Supporting information for

One-pot Efficient Synthesis of PyrrolylBODIPY Dyes from Pyrrole and Acyl Chloride

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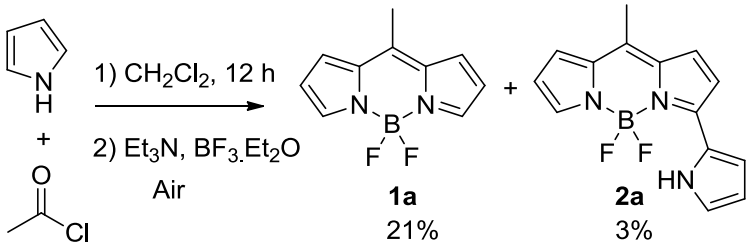
1. Experimental Section



Scheme S1. Initial synthesis of BODIPY **1a** and 3-pyrrolylBODIPY **2a** via pyrrole and acetyl chloride in dichloromethane at room temperature

General: Reagents and solvents were used as received from commercial suppliers unless noted otherwise. All reactions were performed in oven-dried or flame-dried glassware unless otherwise stated, and were monitored by TLC using 0.25 mm silica gel plates with UV indicator (60F-254). ^{1}H and ^{13}C NMR were recorded on a 300 MHz NMR spectrometer at room temperature. Chemical shifts (δ) are given in ppm relative to $CDCl_3$ (7.26 ppm for ^{1}H and 77 ppm for ^{13}C) or to internal TMS. High-resolution mass spectra (HRMS) were obtained using APCI-TOF in positive mode.

UV-visible absorption spectra and Fluorescence emission spectra were recorded on a commercial spectrophotometer (190-1100 nm scan range, Shimadzu UV-2450 and Hitachi F-4500). Relative fluorescence quantum efficiencies of BODIPY derivatives were obtained by comparing the areas under the corrected emission spectrum of the test sample in various solvents with fluorescein (Φ = 0.90 in 0.1 N NaOH aqueous solution) or Rhodamin B (Φ = 0.49 in EtOH).[1] Non-degassed, spectroscopic grade solvents and a 10 mm quartz cuvette were used. Dilute solutions ($0.01<A<0.05$) were used to minimize the reabsorption effects. Quantum yields were determined using the following equation[2]:

$$\Phi_X = \Phi_S (I_X/I_S) (A_S/A_X) (n_X/n_S)^2$$

Where Φ_S stands for the reported quantum yield of the standard, I stands for the integrated emission spectra, A stands for the absorbance at the excitation wavelength and *n* stands for the refractive index of the solvent being used. X subscript stands for the test

sample, and S subscript stands for the standard. Fluorescence lifetimes were measured on a combined steady-state lifetime fluorescence spectrometer and the fluorescence lifetimes were obtained from deconvolution and distribution lifetime analysis. Details of the instrumentation and experimental procedures used have been described elsewhere.[3] When the fluorescence decays were single exponential, the rate constants of radiative (k_f) and nonradiative (k_{nr}) deactivation were calculated from the measured fluorescence quantum yield and fluorescence lifetime using the following equation:

$k_f = \phi/\tau$ and $k_{nr} = (1- \phi)/\tau$.

Crystals of BODIPYs **1a**, **2a** and **2i** suitable for X-ray analysis were obtained by slow evaporation of their dichloromethane solutions. The vial containing this solution was placed, loosely capped, to promote the crystallization. The structure was solved by the direct method using the SHELXS-974 program and refined by the least-squares method on F^2, SHELXL-97, [4] incorporated in SHELXTL V5.10.[5] CCDC- 881436 (**1a**), 881437 (**2a**), and 881438 (**2i**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Fluorescence Imaging: Human gastric cancer SGC7901 cells were cultured in Dulbecco's Modified Eagle Medium (DMEM) supplemented with 10% fetal bovine serum, penicillin (100 U/ml), streptomycin sulfate (100 μg/ml), and maintained at 37°C with 5% CO_2 in a humidified incubator. One day before imaging, cells were seeded in 6-well flat-bottomed plates in an atmosphere of 5% CO_2, 95% air at 37 ℃. Fluorescence imaging of intracellular dyes was observed under OLYMPUS-IX71 inverted fluorescence microscope and imaged using FITC channel or TRITC channel. The cells were treated with 10 μM of dyes in culture media for 30 min at 37 ℃ with 5% CO_2 in a humidified incubator. Fluorescence imaging was then carried out after washing the cells with the

phosphate buffered saline. For the control experiment, the cells without treatment of dyes did not show any noticeable fluorescence under the same conditions.

General procedure for the synthesis of BODIPYs 2: To freshly distilled pyrrole (10 mmol) in dried 1,2-dichloroethane (1.5 mL) was dropwisely added acyl chloride (1 mmol in 0.5 mL 1,2-dichloroethane)**.** The reaction mixture was stirred at room temperature for 6 h under oxygen atmosphere. Triethylamine (0.8 mL) and $BF_3.Et_2O$ (2 mL) were then added, and the reaction mixture was heated at 50 ℃ for 10 h under oxygen atmosphere. The reaction mixture was concentrated in vacuum, and diluted with dichloromethane. Organic layer was washed with water, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v). The first to vivid pink band was collected to give BODIPYs **2**.

2a: 52 mg**,** yield 19%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.61 (s, 1H), 7.32 (d, *J* = 3.0 Hz, 1H), 7.17 (s, 1H), 7.01 (s, 2H), 6.90 (d, *J* = 3.0 Hz, 1H), 6.47 (s, 1H), 6.38 (s, 1H), 2.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.2, 137.9, 137.0, 136.2, 133.9, 130.0, 125.9, 123.5, 121.9, 120.4, 118.1, 115.5, 111.4, 15.6. HRMS (APCI) calcd. for $C_{14}H_{13}BF_2N_3$ $[M+H]^+$: 272.1165, found 272.1167.

2b: 63 mg, yield 21%. ^{1}H NMR(300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.62 (s, 1H), 7.32 (s, 1H), 7.18 (s, 1H), 7.00 (s, 2H), 6.91 (d, *J* = 3.0 Hz, 1H), 6.48 (s, 1H), 6.39 (s, 1H), 2.84 (t, *J* = 6.0 Hz, 2H), 1.81 (m, 2H), 1.05 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.1, 142.1, 137.8, 136.2, 133.5, 129.9, 125.9, 123.6, 121.8, 120.4, 118.0, 115.5, 111.4, 32.5, 26.6, 14.5. HRMS(APCI) calcd. for $C_{16}H_{17}BF_2N_3$ $[M+H]^+$: 300.1484, found 300.1487.

2c: 57 mg, yield 16%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.61 (s, 1H), 7.31 (d, *J* = 3.0 Hz, 1H), 7.17 (s, 1H), 7.01 (s, 2H), 6.91 (s, 1H), 6.47 (s, 1H), 6.38 (s, 1H), 2.85 (t, *J* = 7.5 Hz, 2H), 1.75 (d, *J* = 6.0 Hz, 2H), 1.35 (br, 8H), 0.88 (d, *J* = 6.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 150.0, 141.5, 136.6, 135.1, 132.4, 128.7, 124.8, 122.5, 120.7, 119.3, 116.9, 114.5, 110.4, 32.4, 30.7, 29.7, 28.7, 28.0, 21.6, 13.1. HRMS(APCI) calcd. for $C_{20}H_{25}BF_2N_3$ $[M+H]^+$: 356.2110, found 356.2111.

2d: 66 mg, yield 16%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.49 (s, 1H), 7.60 (s, 1H), 7.31 (d, *J* = 3.0 Hz, 1H), 7.16 (s, 1H), 7.00 (s, 2H), 6.90 (d, *J* = 6.0 Hz, 1H), 6.47 (s, 1H), 6.38 (s, 1H), 2.85 (t, *J* = 7.5 Hz, 2H), 1.78-1.74 (m, 2H), 1.35 (br, 16H), 0.87 (d, *J* = 7.5 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.0, 142.6, 137.7, 136.2, 133.5, 129.8, 125.8, 123.6, 121.7, 120.4, 117.9, 115.5, 111.4, 33.4, 31.9, 30.7, 30.0, 29.6, 29.5, 29.4, 29.3, 22.7, 14.1. HRMS(APCI) calcd. for $C_{24}H_{33}BF_2N_3$ $[M+H]^+$: 412.2736, found 412.2727.

2e: 75 mg, yield 16%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.60 (s, 1H), 7.31 (s, 1H), 7.16 (s, 1H), 7.00 (s, 2H), 6.91 (s, 1H), 6.47 (s, 1H), 6.38 (s, 1H), 2.84 (t, *J* = 7.5 Hz, 2H), 1.75 (s, 2H), 1.34 (br, 24H), 0.88 (s, 3H); ^{13}C NMR (75 MHz, CDCl3) δ 150.0, 141.5, 136.6, 135.1, 132.4, 128.7, 124.8, 122.5, 120.7, 119.3, 116.9, 114.5, 110.4, 32.4, 30.9, 29.7, 29.0, 28.6, 28.5, 28.3, 21.7, 13.1. HRMS(APCI) calcd. for $C_{28}H_{41}BF_2N_3$ $[M+H]^+$: 468.3362, found 468.3355.

2f: 90 mg, yield 27%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.60 (s, 1H), 7.39 (s, 1H), 7.19 (s, 1H), 7.03 (s, 2H), 6.94 (d, *J* = 3.0 Hz, 1H), 6.48 (s, 1H), 6.39 (s, 1H), 3.62 (s, 2H), 3.06 (s, 2H), 2.23 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.5, 138.5, 136.9, 135.3, 132.2, 128.9, 125.3, 122.4, 120.6, 119.9, 117.6, 114.7, 110.6, 43.2, 34.1, 26.2. HRMS(APCI) calcd. for $C_{16}H_{16}BClF_2N_3$ $[M+H]^+$: 334.1094, found 334.1096.

2g: 89 mg, yield 22%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.47 (s, 1H), 7.58 (s, 1H), 7.25 (s, 1H), 7.14 (s, 1H), 6.97 (s, 2H), 6.87 (s, 1H), 6.44 (s), 6.35 (s, 1H), 3.37 (s, 2H), 2.82 (s, 2H), 1.86 (s, 2H), 1.75 (s, 2H), 1.54 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.2, 141.6, 137.6, 136.2, 133.3, 129.7, 126.0, 123.5, 121.6, 120.6, 118.2, 115.6, 111.5, 33.4, 32.4, 30.4, 29.7, 28.5. HRMS(APCI) calcd. for $C_{18}H_{20}B^{79}BrF_2N_3$ $[M+H]^+$: 406.0896, found 406.0893; HRMS(APCI) calcd. for $C_{18}H_{20}B^{81}BrF_2N_3$ $[M+H]^+$: 408.0876, found 408.0874;

HRMS(APCI) calcd. for $C_{18}H_{19}B^{79}BrFN_3$ $[M-F]^+$: 386.0834, found 386.0831; HRMS(APCI) calcd. for $C_{18}H_{20}B^{81}BrF_2N_3$ $[M-F]^+$: 388.0814, found 388.0815.

2h: 78 mg, yield 21%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.49 (s, 1H), 7.60 (s, 1H), 7.30 (s, 1H), 7.17 (s, 1H), 7.00 (s, 2H), 6.90 (s, 1H), 6.47 (s, 1H), 6.38 (s, 1H), 3.67 (s, 3H), 2.86 (s, 2H), 2.36 (s, 2H), 1.78 (s, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.6, 151.2, 141.4, 137.7, 136.2, 133.3, 129.8, 126.0, 123.5, 121.6, 120.6, 118.2, 115.6, 111.5, 51.6, 33.6, 32.5, 30.2, 25.1. HRMS(APCI) calcd. for $C_{19}H_{21}BF_2N_3O_2$ $[M+H]^+$: 372.1689, found 372.1686. HRMS(EI) calcd. for $C_{19}H_{20}BFN_3O_2$ $[M-F]^+$: 352.1627, found 352.1630.

2i: 57 mg, yield 17%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.57 (s, 1H), 7.70 (s, 1H), 7.53 (br, 5H), 7.22 (s, 1H), 7.04 (s, 1H), 6.93 (d, J = 7.5 Hz, 2H), 6.67 (s, 1H), 6.47 (s, 1H), 6.41 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.6, 144.1, 139.7, 136.7, 134.5, 133.4, 133.2, 130.4, 129.9, 128.3, 126.5, 125.1, 123.6, 121.1, 118.6, 116.0, 111.7. HRMS(APCI) calcd. for $C_{19}H_{15}BF_2N_3$ $[M+H]^+$: 334.1327, found 334.1326.

2j: 60 mg, yield 16%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.56 (s, 1H), 7.65 (s, 1H), 7.20 (s, 1H), 7.01-6.95 (br, 3H), 6.84 (s, 1H), 6.67 (s, 1H), 6.39 (s, 3H), 2.36 (s, 3H), 2.11 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.7, 139.3, 138.4, 138.0, 136.8, 136.7, 133.4, 131.8, 130.3, 128.1, 126.4, 123.8, 123.7, 121.1, 118.5, 116.0, 111.7, 21.2, 20.0. HRMS calcd. for $C_{22}H_{21}BF_2N_3$ $[M+H]^+$: 376.1797, found 376.1795.

2k: 119 mg, yield 19%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.69 (s, 1H), 7.62 (s, 1H), 7.36 (s, 2H), 7.22 (s, 1H), 7.06 (d, J = 5.1 Hz), 6.50 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.3, 137.1, 133.2, 133.1, 133.0, 130.2, 129.7, 125.1, 124.4, 123.5, 122.9, 116.8, 113.2. HRMS(EI) calcd. for $C_{20}H_{10}BF_{17}N_3$ $[M+H]^+$: 626.0691, found 626.0681; HRMS(EI) calcd. for $C_{20}H_9BF_{16}N_3$ $[M-F]^+$: 606.0629, found 606.0618.

General procedure for the synthesis of BODIPYs 1: To freshly distilled pyrrole (7 mmol) in dried dichloroethane (100 mL) was dropwisely added acyl chloride (3.5 mmol)**.** The reaction mixture was stirred at room temperature for 12 h under argon. Then

triethylamine (3 mL) and $BF_3.Et_2O$ (8 mL) were then added at ice cold bath, and the reaction mixture was stirred at room temperature for 2 h. The reaction mixture was washed with water, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1, v/v) and the greenish yellow band was collected to give BODIPYs **1**.

1a: 238 mg, yield 33%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (s, 2H), 7.28 (s, 2H), 6.52 (s, 1H), 2.61 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.0, 134.4, 135.5, 128.1, 118.0, 16.1. HRMS (APCI) calcd. for $C_{10}H_{10}BF_2N_2$ $[M+H]^+$: 207.0905, found 207.0916.

1g: 357 mg, yield 30%, ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (s, 2H), 7.26 (s, 2H), 6.54 (s, 2H), 3.40 (t, *J* = 6.0 Hz, 2H), 2.94 (t, *J* = 7.5 Hz, 2H), 1.97-1.74 (m, 2H), 1.61 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.4, 143.5, 135.1, 127.8, 118.1, 33.3, 32.9, 32.2, 31.0, 28.5. HRMS(APCI) calcd. for $C_{14}H_{17}B^{79}BrF_2N_2$ $[M+H]^+$: 341.0631, found 341.0626; HRMS(APCI) calcd. for $C_{14}H_{16}B^{79}BrFN_2$ $[M-F]^+$: 321.0569, found 321.0573. HRMS(APCI) calcd. for $C_{14}H_{16}B^{81}BrFN_2$ $[M-F]^+$: 323.0548, found 323.0547.

Synthesis of BODIPY 3: To a 10 mL dry Schlenk flask were added BODIPY **1g** (34.0 mg, 0.1 mmol), triphenylphosphine (263.0 mg, 1.0 mmol) dissolved in 5 mL toluene. The mixture was heated to reflux for 24 h under argon atmosphere. The mixture was then cooled to room temperature and washed with toluene until the triphenylphosphine was completely removed. The crude product was dissolved in a 1 mL dichloromethane solution and was layered with petroleum ether to give brown powder **3** in 79% yield (48 mg). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (s, 11H), 7.67 (s, 6H), 7.36 (s, 2H), 6.48 (s, 2H), 3.78 (s, 2H), 2.97 (s, 2H), 1.81 (s, 2H), 1.60 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.8, 143.2, 135.0, 133.7, 133.6, 130.6, 130.4, 128.6, 118.8, 118.1, 117.6, 33.1, 30.8, 30.4, 22.8, 22.6. HRMS (ESI) calcd. for $C_{32}H_{31}BF_2N_2P$ $[M^+]$: 523.2286, found 523.2286.

Synthesis of BODIPY 4: BODIPY **2g** (40.5, 0.1mmol) was used for the above reaction to give purple powder **4** in 87% yield (58 mg) using the above procedure. ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.50 (s, 1H), 7.72-7.62 (m, 15H), 7.49 (s, 1H), 3.63 (s, 2H), 2.81 (s, 2H), 1.70 (s, 2H), 1.55 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.4, 141.6, 137.9, 135.6, 135.0, 133.6, 133.5, 133.2, 130.9, 130.6, 130.4, 125.9, 123.5, 121.7, 121.0, 118.6, 118.3, 117.5, 115.4, 111.5, 32.4, 30.4, 22.8, 22.6, 22.1. HRMS (ESI) calcd. for $C_{36}H_{34}BF_2N_3P$ [M^+]: 588.2551, found 588.2550.

References:

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4. SHELXL-97, Program for the Refinement of Crystal Structure, University of Gottingen, Germany, 1997.

5. SHELXTL 5.10 (PC/NT-Version), Program Library for Structure Solution and Molecular Graphics, Bruker Analytical X-ray Systems, Madison, WI, 1998.

2.Table S1: Photophysical properties of BODIPYs 1a, 2a-k, 3 and 4 in different solvents at room temperature (THF: Tetrahydrofuran).

BODIPYs	solvents	λ_{abs}^{max} (nm)	λ_{em}^{max} (nm)	logε_{max}	ϕ^{c}	Stokes Shift (cm^{-1})
	dichloromethane	494	512	4.93	0.87	712
	toluene	497	517	4.90	0.82	778
1a	acetonitrile	488	507	4.97	0.75	768
	methanol	489	508	5.04	0.94	765
	hexane	495	511	4.60	0.81	633
	THF	492	511	4.93	0.74	756
	dichloromethane	565	594	4.72	0.57	864
	toluene	571	597	4.92	0.45	763
2a	acetonitrile	558	591	4.95	0.45	1001
	methanol	560	590	4.87	0.45	908
	hexane	567	587	4.97	0.52	601
	THF	565	594	4.92	0.45	864
	dichloromethane	567	593	4.50	0.34	773
	toluene	573	596	4.55	0.45	673
2b	acetonitrile	560	582	4.56	0.34	675
	methanol	563	590	4.25	0.45	813
	hexane	569	586	4.68	0.47	510
	THF	568	594	4.67	0.35	771
	dichloromethane	567	588	4.76	0.39	630
	toluene	574	596	4.80	0.47	643
2c	acetonitrile	561	590	4.34	0.46	876
	methanol	563	590	4.48	0.49	813
	hexane	569	588	4.94	0.46	568
	THF	568	594	4.90	0.49	771
	dichloromethane	567	588	4.61	0.45	630
	toluene	574	597	4.78	0.47	671
2d	acetonitrile	561	590	4.78	0.49	876
	methanol	563	589	4.53	0.48	784
	hexane	569	586	4.87	0.50	510
	THF	568	594	4.51	0.34	771
	dichloromethane	567	594	4.44	0.48	802
	toluene	574	597	4.57	0.47	671
2e	acetonitrile	561	590	4.37	0.47	876
	methanol	563	590	4.36	0.33	813
	hexane	569	587	4.52	0.50	539
	THF	568	594	4.39	0.47	771
	dichloromethane	570	597	4.69	0.36	793
	toluene	575	600	4.78	0.48	725
2f	acetonitrile	563	593	4.87	0.30	899
	methanol	566	593	4.58	0.30	804
	hexane	570	590	4.82	0.54	595
	THF	570	596	4.57	0.35	765
	dichloromethane	568	594	4.65	0.55	771
	toluene	574	597	4.80	0.38	671
2g	acetonitrile	561	589	4.77	0.32	847
	methanol	564	592	4.70	0.40	839
	hexane	570	589	4.51	0.54	566
	THF	568	594	4.67	0.42	771
	dichloromethane	568	594	4.94	0.49	771
	toluene	574	596	4.56	0.40	643
2h	acetonitrile	561	590	4.76	0.35	876
	methanol	564	593	4.80	0.72	867
	hexane	569	587	4.81	0.46	539
	THF	568	595	4.72	0.42	799

	dichloromethane	576	609	4.52	0.24	941
2i	toluene	581	611	4.51	0.35	845
	acetonitrile	570	606	4.73	0.16	1042
	methanol	573	604	4.81	0.16	896
	hexane	576	601	4.59	0.41	722
	THF	577	609	4.51	0.25	911
	dichloromethane	573	600	4.68	0.60	785
2j	toluene	579	602	4.70	0.57	660
	acetonitrile	568	598	4.62	0.50	883
	methanol	570	596	4.60	0.56	795
	hexane	573	598	4.75	0.50	730
	THF	575	601	4.72	0.57	752
	dichloromethane	602	632	4.24	0.27	789
	toluene	610	638	4.29	0.19	719
2k	acetonitrile	591	637	4.19	0.02	1222
	methanol	597	624	4.29	0.02	725
	hexane	604	624	4.33	0.38	531
	THF	601	639	4.35	0.02	989
	dichloromethane	497	515	4.30	0.90	703
3	acetonitrile	491	510	4.30	0.85	759
	methanol	493	514	4.31	0.92	829
	THF	493	511	4.27	0.39	715
	dichloromethane	571	597	4.29	0.71	763
4	acetonitrile	562	590	4.32	0.59	844
	methanol	565	592	4.34	0.58	807
	THF	566	595	4.34	0.57	861

[a]All ϕ_f values are corrected for changes in refractive indexes of different solvents. [b]Molar absorption coefficient are in the maximum of the highest peak. [c]Fluorescence quantum yields were calculated using Rhodamine B (ϕ = 0.49 in ethanol) and fluorescein (ϕ = 0.90 in 0.1 N NaOH aqueous solution) as the reference.

3. UV-vis and fluorescence emission spectra

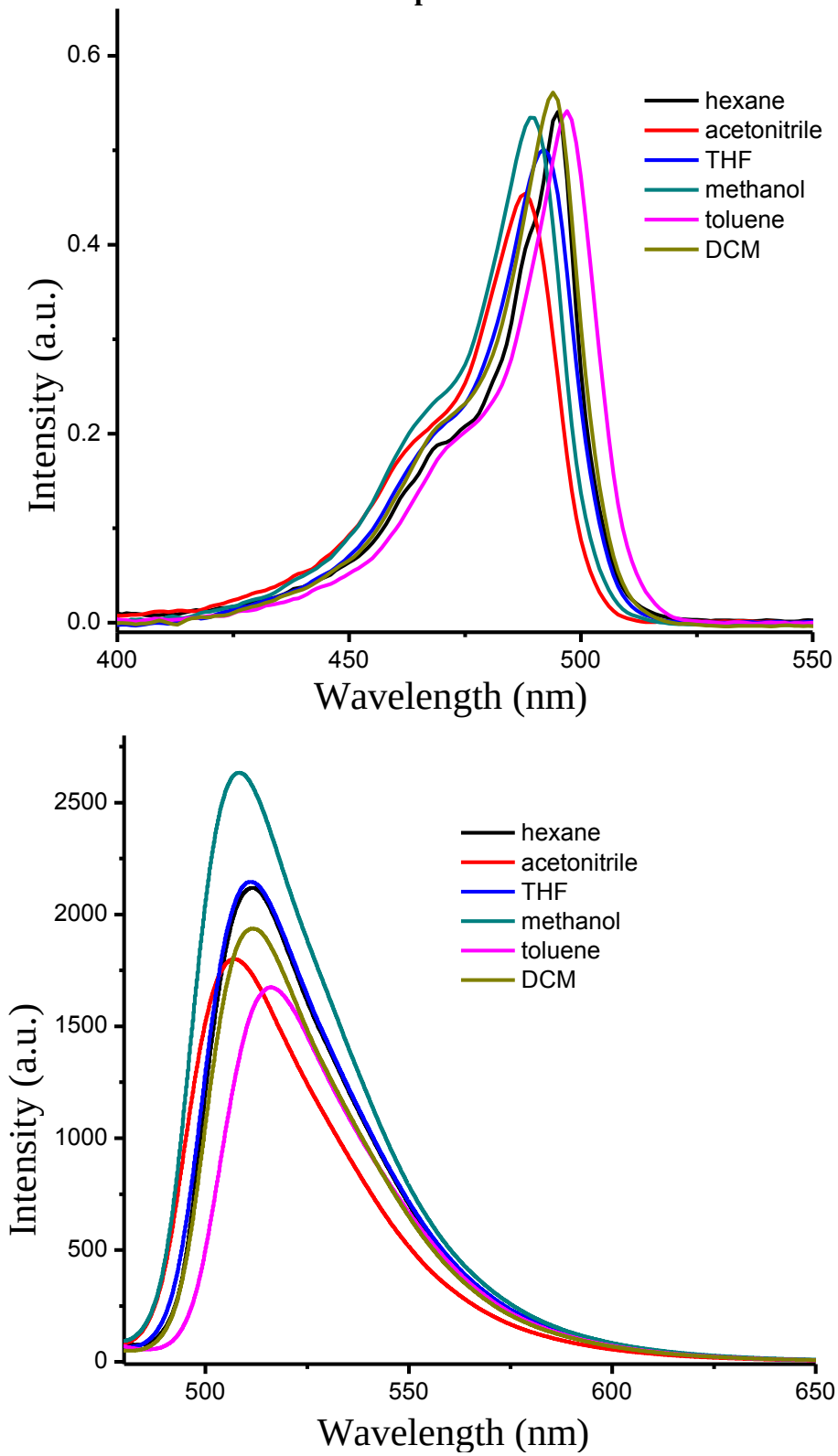


Figure S1: Absorption (top) and emission (bottom) spectra of BODIPY **1a** recorded in different solvents. Excited at 470 nm

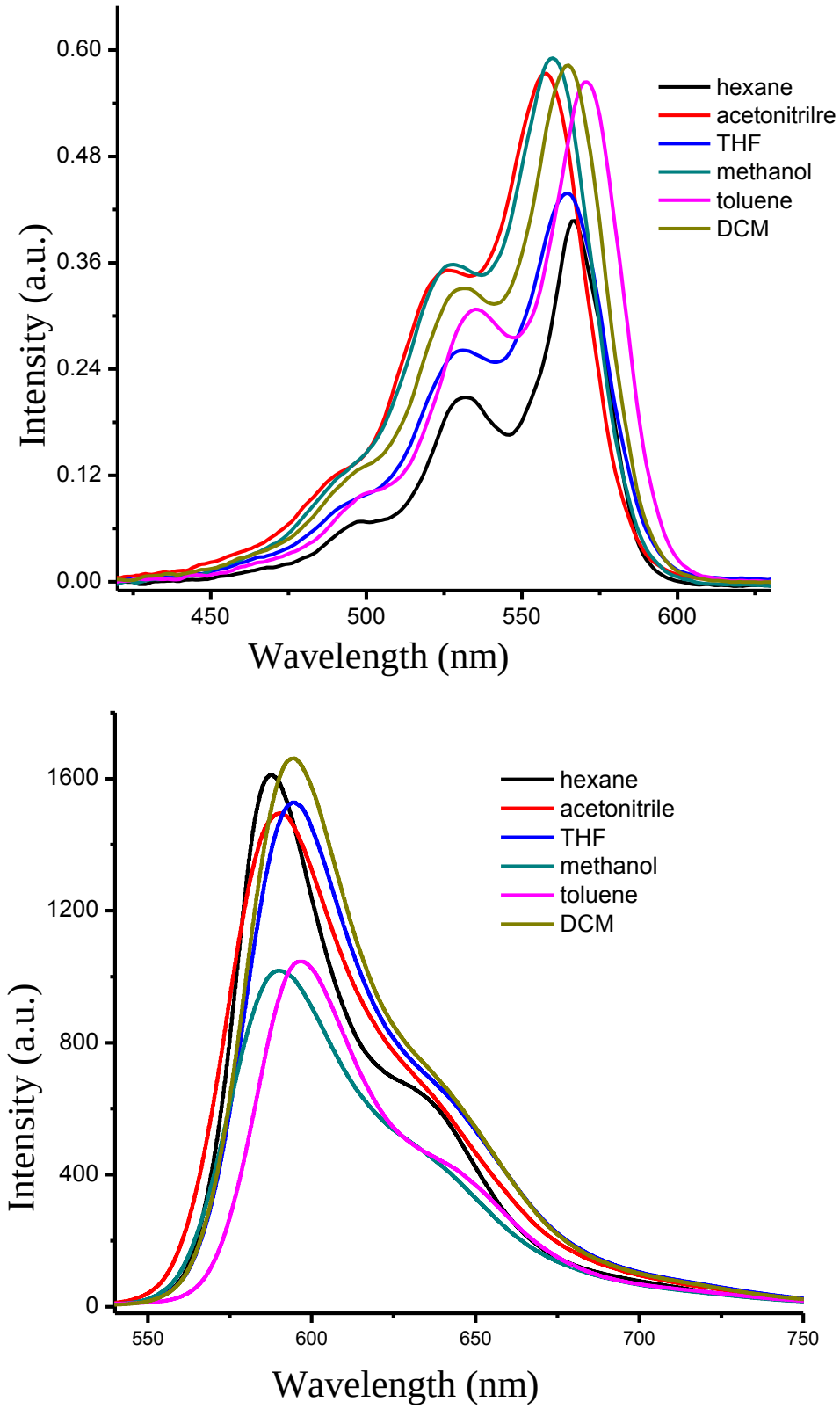


Figure S2: Absorption (top) and emission (bottom) spectra of BODIPY **2a** recorded in different solvents. Excited at 520 nm

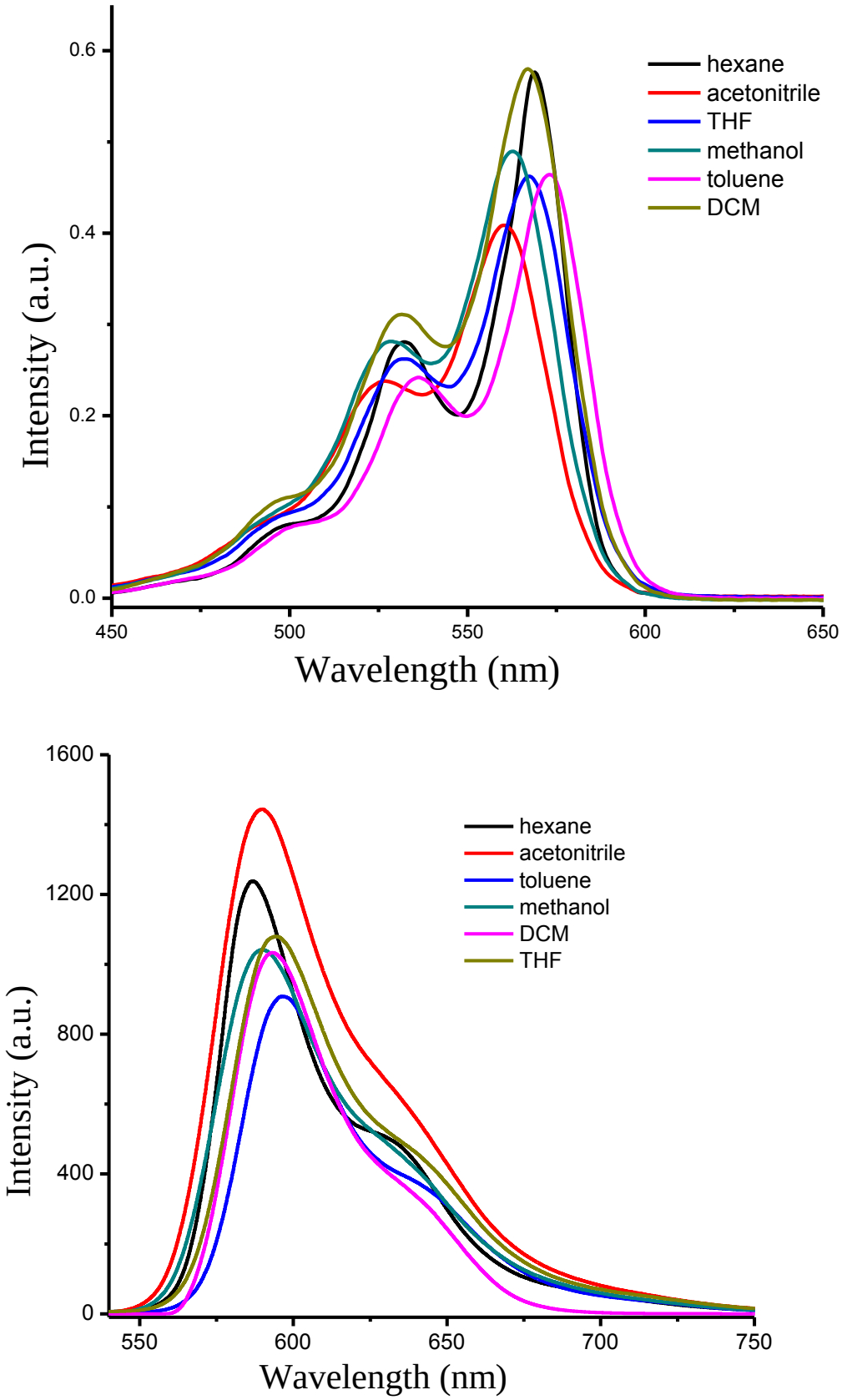


Figure S3: Absorption (top) and emission (bottom) spectra of BODIPY **2b** recorded in different solvents. Excited at 520 nm

