Supporting Information for

Synthesis, Structure and Photophysical Properties of Near-infrared 3,5-DiarylbenzoBODIPY Fluorophores

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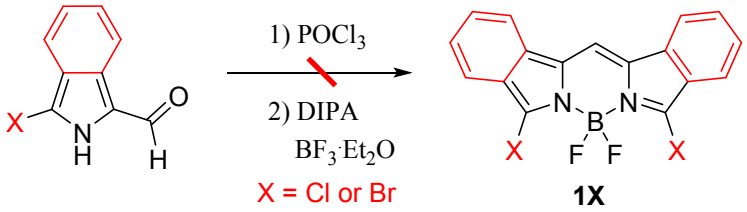
Contents:

1. **Scheme S1**. Attempted Syntheses of BODIPY **1X**.



2. **Crystal Structure**

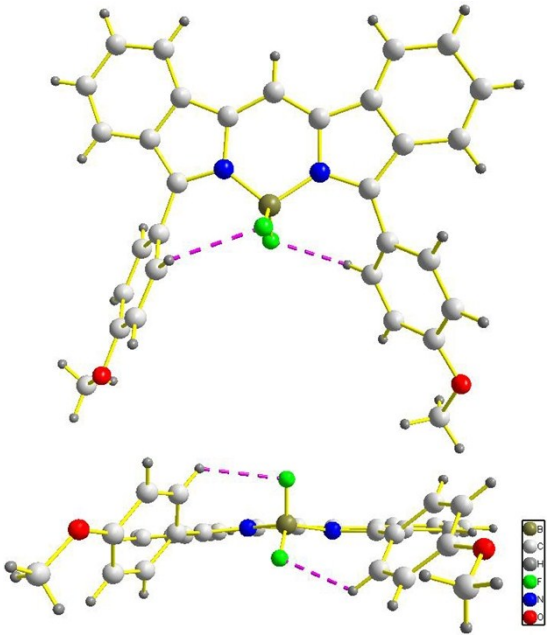


Figure S1: X-ray structures of **1a**. C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

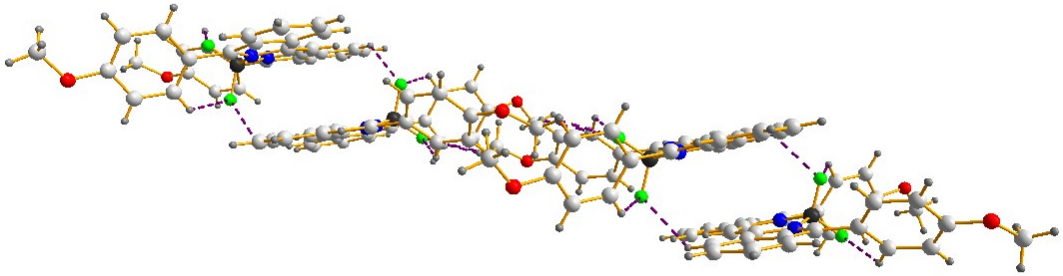


Figure S2: Intermolecular crystal packing of **1a** through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

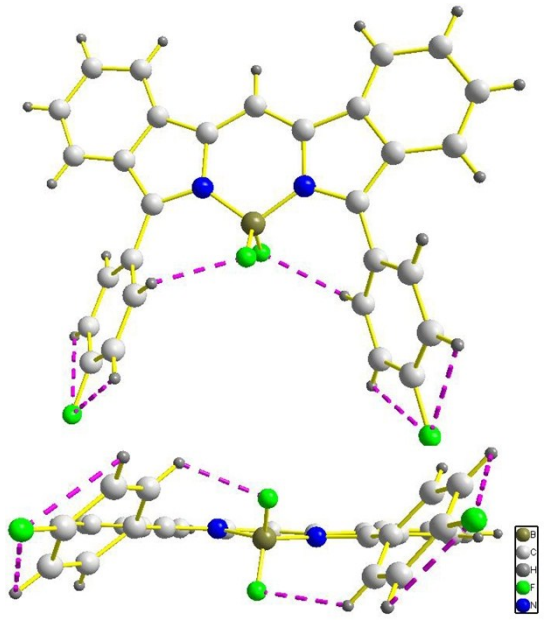


Figure S3: X-ray structures of **1c**. C, light gray; H, gray; N, blue; B, yellow; F, light green.

