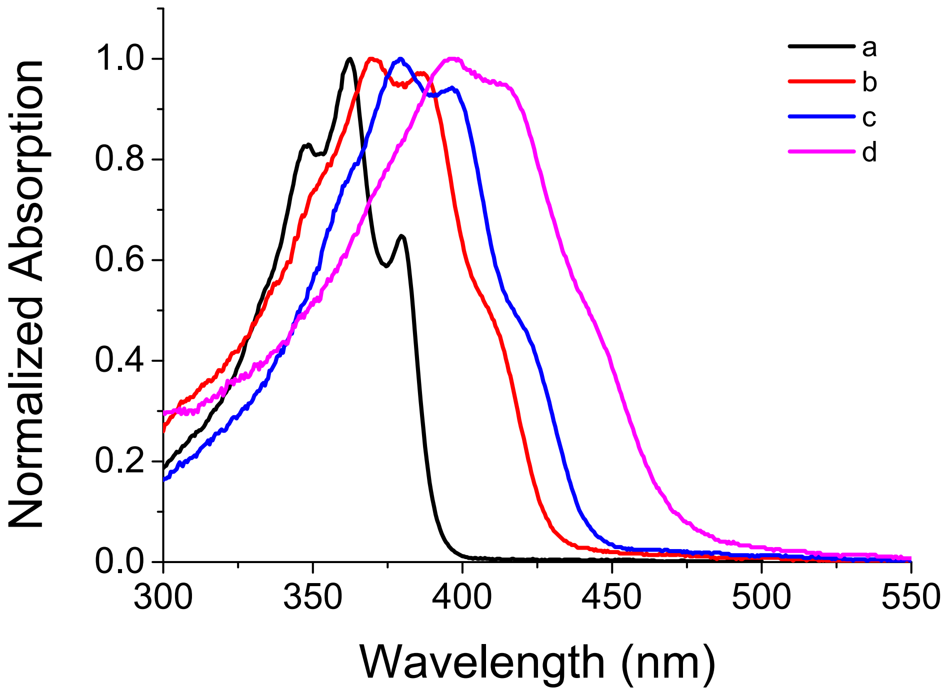


Fig. S8. Absorption (top) and emission (bottom) spectra of **1a** (black), **1b** (red), **1c** (blue) and **1d** (magenta) in tetrahydrofuran.



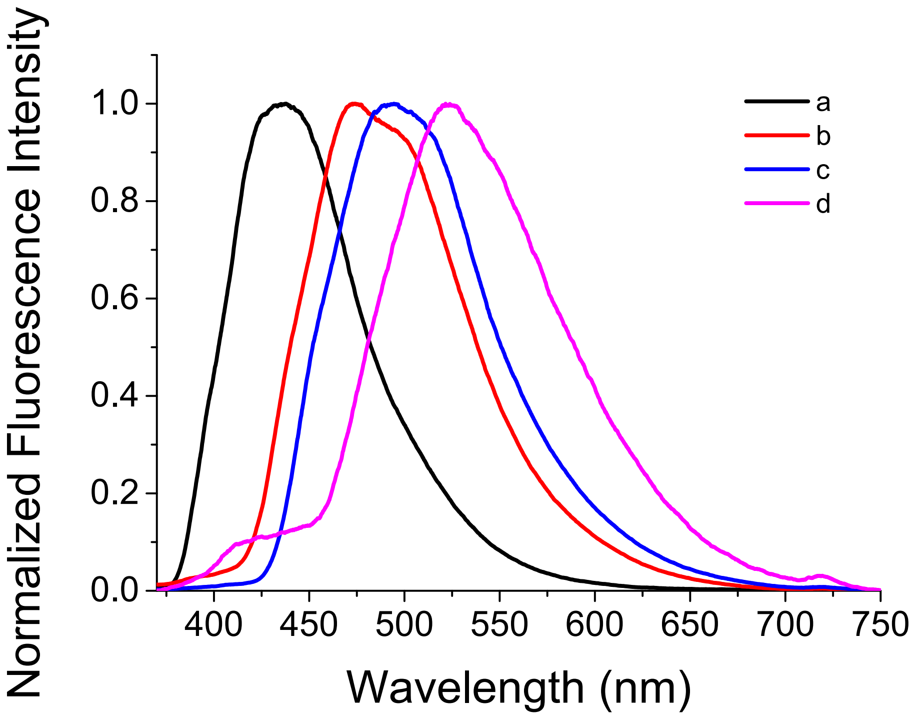


Fig. S9. Absorption (top) and emission (bottom) spectra of **1a** (black), **1b** (red), **1c** (blue) and **1d** (magenta) in toluene.

4. Fluorescence lifetime decay curves

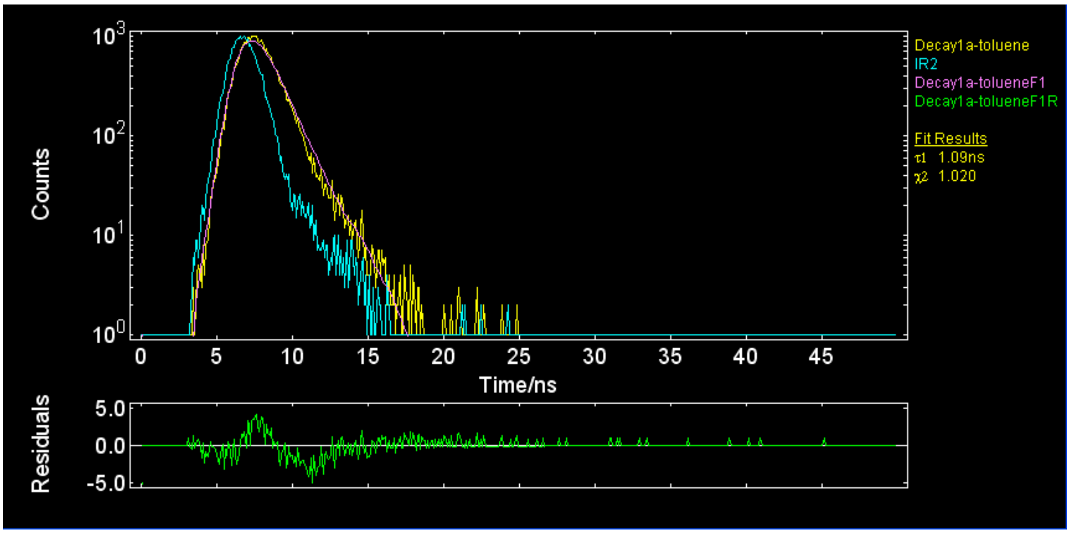


Fig. S10. The fluorescence decay of dye **1a** in toluene excited at 360 nm and measured by single photon counting method whose emission at 435 nm.

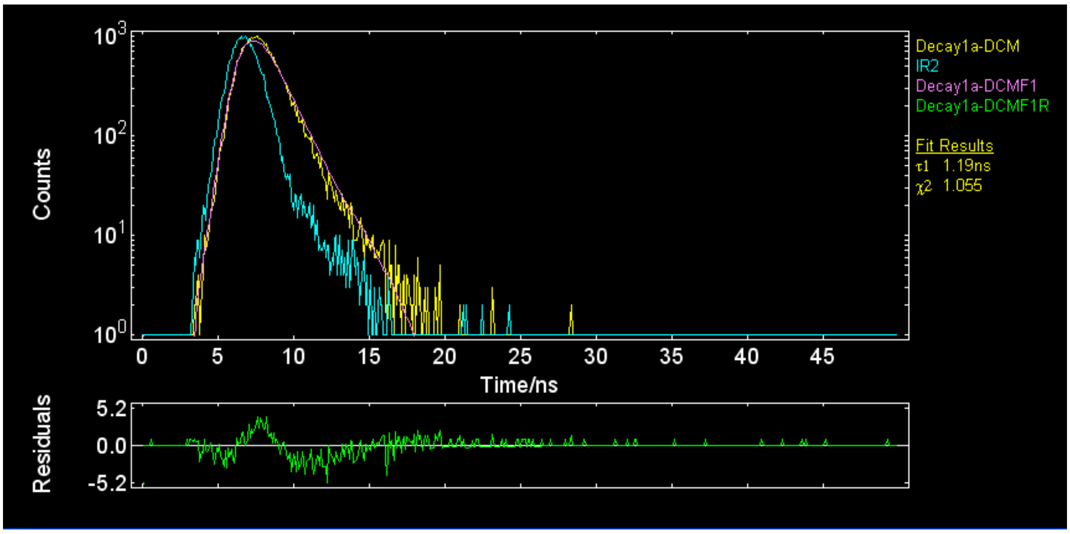


Fig. S11. The fluorescence decay of dye **1a** in dichloromethane excited at 360 nm and measured by single photon counting method whose emission at 435 nm.

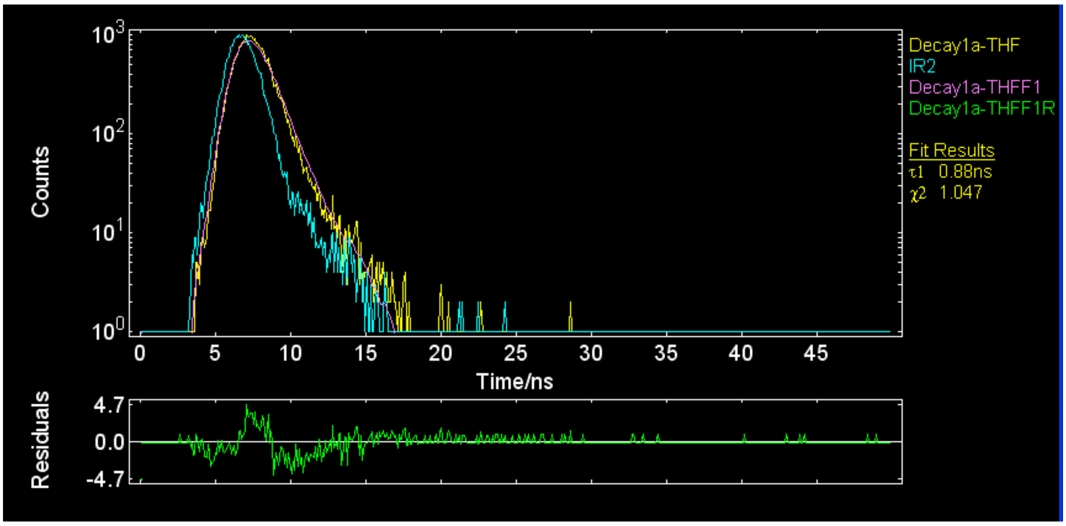


Fig. S12. The fluorescence decay of dye **1a** in tetrahydrofuran excited at 360 nm and measured by single photon counting method whose emission at 435 nm.