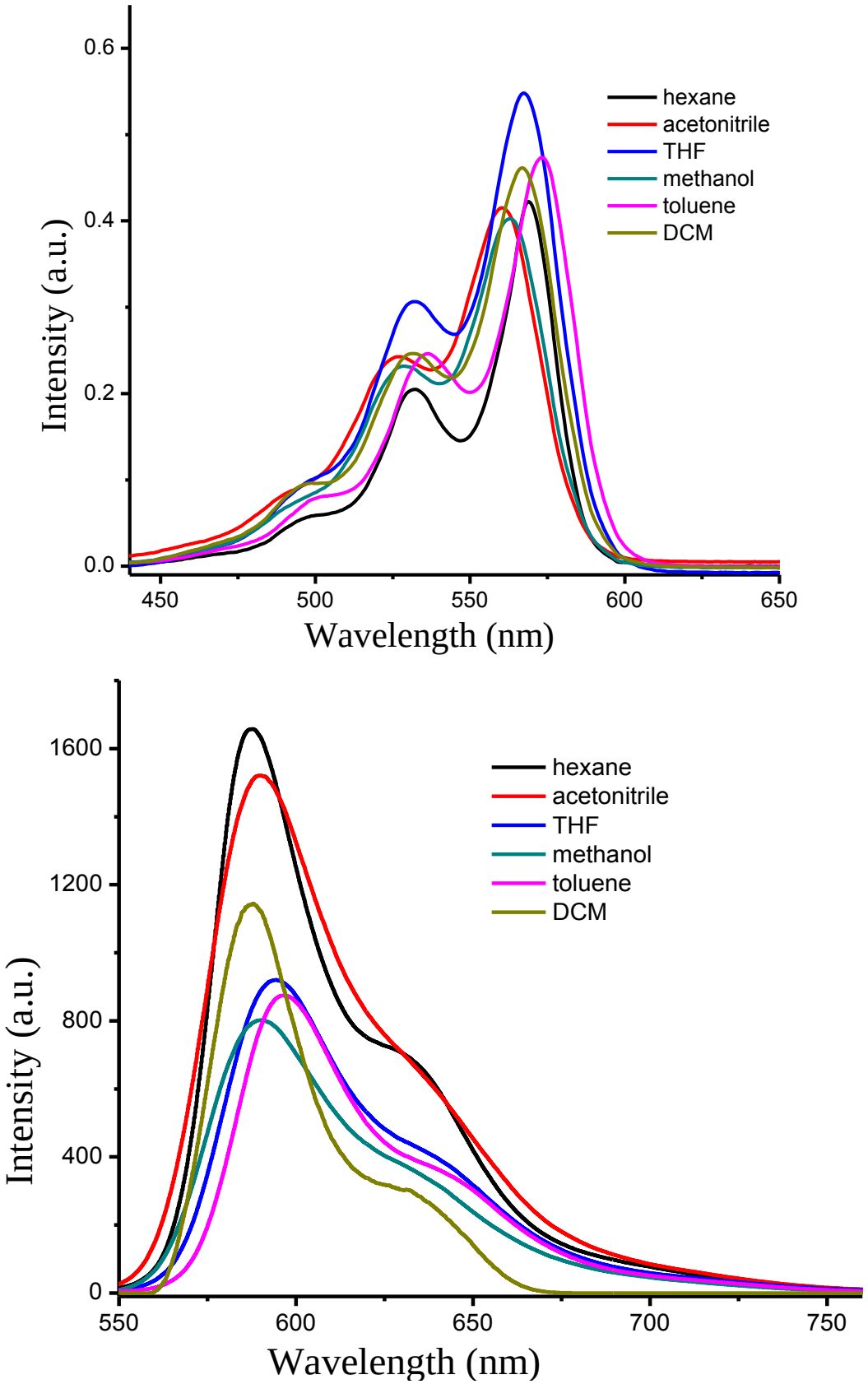


Figure S4: Absorption (top) and emission (bottom) spectra of BODIPY **2c** recorded in different solvents. Excited at 520 nm

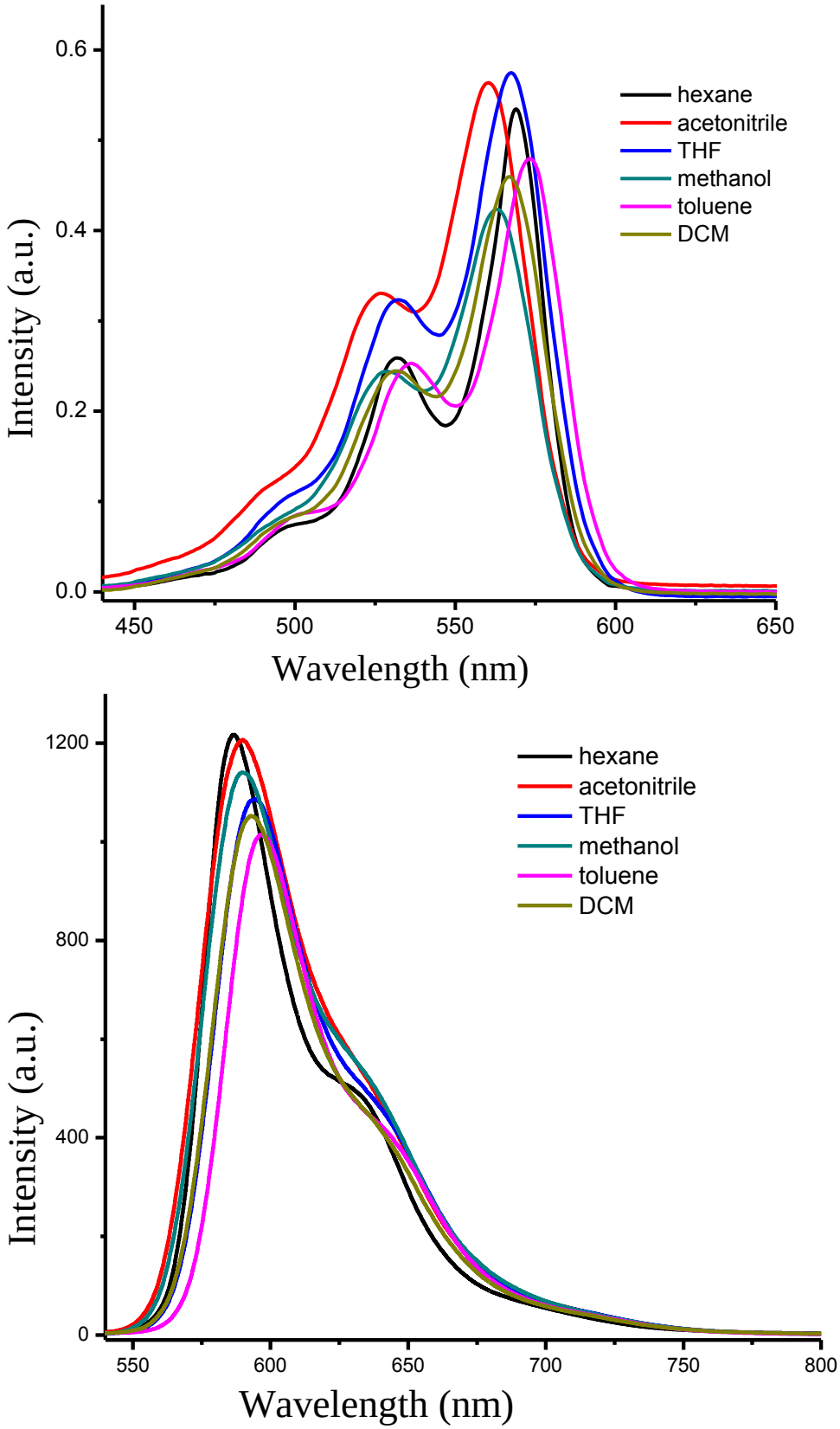


Figure S5: Absorption (top) and emission spectra (bottom) of BODIPY **2d** recorded in different solvents. Excited at 520 nm

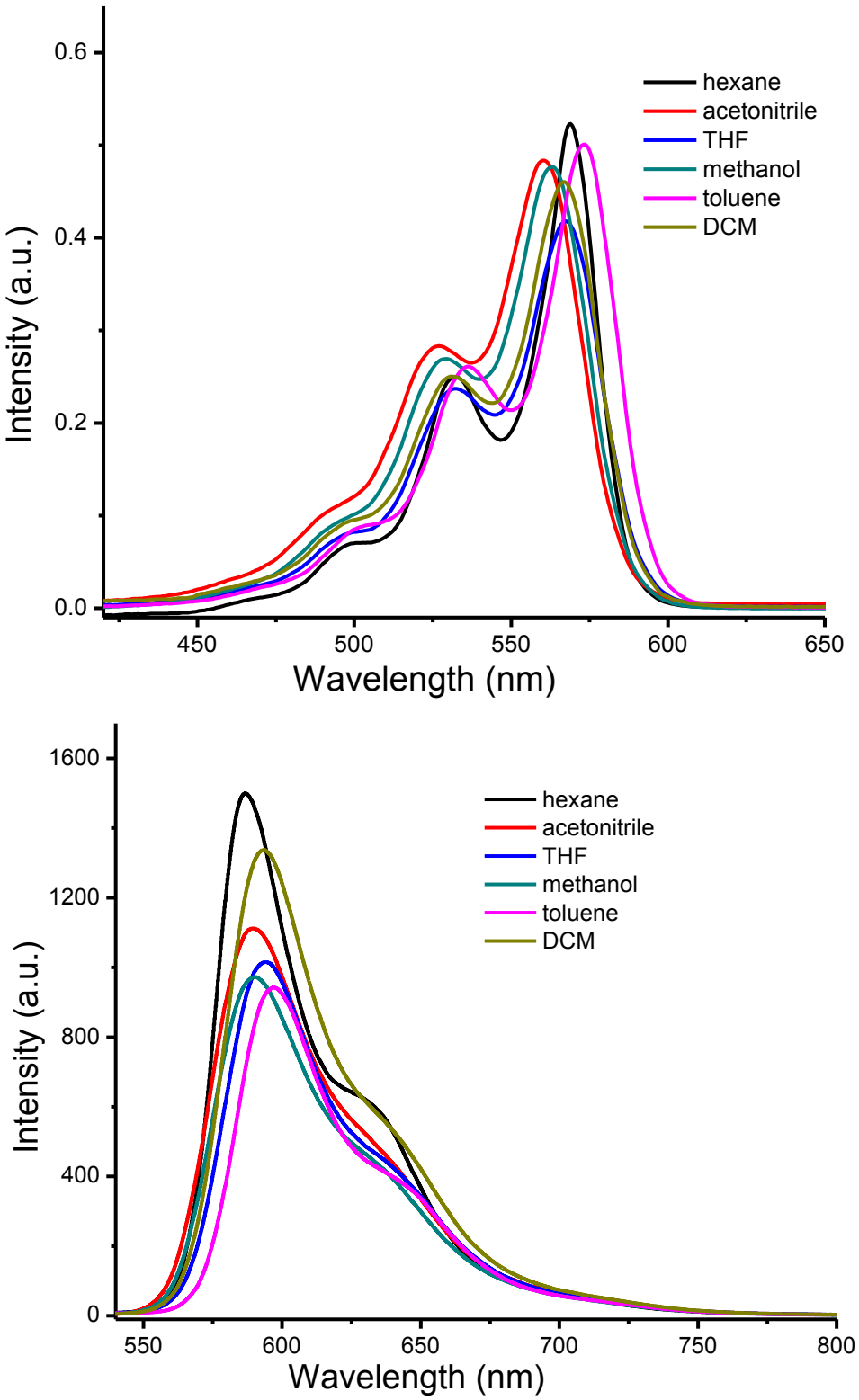


Figure S6: Absorption (top) and emission (bottom) spectra of BODIPY **2e** recorded in different solvents. Excited at 520 nm

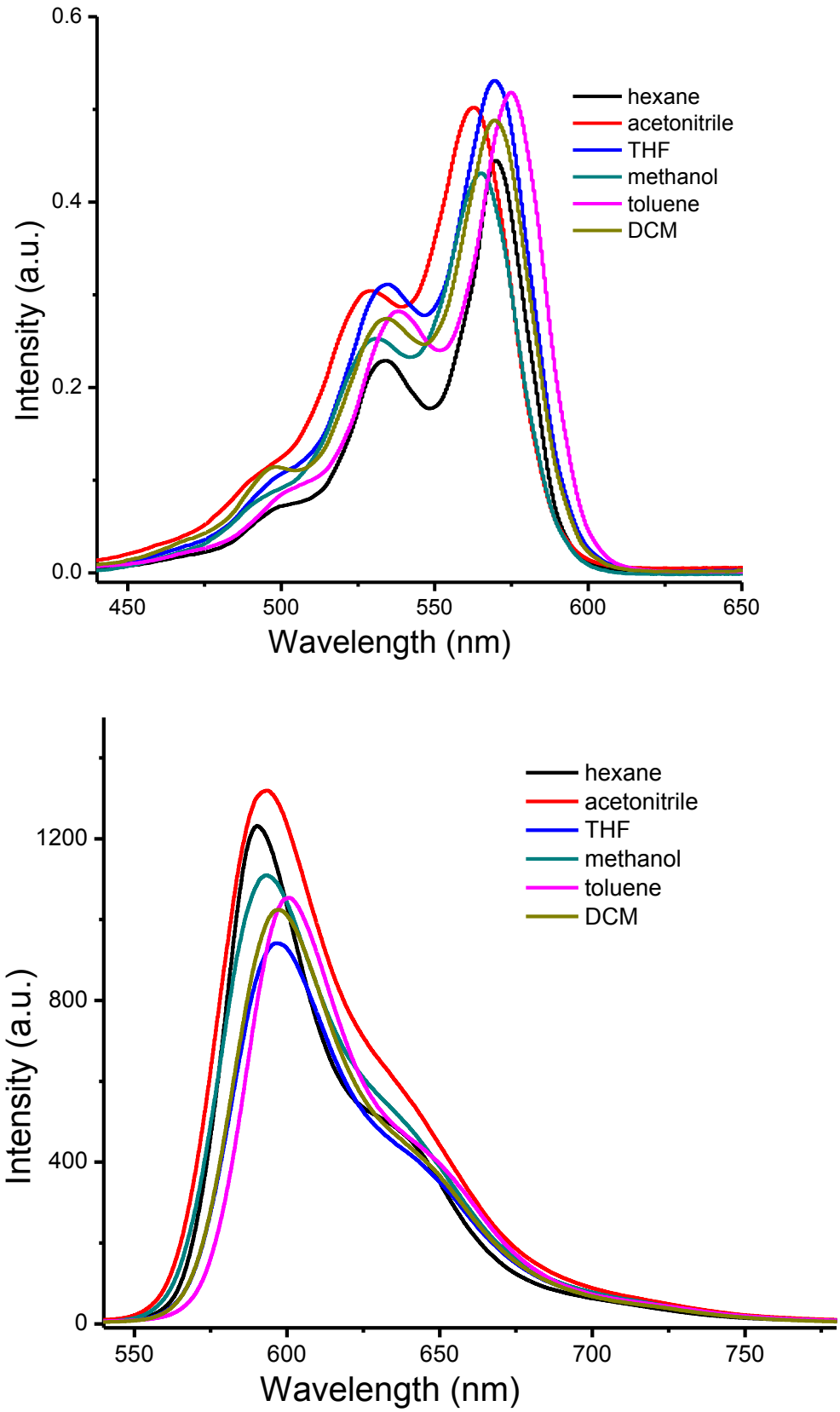


Figure S7: Absorption (top) and emission (bottom) spectra of BODIPY **2f** recorded in different solvents. Excited at 520 nm

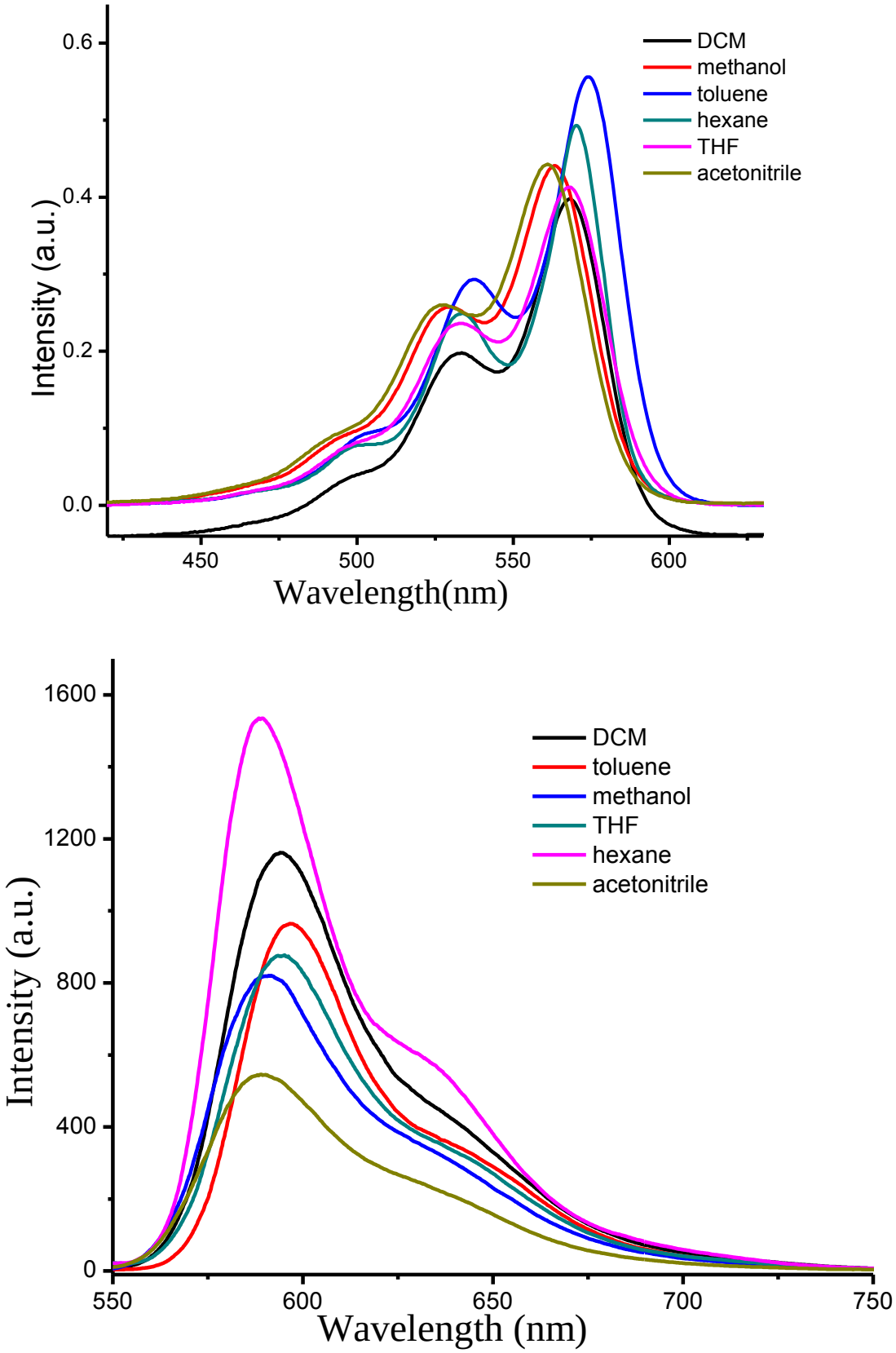


Figure S8: Absorption (top) and emission (bottom) spectra of BODIPY **2g** recorded in different solvents. Excited at 540 nm

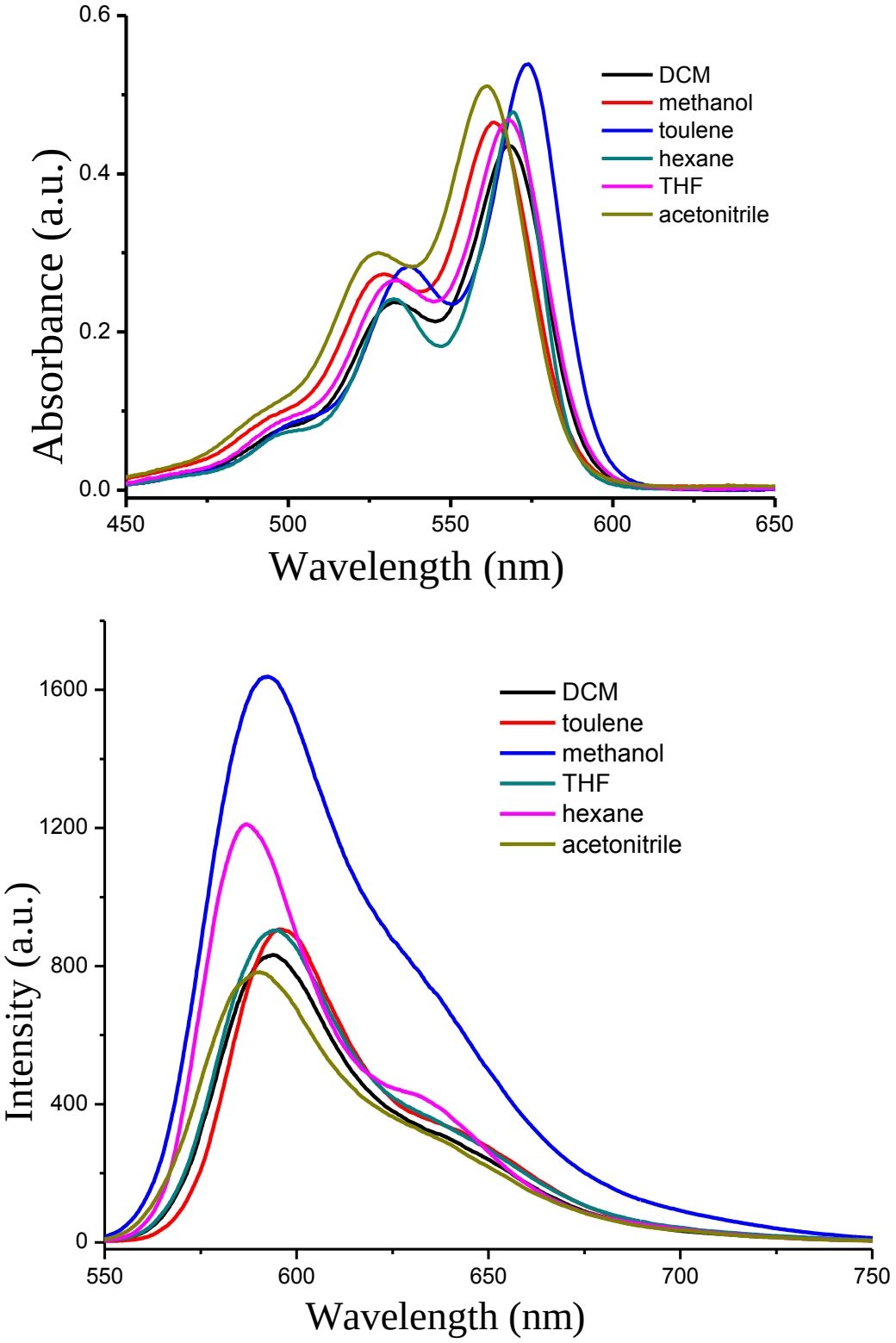


Figure S9: Absorption (top) and emission spectra (bottom) of BODIPY **2h** recorded in different solvents. Excited at 540 nm

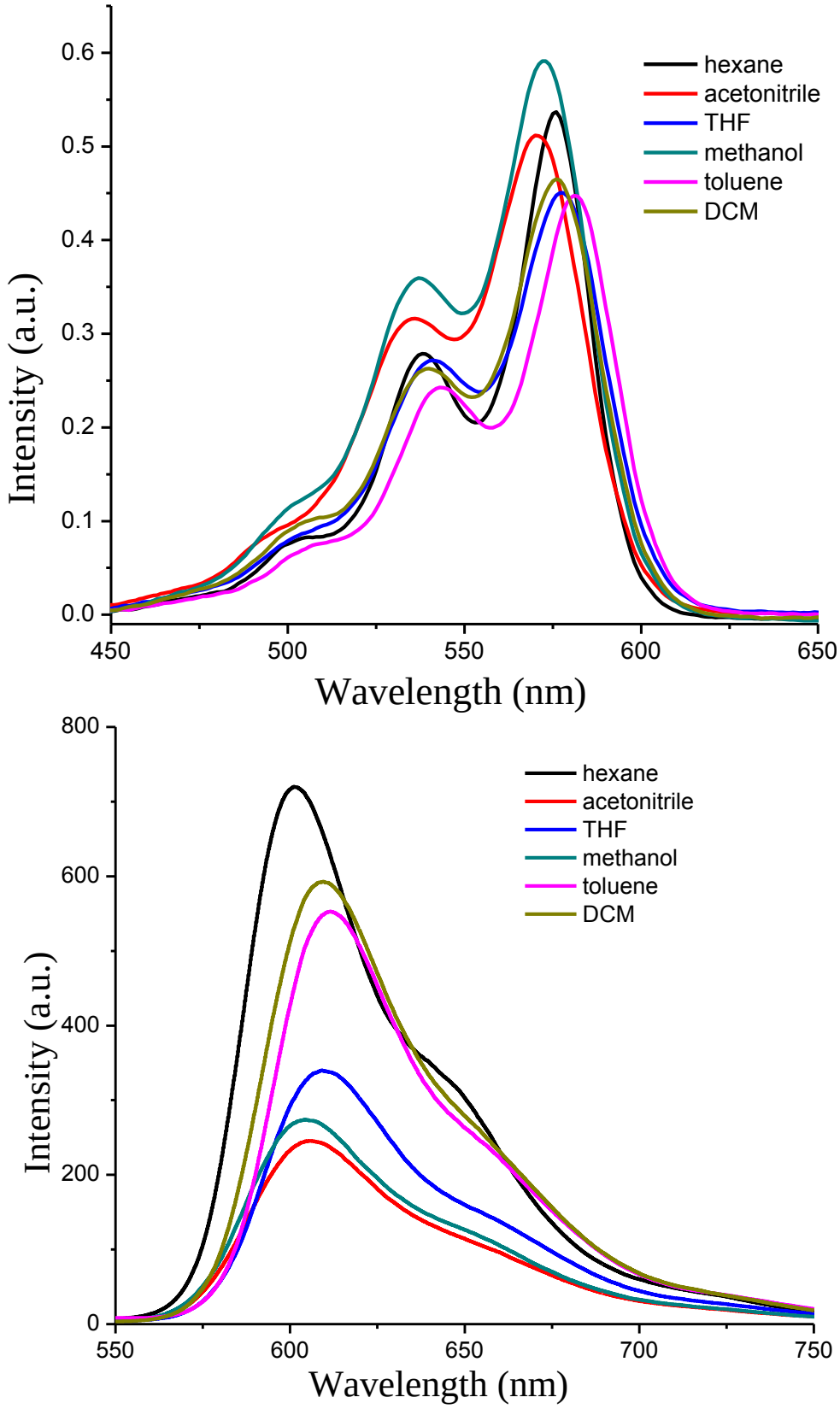


Figure S10: Absorption (top) and emission (bottom) spectra of BODIPY **2i** recorded in different solvents. Excited at 520 nm.

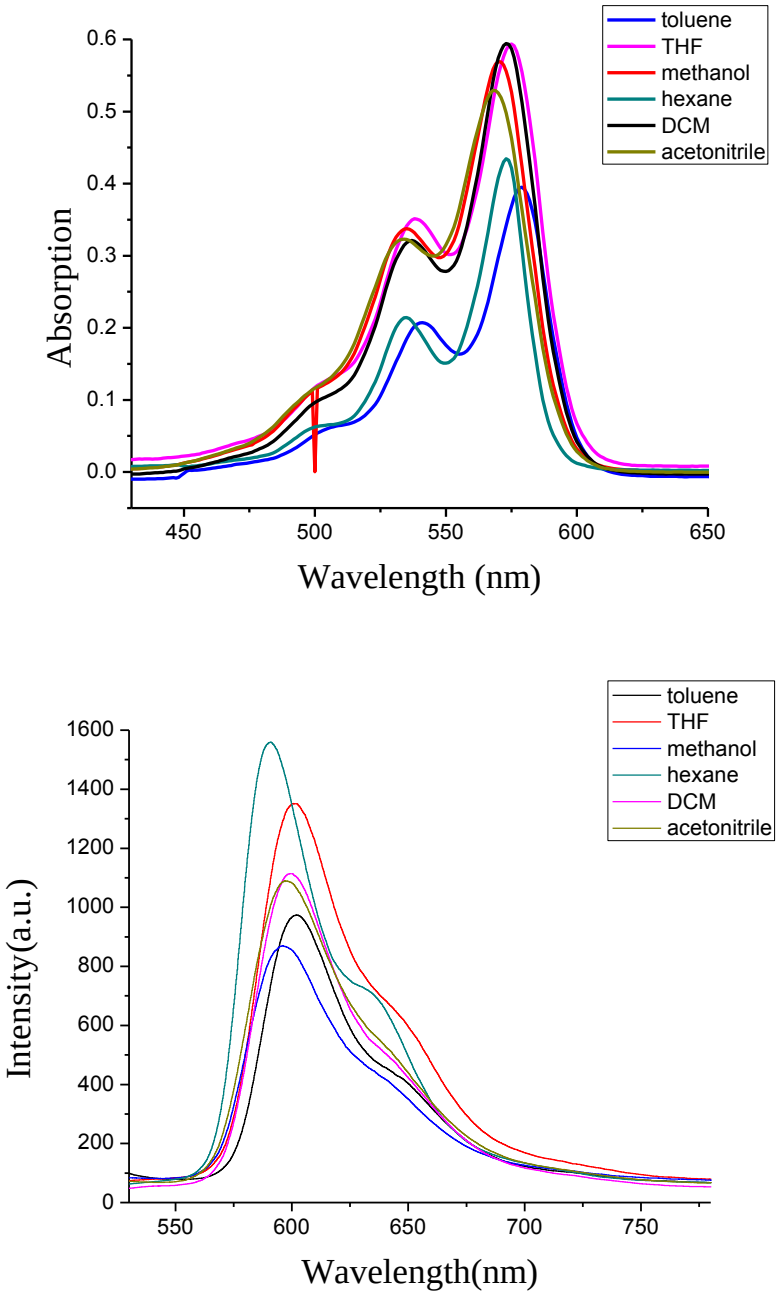


Figure S11: Absorption (top) and emission (bottom) spectra of BODIPY **2j** recorded in different solvents. Excited at 570 nm.

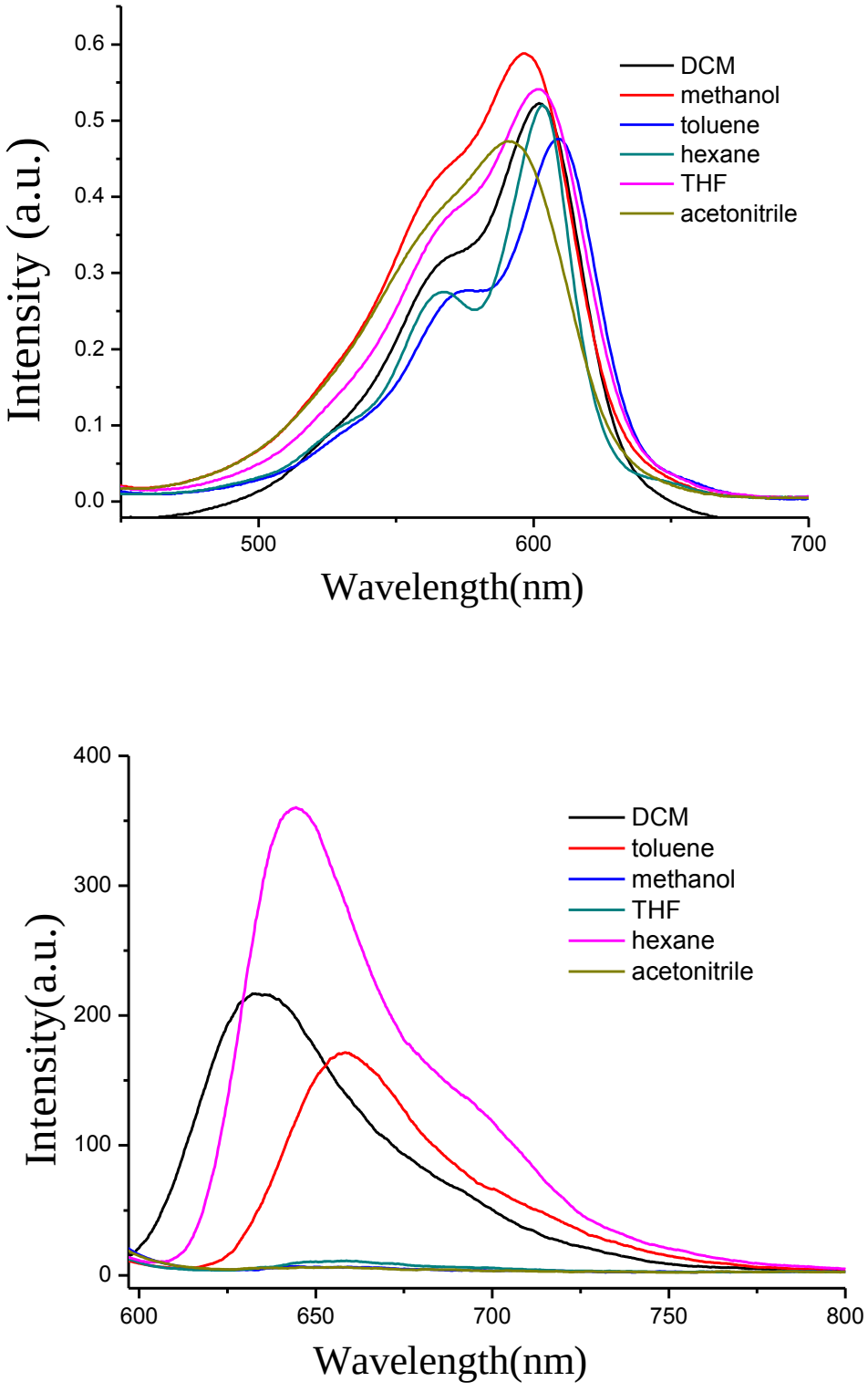


Figure S12: Absorption (top) and emission (bottom) spectra of BODIPY **2k** recorded in different solvents. Excited at 570 nm.