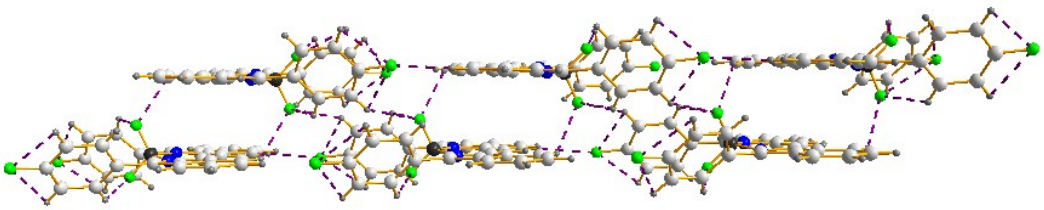


Figure S4: Intermolecular crystal packing of **1c** through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green.

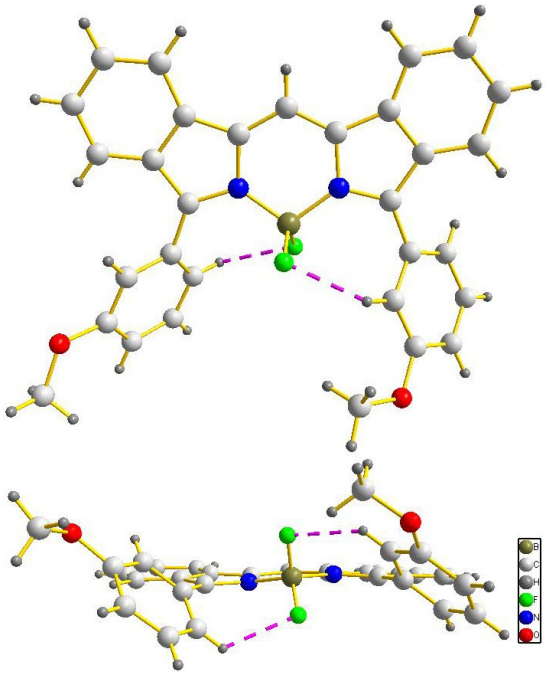


Figure S5: X-ray structures of **1d**. C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

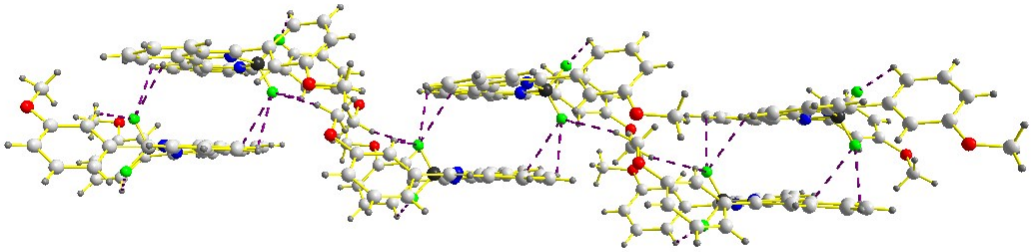


Figure S6: Intermolecular crystal packing of **1d** through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

Table S1. Crystallographic data and details of the structure determinations of the compounds **1a**, **1c** and **1d**