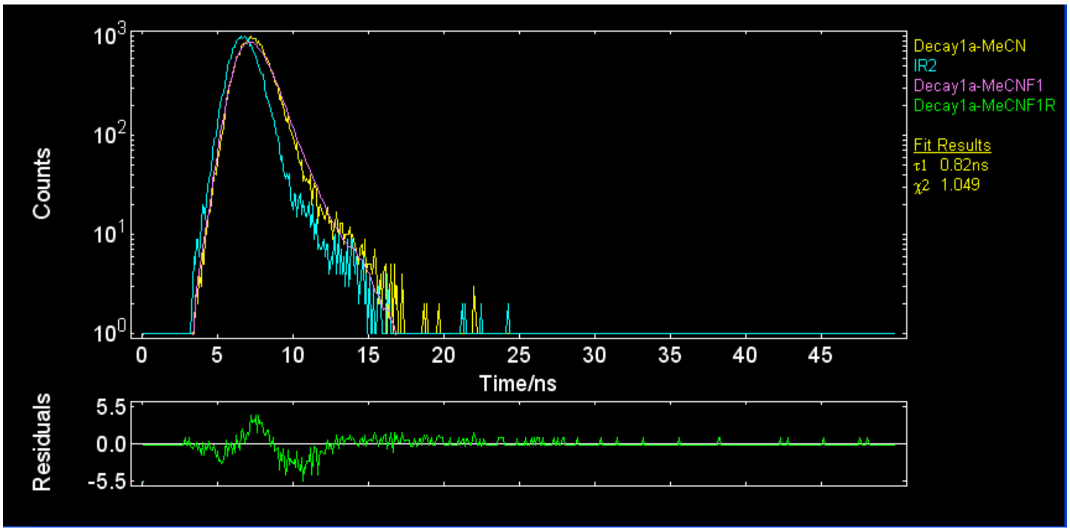


Fig. S13. The fluorescence decay of dye **1a** in acetonitrile excited at 360 nm and measured by single photon counting method whose emission at 435 nm

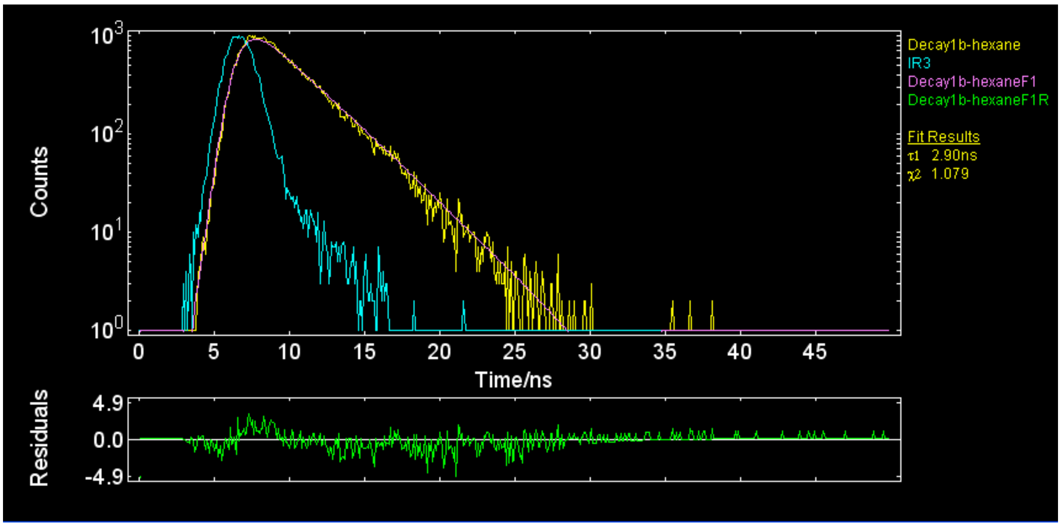


Fig. S14. The fluorescence decay of dye **1b** in hexane excited at 370 nm and measured by single photon counting method whose emission at 455 nm

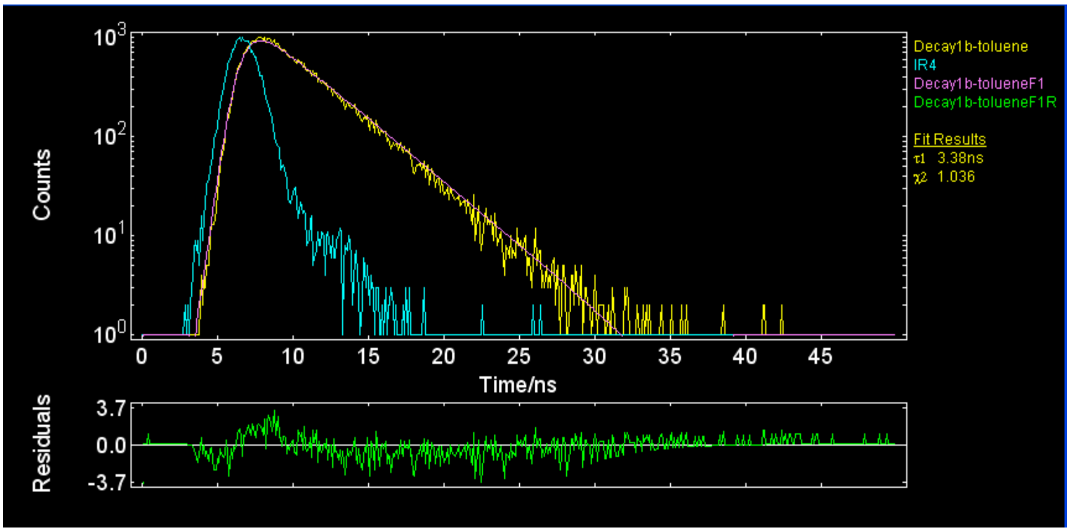


Fig. S15. The fluorescence decay of dye **1b** in toluene excited at 370 nm and measured by single photon counting method whose emission at 480 nm

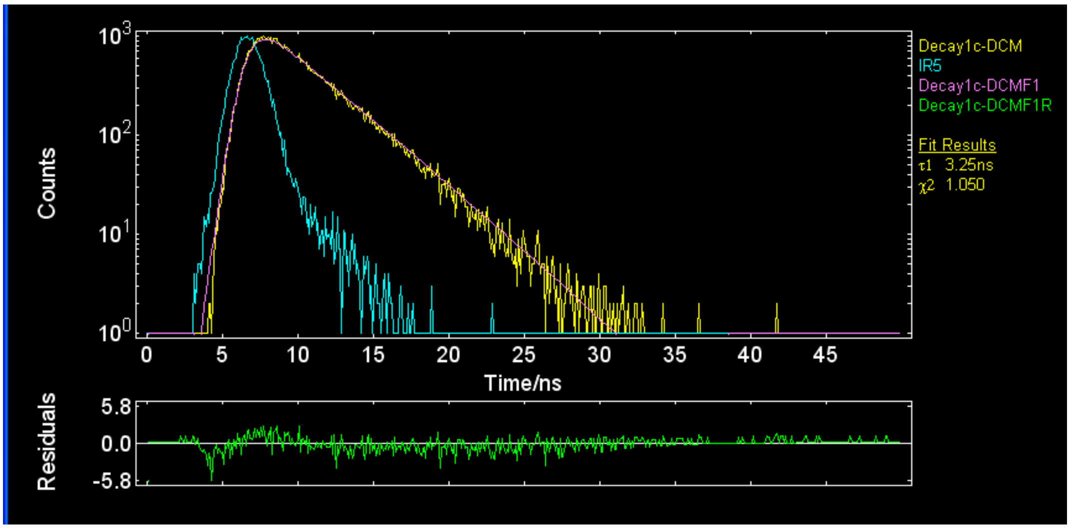


Fig. S16. The fluorescence decay of dye **1b** in dichloromethane excited at 370 nm and measured by single photon counting method whose emission at 480 nm

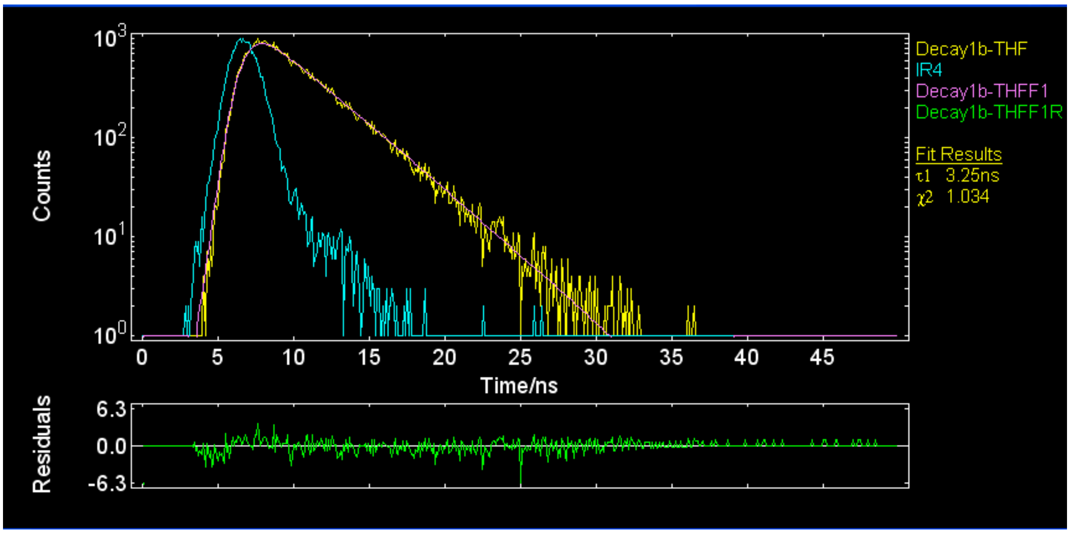


Fig. S17. The fluorescence decay of dye **1b** in tetrahydrofuran excited at 370 nm and measured by single photon counting method whose emission at 480 nm.