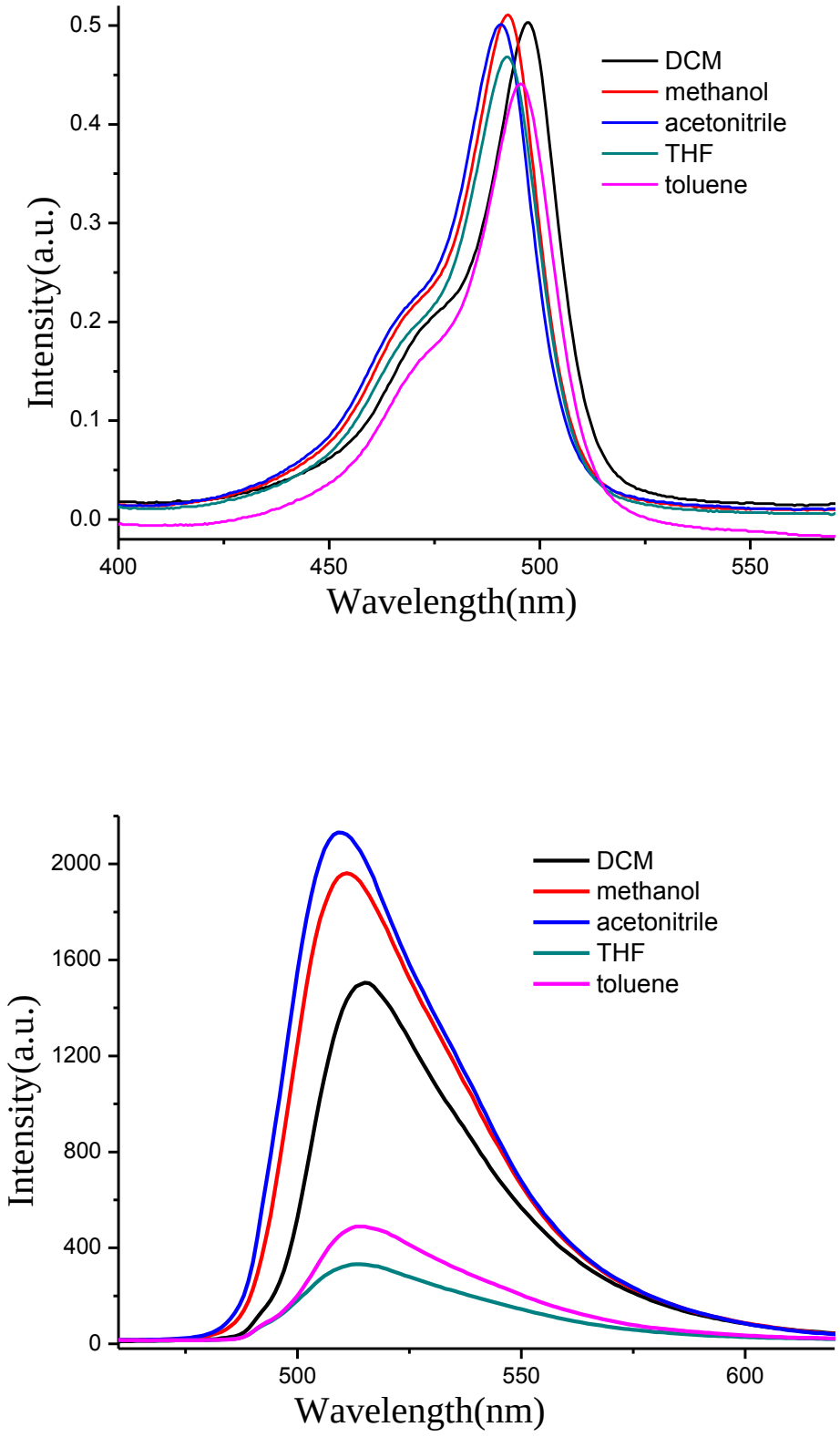


Figure S13: Absorption (top) and emission (bottom) spectra of BODIPY **3** recorded in different solvents. Excited at 490 nm.

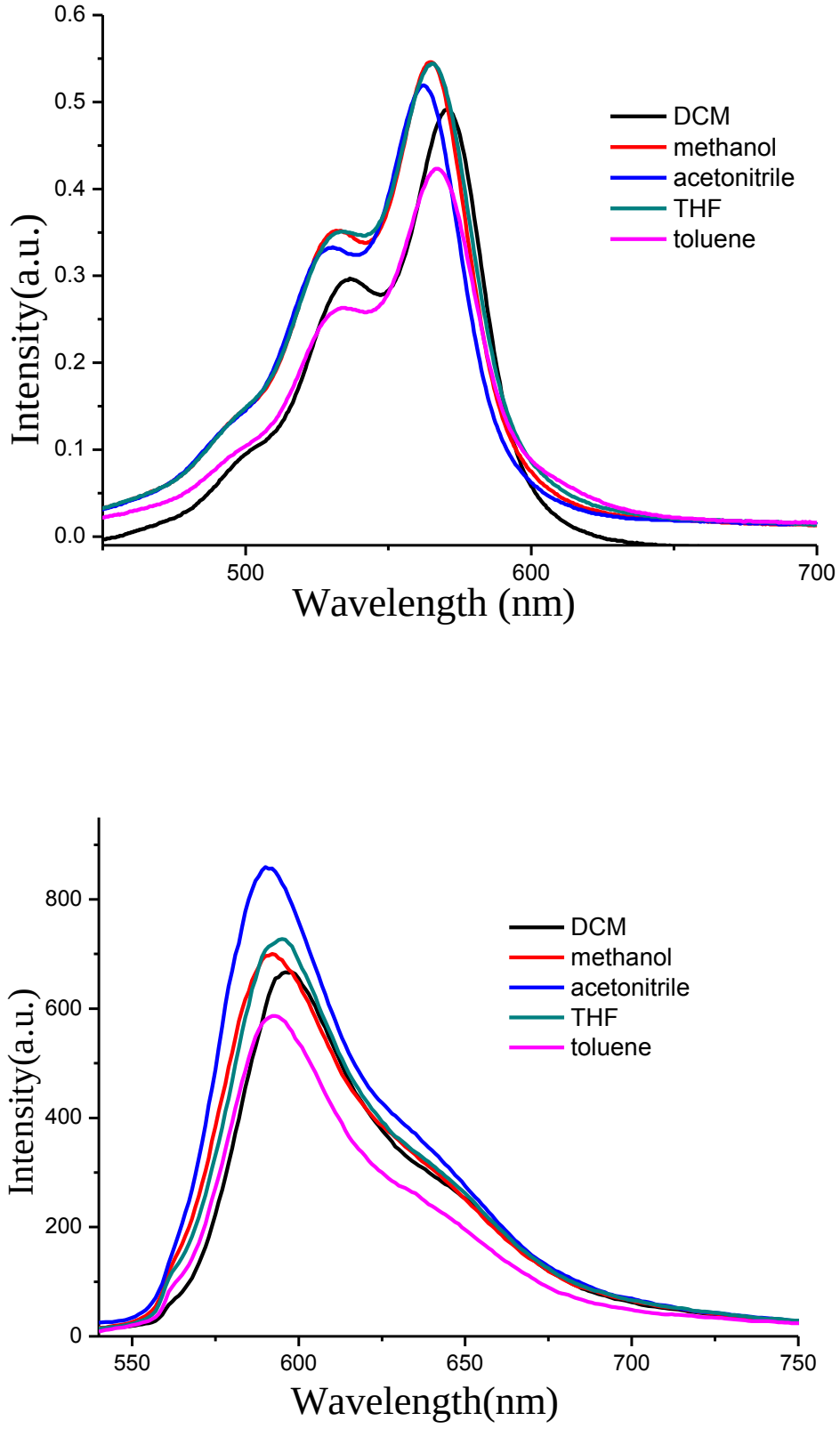


Figure S14: Absorption (top) and emission (bottom) spectra of BODIPY **4** recorded in different solvents. Excited at 560 nm.

4. Photostability of BODIPY 4

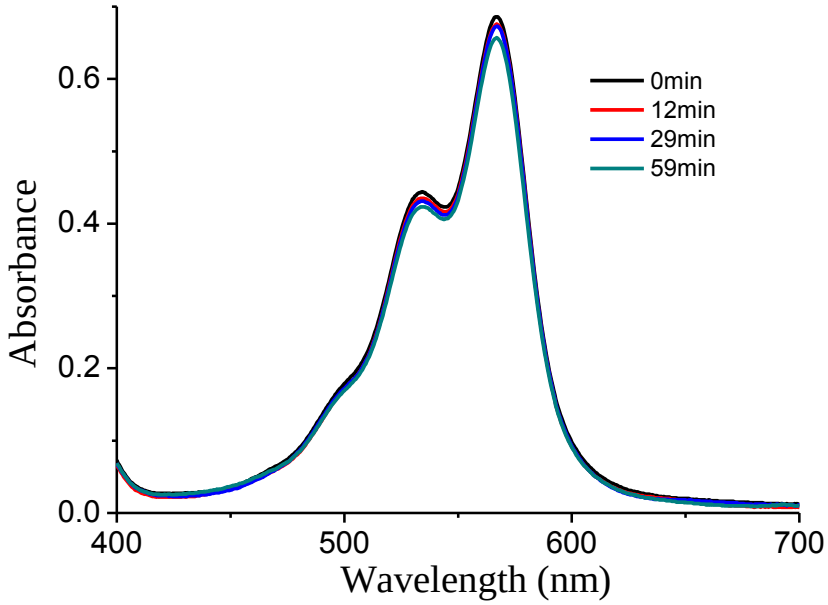


Figure S15. Absorbance changes of BODIPY **4** in ethanol under continuous irradiation with light (500W Xe) after different irradiation times.

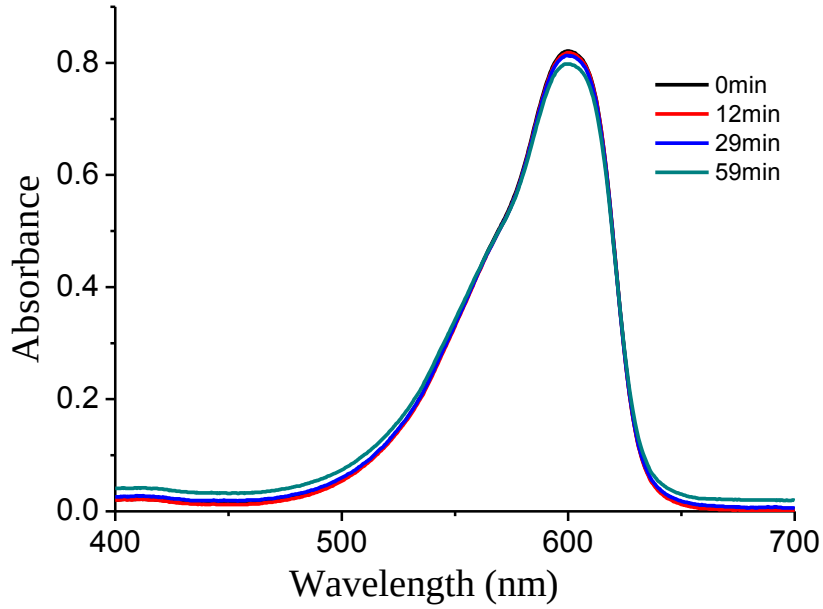


Figure S16. Absorbance changes of Cresyl violet perchlorate in EtOH under continuous irradiation with light (500W Xe) after different irradiation times.