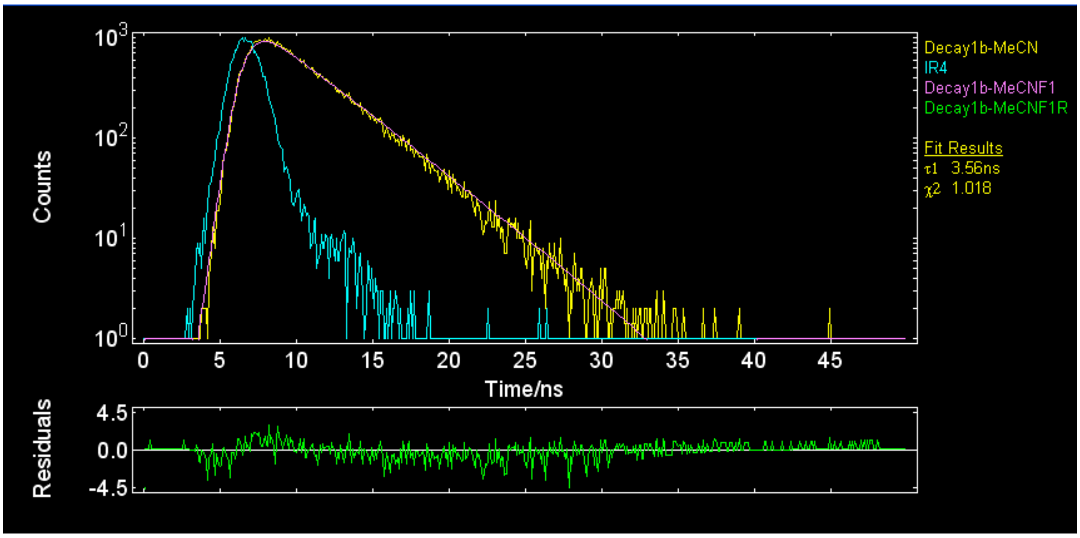


Fig. S18. The fluorescence decay of dye **1b** in acetonitrile excited at 370 nm and measured by single photon counting method whose emission at 480 nm

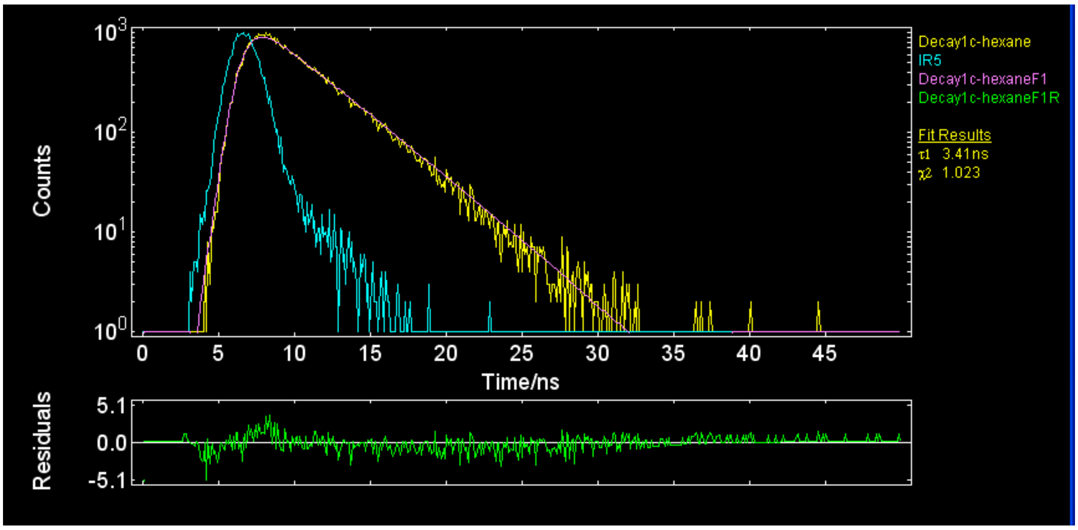


Fig. S19. The fluorescence decay of dye **1c** in hexane excited at 370 nm and measured by single photon counting method whose emission at 469 nm

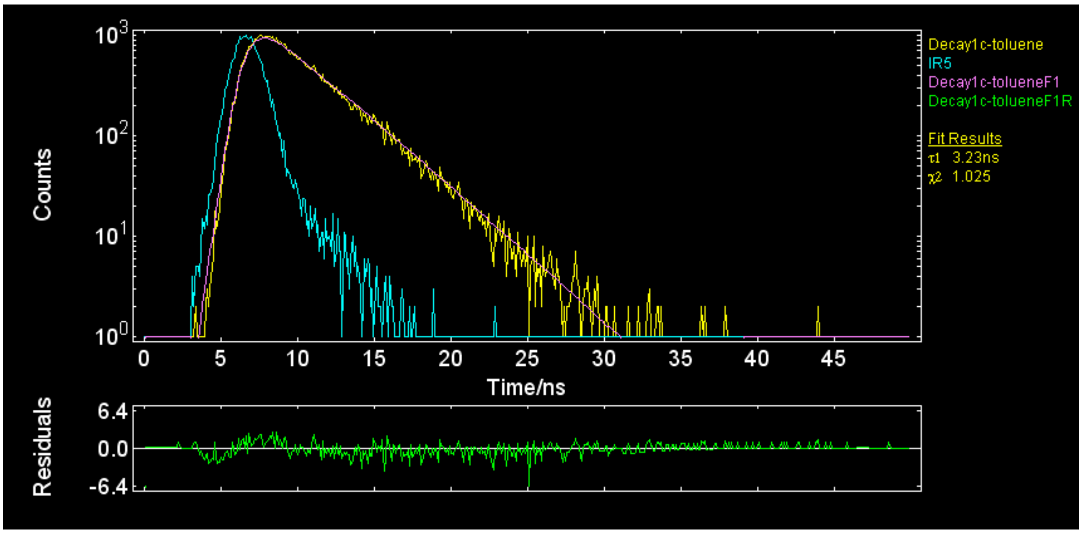


Fig. S20. The fluorescence decay of dye **1c** in toluene excited at 370 nm and measured by single photon counting method whose emission at 500 nm

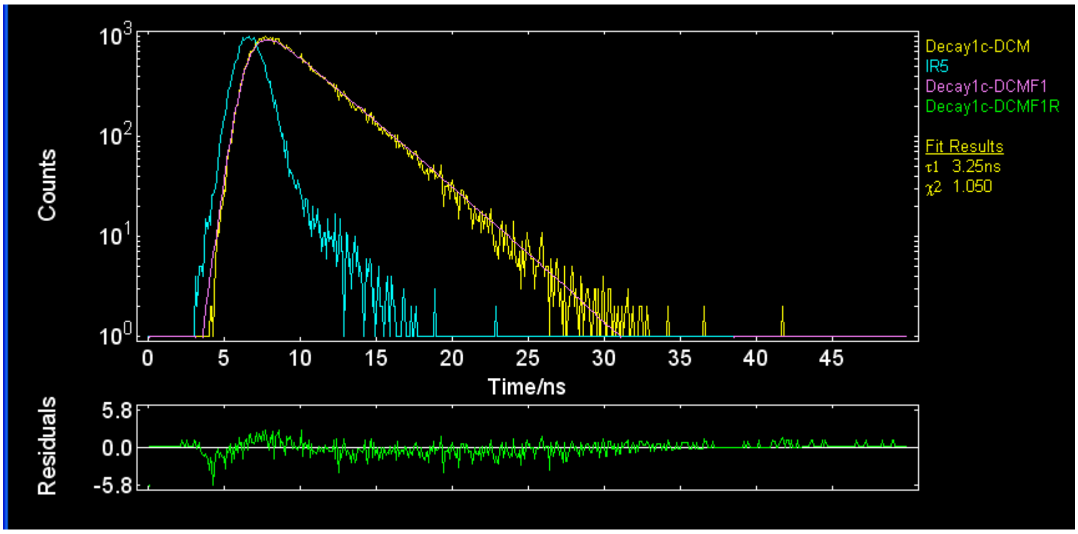


Fig. S21. The fluorescence decay of dye **1c** in dichloromethane excited at 370 nm and measured by single photon counting method whose emission at 500 nm

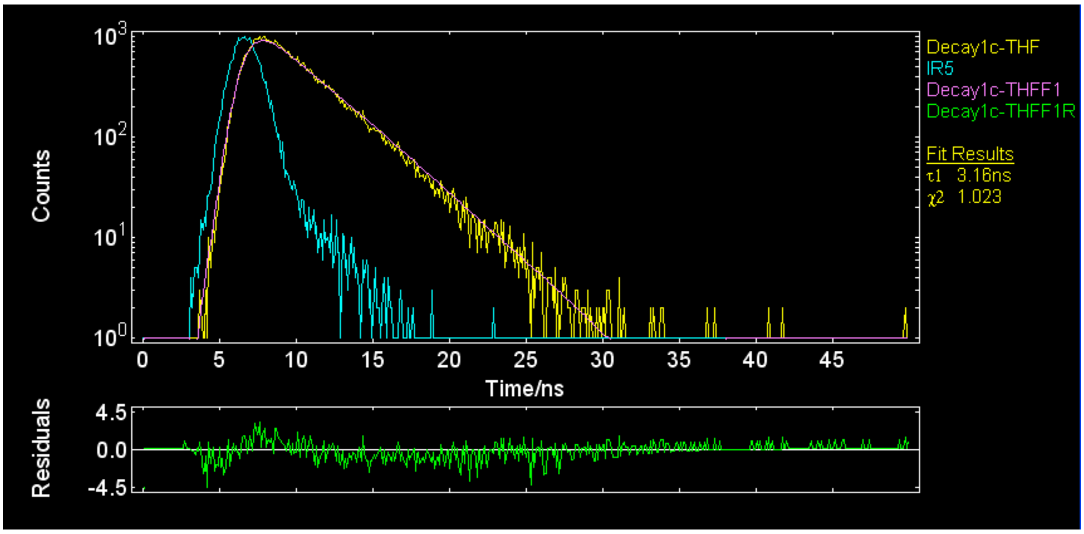


Fig. S22. The fluorescence decay of dye **1c** in tetrahydrofuran excited at 370 nm and measured by single photon counting method whose emission at 500 nm.