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

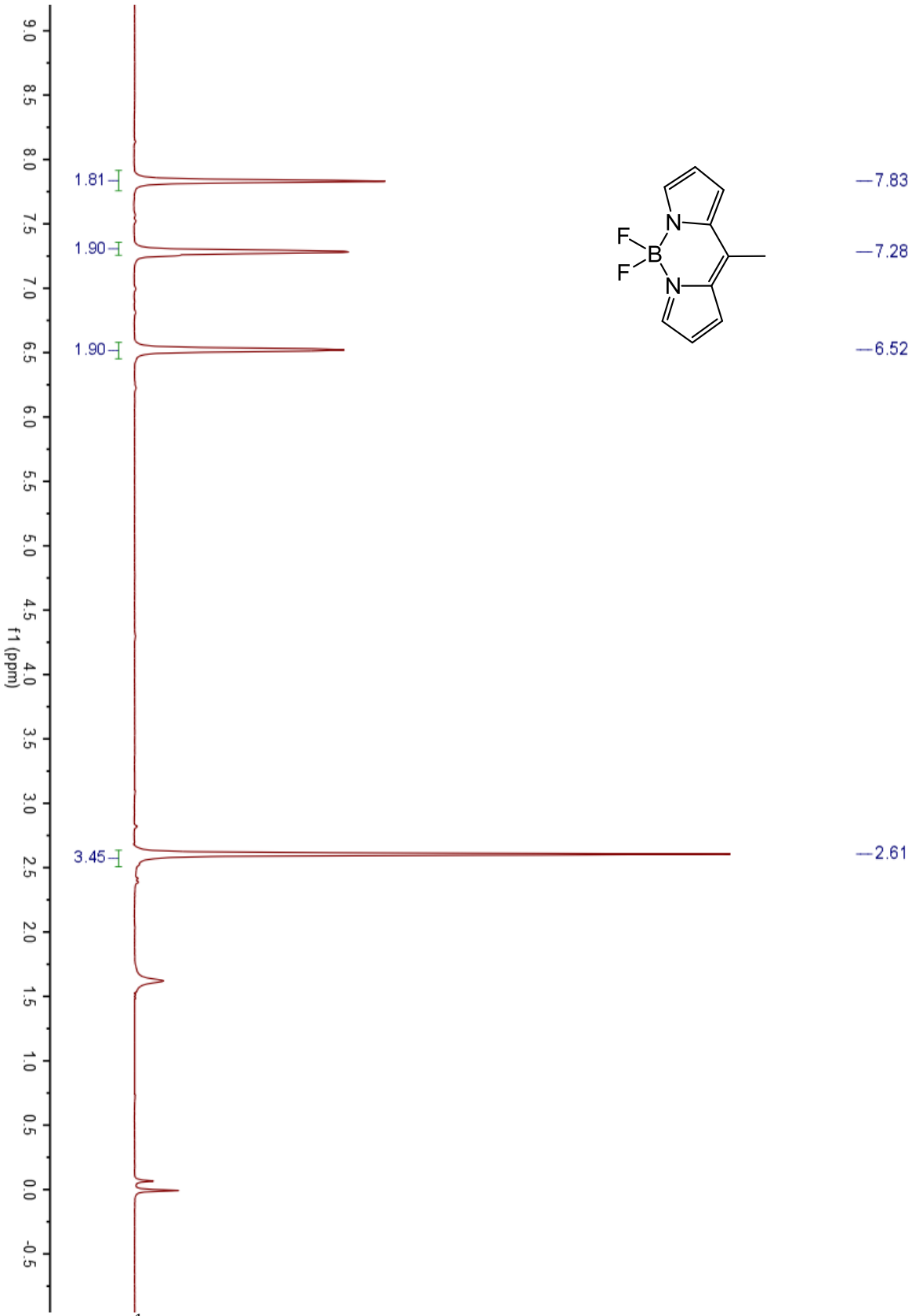


Figure S17: ^{1}H NMR spectrum of BODIPY dye **1a** in $CDCl_3$ solution

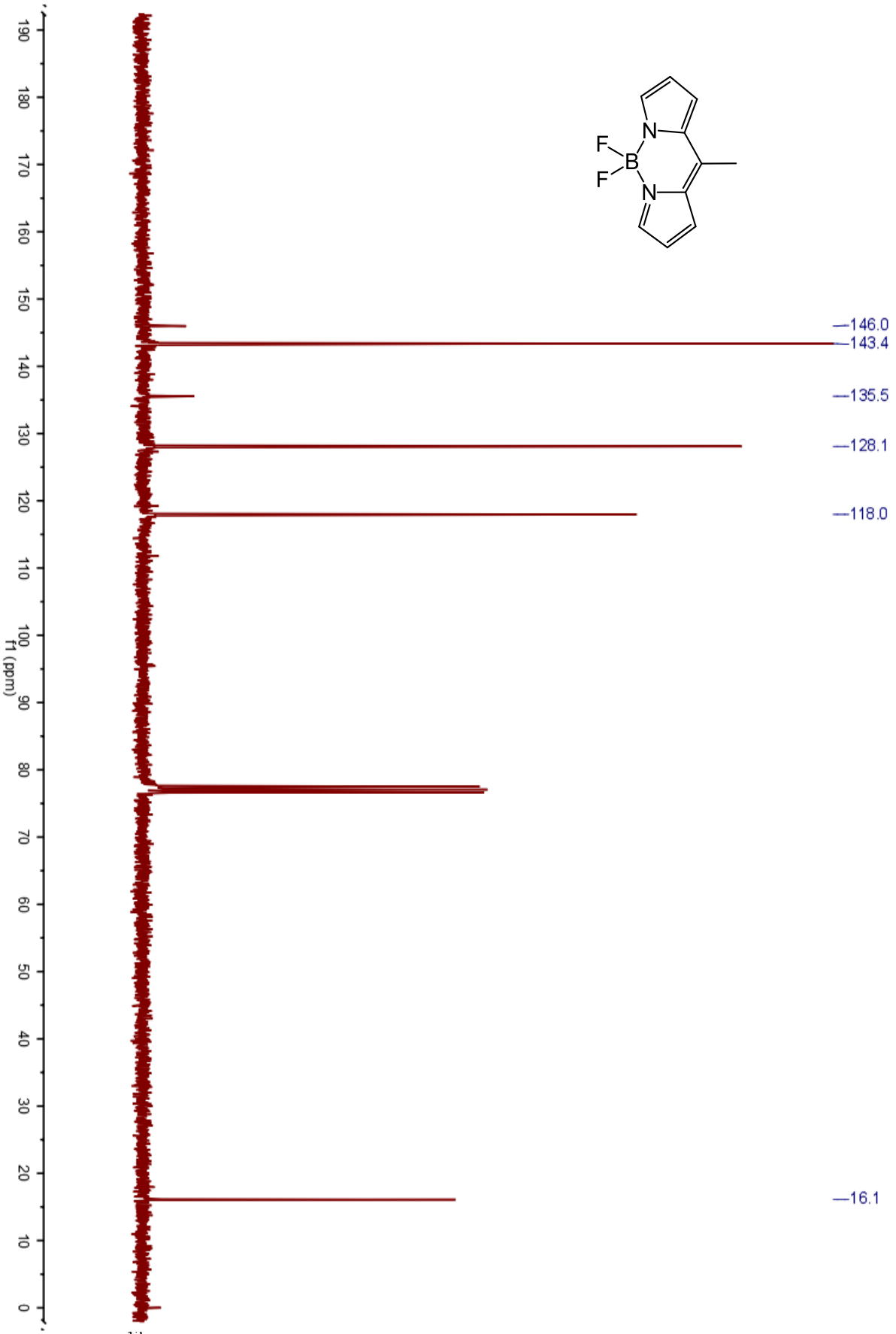


Figure S18: ^{13}C NMR spectrum of BODIPY dye **1a** in $CDCl_3$ solution

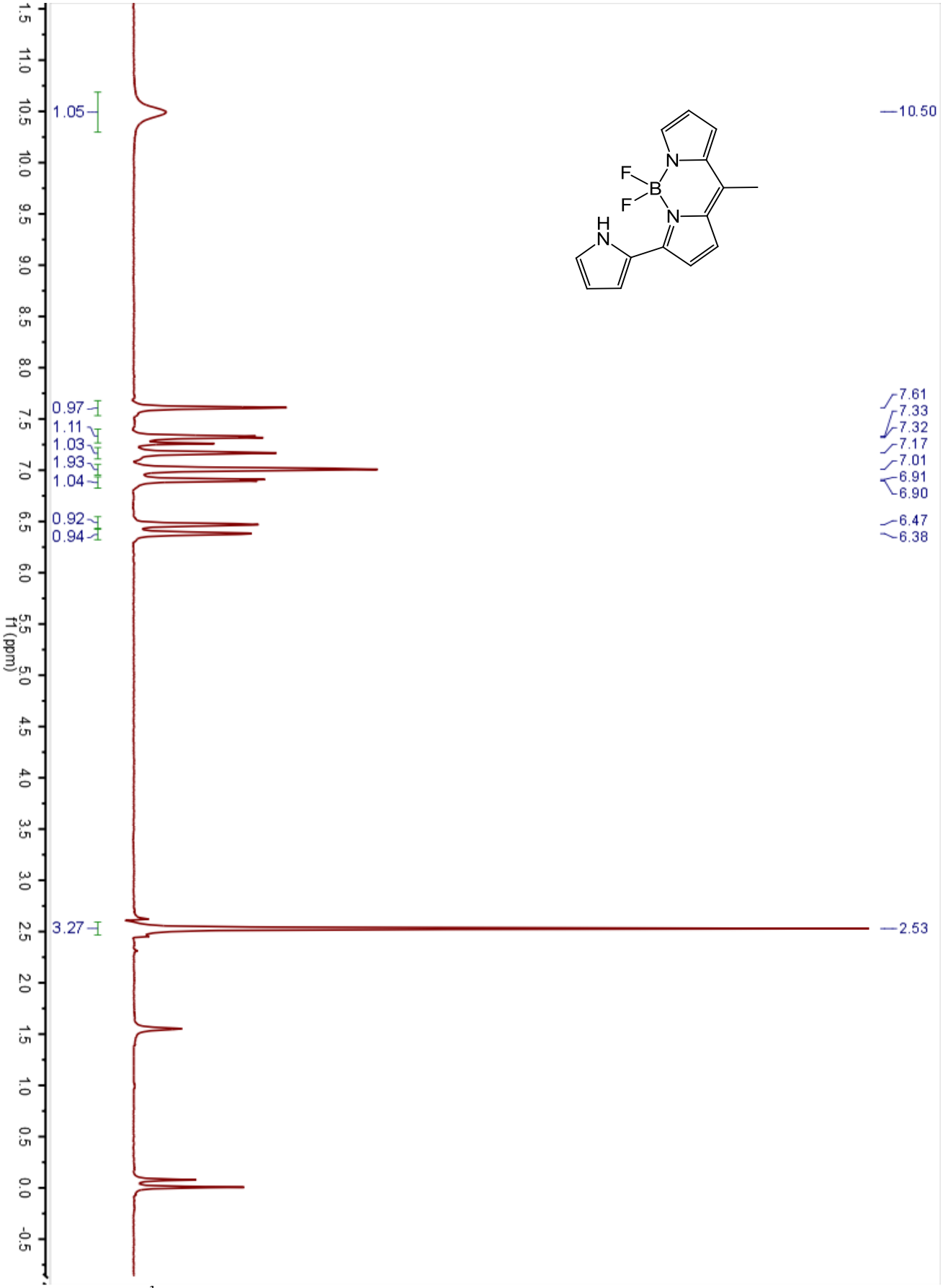


Figure S19: ^{1}H NMR spectrum of BODIPY dye **2a** in $CDCl_3$ solution

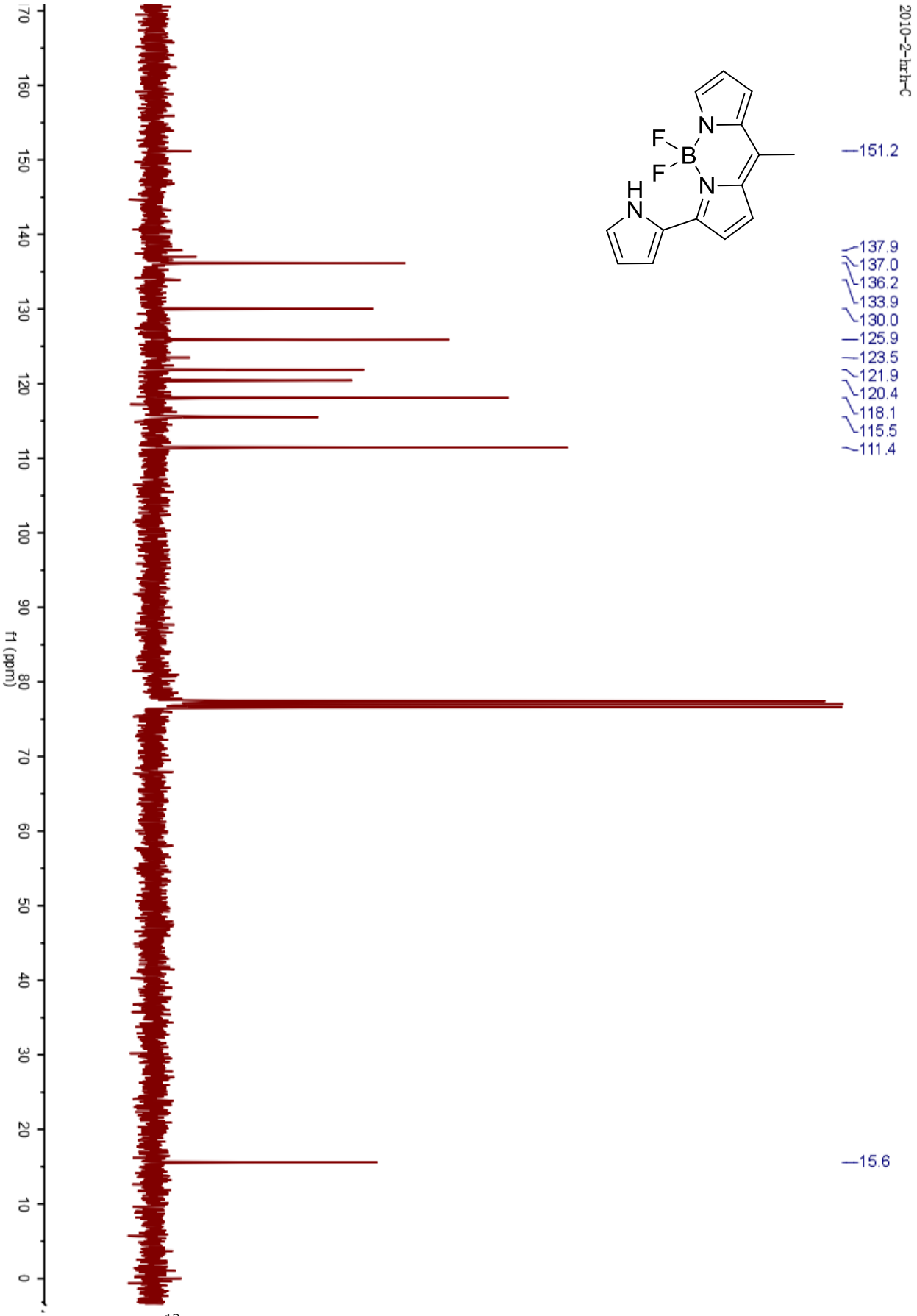


Figure S20: ^{13}C NMR spectrum of BODIPY dye **2a** in $CDCl_3$ solution

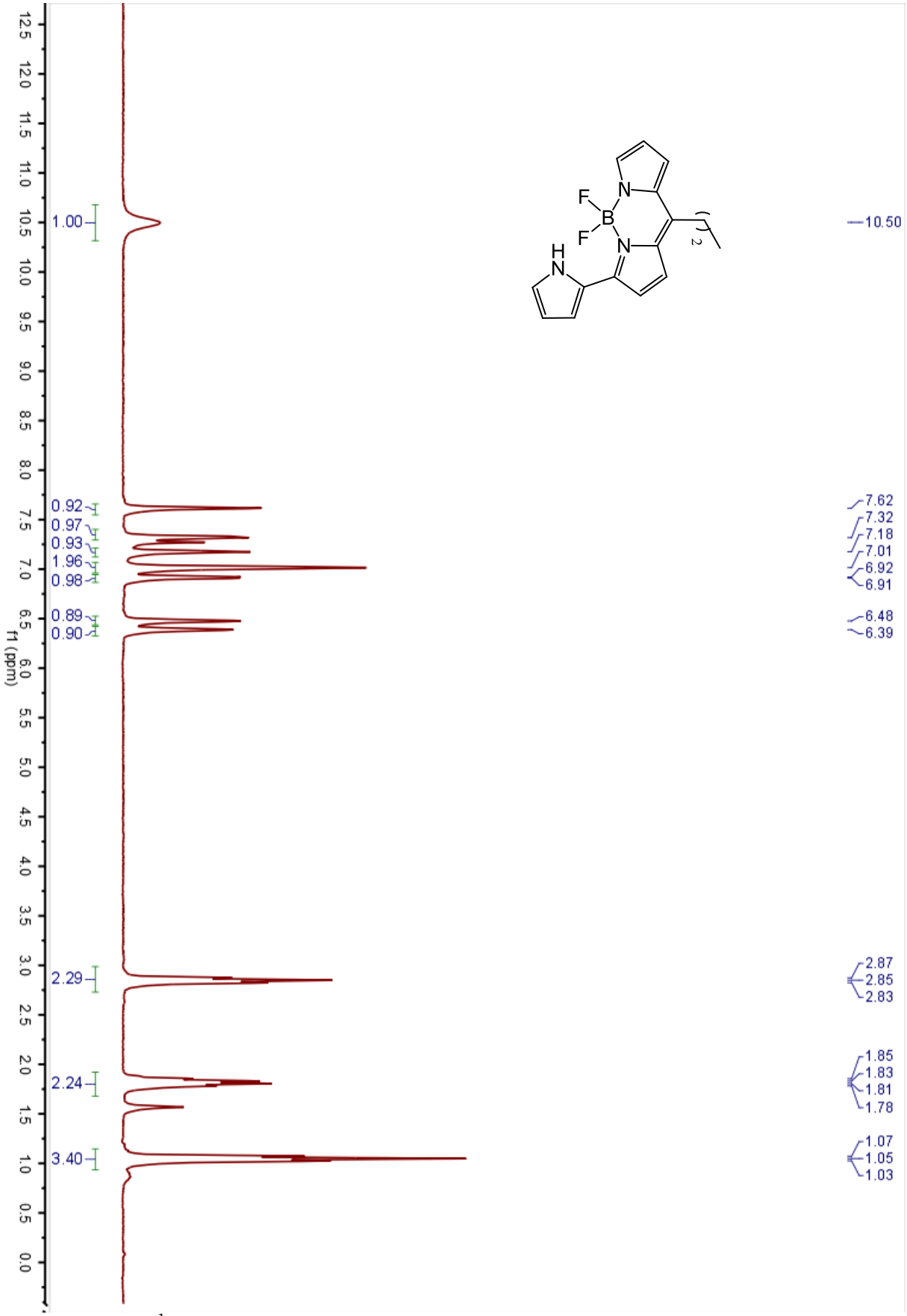


Figure S21: ^{1}H NMR spectrum of BODIPY dye **2b** in $CDCl_3$ solution

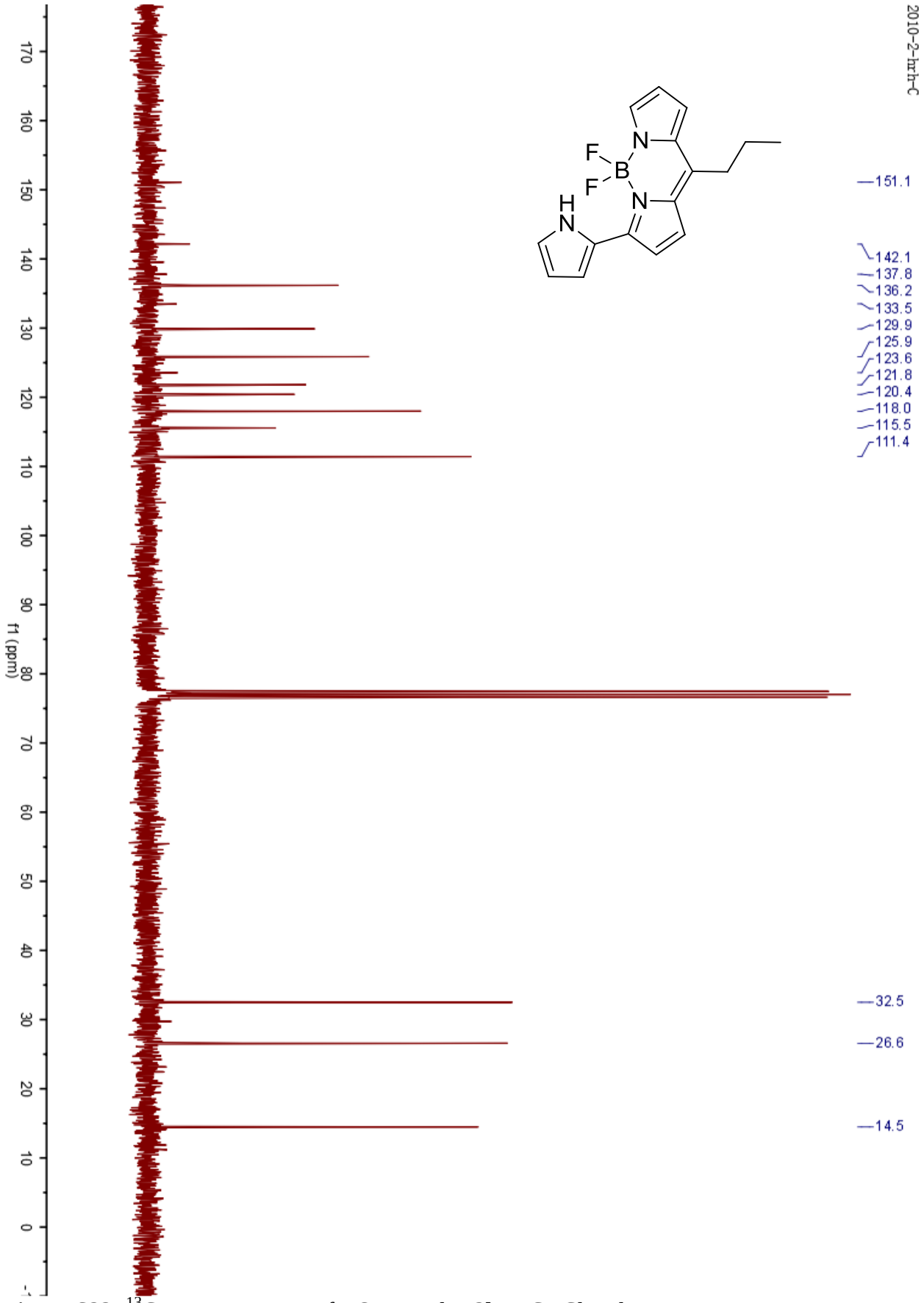


Figure S22: ^{13}C NMR spectrum of BODIPY dye **2b** in $CDCl_3$ solution

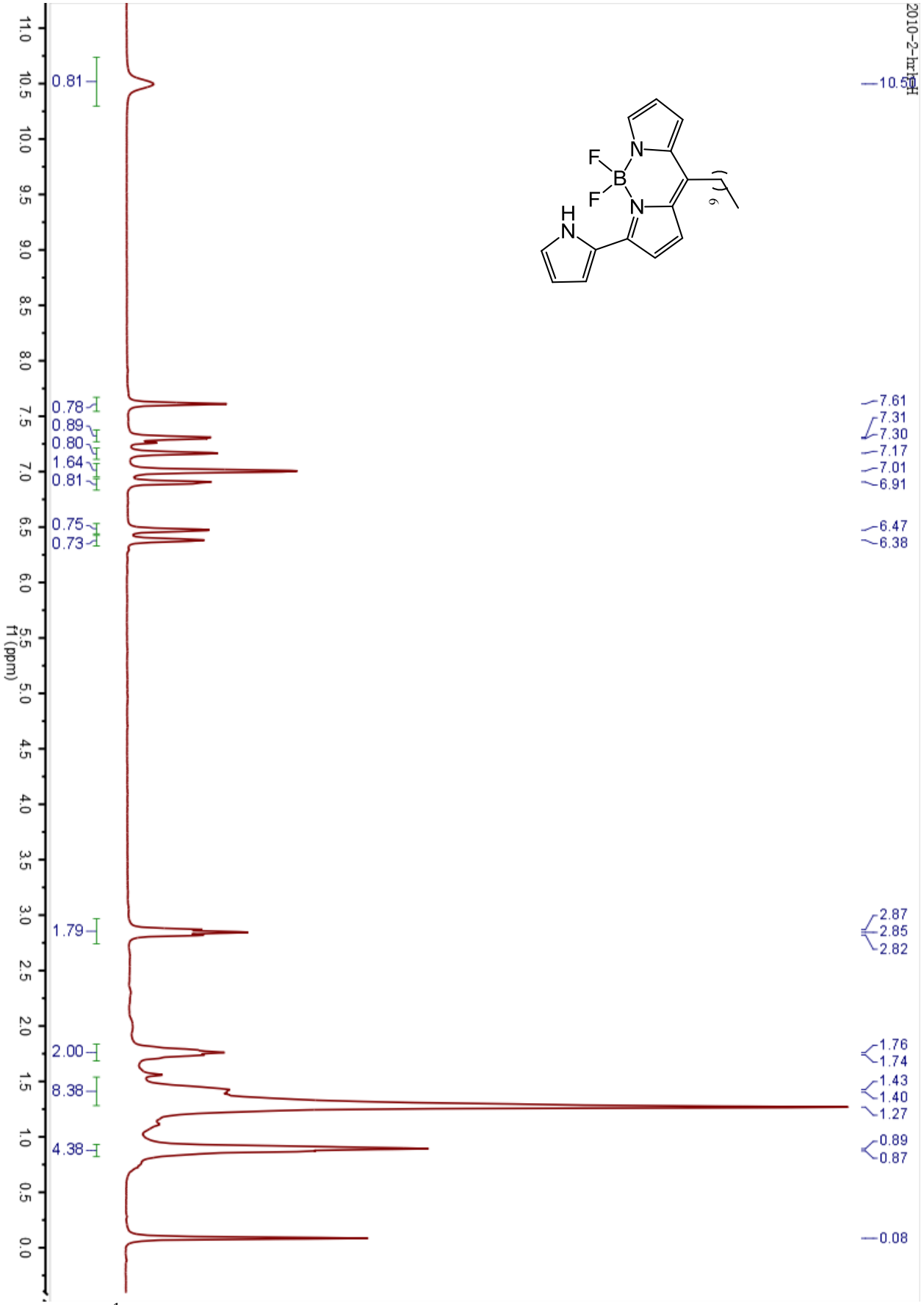


Figure S23: ^{1}H NMR spectrum of BODIPY dye **2c** in $CDCl_3$ solution

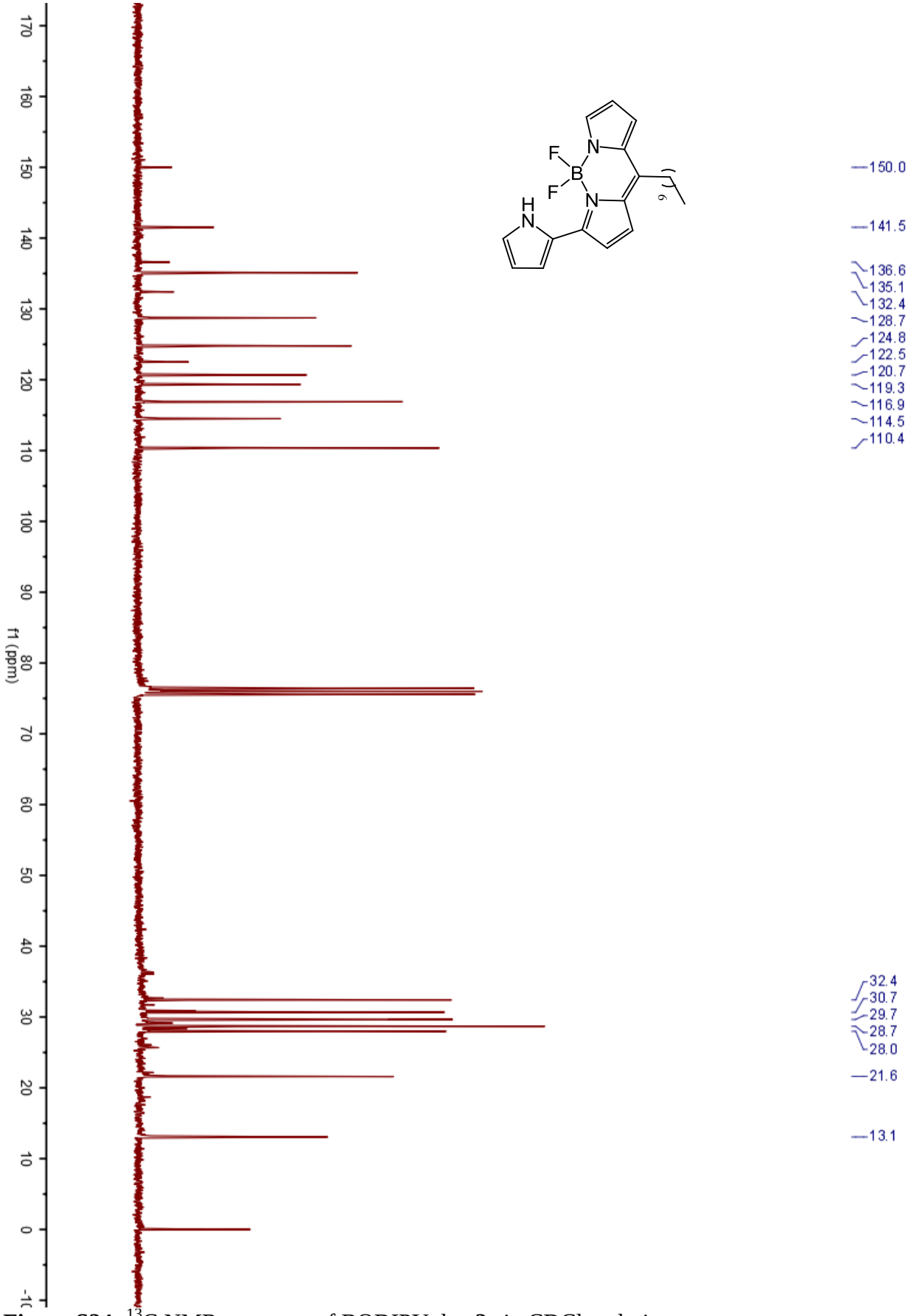


Figure S24: ^{13}C NMR spectrum of BODIPY dye **2c** in $CDCl_3$ solution

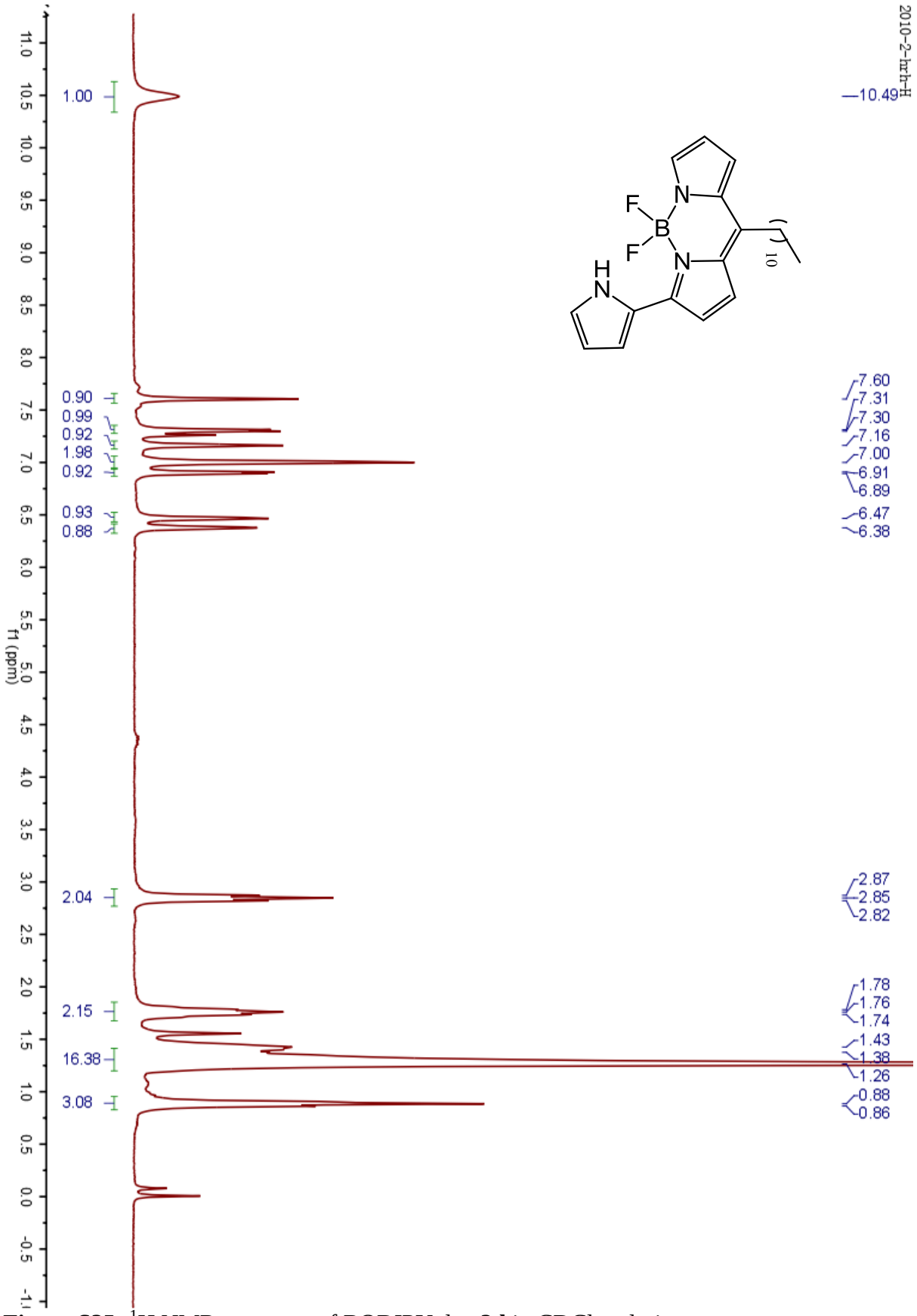


Figure S25: ^{1}H NMR spectrum of BODIPY dye **2d** in $CDCl_3$ solution

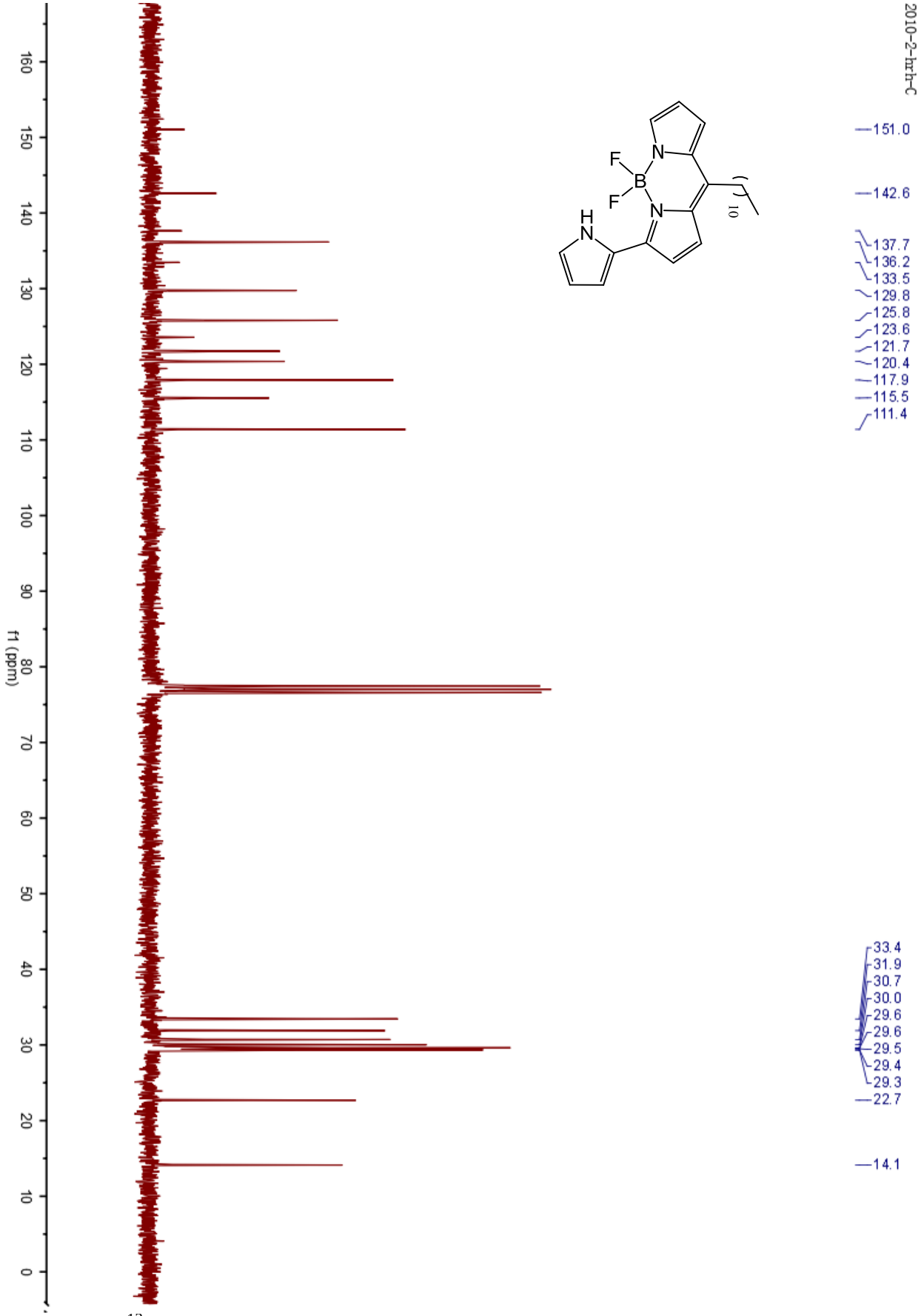


Figure S26: ^{13}C NMR spectrum of BODIPY dye **2d** in $CDCl_3$ solution

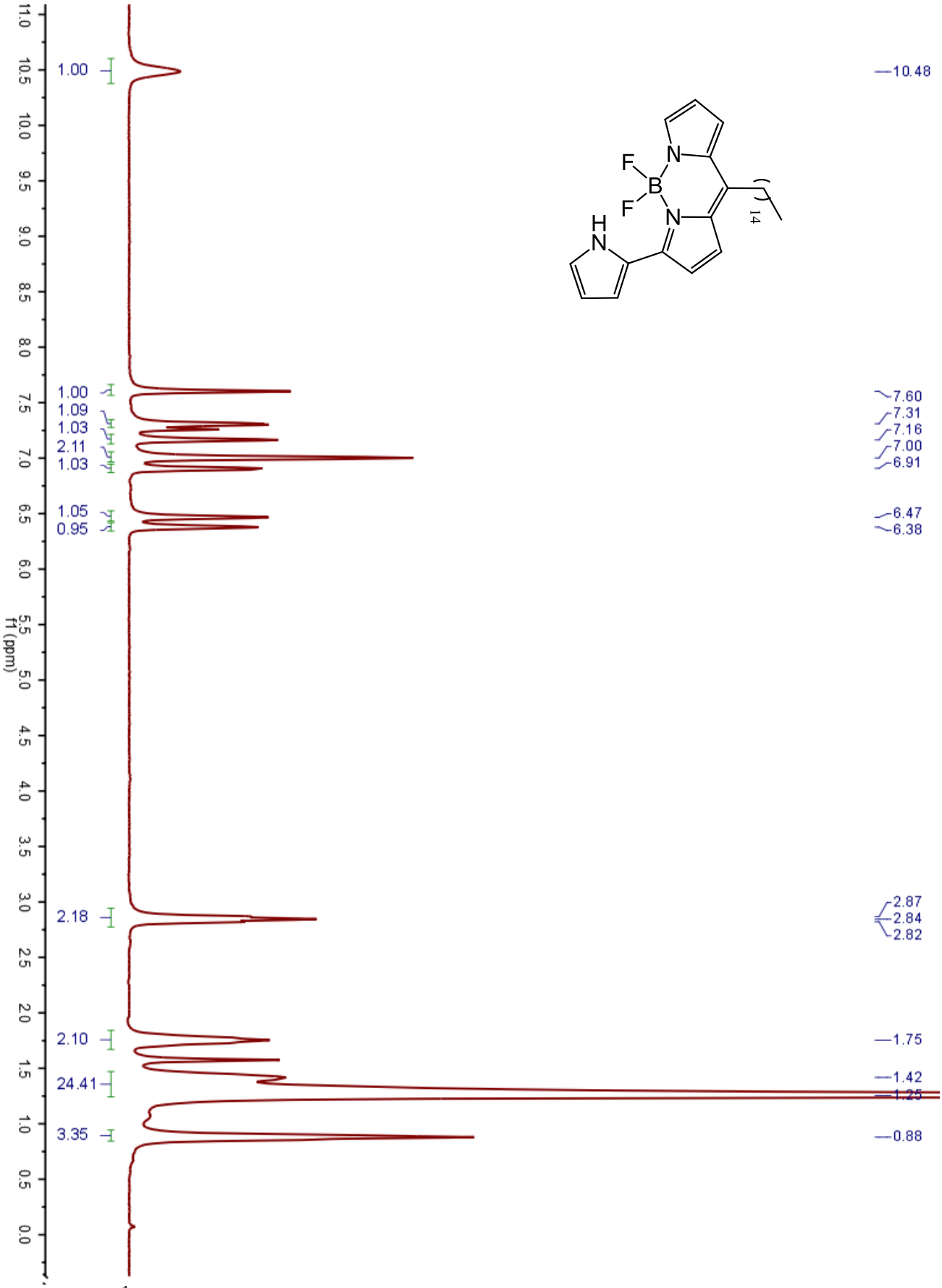


Figure S27: ^{1}H NMR spectrum of BODIPY dye **2e** in $CDCl_3$ solution

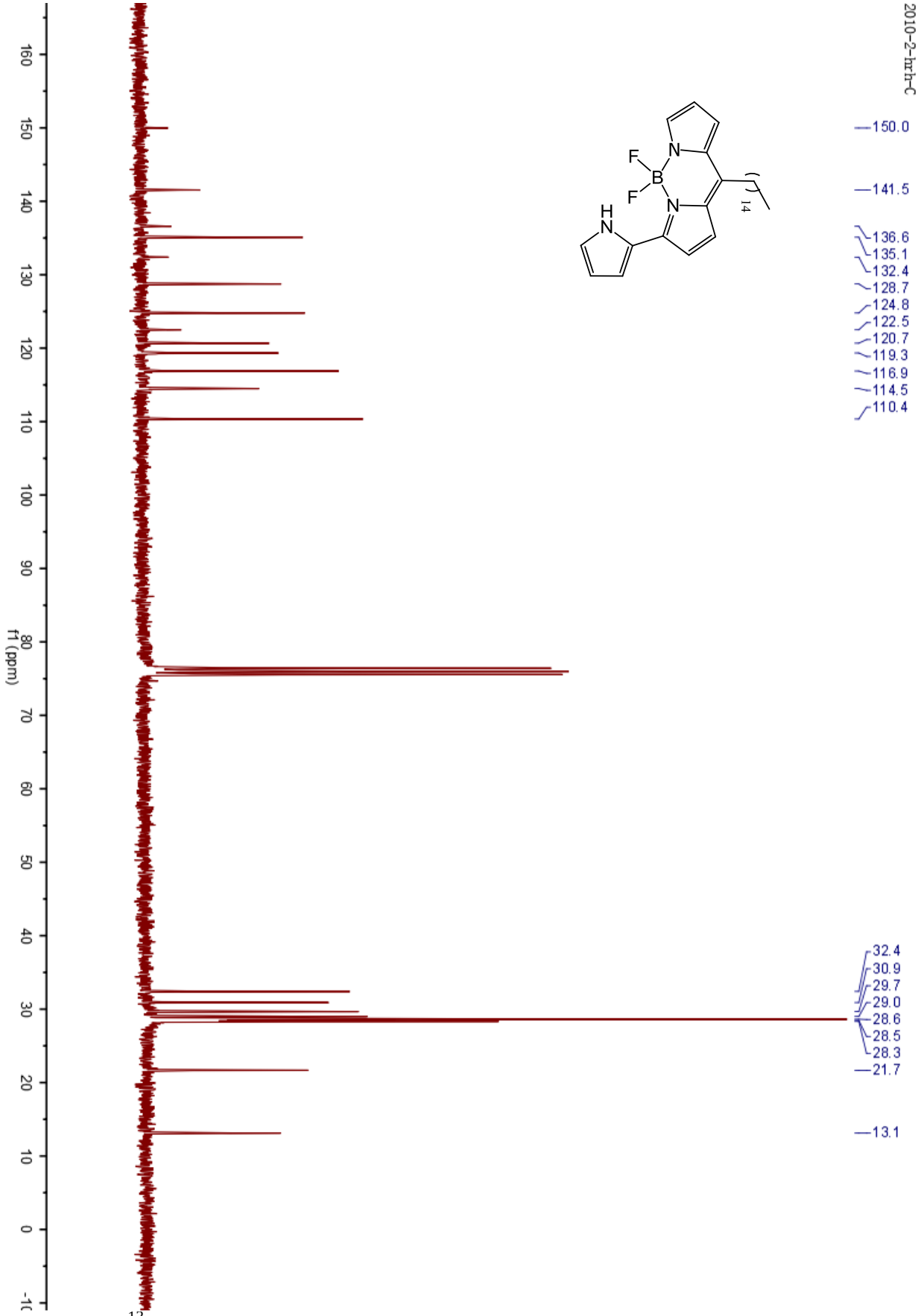


Figure S28: ^{13}C NMR spectrum of BODIPY dye **2e** in $CDCl_3$ solution

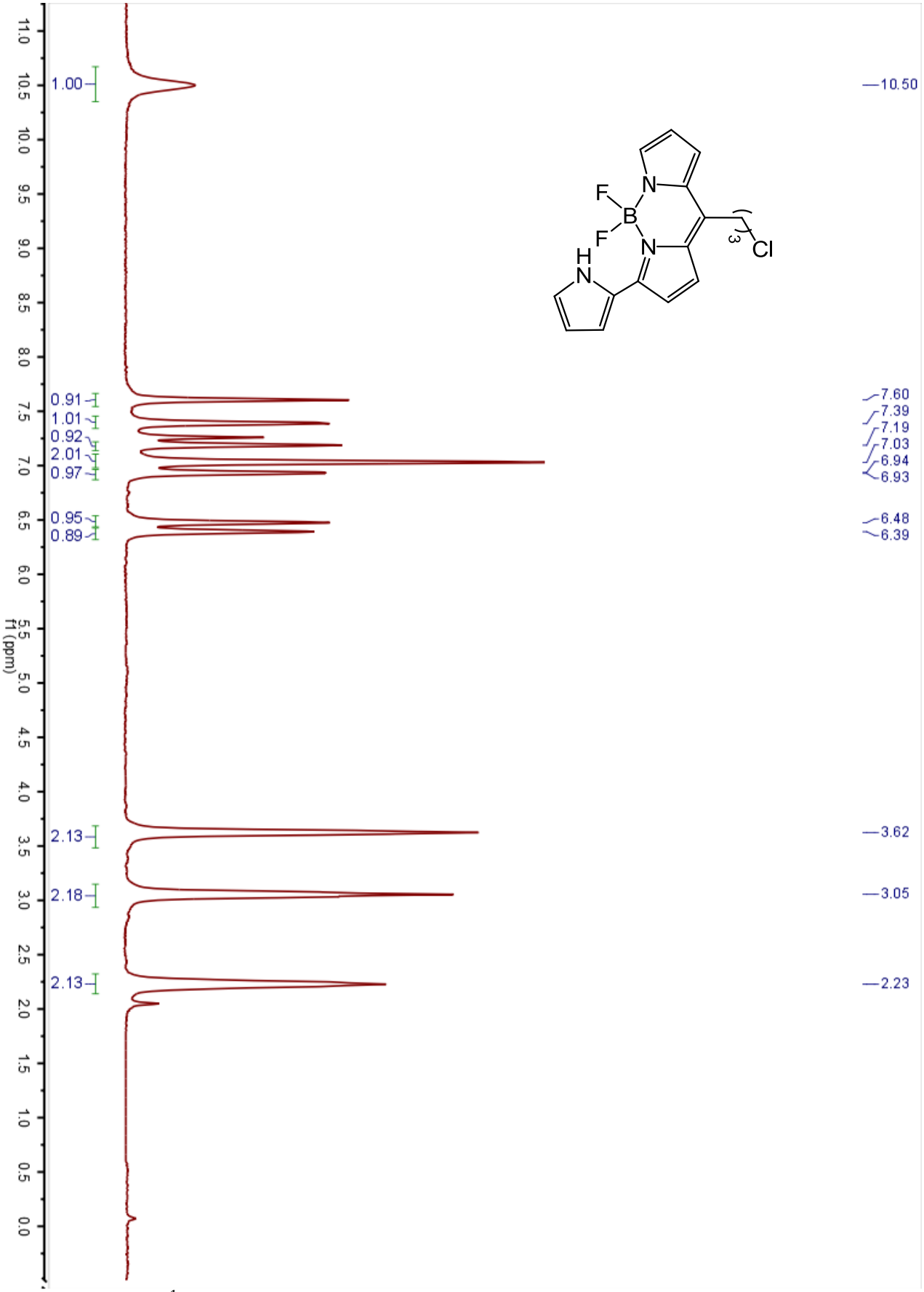


Figure S29: ^{1}H NMR spectrum of BODIPY dye **2f** in $CDCl_3$ solution

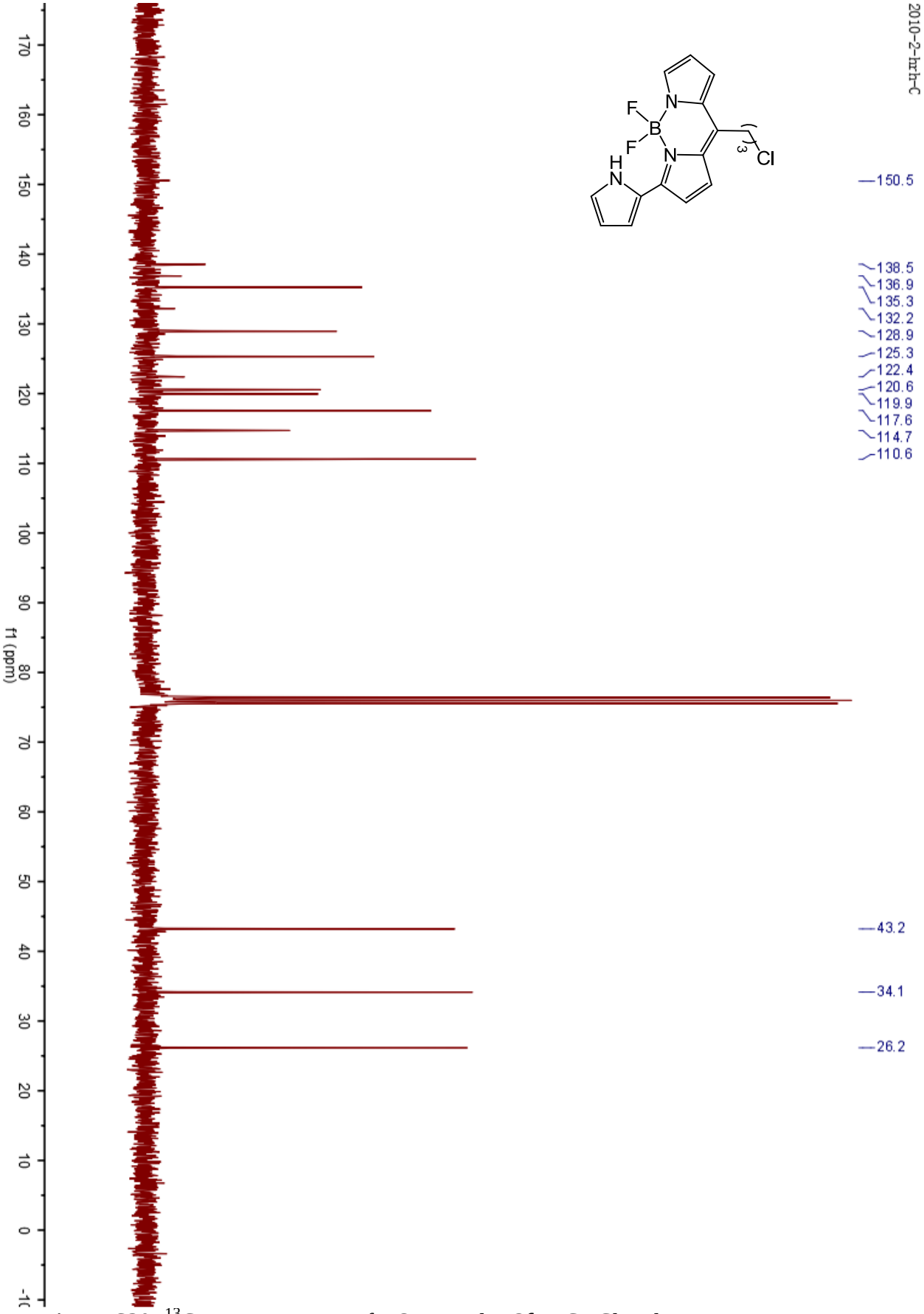


Figure S30: ^{13}C NMR spectrum of BODIPY dye **2f** in $CDCl_3$ solution

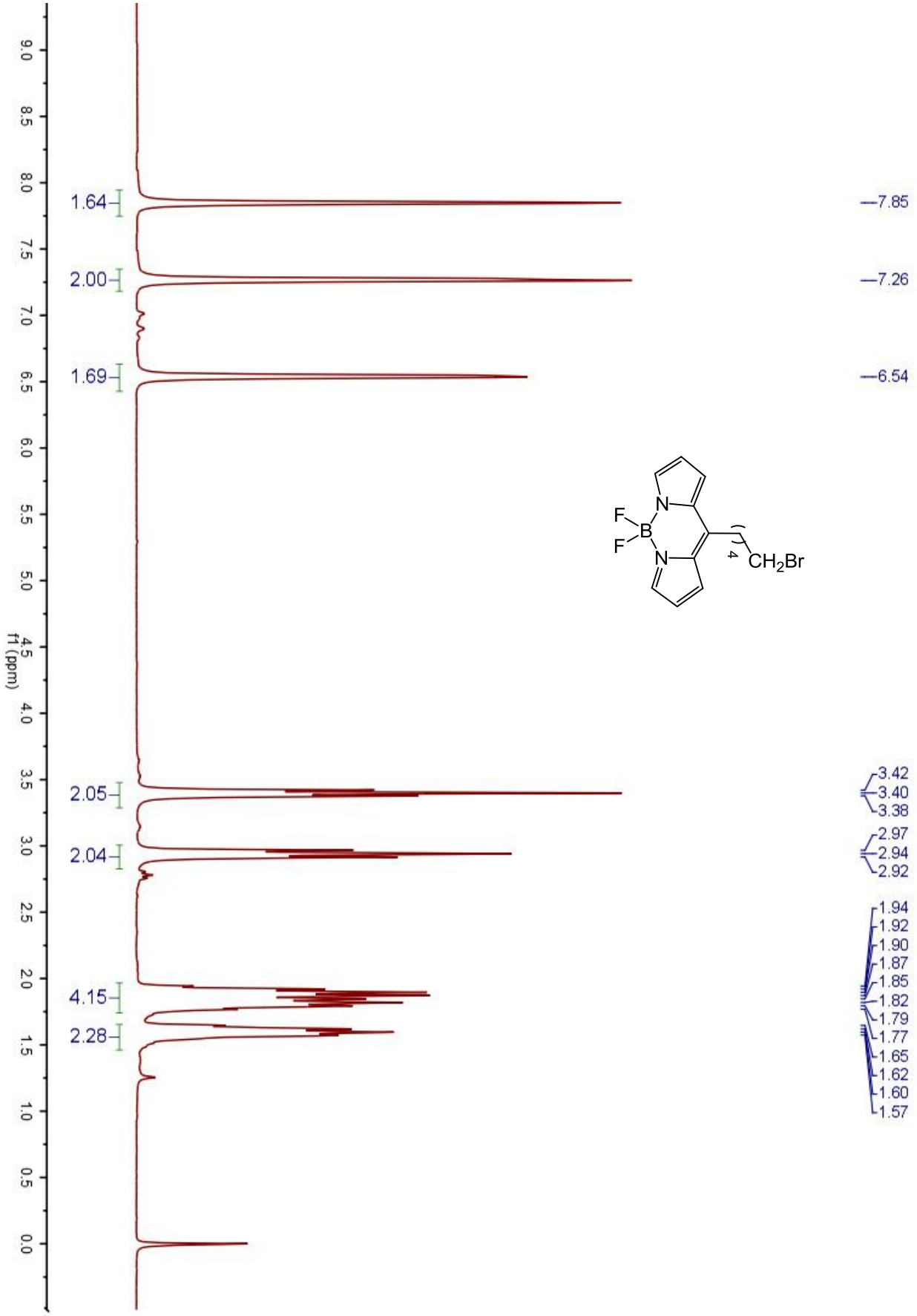


Figure S31: ^{1}H NMR spectrum of BODIPY dye **1g** in $CDCl_3$ solution

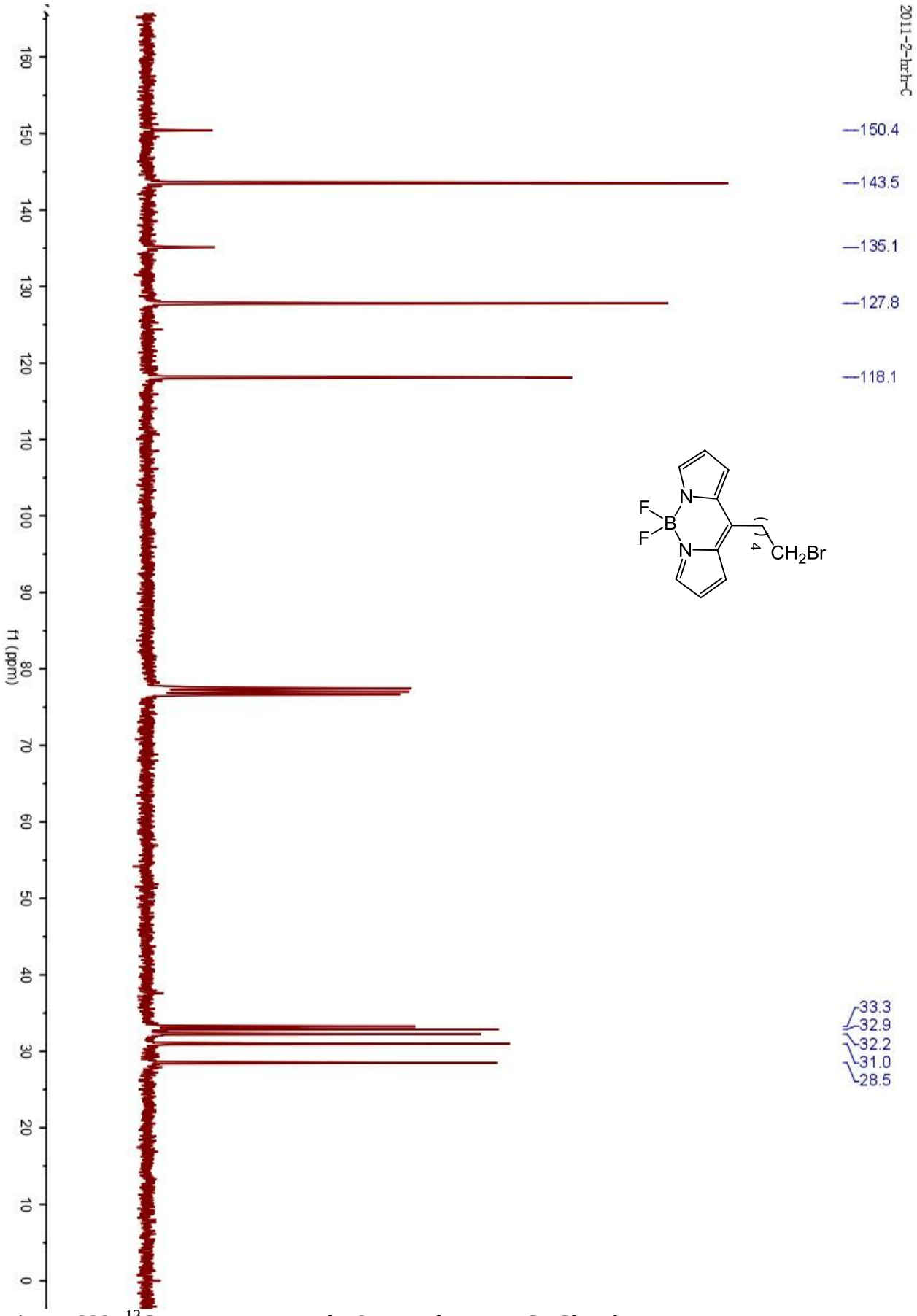


Figure S32: ^{13}C NMR spectrum of BODIPY dye **1g** in $CDCl_3$ solution

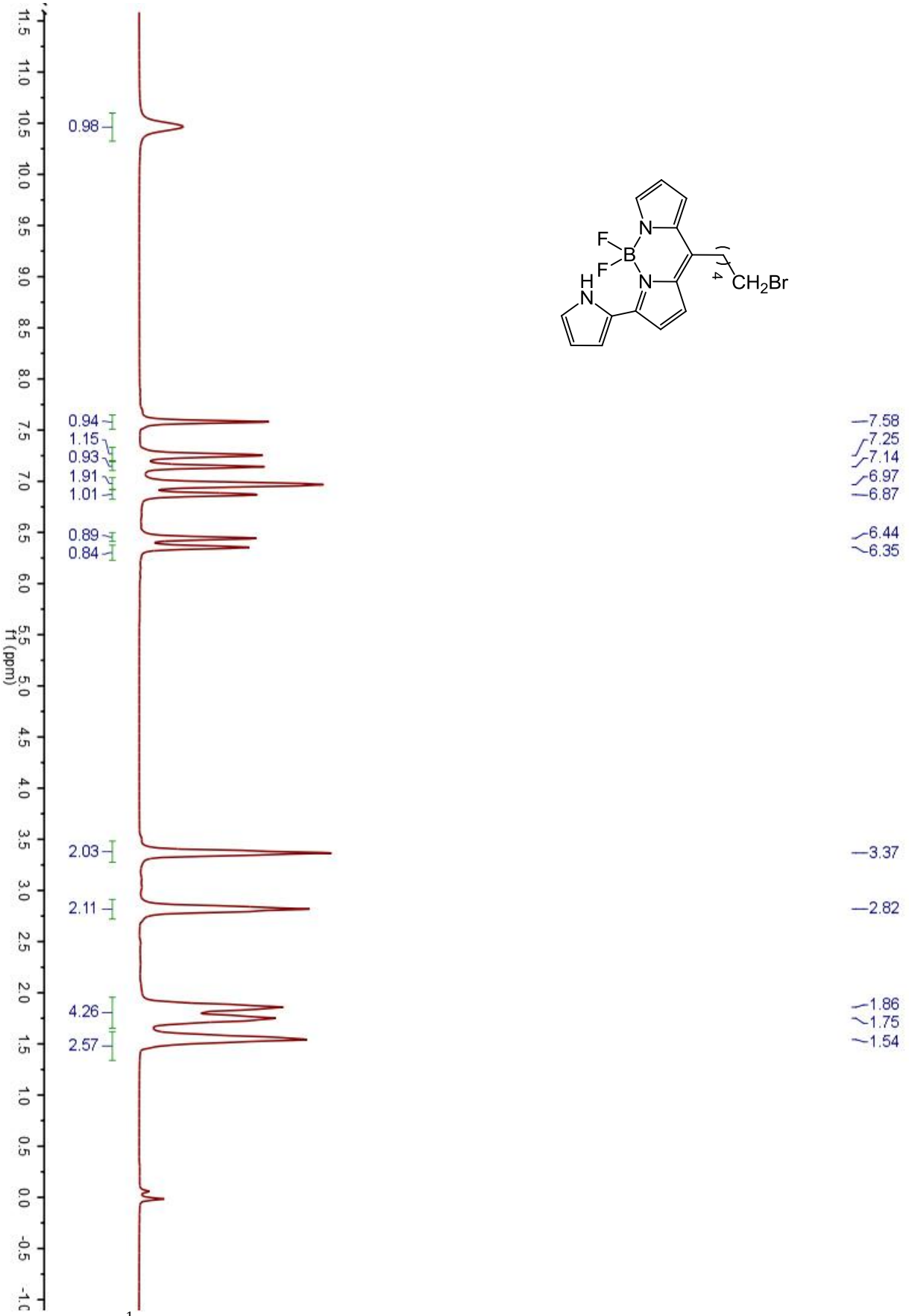


Figure S33: ^{1}H NMR spectrum of BODIPY dye **2g** in $CDCl_3$ solution

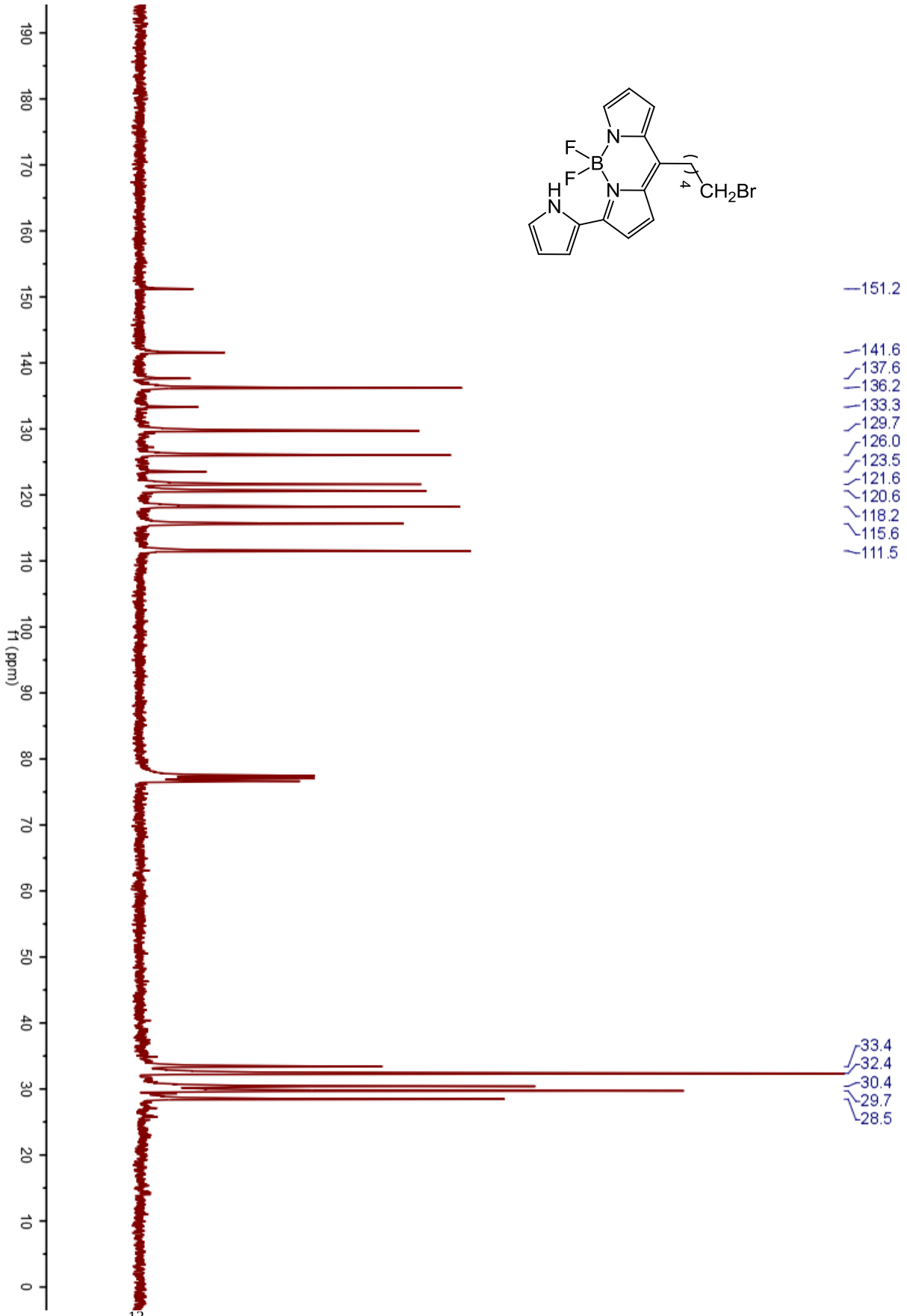


Figure S34: ^{13}C NMR spectrum of BODIPY dye **2g** in $CDCl_3$ solution

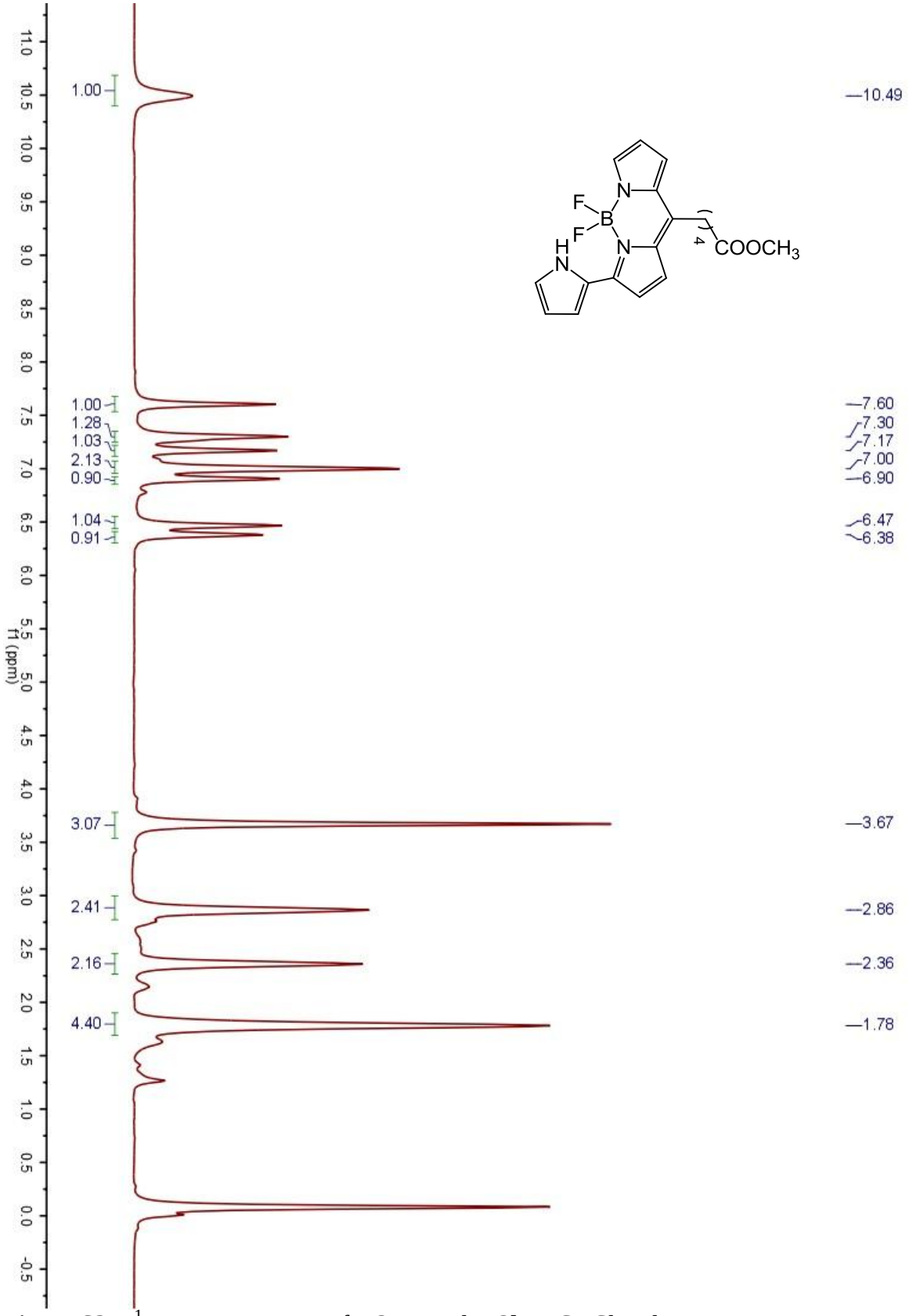


Figure S35: ^{1}H NMR spectrum of BODIPY dye **2h** in $CDCl_3$ solution

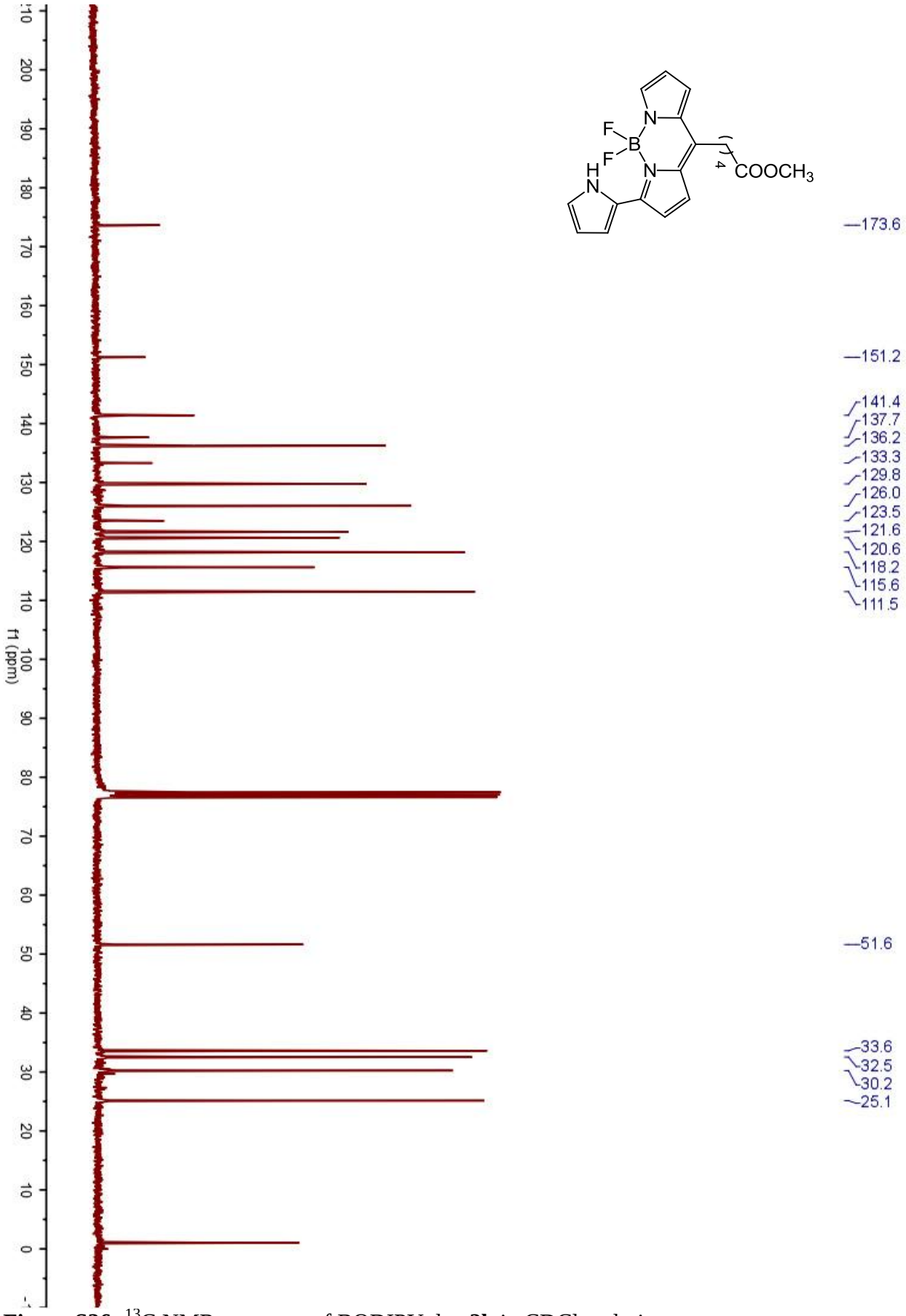


Figure S36: ^{13}C NMR spectrum of BODIPY dye **2h** in $CDCl_3$ solution

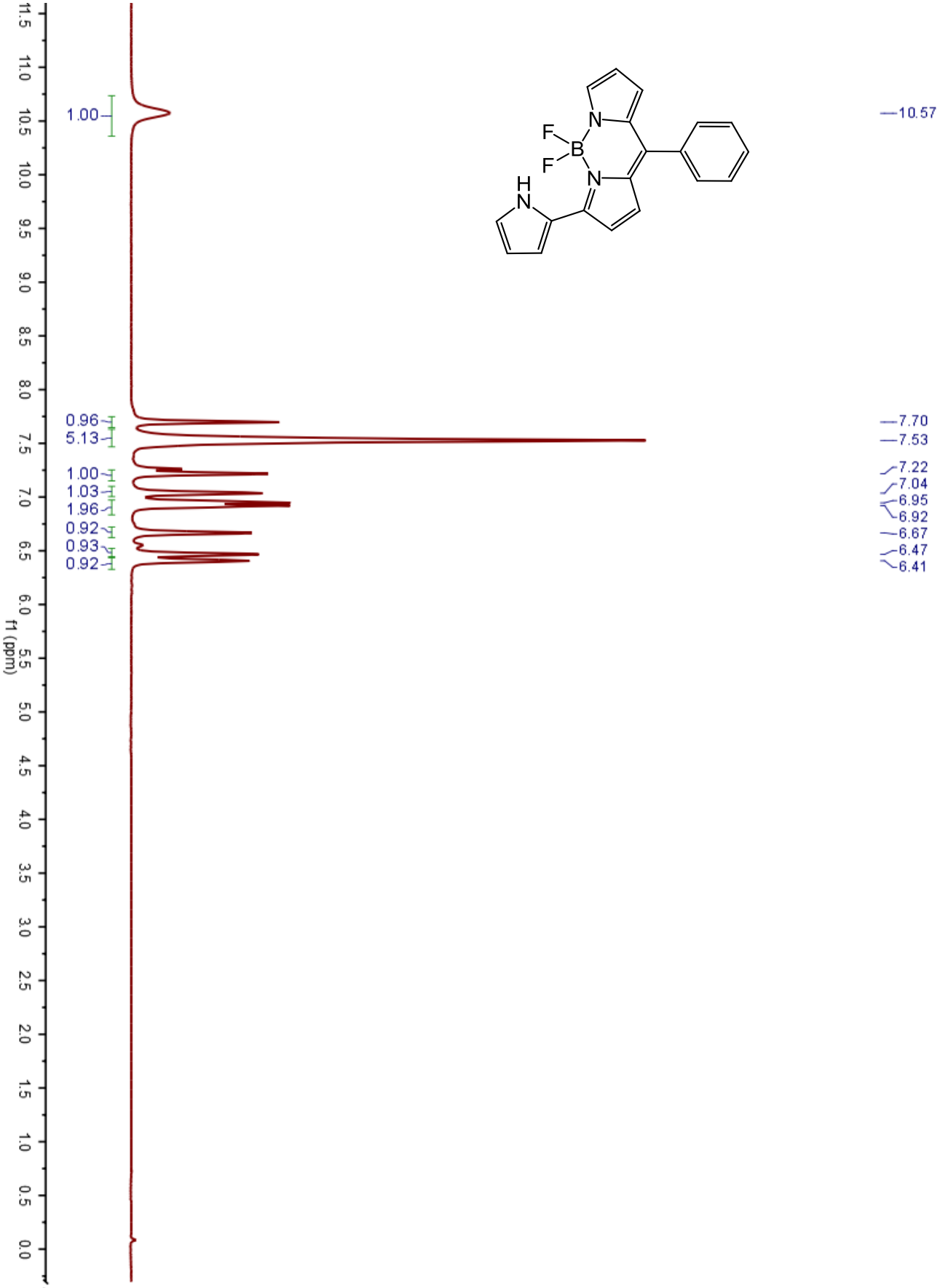


Figure S37: ^{1}H NMR spectrum of BODIPY dye **2i** in $CDCl_3$ solution

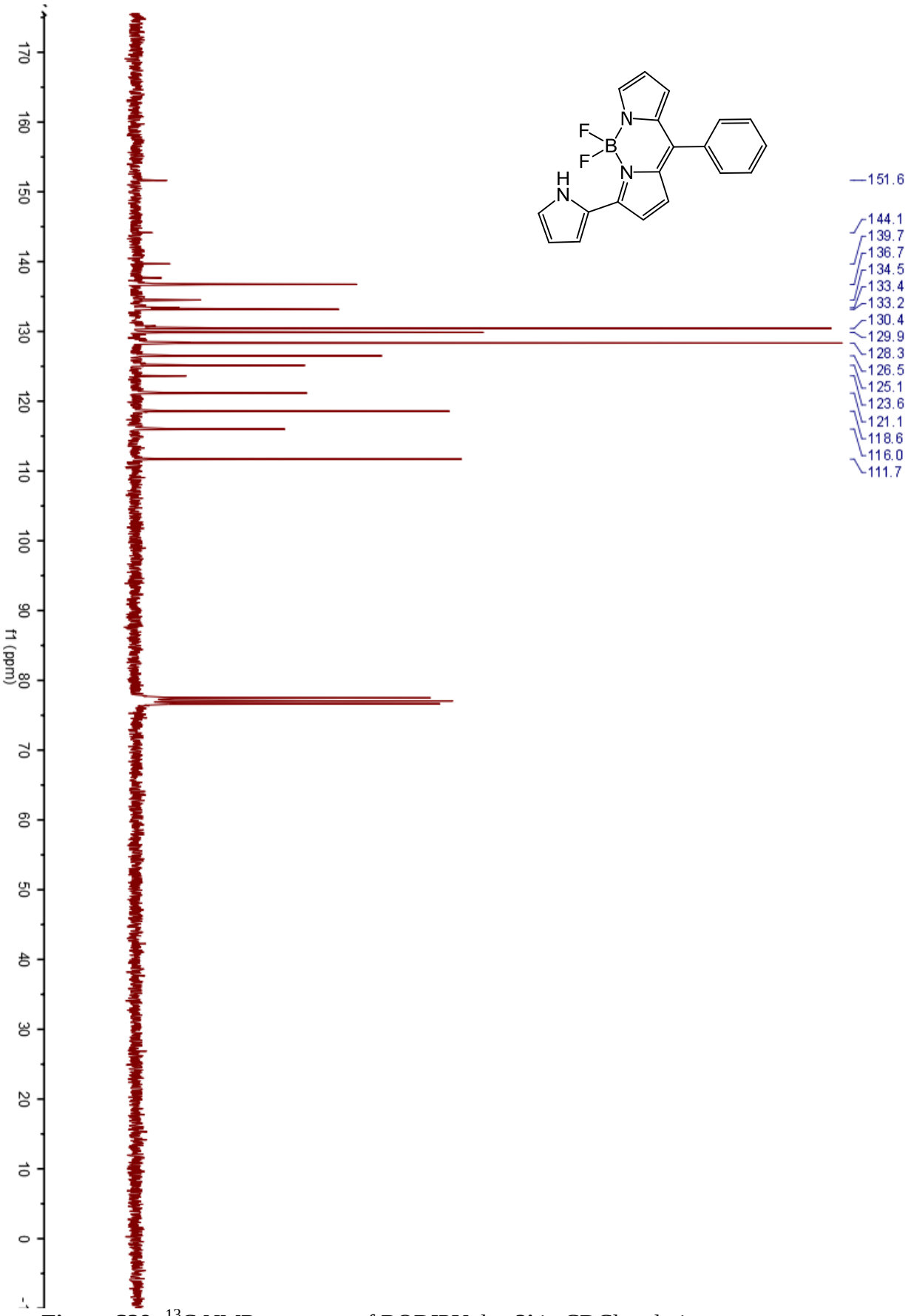


Figure S38: ^{13}C NMR spectrum of BODIPY dye **2i** in $CDCl_3$ solution

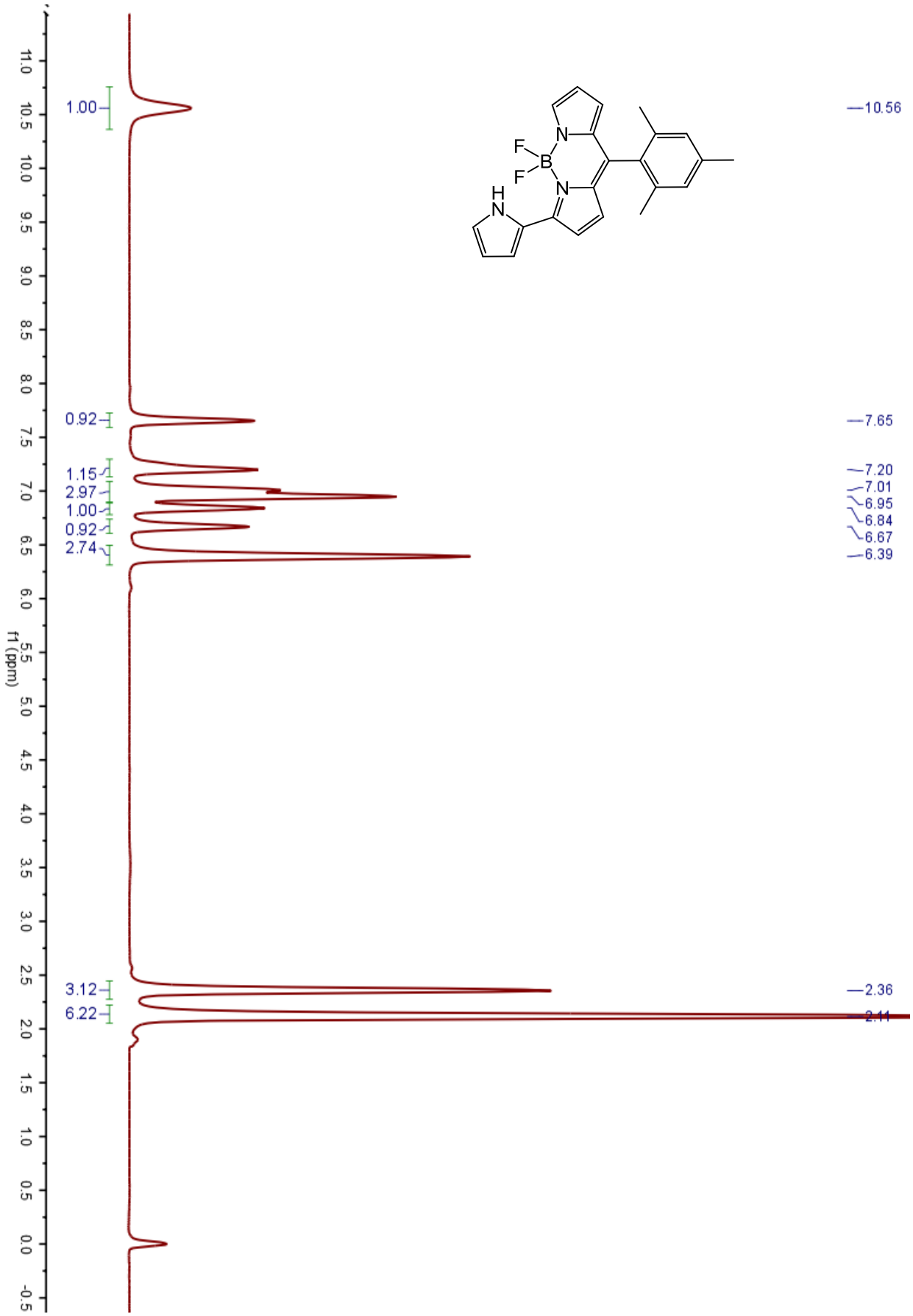


Figure S39: ^{1}H NMR spectrum of BODIPY dye **2j** in $CDCl_3$ solution

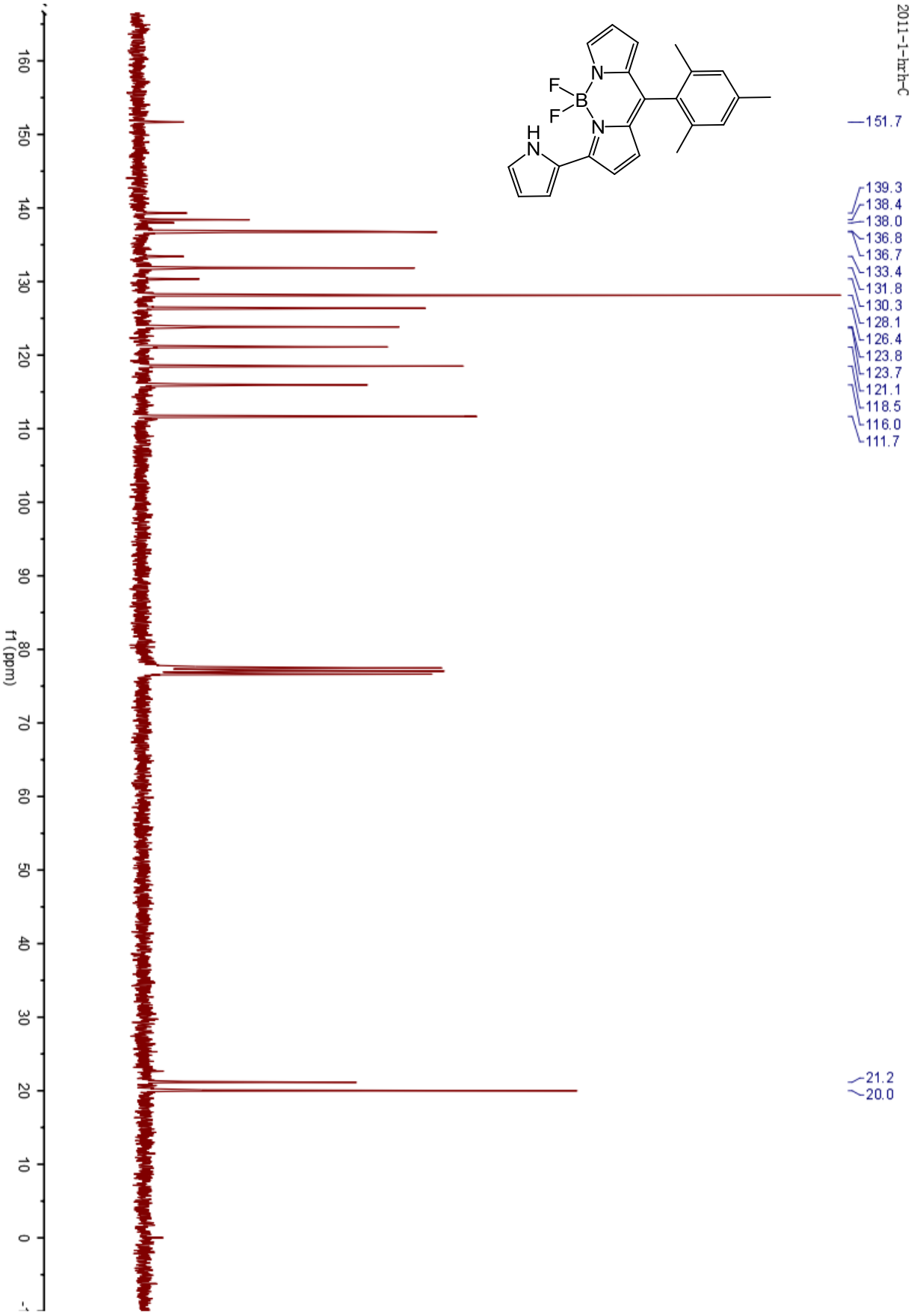


Figure S40: ^{13}C NMR spectrum of BODIPY dye **2j** in $CDCl_3$ solution

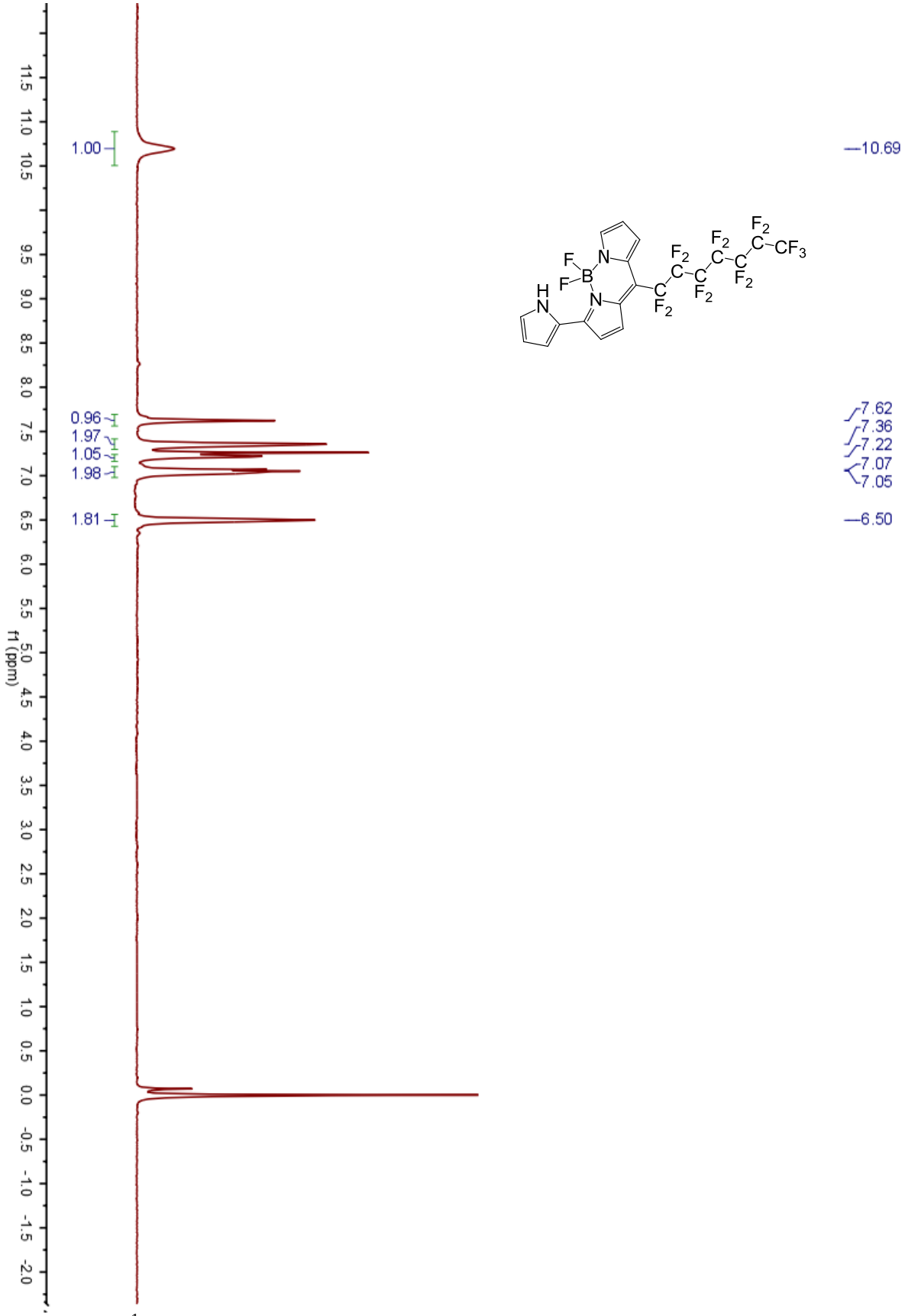


Figure S41: ^{1}H NMR spectrum of BODIPY dye **2k** in $CDCl_3$ solution

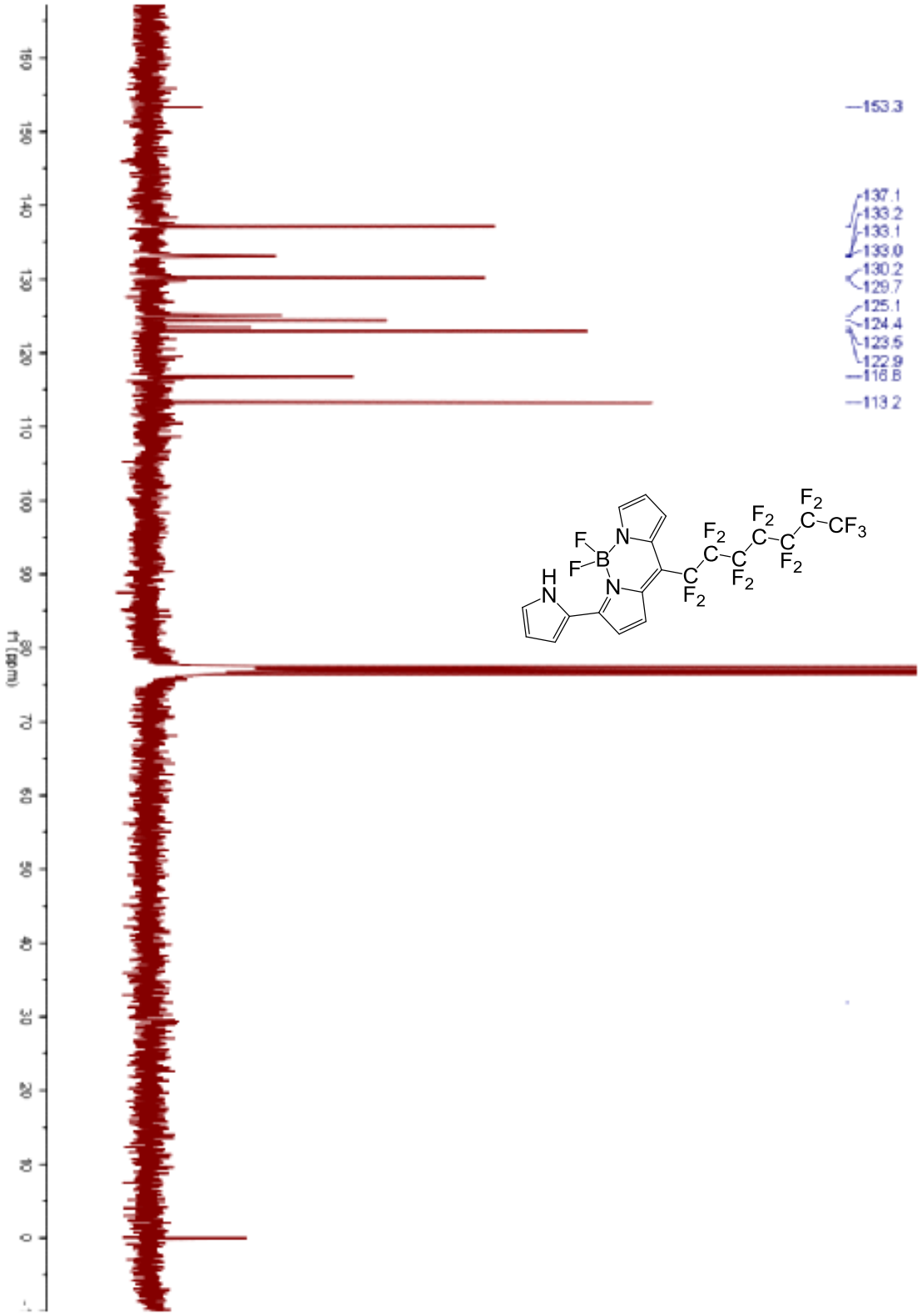


Figure S42: ^{13}C NMR spectrum of BODIPY dye **2k** in $CDCl_3$ solution