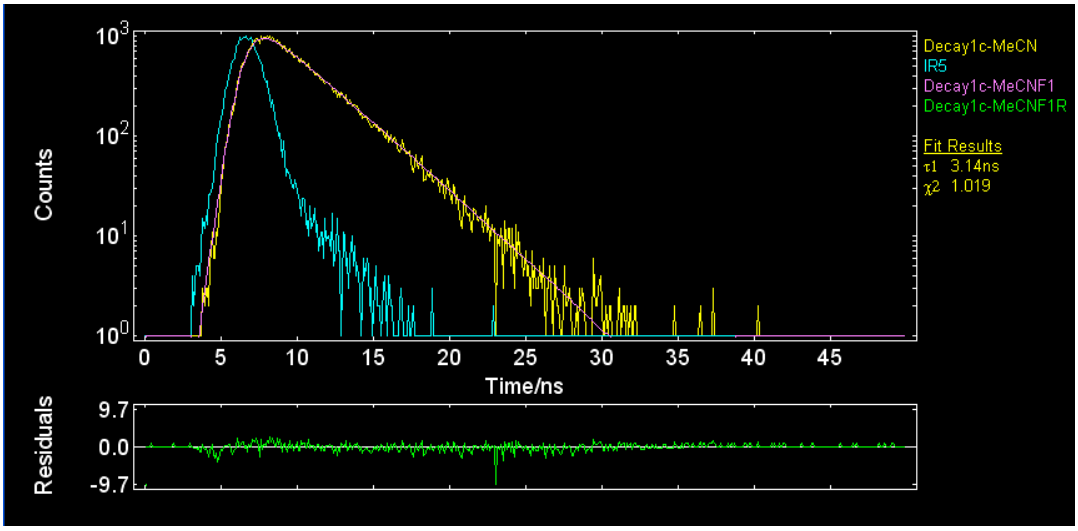


Fig. S23. The fluorescence decay of dye **1c** in acetonitrile excited at 370 nm and measured by single photon counting method whose emission at 500 nm

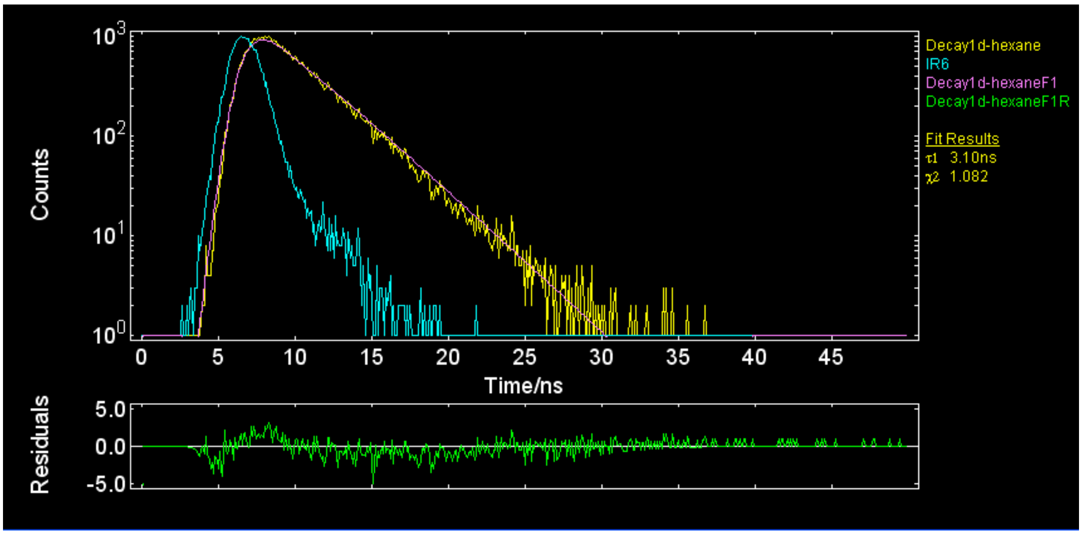


Fig. S24. The fluorescence decay of dye **1d** in hexane excited at 390 nm and measured by single photon counting method whose emission at 520 nm

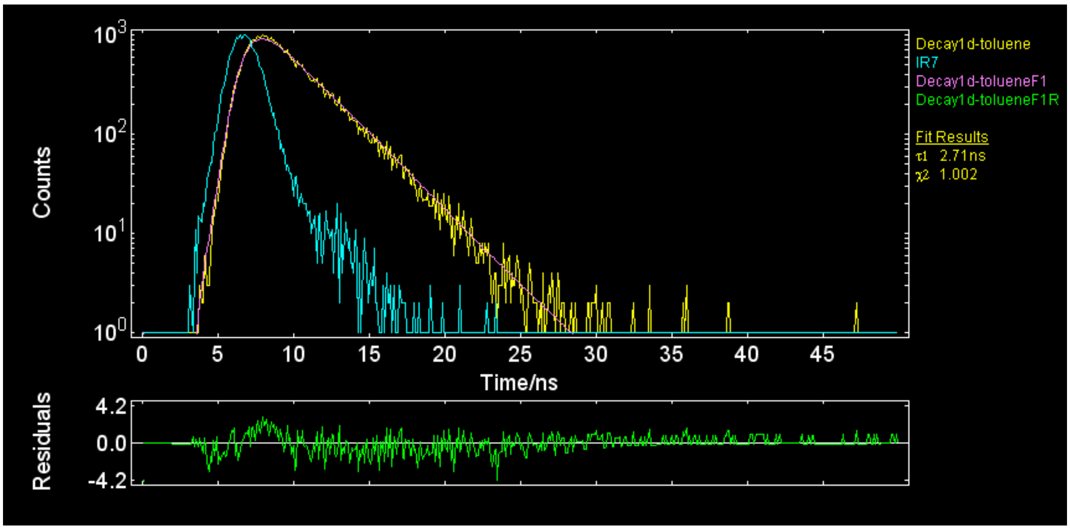


Fig. S25. The fluorescence decay of dye **1d** in toluene excited at 390 nm and measured by single photon counting method whose emission at 524 nm

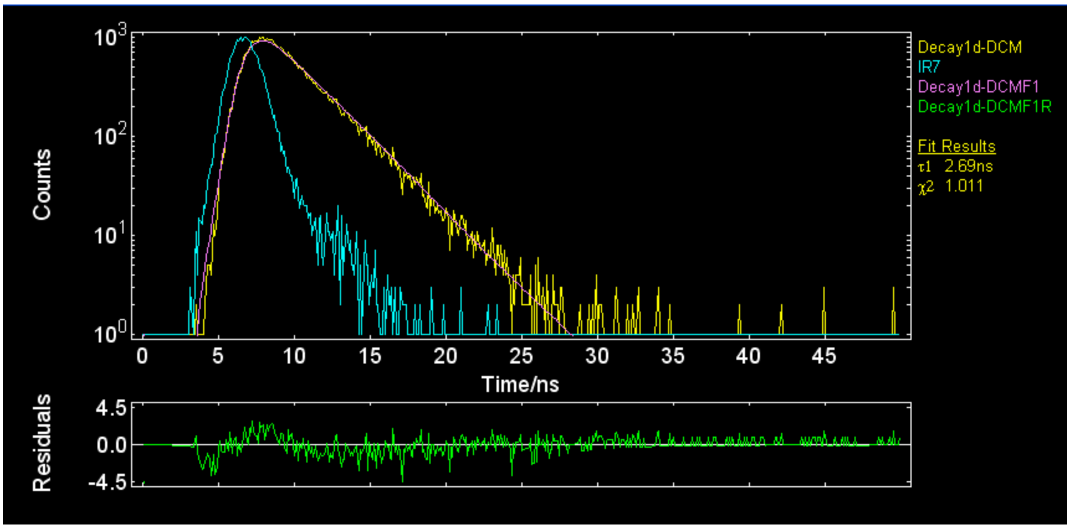


Fig. S26. The fluorescence decay of dye **1d** in dichloromethane excited at 390 nm and measured by single photon counting method whose emission at 540 nm

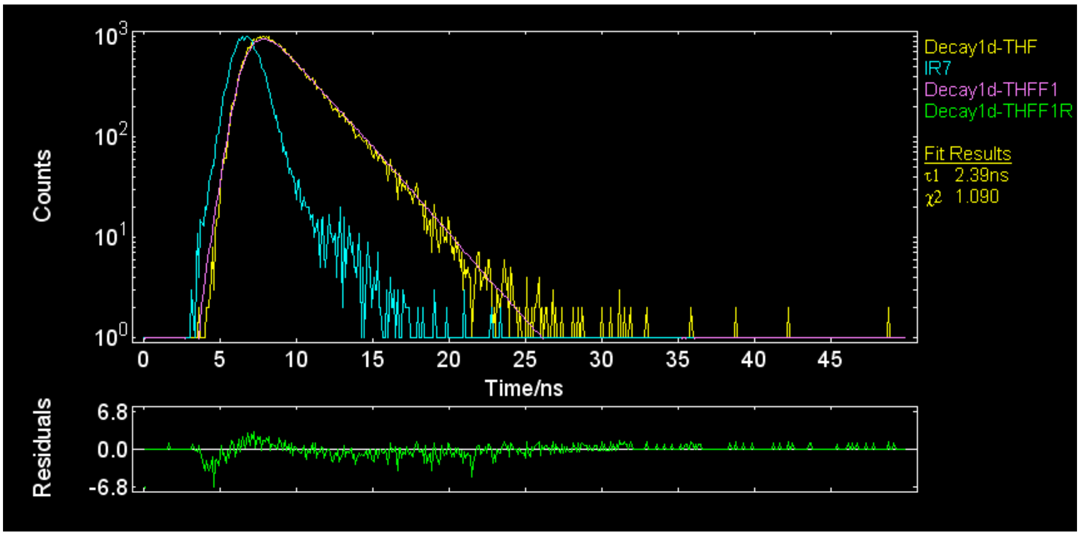


Fig. S27. The fluorescence decay of dye **1d** in tetrahydrofuran excited at 390 nm and measured by single photon counting method whose emission at 540 nm

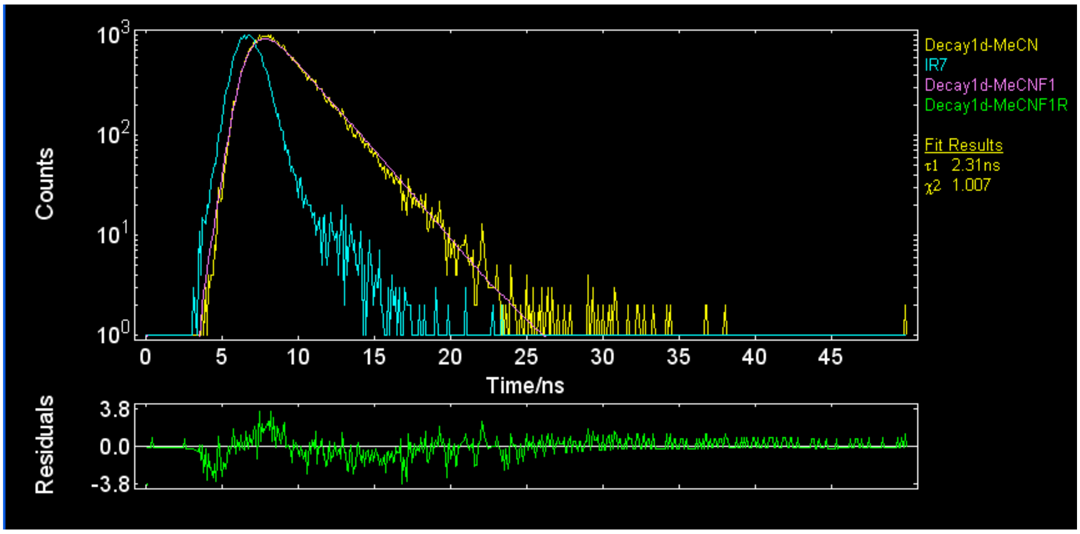


Fig. S28. The fluorescence decay of dye **1d** in acetonitrile excited at 390 nm and measured by single photon counting method whose emission at 560 nm