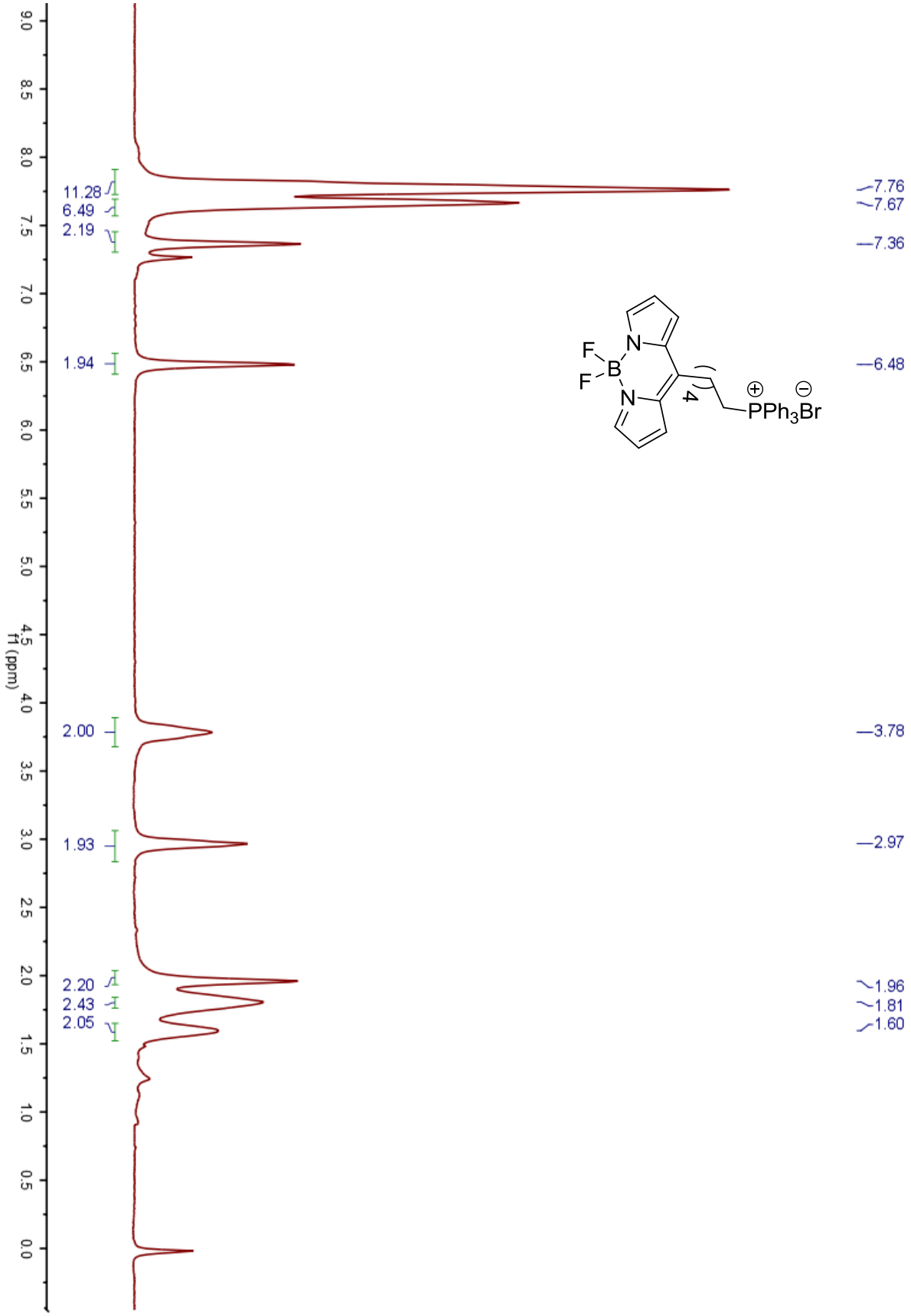


Figure S43: ^{1}H NMR spectrum of BODIPY dye **3** in $CDCl_3$ solution

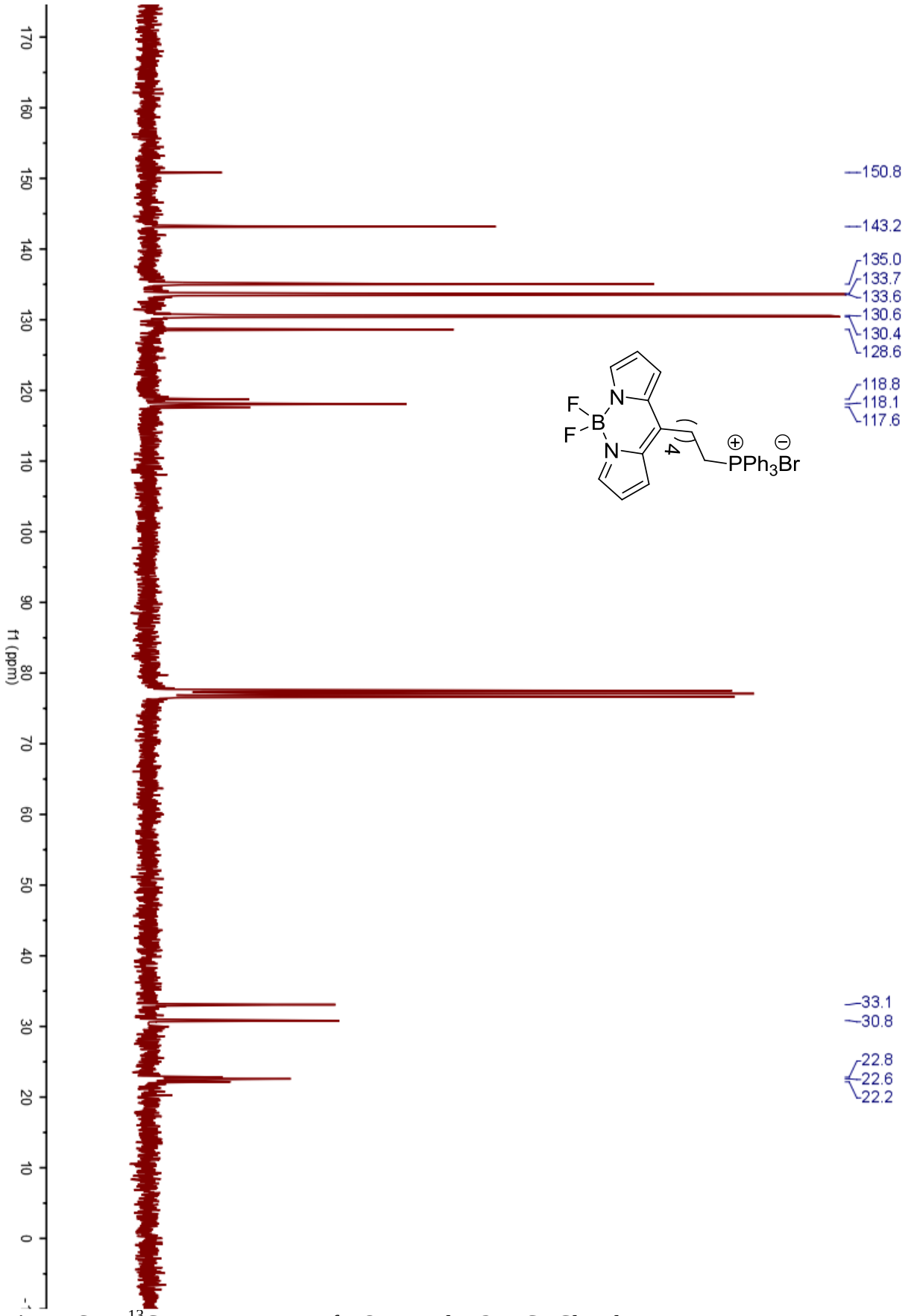


Figure S44: ^{13}C NMR spectrum of BODIPY dye **3** in $CDCl_3$ solution

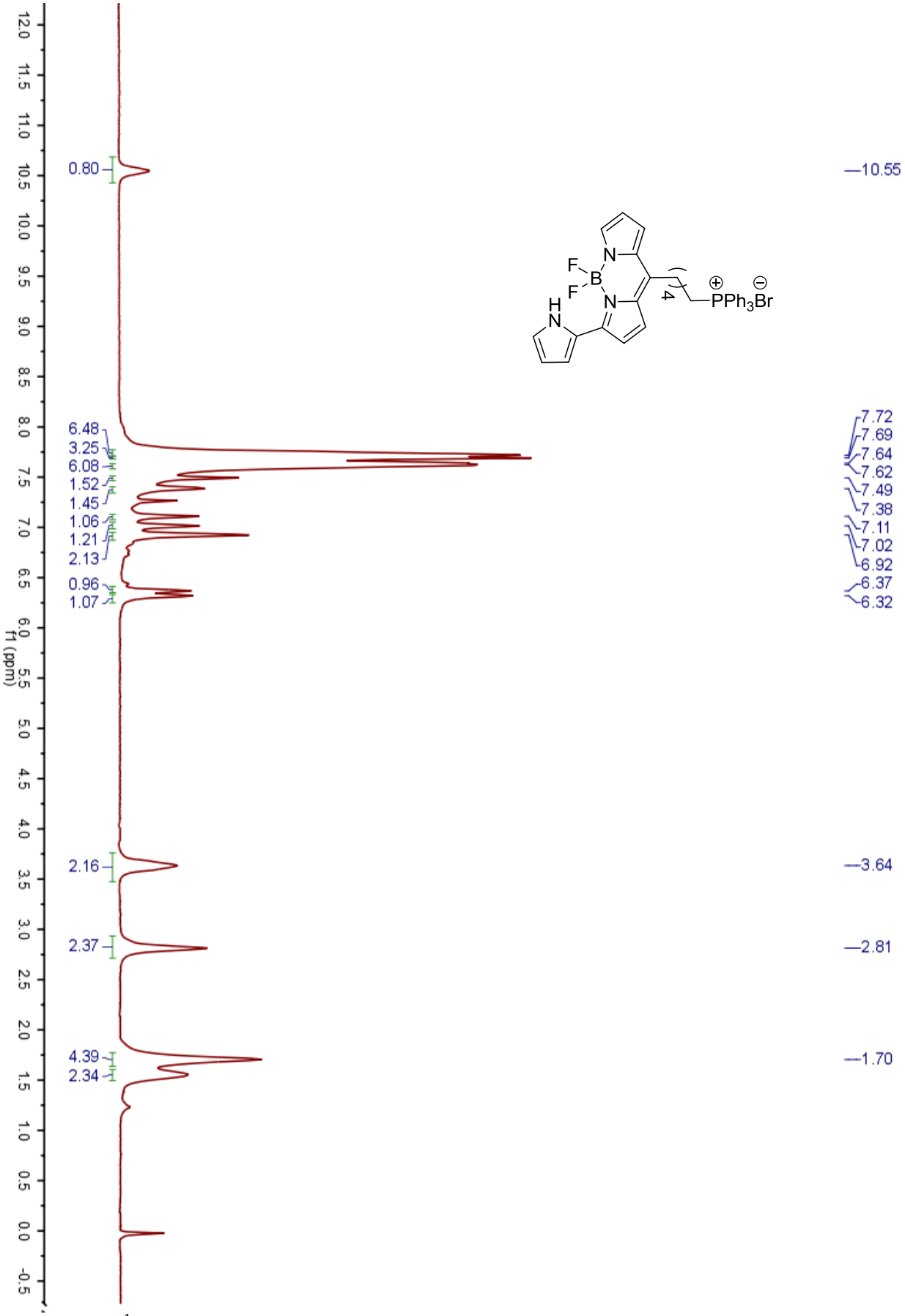


Figure S45: ^{1}H NMR spectrum of BODIPY dye **4** in $CDCl_3$ solution

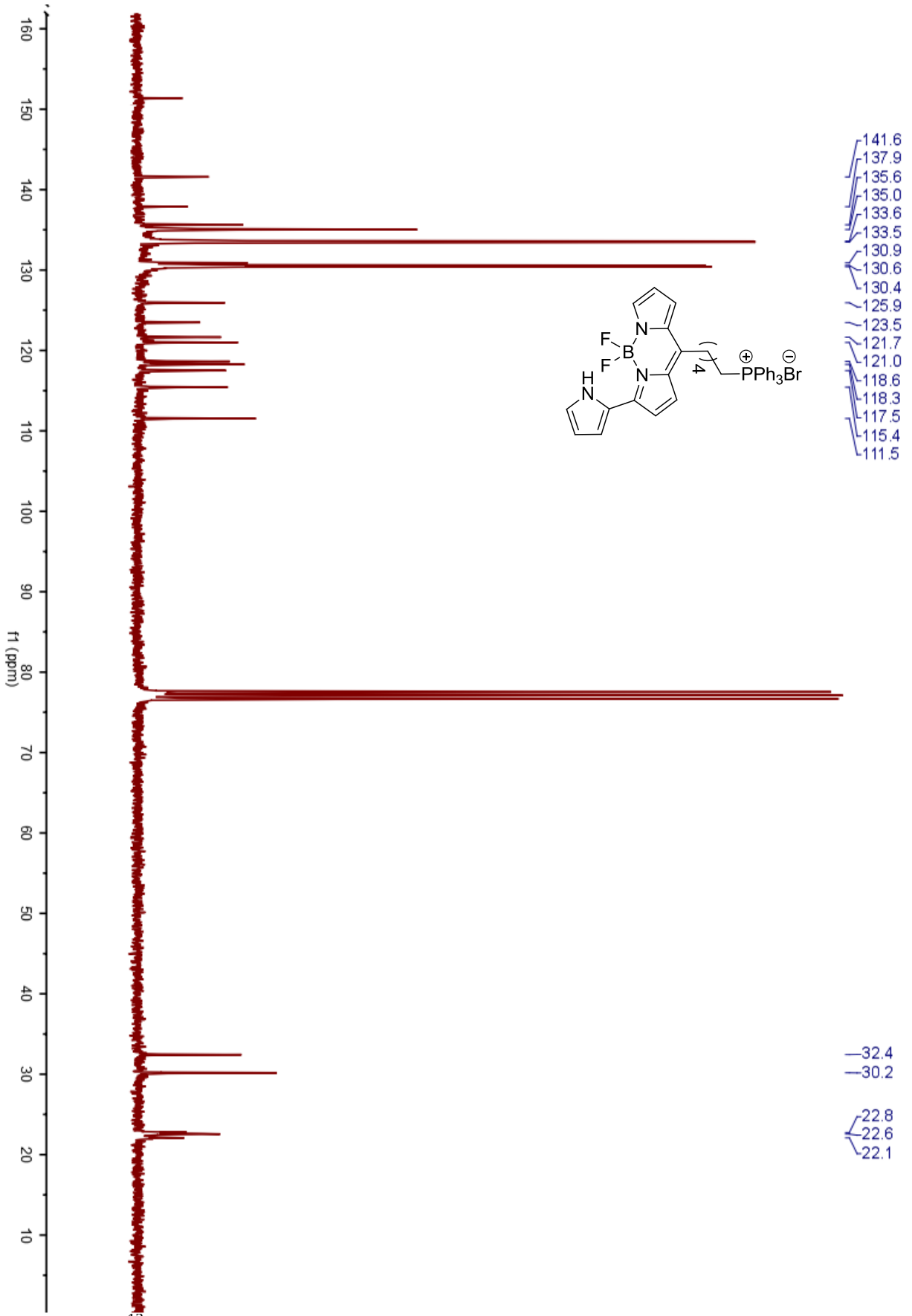
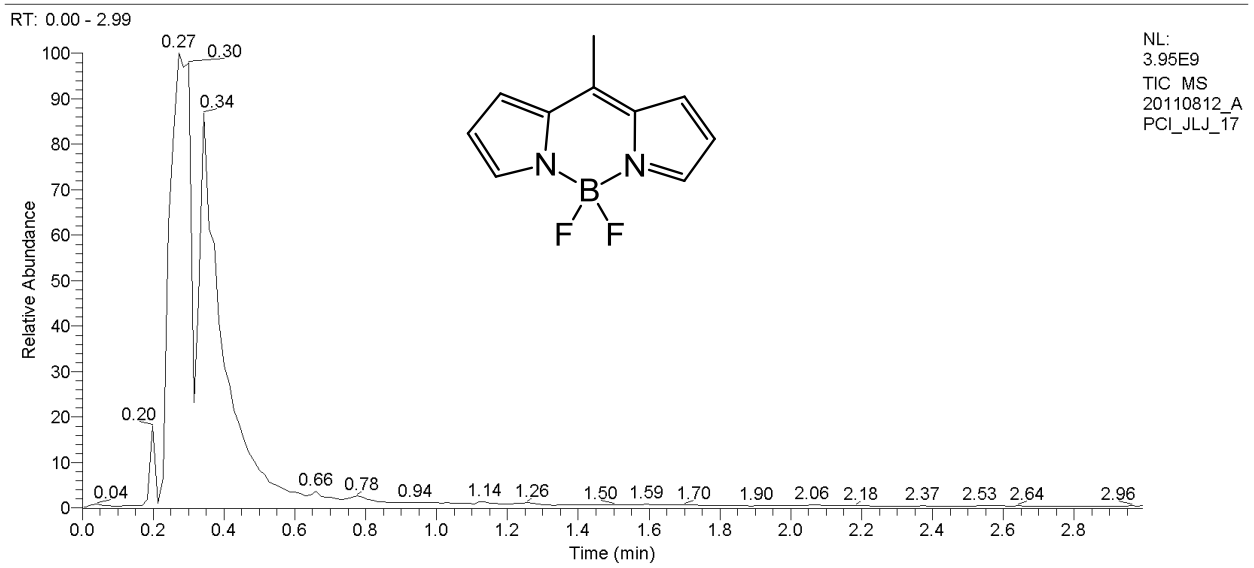
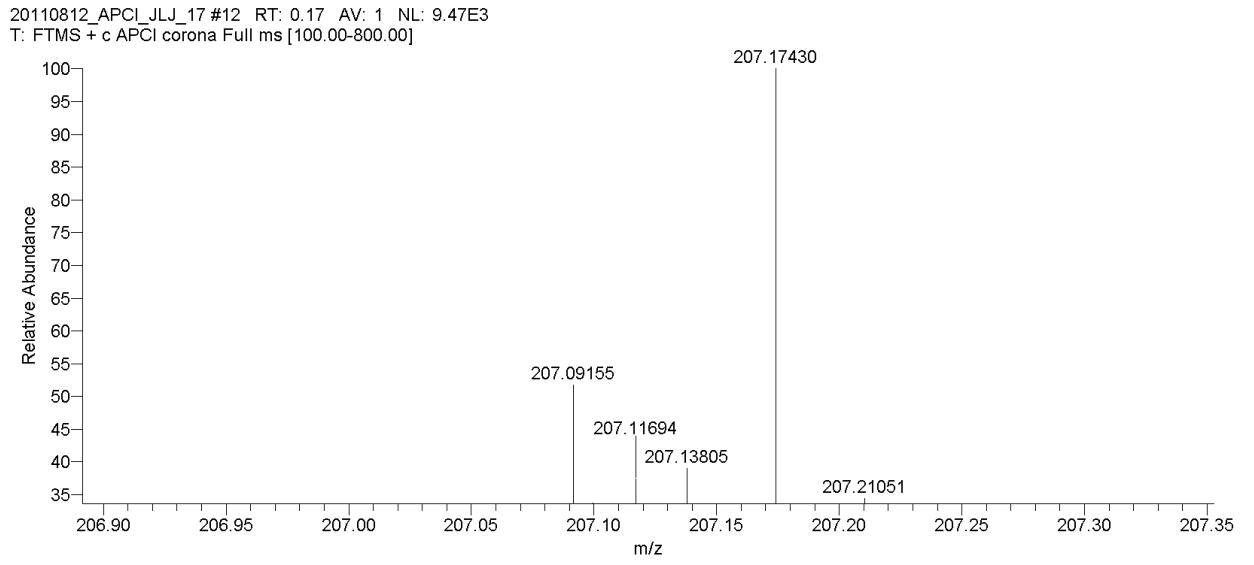


Figure S46: ^{13}C NMR spectrum of BODIPY dye **4** in $CDCl_3$ solution

6. High resolution mass spectroscopes for all new compounds

E:\data\20110812\20110812_APCI_JLJ_17 2011-8-12 13:33:57





20110812_APCI_JLJ_17#12 RT: 0.17
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
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207.09972	3189.1	0.08	207.09717	2.54	$C_4H_{10}ON_6BF_2$
207.11694	3543.4	0.09	207.11511	1.83	$C_{12}H_{14}BF_2$
207.13805	3689.1	0.09	207.13490	3.15	$C_7H_{16}ON_3BF_2$
207.17430	9468.8	0.24	207.17263	1.67	$C_{10}H_{22}OBF_2$
207.21051	3264.6	0.08	207.18386	26.65	$C_9H_{22}N_2BF_2$
207.89641	2698.9	0.07	207.91984	-23.44	$C_4ONB^{81}BrF_2$
208.08688	37114.0	0.92	208.08655	0.33	$C_{11}H_{11}OBF_2$
208.11197	4030.3	0.10	208.11036	1.61	$C_{11}H_{13}NBF_2$
209.09013	4241.0	0.11	209.08767	2.46	$C_2H_8ON_8BF_2$
209.09637	6130.2	0.15	209.09438	2.00	$C_{11}H_{12}OBF_2$
209.13252	5737.4	0.14	209.13076	1.76	$C_{12}H_{16}BF_2$

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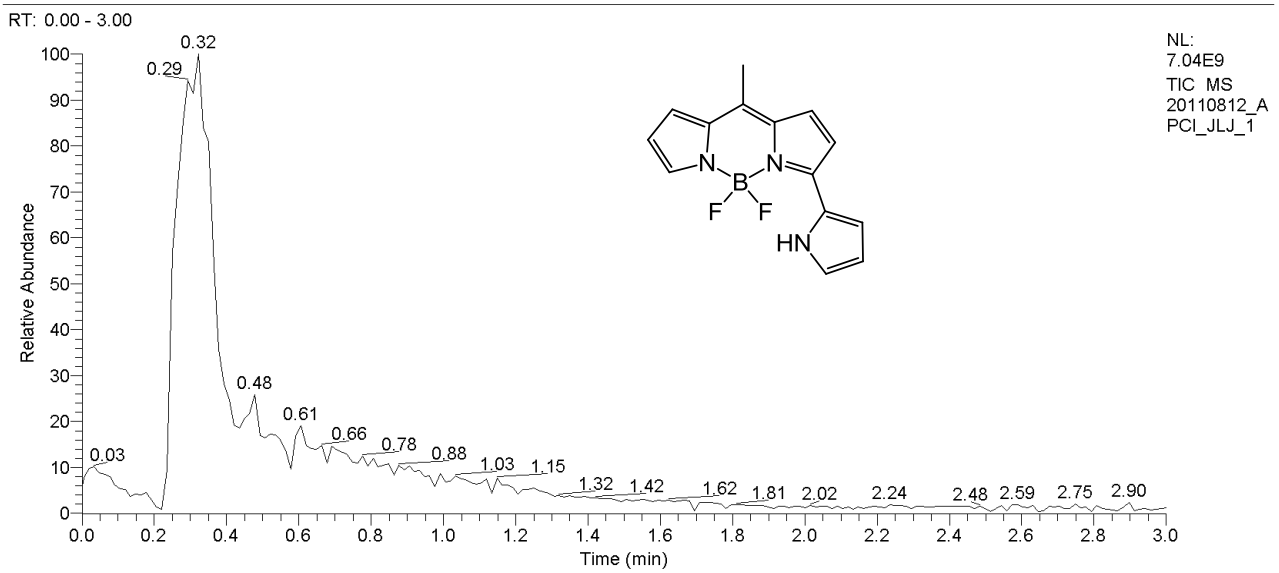