5. Electrochemical spectra for all compounds

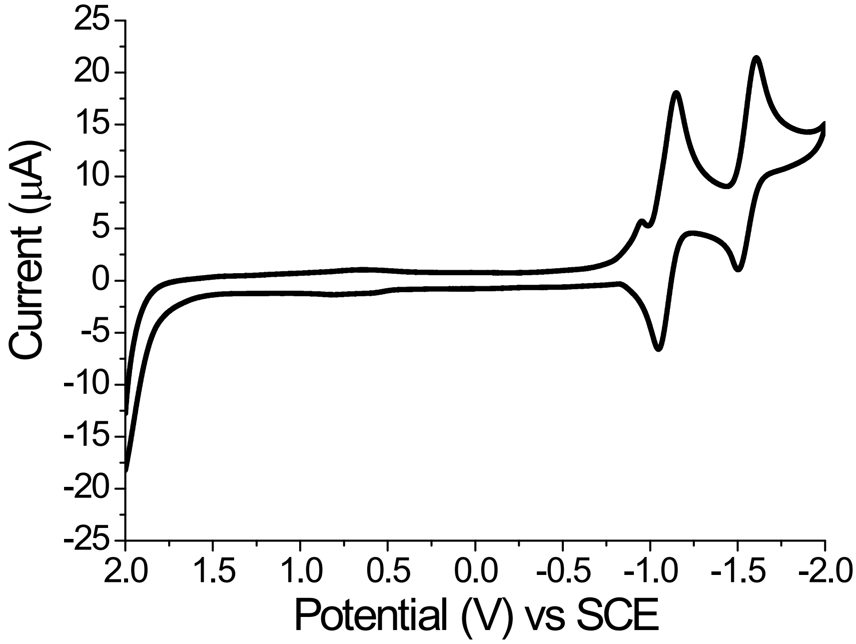


Fig. S29. Cyclic voltammograms of 1mM **1a** measured in dichloromethane solution, containing 0.1 M $TBAPF_6$ as the supporting electrolyte at room temperature. Glassy carbon electrode as a working electrode, and the scan rate at 50 mV s^{-1}.

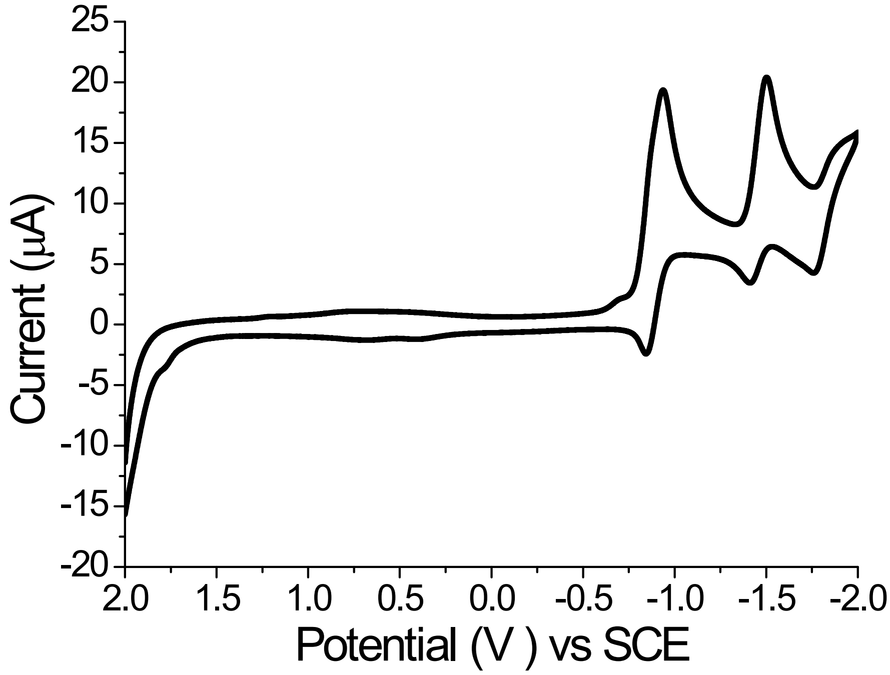


Fig. S30. Cyclic voltammograms of 1mM **1b** measured in dichloromethane solution, containing 0.1 M $TBAPF_6$ as the supporting electrolyte at room temperature. Glassy carbon electrode as a working electrode, and the scan rate at 50 mV s^{-1}.

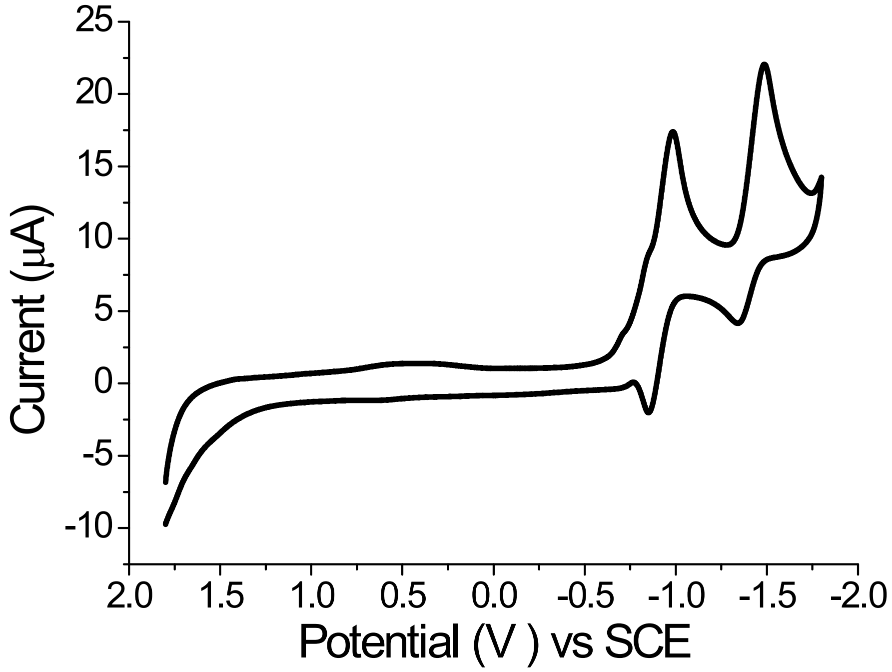


Fig. S31. Cyclic voltammograms of 1mM **1c** measured in dichloromethane solution, containing 0.1 M $TBAPF_6$ as the supporting electrolyte at room temperature. Glassy carbon electrode as a working electrode, and the scan rate at 50 mV s^{-1}.

6. Copies of ^{1}H and ^{13}C NMR spectra

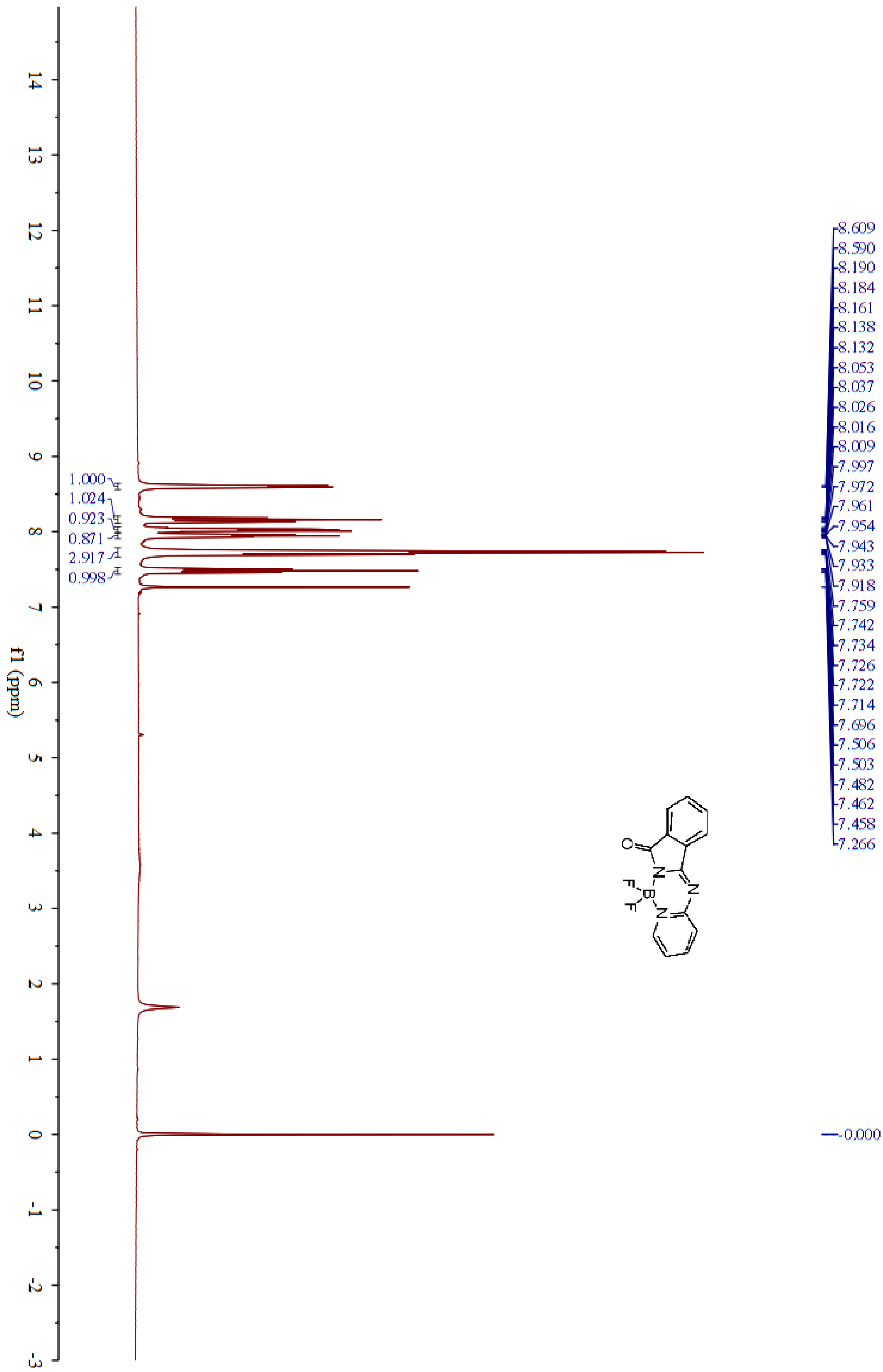


Fig. S32. ^{1}H NMR spectrum of **1a** in $CDCl_3$ solution

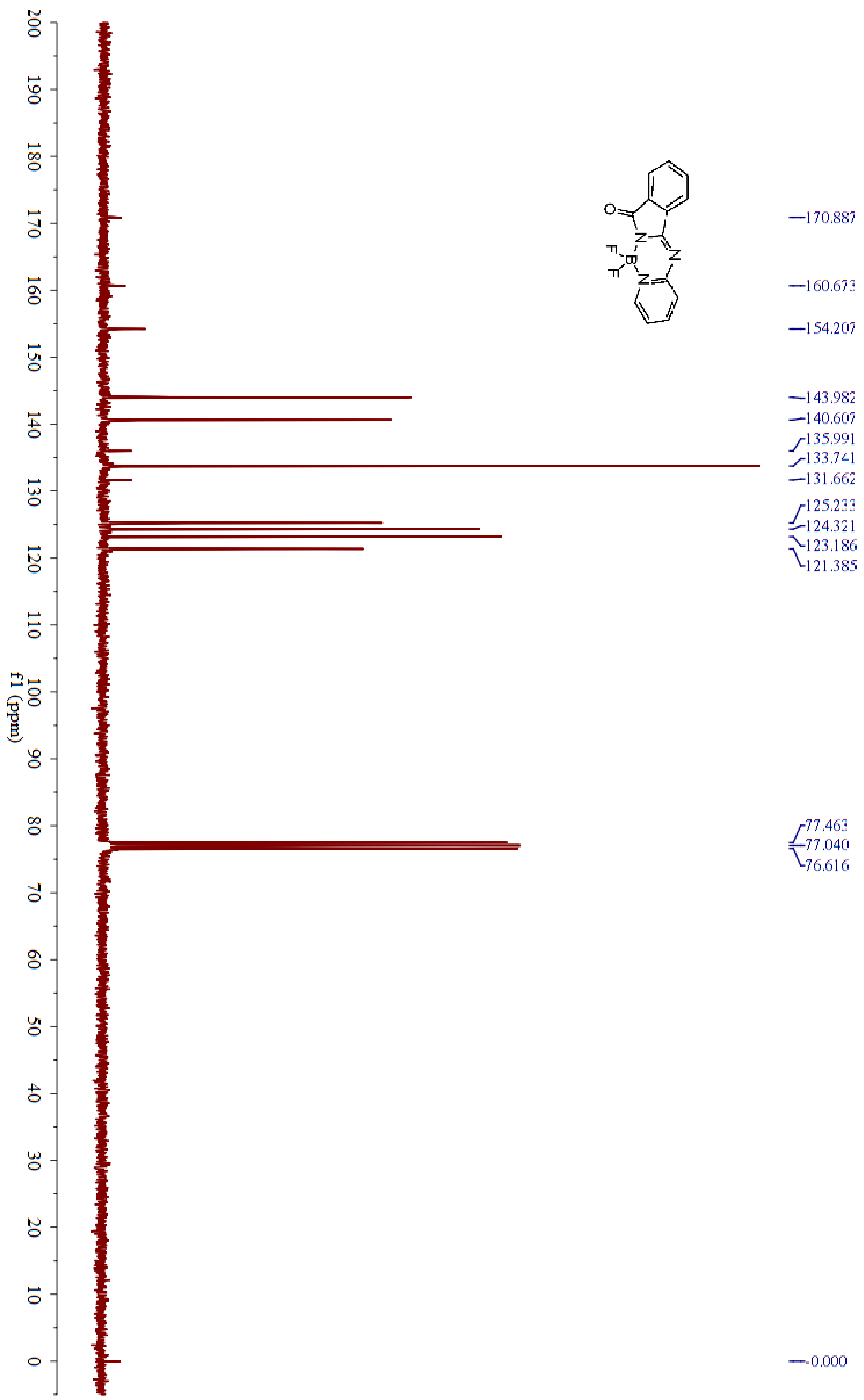


Fig. S33. ^{13}C NMR spectrum of **1a** in $CDCl_3$ solution

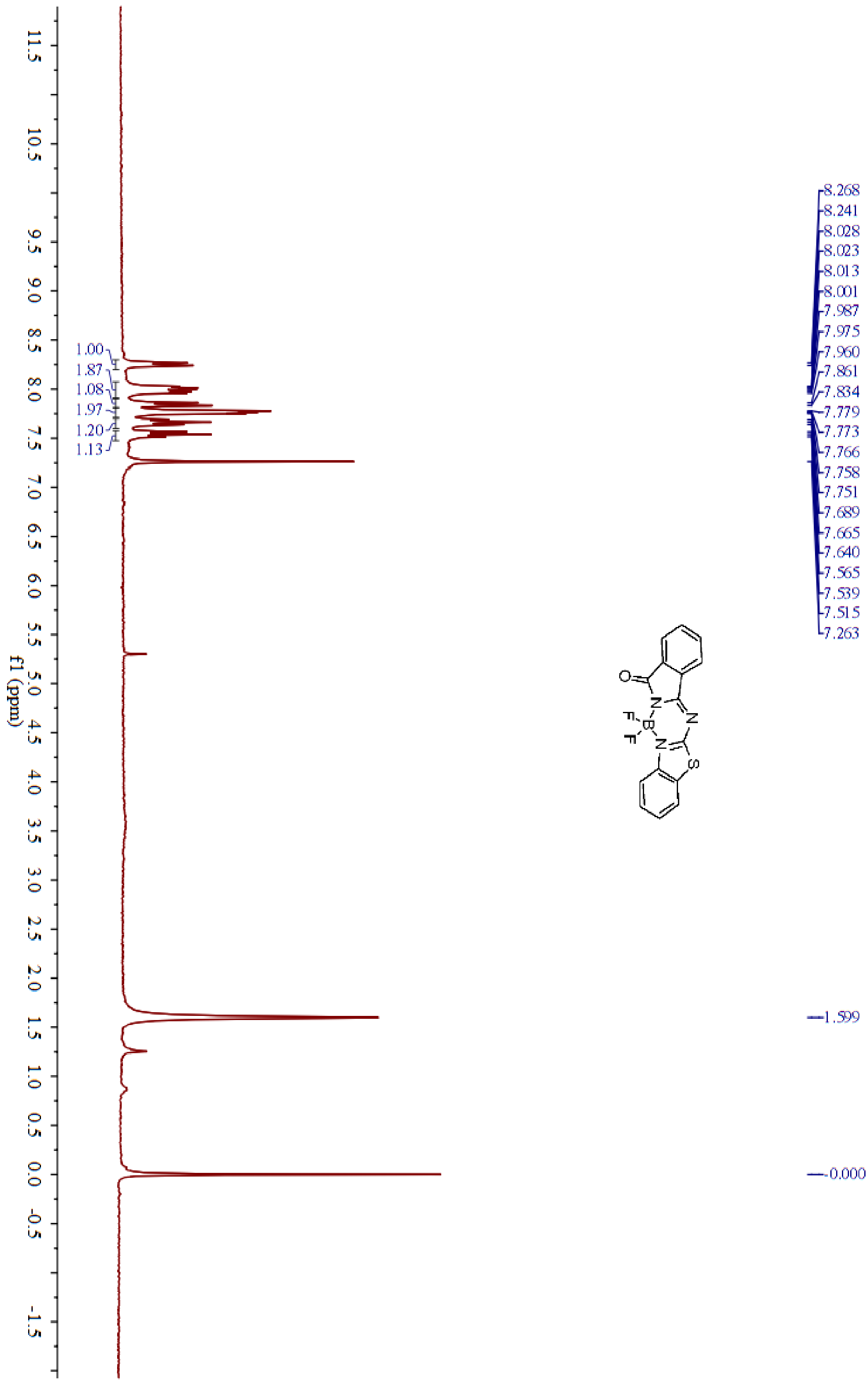


Fig. S34. ^{1}H NMR spectrum of **1b** in $CDCl_3$ solution