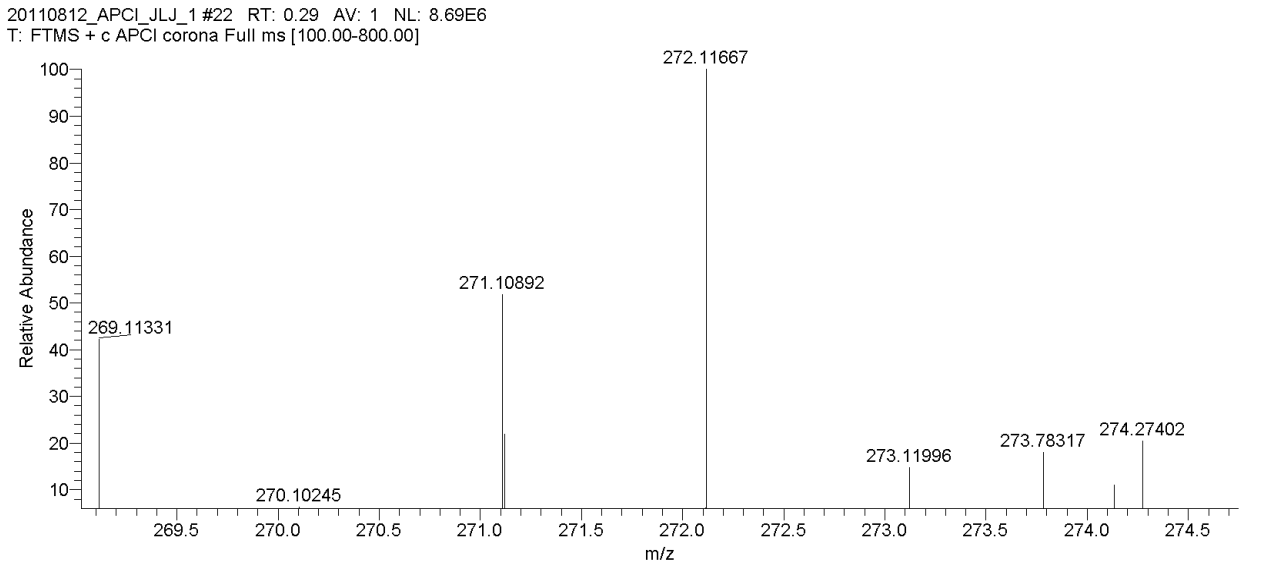

20110812_APCI_JLJ_1#22 RT: 0.29
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
263.13409	22592186.0	1.23	263.13462	-0.53	$C_6H_{14}ON_8BF_2$
264.13046	100815024.0	5.47	264.12987	0.59	$C_5H_{13}ON_9BF_2$
265.13376	14138010.0	0.77	265.13183	1.93	$C_{13}H_{16}ON_2BF_2$
272.11667	8692419.0	0.47	272.11651	0.16	$C_{14}H_{13}N_3BF_2$
307.17703	8663618.0	0.47	307.17743	-0.40	$C_{14}H_{20}N_5BF_2$
308.17325	46491636.0	2.52	308.17268	0.57	$C_{13}H_{19}N_6BF_2$
479.21899	35924984.0	1.95	479.21914	-0.14	$C_{12}H_{30}O_9N_8BF_2$
480.21533	312605856.0	16.97	480.21522	0.11	$C_{27}H_{29}O_4NBF_2$
481.21176	595986048.0	32.35	481.21181	-0.05	$C_{27}H_{24}N_6BF_2$
482.21497	184487664.0	10.01	482.21561	-0.64	$C_{22}H_{25}O_2N_8BF_2$
483.21829	23407258.0	1.27	483.21808	0.22	$C_{16}H_{30}O_8N_6BF_2$
495.22717	9407821.0	0.51	495.22746	-0.29	$C_{28}H_{26}N_6BF_2$
579.53522	18781084.0	1.02	579.50514	30.08	$C_{27}H_{62}O_2N_8BF_2$

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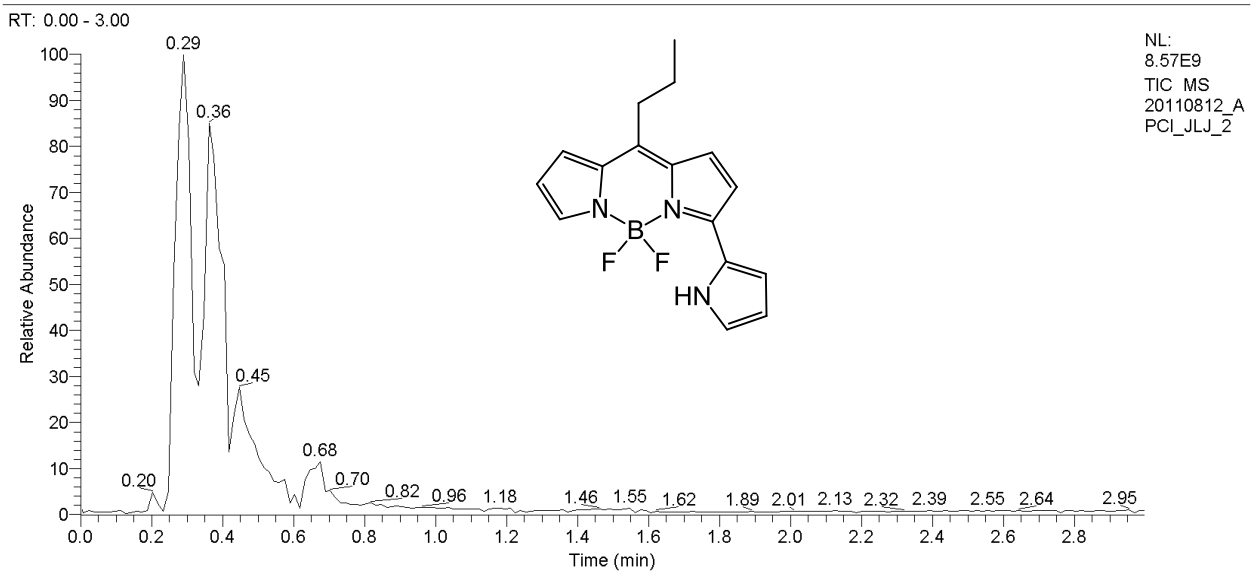

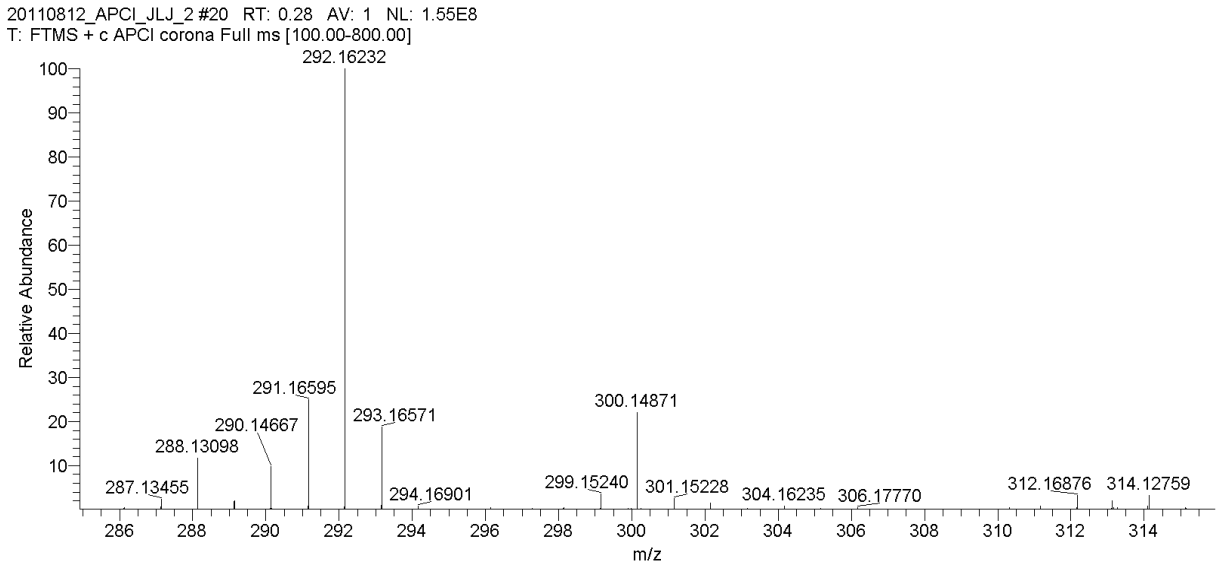

20110812_APCI_JLJ_2#20 RT: 0.28
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
292.16232	155280976.0	6.72	292.16654	-4.21	$C_{14}H_{19}N_4BF_2$
292.16861	6068174.0	0.26	292.16654	2.07	$C_{14}H_{19}N_4BF_2$
293.16571	29188022.0	1.26	293.16178	3.93	$C_{13}H_{18}N_5BF_2$
299.15240	5688538.5	0.25	299.15843	-6.03	$C_9H_{16}N_9BF_2$
300.14871	34242248.0	1.48	300.14781	0.90	$C_{16}H_{17}N_3BF_2$
312.16876	4958324.0	0.21	312.16626	2.51	$C_{10}H_{17}N_9BF_2$
314.12759	5109665.5	0.22	314.12573	1.86	$C_{14}H_{13}N_6BF_2$
509.24442	4411931.0	0.19	509.24311	1.31	$C_{29}H_{28}N_6BF_2$
532.24792	10341207.0	0.45	532.22271	25.22	$C_{30}H_{25}N_7BF_2$
533.24438	23853666.0	1.03	533.23053	13.85	$C_{30}H_{26}N_7BF_2$
533.26733	7749823.5	0.34	533.28670	-19.37	$C_{26}H_{32}N_{10}BF_2$
534.24744	6750095.0	0.29	534.23836	9.08	$C_{30}H_{27}N_7BF_2$
534.26343	76023976.0	3.29	534.23836	25.07	$C_{30}H_{27}N_7BF_2$

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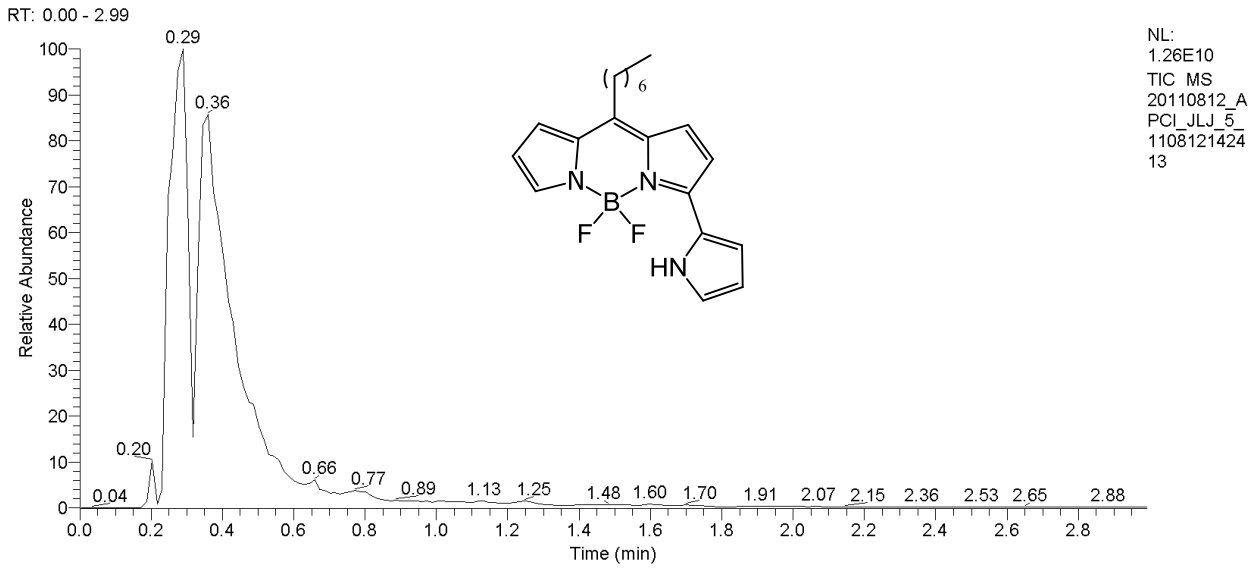

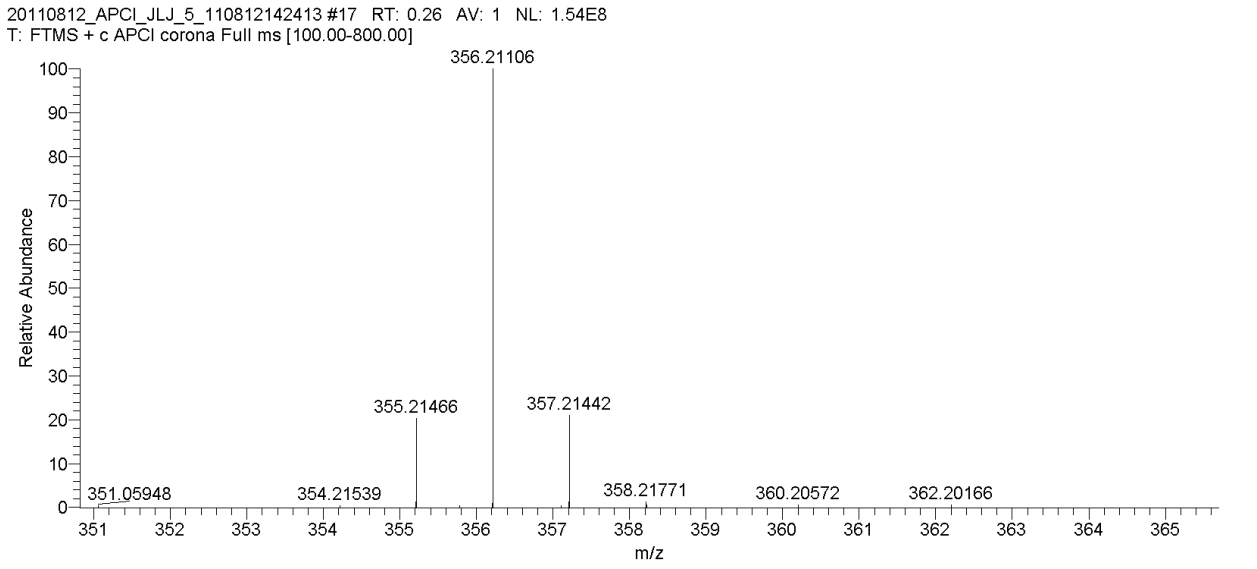

20110812_APCI_JLJ_5_110812142413#17 RT: 0.26
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
335.20920	976455808.0	26.52	335.20873	0.46	$C_{16}H_{24}N_5BF_2$
336.20499	3682384896.0	100.00	336.20398	1.00	$C_{15}H_{23}N_6BF_2$
337.20825	767099136.0	20.83	337.21181	-3.56	$C_{15}H_{24}N_6BF_2$
348.22476	516778752.0	14.03	348.22914	-4.37	$C_{18}H_{27}N_4BF_2$
356.21106	153955536.0	4.18	356.21041	0.65	$C_{20}H_{25}N_3BF_2$
648.40393	135509120.0	3.68			
649.40033	270146592.0	7.34			

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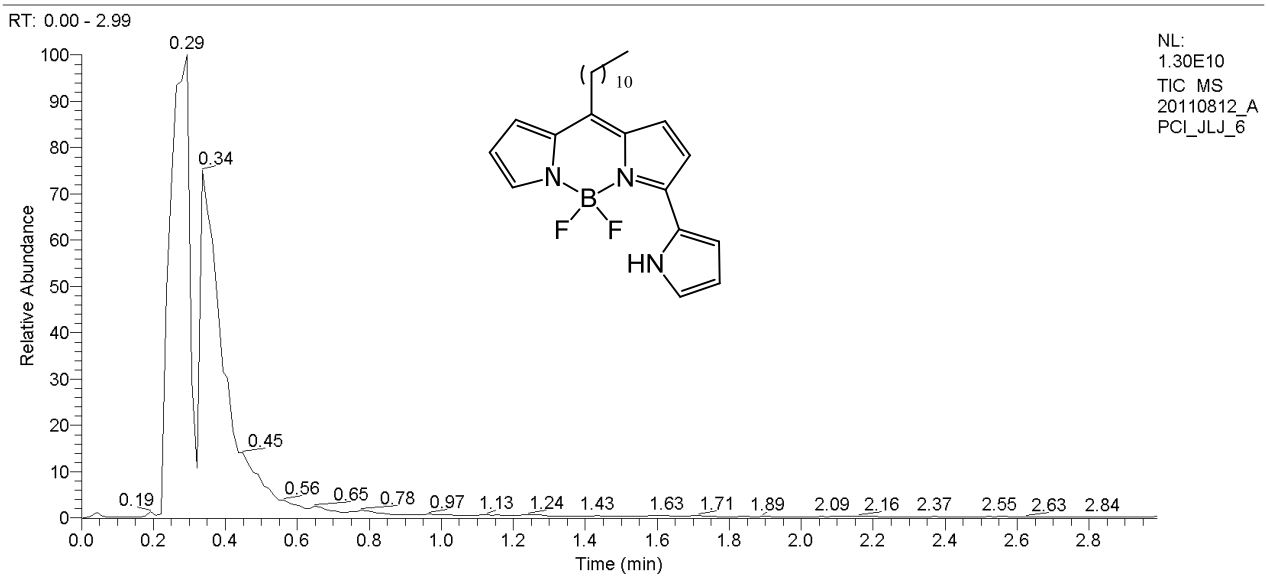

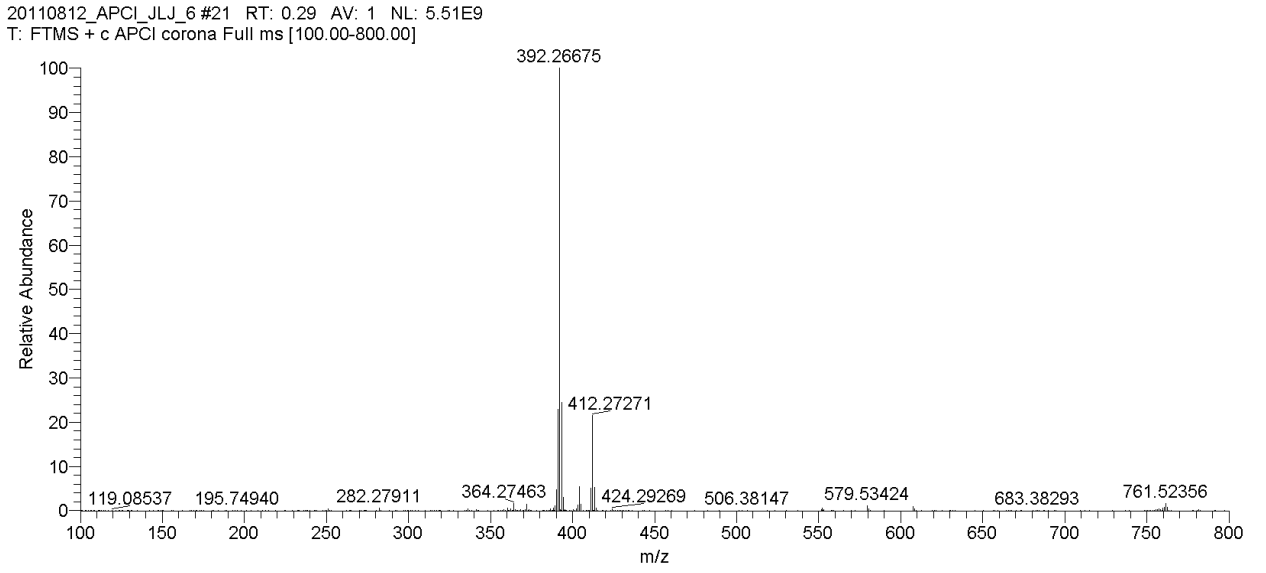

20110812_APCI_JLJ_6#21 RT: 0.29
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
393.26981	1351773184.0	24.52	393.27021	-0.41	$C_{19}H_{37}N_3B^{37}ClF_2$
394.27304	169126288.0	3.07	394.27149	1.55	$C_{17}H_{36}N_5BClF_2$
404.28638	300594240.0	5.45	404.28754	-1.16	$C_{22}H_{40}NB^{37}ClF_2$
411.27621	281265664.0	5.10	411.27776	-1.55	$C_{25}H_{34}N_2BF_2$
412.27271	1188476032.0	21.55	412.27301	-0.31	$C_{24}H_{33}N_3BF_2$
413.27588	287708096.0	5.22	413.27596	-0.08	$C_{14}H_{35}N_9BClF_2$
761.52356	88284776.0	1.60			

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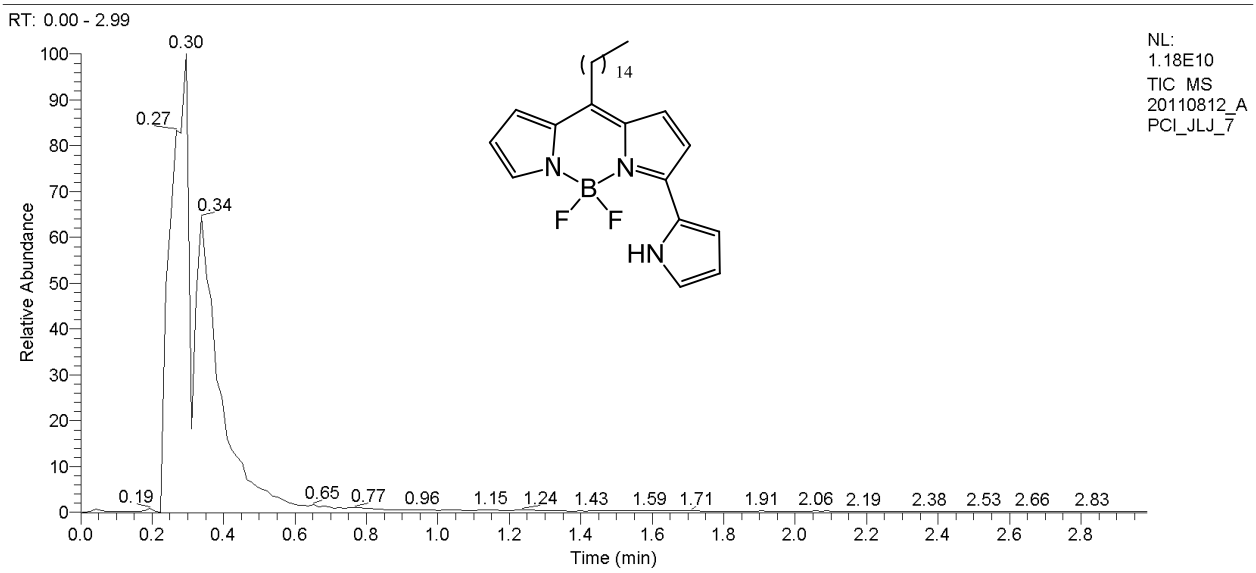

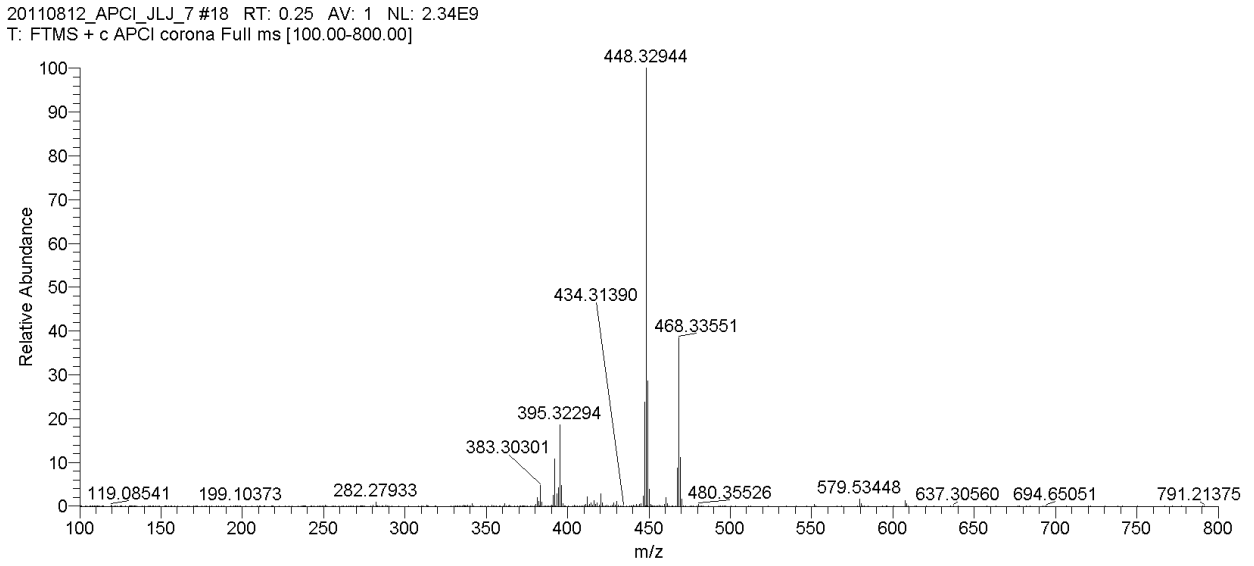

20110812_APCI_JLJ_7#18 RT: 0.25
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
396.32617	111111584.0	4.75	396.32304	3.14	$C_{21}H_{39}N_4BF_2$
447.33319	556929600.0	23.81	447.33393	-0.74	$C_{24}H_{40}N_5BF_2$
448.32944	2338852096.0	100.00	448.32918	0.25	$C_{23}H_{39}N_6BF_2$
449.33252	670229504.0	28.66	449.33281	-0.29	$C_{23}H_{45}N_3B^{37}ClF_2$
467.33884	203332896.0	8.69	467.34036	-1.53	$C_{29}H_{42}N_2BF_2$
468.33551	898678208.0	38.42	468.33561	-0.10	$C_{28}H_{41}N_3BF_2$
469.33853	261394688.0	11.18	469.33856	-0.03	$C_{18}H_{43}N_9BClF_2$

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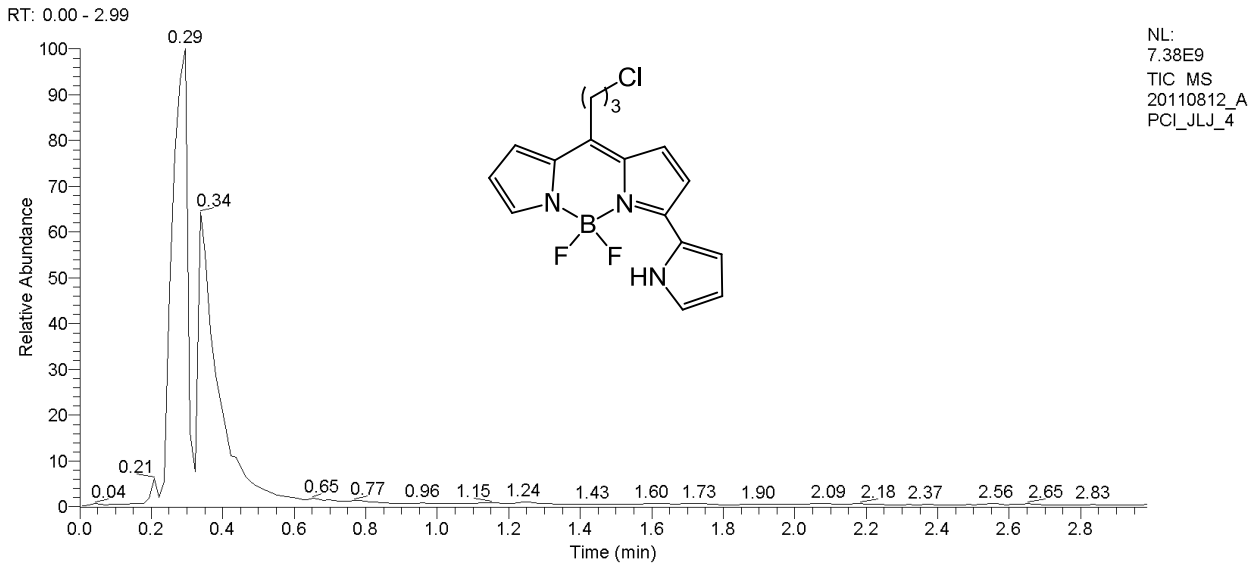
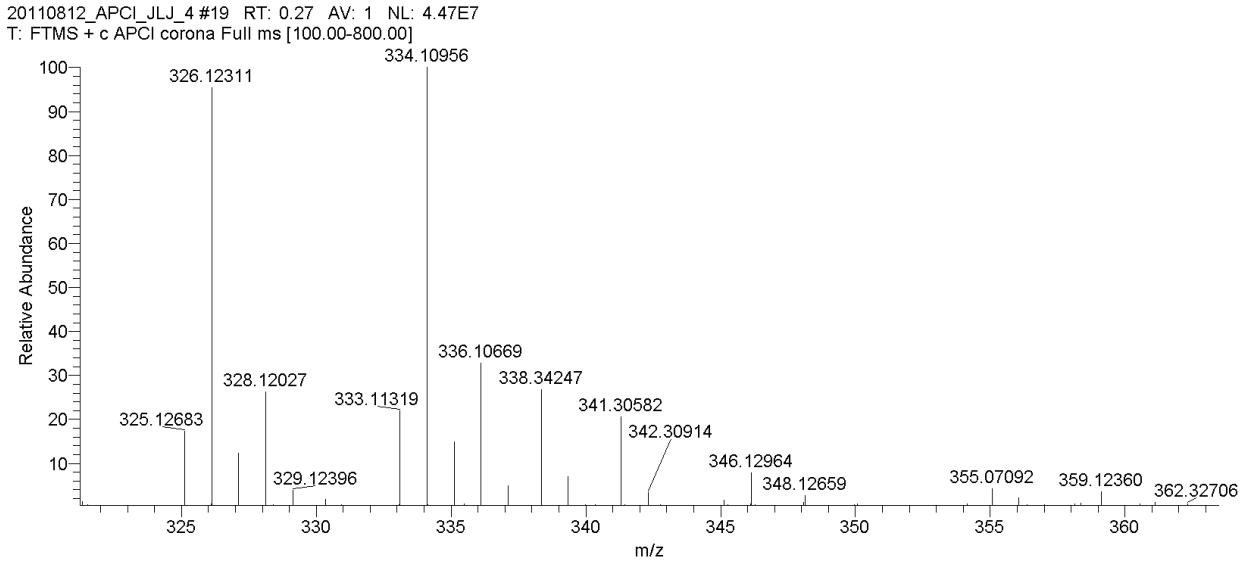
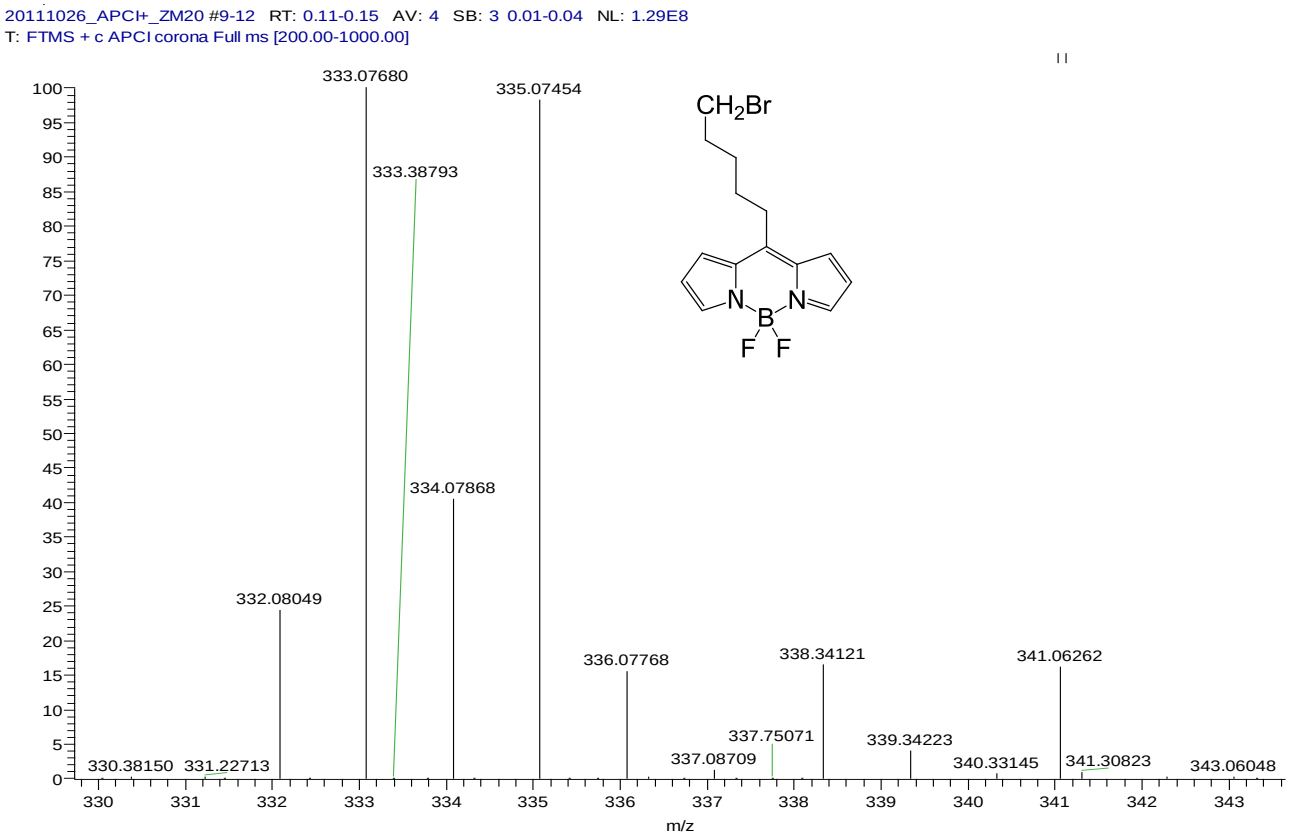