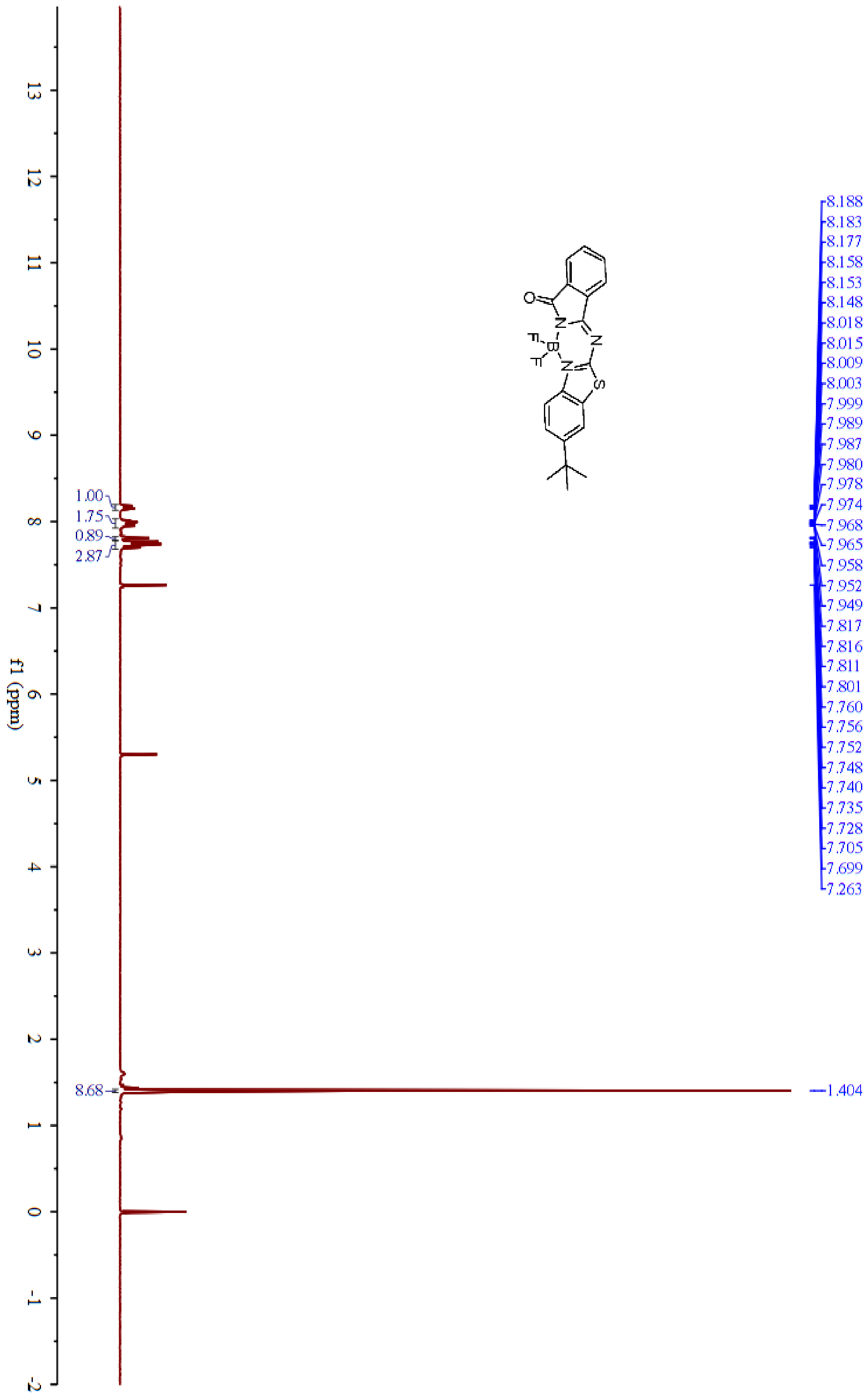


Fig. S35. ^{1}H NMR spectrum of **1c** in $CDCl_3$ solution

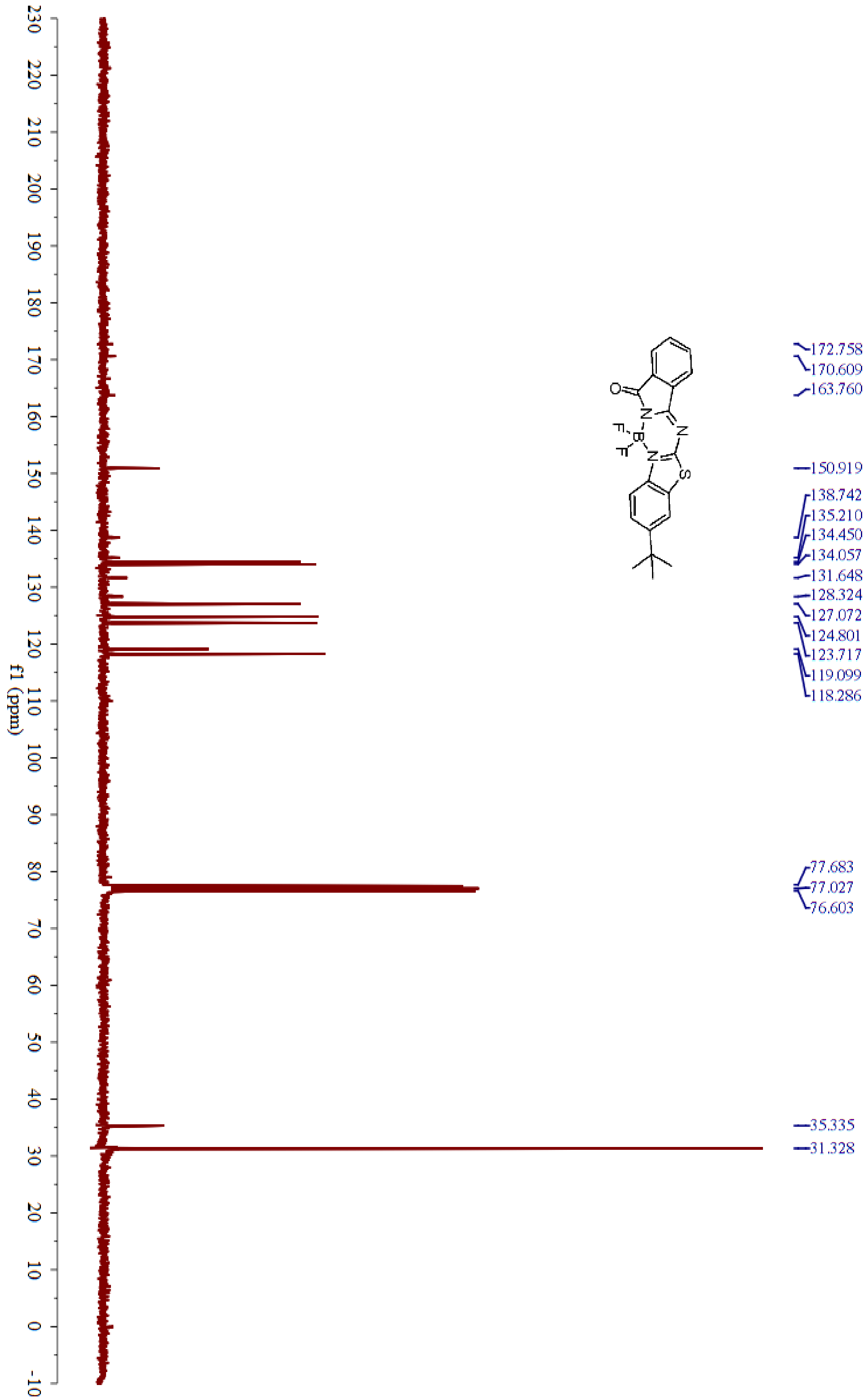


Fig. S36. ^{13}C NMR spectrum of **c** in $CDCl_3$ solution

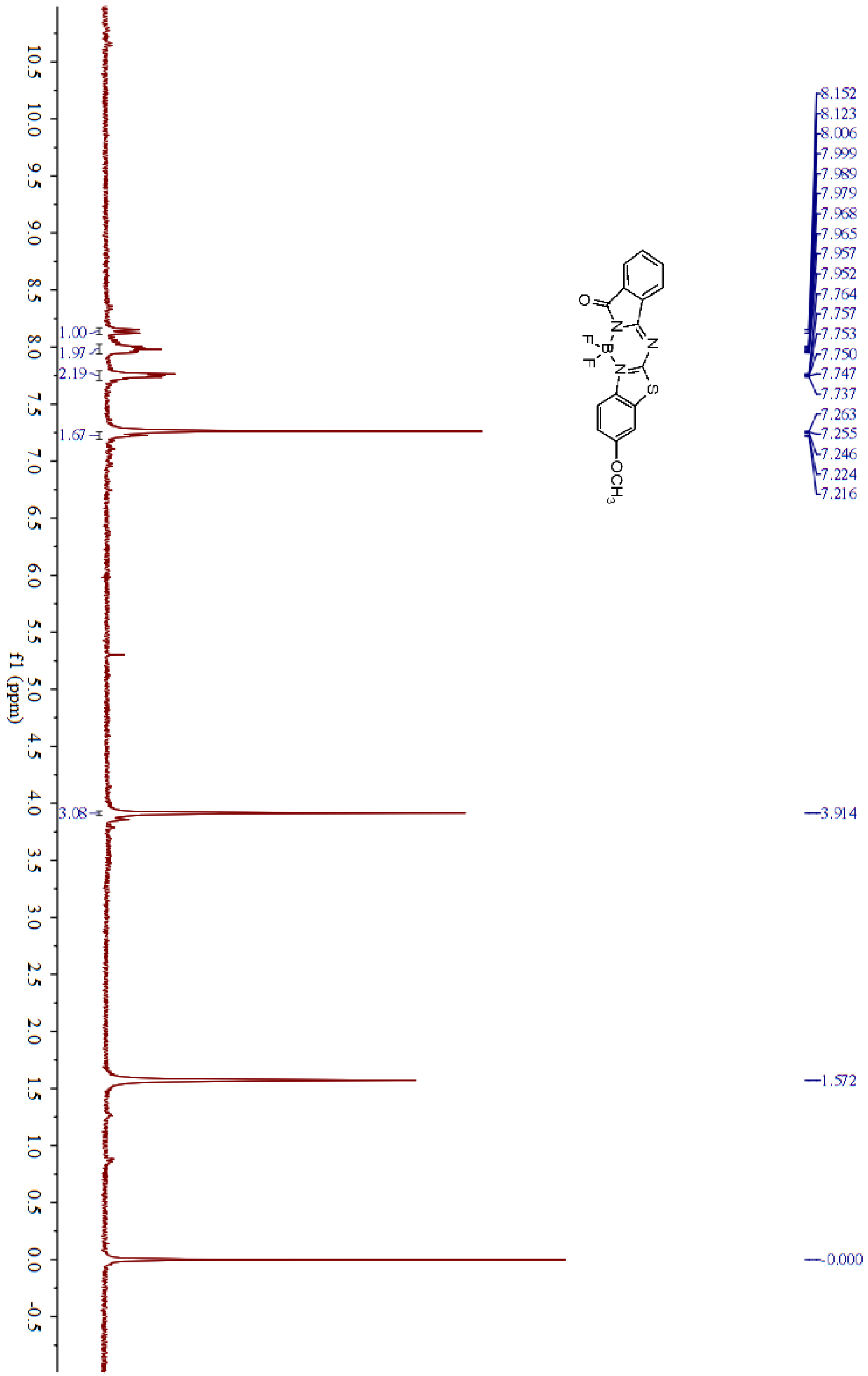
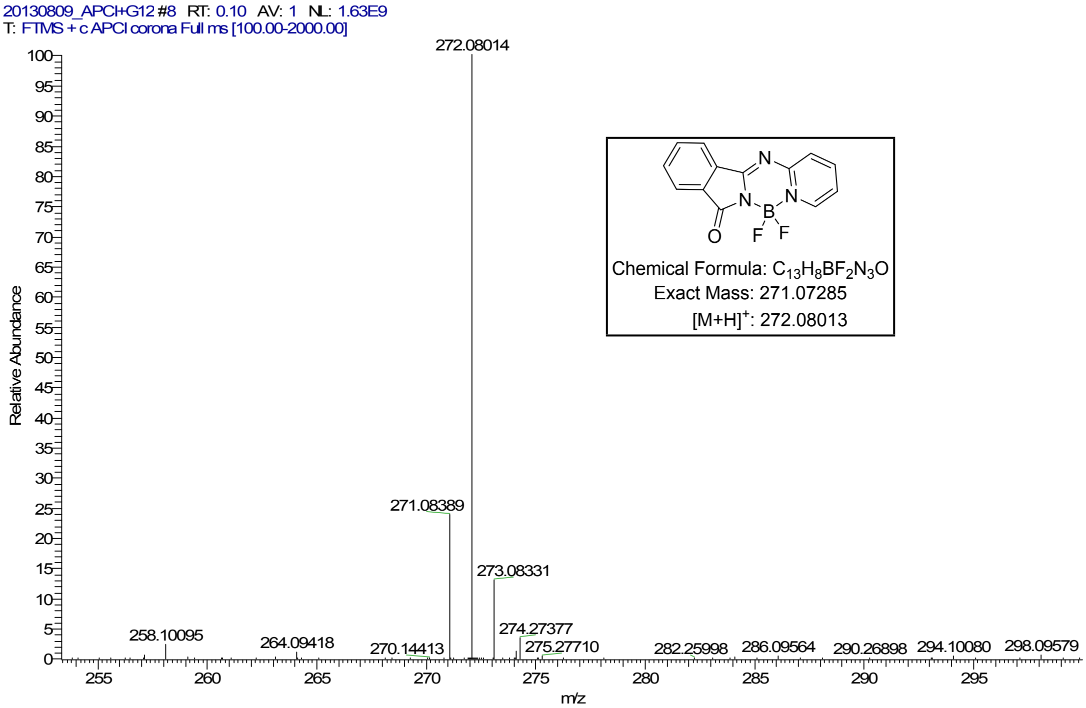
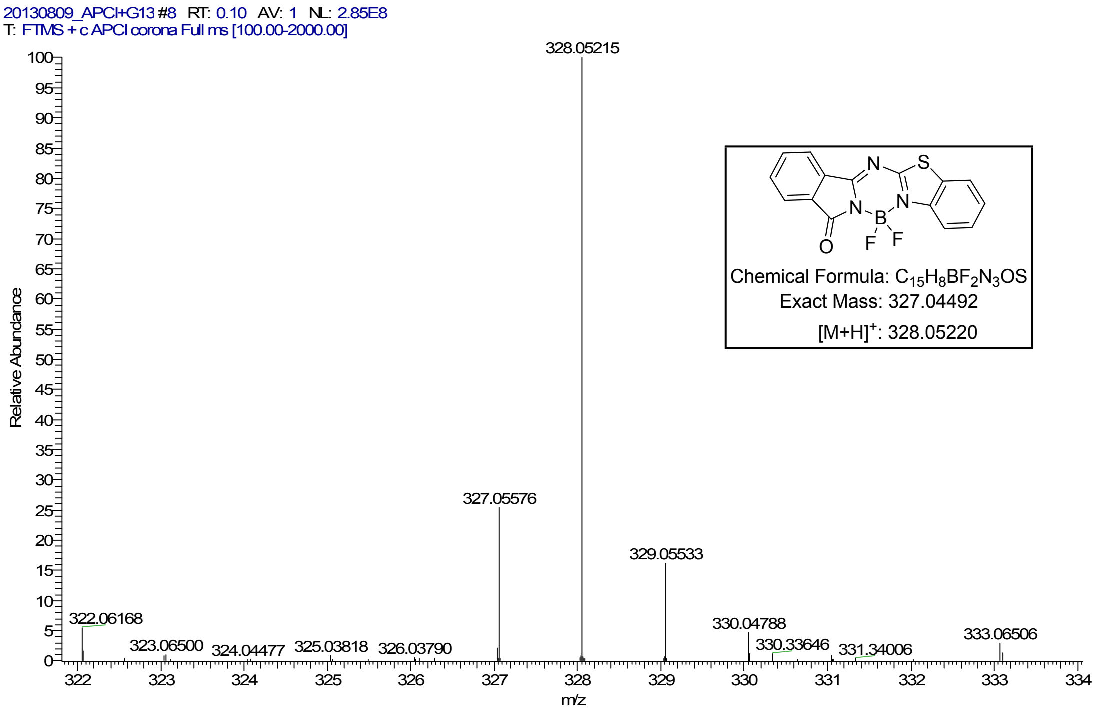


Fig. S37. ^{1}H NMR spectrum of **d** in $CDCl_3$ solution

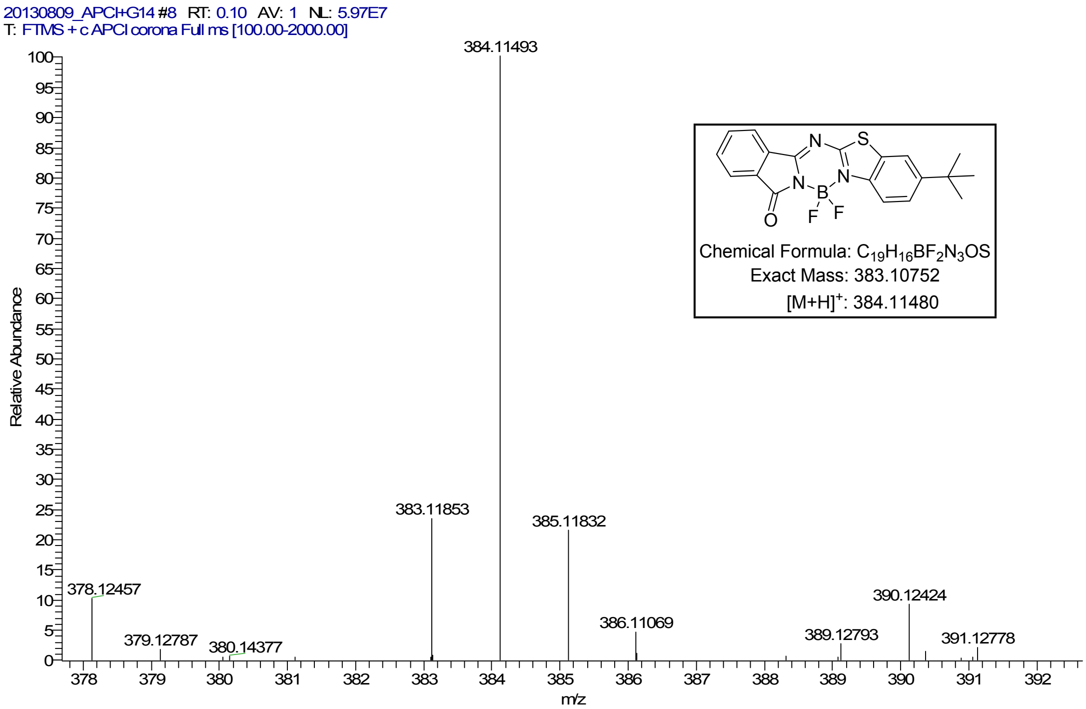
7. High resolution mass spectroscopes for all new compounds



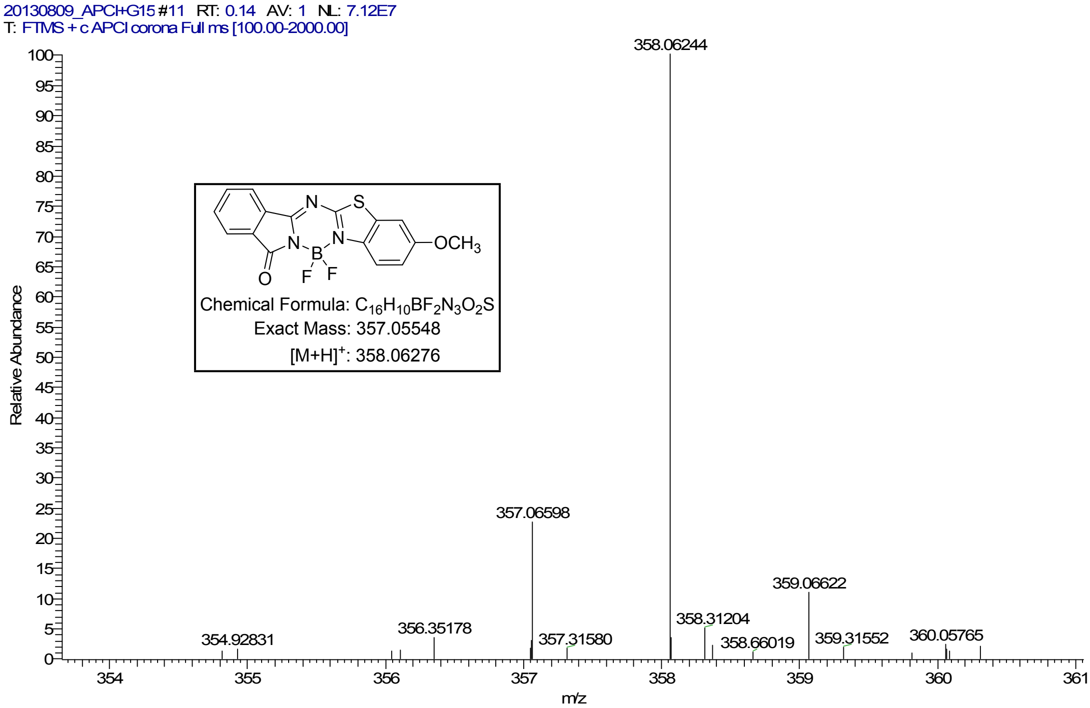
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
258.101	38395448	2.35	258.1009	0.09	C13 H11 N3 B F2
271.0839	3.9E+08	23.89	271.0723	11.59	C13 H8 O N3 B F2
272.0801	1.63E+09	100	272.0801	0.01	C13 H9 O N3 B F2
273.0833	2.13E+08	13.04	273.088	-4.64	C13 H10 O N3 B F2
274.2738	55143160	3.38	274.2461	27.73	C13 H30 O N3 B F



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
322.0617	15226524	5.34	322.08202	-20.34	C15 H14 O N3 F2 S
327.0558	72094888	25.26	327.04437	11.38	C15 H8 O N3 B F2 S
328.0522	2.85E+08		328.0522	-0.04	C15 H9 O N3 B F2 S
329.0553	45590876	15.98	329.06002	-4.69	C15 H10 O N3 B F2 S
330.0479	12984702	4.55	330.06785	-19.96	C15 H11 O N3 B F2 S



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
378.1246	6013933	10.07	378.14462	-20.04	C19 H22 O N3 F2 S
383.1185	13930802	23.32	383.10697	11.56	C19 H16 O N3 B F2 S
384.1149	59734448	100	384.1148	0.13	C19 H17 O N3 B F2 S
385.1183	12828146	21.48	385.12262	-4.3	C19 H18 O N3 B F2 S
390.1242	5503058	9.21	390.16175	-37.51	C19 H23 O N3 B F2 S



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
356.3518	2462844	3.46	356.25417	97.61	C16 H36 O N3 F2 S
357.066	16112895	22.62	357.05494	11.04	C16 H10 O2 N3 B F2 S
358.0624	71245960	100	358.06276	-0.32	C16 H11 O2 N3 B F2 S
358.312	3563560	5	358.24601	66.04	C16 H36 O2 N2 F2 S
359.0662	7839142	11	359.07059	-4.36	C16 H12 O2 N3 B F2 S