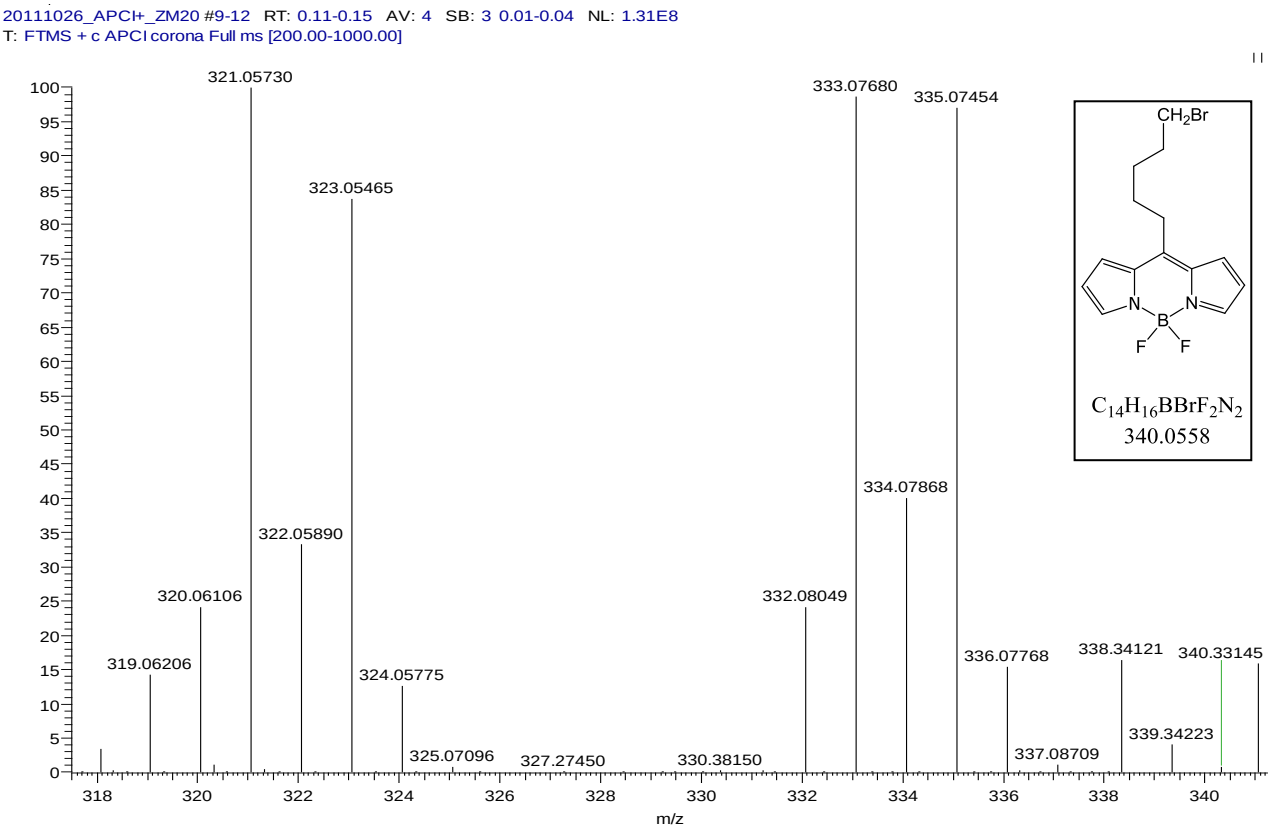


20110812_APCI_JLJ_4#19 RT: 0.27
T: FTMS + c APCI corona Full ms [100.00-800.00]

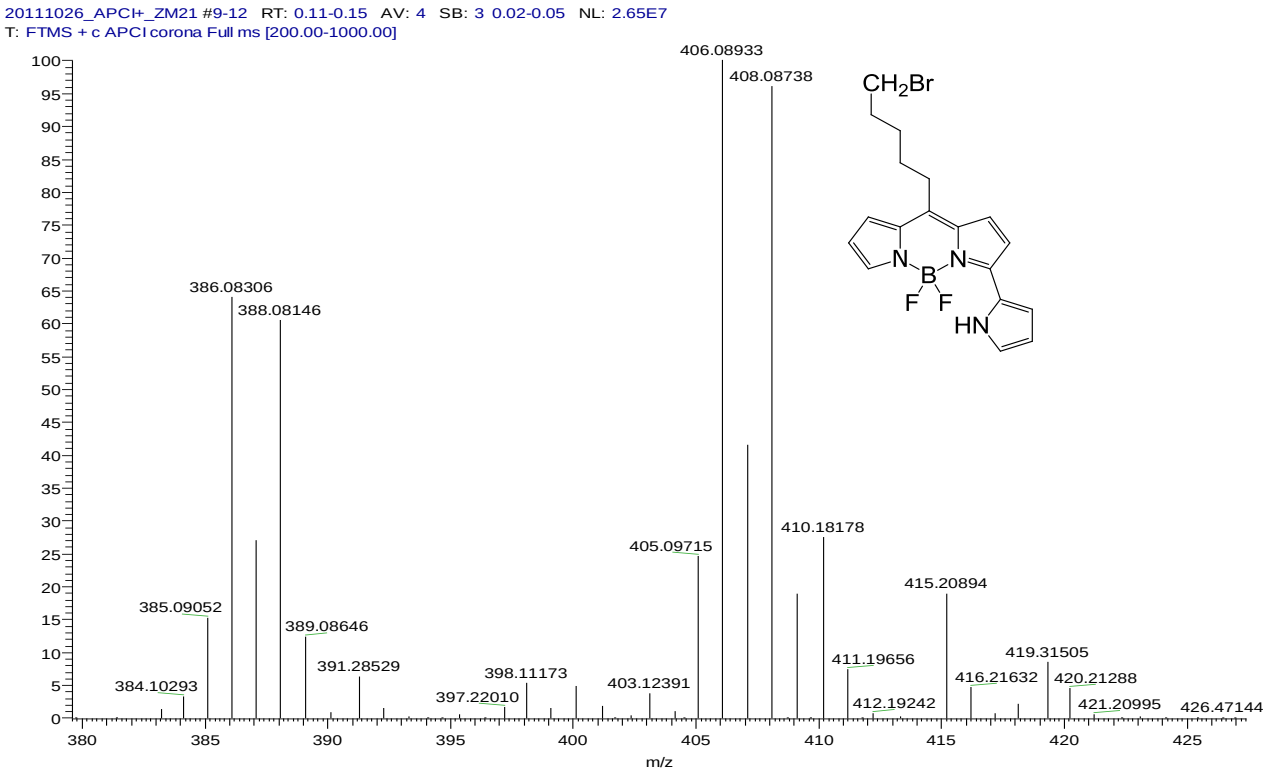
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
333.11319	9823366.0	0.53	333.11343	-0.24	$C_{10}H_{15}N_8B^{37}ClF_2$
334.10956	44683144.0	2.39	334.10884	0.72	$C_{16}H_{16}N_3BClF_2$
335.11328	6651089.5	0.36	335.11247	0.81	$C_{16}H_{22}BCl^{37}ClF_2$
336.10669	14633540.0	0.78	336.10589	0.80	$C_{16}H_{16}N_3B^{37}ClF_2$
338.34247	11968630.0	0.64	338.30096	41.51	$C_{13}H_{35}N_7BF_2$
341.30582	9194383.0	0.49	341.30599	-0.17	$C_{20}H_{38}NBF_2$
346.12964	3540292.3	0.19	346.12797	1.67	$C_{20}H_{20}B^{37}ClF_2$
532.24762	9522088.0	0.51	532.24953	-1.91	$C_{24}H_{32}N_9B^{37}ClF_2$
533.24377	19848004.0	1.06	533.24478	-1.01	$C_{23}H_{31}N_{10}B^{37}ClF_2$
534.24731	6464708.5	0.35	534.24857	-1.25	$C_{30}H_{39}NBCl^{37}ClF_2$
551.50476	6635910.5	0.36	551.47786	26.90	$C_{30}H_{58}N_6BF_2$
569.22052	3930014.5	0.21	569.22146	-0.94	$C_{23}H_{32}N_{10}BCl^{37}ClF_2$
579.53595	29380608.0	1.57	579.48401	51.94	$C_{30}H_{58}N_8BF_2$



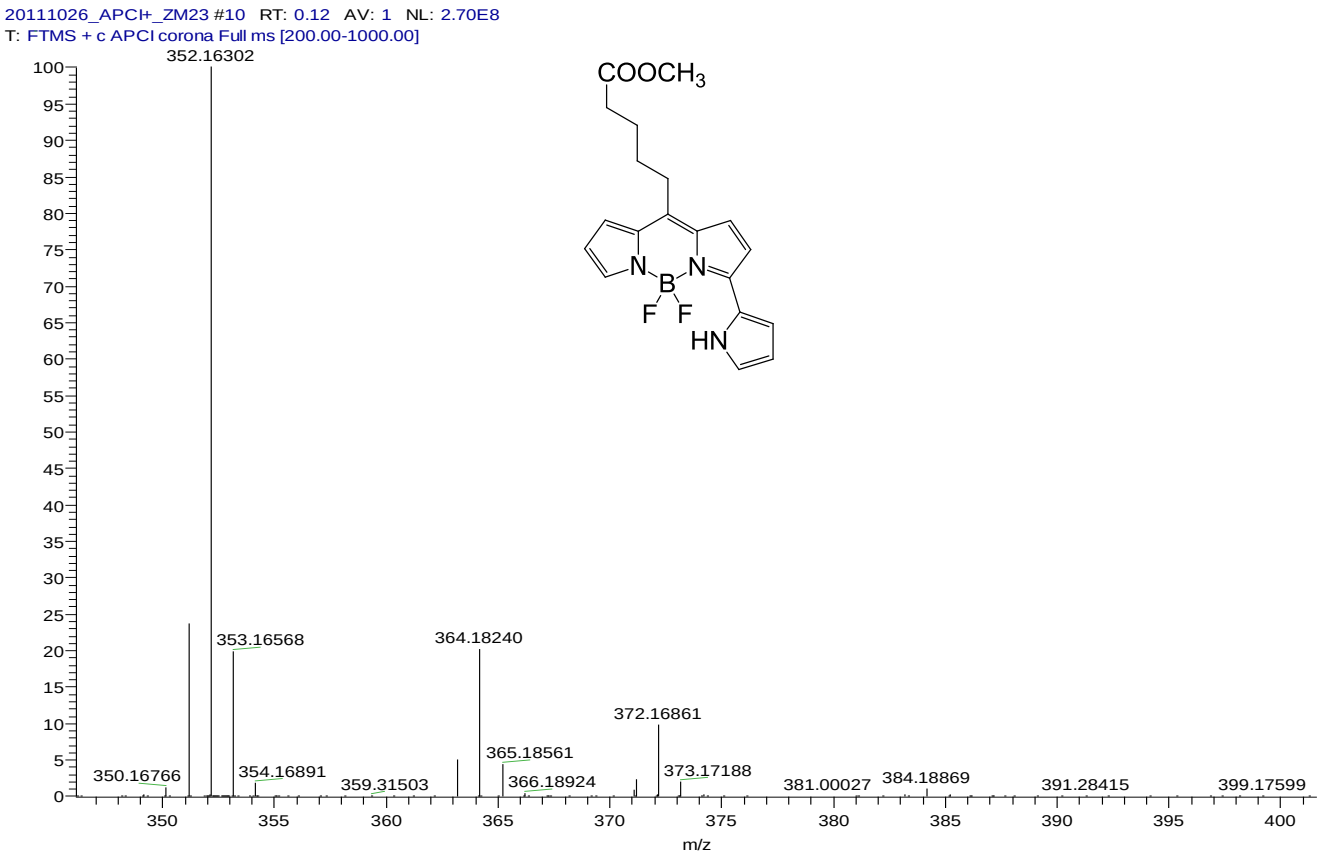
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
331.2271	230376	0.18	331.1915	35.66	C15 H33 N2 B Br
332.0805	31406822	24.36	332.0814	-0.94	C14 H20 N B [81]Br F2
333.0768	1.29E+08	100	333.0768	-0.04	C15 H19 O N2 B Br
334.0787	52253420	40.53	334.0784	0.29	C13 H20 O N B Br F2
335.0745	1.27E+08	98.33	335.0748	-0.25	C15 H19 O N2 B [81]Br
335.7362	156986.9	0.12	335.8289	-92.72	C9 O N Br [81]Br F2
336.0777	20003884	15.52	336.0769	0.77	C14 H21 O N Br F2
336.3257	407898.8	0.32	336.1891	136.6	C15 H34 O N B [81]Br
337.0871	1484248	1.15	337.0882	-1.05	C15 H20 N2 B Br F
341.0626	207471.4	0.16	341.0631	-0.46	C14 H17 N2 B Br F2



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
318.0682	4495372.5	3.44	318.0686	-0.47	C14 H20 O N [81]Br F
319.0621	18581756	14.21	319.0616	0.47	C13 H18 N2 Br F2
320.0611	31356950	23.97	320.0616	-0.54	C15 H17 N B Br F
320.3317	1443146.4	1.1	320.1942	137.48	C15 H34 N B [81]Br
321.0573	130790936	100	321.0569	0.45	C14 H16 N2 B Br F
321.3289	484513.1	0.37	321.19	138.94	C15 H34 N2 Br
322.0589	43570044	33.31	322.0596	-0.65	C15 H17 N B [81]Br F
323.0547	109451040	83.68	323.0548	-0.15	C14 H16 N2 B [81]Br F
324.0578	16482730	12.6	324.0565	1.24	C14 H17 O N B Br F
325.071	1012121.5	0.77	325.071	-0.05	C15 H19 N2 Br F
332.0805	31406822	24.01	332.0814	-0.94	C14 H20 N B [81]Br F2
333.0768	128910768	98.56	333.0768	-0.04	C15 H19 O N2 B Br
334.0787	52253420	39.95	334.0784	0.29	C13 H20 O N B Br F2
335.0745	126751976	96.91	335.0748	-0.25	C15 H19 O N2 B [81]Br
336.0777	20003884	15.29	336.0769	0.77	C14 H21 O N Br F2
336.3257	407898.8	0.31	336.1891	136.6	C15 H34 O N B [81]Br
337.0871	1484247.9	1.13	337.0882	-1.05	C15 H20 N2 B Br F



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
385.0905	4040107	15.25	385.0909	-0.32	C18 H22 N2 [81]Br F2
386.0831	16974114	64.05	386.0834	-0.33	C18 H19 N3 B Br F
387.0887	7177349	27.08	387.0912	-2.57	C18 H20 N3 B Br F
388.0815	16024782	60.47	388.0814	0.11	C18 H19 N3 B [81]Br F
389.0865	3267146	12.33	389.0859	0.58	C13 H31 N3 Br [81]Br
391.2853	1655935	6.25	391.2551	30.19	C18 H41 N3 B [81]Br
398.1117	1411202	5.33	398.1158	-4.07	C18 H24 N2 B [81]Br F2
400.1047	1277008	4.82	400.1032	1.49	C16 H34 N Br [81]Br
403.1239	984055.8	3.71	403.1252	-1.31	C18 H26 N3 [81]Br F2
405.0972	6513800	24.58	405.086	11.19	C15 H32 N Br [81]Br F
406.0893	26500826	100	406.0896	-0.29	C18 H20 N3 B Br F2
407.0917	11002784	41.52	407.0938	-2.04	C17 H32 B Br [81]Br
408.0874	25453418	96.05	408.0876	-0.19	C18 H20 N3 B [81]Br F2
409.0959	5002697	18.88	409.0954	0.53	C18 H21 N3 B [81]Br F2
410.1818	7308281	27.58	410.18	1.79	C18 H33 N3 [81]Br F2
411.1966	1960773	7.4	411.205	-8.39	C17 H35 N3 B [81]Br F2
415.2089	5028621	18.98	415.2191	-10.18	C18 H38 N3 [81]Br F2
416.2163	1232166	4.65	416.227	-10.63	C18 H39 N3 [81]Br F2



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
351.1669	64041084	23.74	351.1675	-0.59	C20 H21 O2 N2 B F
352.1630	2.7E+08	100	352.1627	0.31	C19 H20 O2 N3 B F
353.1657	53418368	19.8	353.1671	-1.45	C18 H23 O3 N2 F2
354.1689	5009380	1.86	354.1671	1.79	C20 H22 O3 N B F
363.1859	13488829	5	363.1879	-1.98	C20 H25 O2 N2 F2
364.1824	54277276	20.12	364.1827	-0.3	C20 H23 O3 N3 B
365.1856	11990389	4.44	365.1843	1.35	C18 H24 O3 N2 B F2
371.1722	6385916	2.37	371.1737	-1.48	C20 H22 O2 N2 B F2
372.1686	26403770	9.79	372.1689	-0.33	C19 H21 O2 N3 B F2
373.1719	5230181	1.94	373.1768	-4.89	C19 H22 O2 N3 B F2

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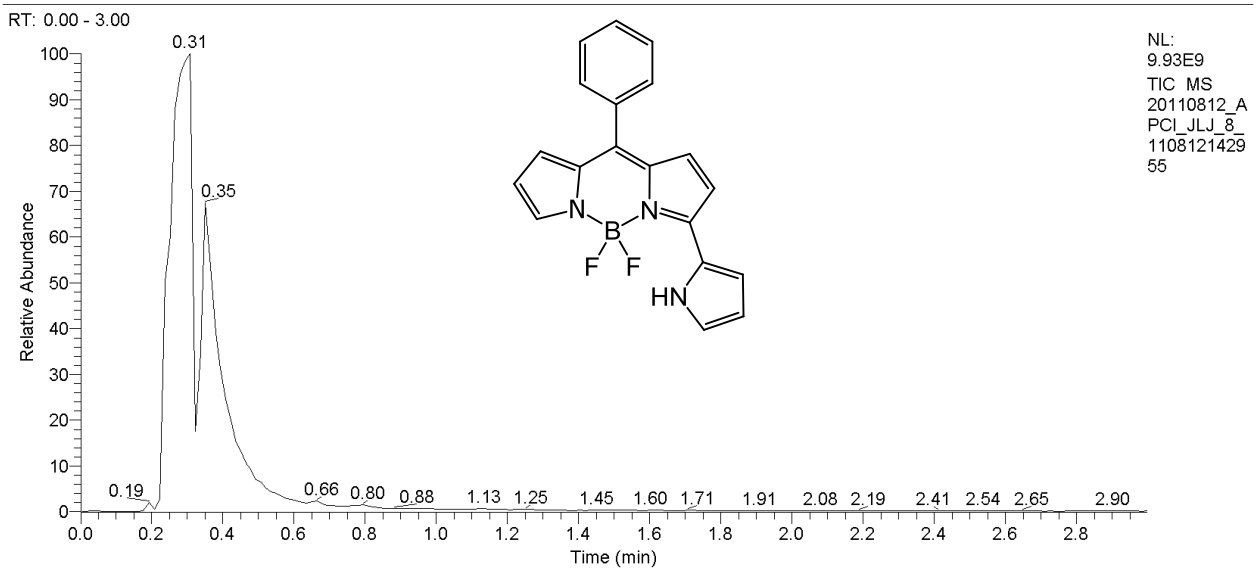
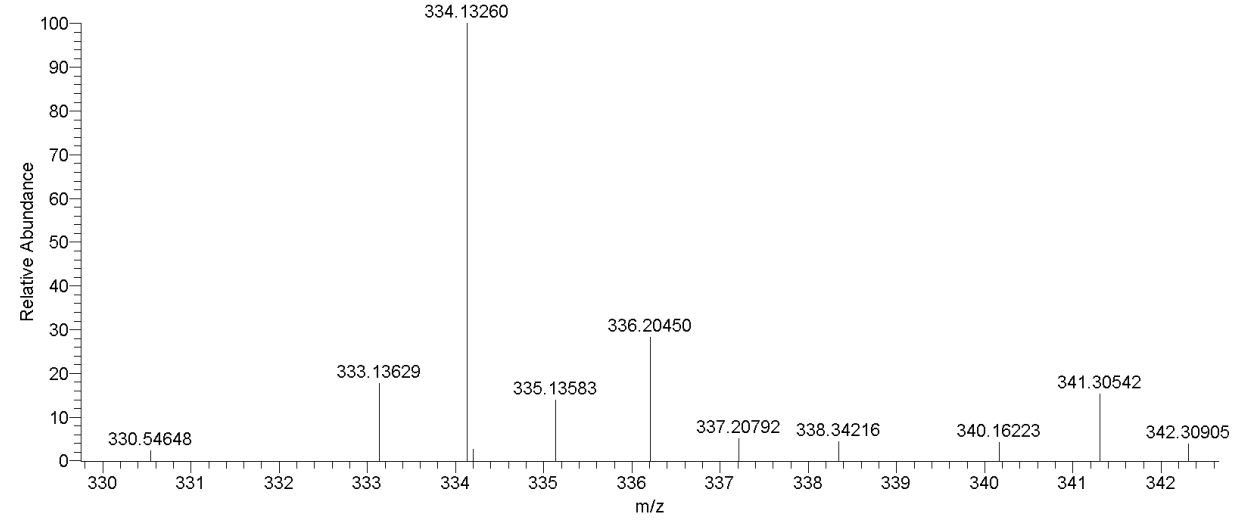


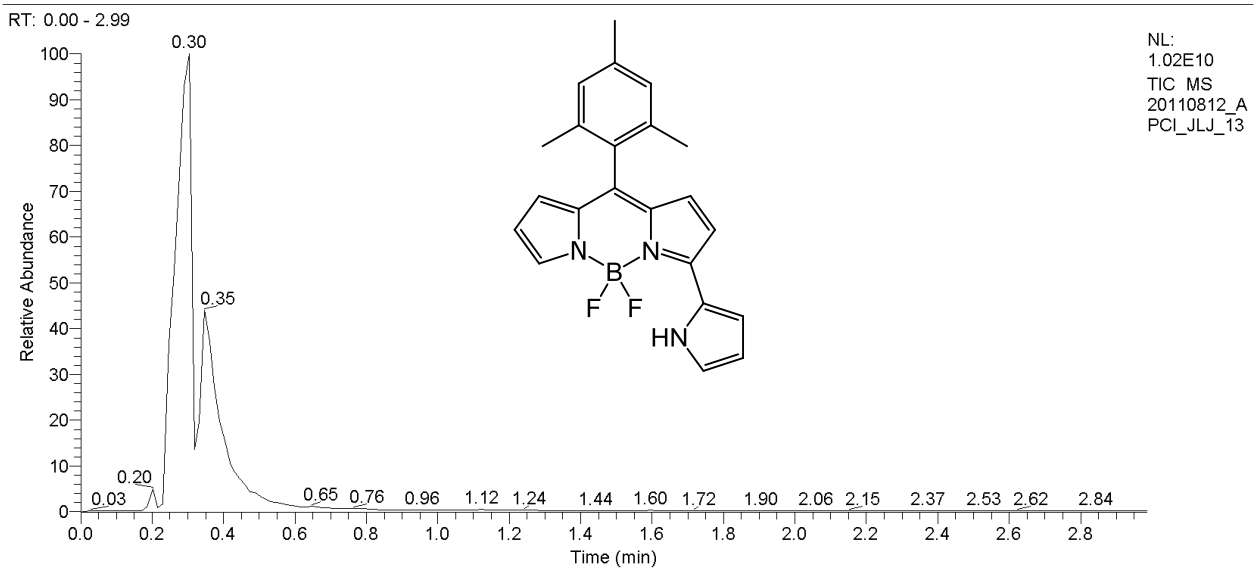
20110812_APCI_JLJ_8_110812142955 #20 RT: 0.29 AV: 1 NL: 4.33E7
T: FTMS + c APCI corona Full ms [100.00-800.00]

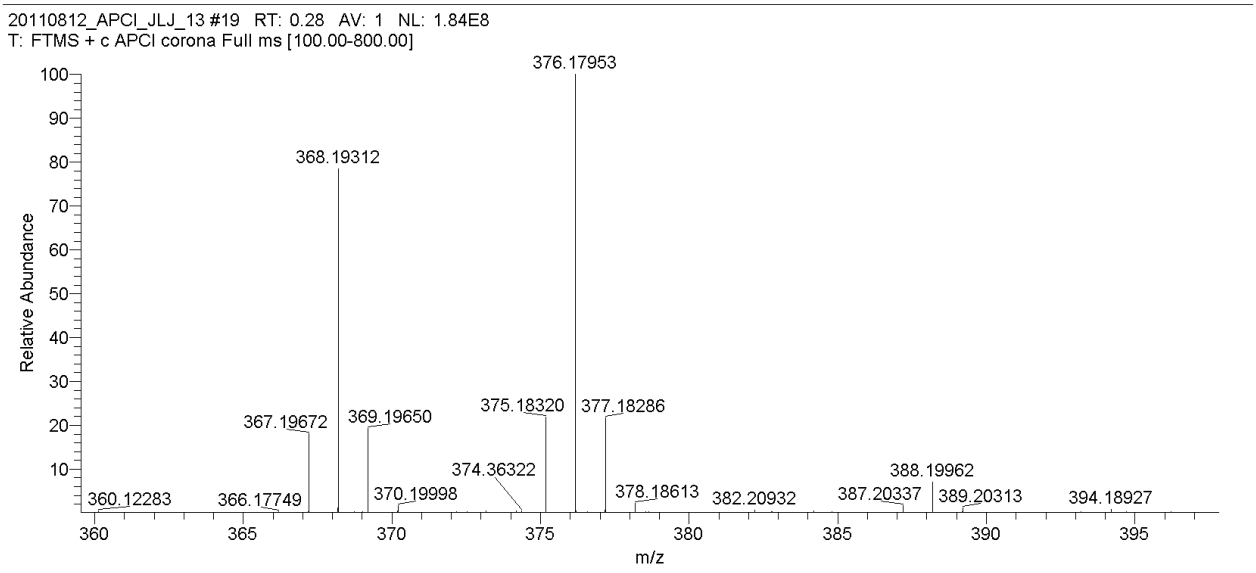


20110812_APCI_JLJ_8_110812142955#20 RT: 0.29
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
333.13629	7715913.5	0.20	333.13691	-0.62	$C_{20}H_{16}N_2BF_2$
334.13260	43326648.0	1.11	334.13216	0.44	$C_{19}H_{15}N_3BF_2$
334.19949	1175933.3	0.03	334.20091	-1.42	$C_{16}H_{23}N_5BF_2$
335.13583	6008603.5	0.15	335.13999	-4.15	$C_{19}H_{16}N_3BF_2$
336.20450	12272509.0	0.31	336.20398	0.52	$C_{15}H_{23}N_6BF_2$
337.20792	2225465.3	0.06	337.21181	-3.89	$C_{15}H_{24}N_6BF_2$
338.34216	1880872.9	0.05	338.30096	41.21	$C_{13}H_{35}N_7BF_2$
340.16223	1846292.9	0.05	340.16654	-4.30	$C_{18}H_{19}N_4BF_2$
341.30542	6645545.0	0.17	341.30599	-0.57	$C_{20}H_{38}NBF_2$
342.30905	1717402.6	0.04	342.31381	-4.76	$C_{20}H_{39}NBF_2$
345.14404	3169334.8	0.08	345.14278	1.26	$C_{13}H_{14}N_9BF_2$
346.09192	3134744.5	0.08	346.09443	-2.51	$C_{17}H_9N_6BF_2$
346.15268	6581354.0	0.17	346.15060	2.07	$C_{13}H_{15}N_9BF_2$

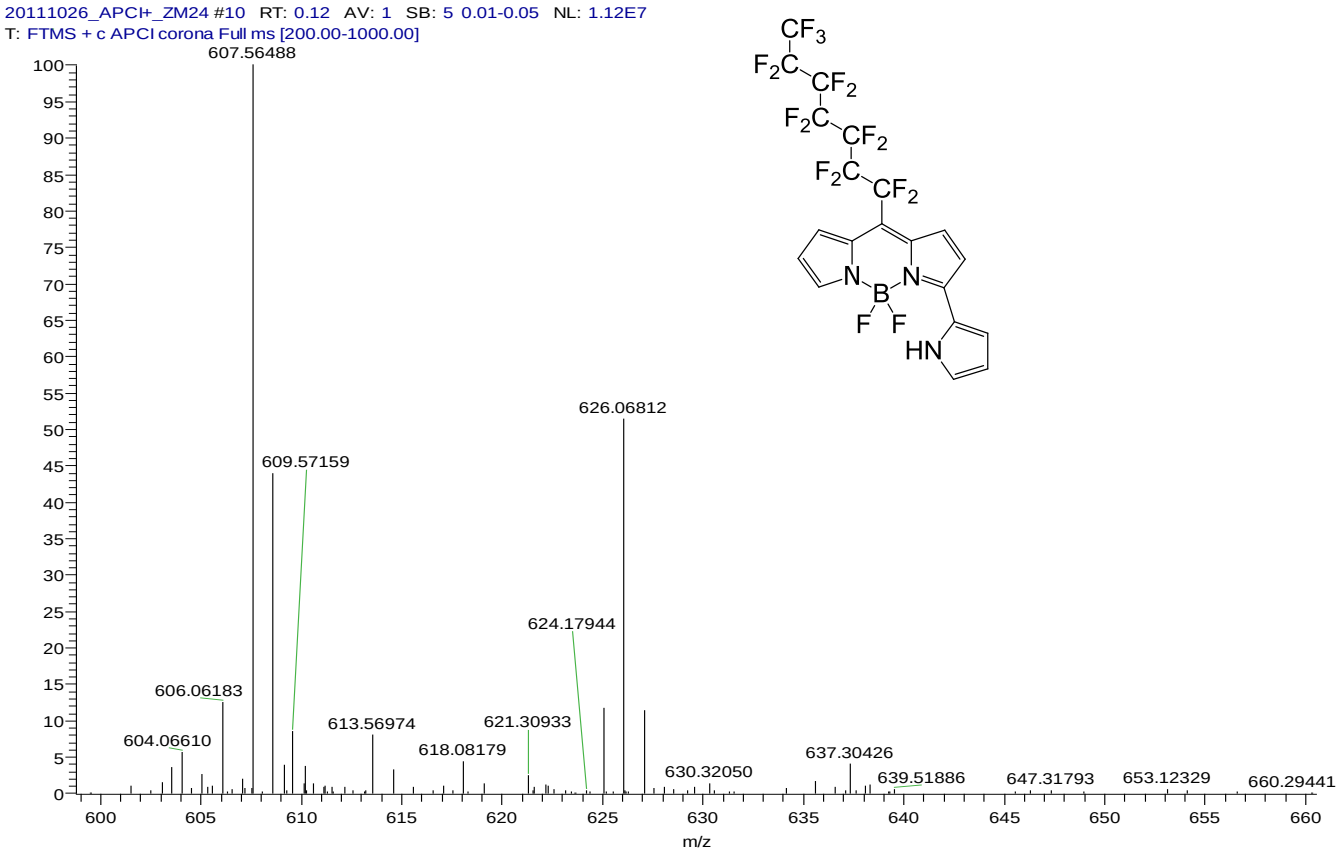
E:\data\20110812\20110812_APCI_JLJ_13 2011-8-12 13:18:57





20110812_APCI_JLJ_13#32 RT: 0.46
T: FTMS + c APCI corona Full ms [100.00-800.00]

m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
354.17776	17713906.0	6.35	354.17682	0.95	$C_{12}H_{19}ON_9BF_2$
355.17715	66948380.0	24.01	355.17743	-0.28	$C_{18}H_{20}N_5BF_2$
356.17334	278829120.0	100.00	356.17268	0.66	$C_{17}H_{19}N_6BF_2$
357.17636	63413432.0	22.74	357.18051	-4.15	$C_{17}H_{20}N_6BF_2$
358.17963	6736812.5	2.42	358.17710	2.53	$C_{18}H_{21}ON_4BF_2$
368.19287	11945678.0	4.28	368.19247	0.40	$C_{13}H_{21}ON_9BF_2$
376.17923	11848446.0	4.25	376.17911	0.12	$C_{22}H_{21}N_3BF_2$



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	Composition
604.0661	633688.9	5.67	604.0672	-1.09	C20 H10 O N3 B F15
606.0618	1404296	12.55	606.0629	-1.03	C20 H9 N3 B F16
607.5649	11185586	100			
608.5683	4917023	43.96			
609.5716	946420.2	8.46			
613.5697	899234.6	8.04			
618.0818	499338.3	4.46	618.0828	-1.05	C21 H12 O N3 B F15
625.0717	1311391	11.72	625.0738	-2.18	C21 H11 N2 B F17
626.0681	5748613	51.39	626.0691	-0.97	C20 H10 N3 B F17
627.0716	1281051	11.45	627.0769	-5.31	C20 H11 N3 B F17