	1a	1c	1d
Empirical formula	$C_{31}H_{23}BF_2N_2O_2$	$C_{29}H_{17}BF_4N_2$	$C_{31}H_{23}BF_2N_2O_2$
Formula weight	504.32	480.26	504.32
Temperature [K]	293(2)	293(2)	293(2)
Wavelength	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Triclinic
space group	P-1	P2(1)/n	P-1
a[]	10.2591(10)	12.1936(18)	7.683(4)
b[]	10.3442(10)	15.062(2)	12.170(6)
c[]	12.7331(12)	12.2515(18)	13.064(6)
α [°]	96.5350(10)	90	85.699(6)
β [°]	104.5740(10)	97.131(2)	81.017(7)
γ [°]	104.6180(10)	90	86.489(6)
V[]	1242.6(2)	2232.7(6)	1201.6(10)
Z	2	4	2
Calculated density [g.cm-3]	1.348	1.429	1.394
Absorption coefficient (mm^{-1})	0.094	0.107	0.097
F(000)	524	984	524
Crystal size (mm)	0.19×0.18×0.16	0.15×0.13×0.12	0.16×0.13×0.12
θ_{max} [°]	27.70	27.61	27.64
Index ranges	-13 ≤ h ≤13	-15≤ h ≤15	-9 ≤ h ≤ 10
	-13 ≤ k ≤13	-19 ≤ k ≤ 19	-15 ≤ k ≤ 15
	-16 ≤ l ≤15	-15 ≤ l ≤ 15	-16 ≤ l ≤ 16
Unique reflections	5665	5131	5338
Reflections observed [$I > 2\sigma(I)$]	4055	3294	3105
Parameters	345	325	345
R1 (on F) [$I > 2\sigma(I)$]	0.0496	0.0517	0.0721
wR2 (on F^2)	0.1321	0.1418	0.2199
Largest diff. peak/hole (eA^{-3})	0.514/-0.431	0.424/-0.530	0.327/-0.328

Table S2. Selected Geometrical Parameters of **1a**, **1c** and **1d** obtained from crystallography

	1a	**1c**	**1d**
the B-N bond distances (Å)	1.5722(27) 1.5729(29)	1.5521(31) 1.5580(27)	1.5777(39) 1.5809(37)
the intramolecular F-H Hydrogen bond distances (Å)	2.2980(16) 2.4856(14)	2.2466(17) 2.3979(15) 2.5169(19) 2.5233(20) 2.5126(15) 2.5249(16)	2.2615(19) 2.3470(18)
the intermolecular F-H Hydrogen bond distances (Å)	2.5482(19) 2.8332(20) 2.7450(16) 2.8740(14)	2.3830(18) 2.4489(17) 2.8012(17) 2.5571(13) 2.5962(20)	2.7480(18) 2.6395(18) 2.7952(19) 2.8226(17)
dihedral angles of two pyrrole rings in dipyyrin core (deg)	6.421(70)	3.864(69)	6.044(96)
dihedral angles between phenyl ring and dipyrrin core (deg)	48.124(68) 56.931(63)	47.329(62) 51.263(65)	40.841(93) 46.090(89)

3. Table S3: Photophysical properties of BODIPYs 1a-e and 5, 6 in different solvents at room temperature.

BODIPYs	Solvent	λ_{abs}^{max}(nm)	λ_{em}^{max}(nm)	logε_{max}	Φ_a	Stokes Shift (cm^{-1})
	Acetonitrile	645	680	4.78	0.74	798
	Methanol	648	680	4.74	0.78	726
1a	THF	653	684	4.92	0.73	694
	Dichloromethane	654	687	4.94	0.76	734
	Toluene	658	690	4.84	0.70	705
	Acetonitrile	640	671	4.86	0.85	722
	Methanol	642	673	4.84	0.99	717
1b	THF	648	677	4.94	0.82	661
	Dichloromethane	648	679	4.97	0.91	704
	Toluene	653	681	5.04	0.76	630
	Acetonitrile	634	663	4.76	0.93	690
	Methanol	635	664	4.74	0.93	688
1c	THF	641	669	4.84	0.82	653
	Dichloromethane	643	671	4.87	0.92	649
	Toluene	646	674	4.94	0.78	643
	Acetonitrile	635	669	4.80	0.90	800
	Methanol	637	671	4.86	0.96	795
1d	THF	643	675	4.85	0.87	737
	Dichloromethane	648	677	4.98	0.87	757
	Toluene	648	679	5.01	0.75	704
	Acetonitrile	690	737	4.69	0.33	924
	Methanol	693	738	4.77	0.30	880
1e	THF	698	742	4.82	0.33	850
	Dichloromethane	699	745	4.96	0.36	815
	Toluene	706	747	4.86	0.35	777

The fluorescence quantum yields were calculated using ZnPc in DMF solution (ϕ = 0.28) as the standards for **1a-d,** and 1,3,5,7-(4-methoxy)phenylazaBODIPY (ϕ = 0.36 in chloroform) for **1e**, respectively.

4. UV-vis and Fluorescence Spectra

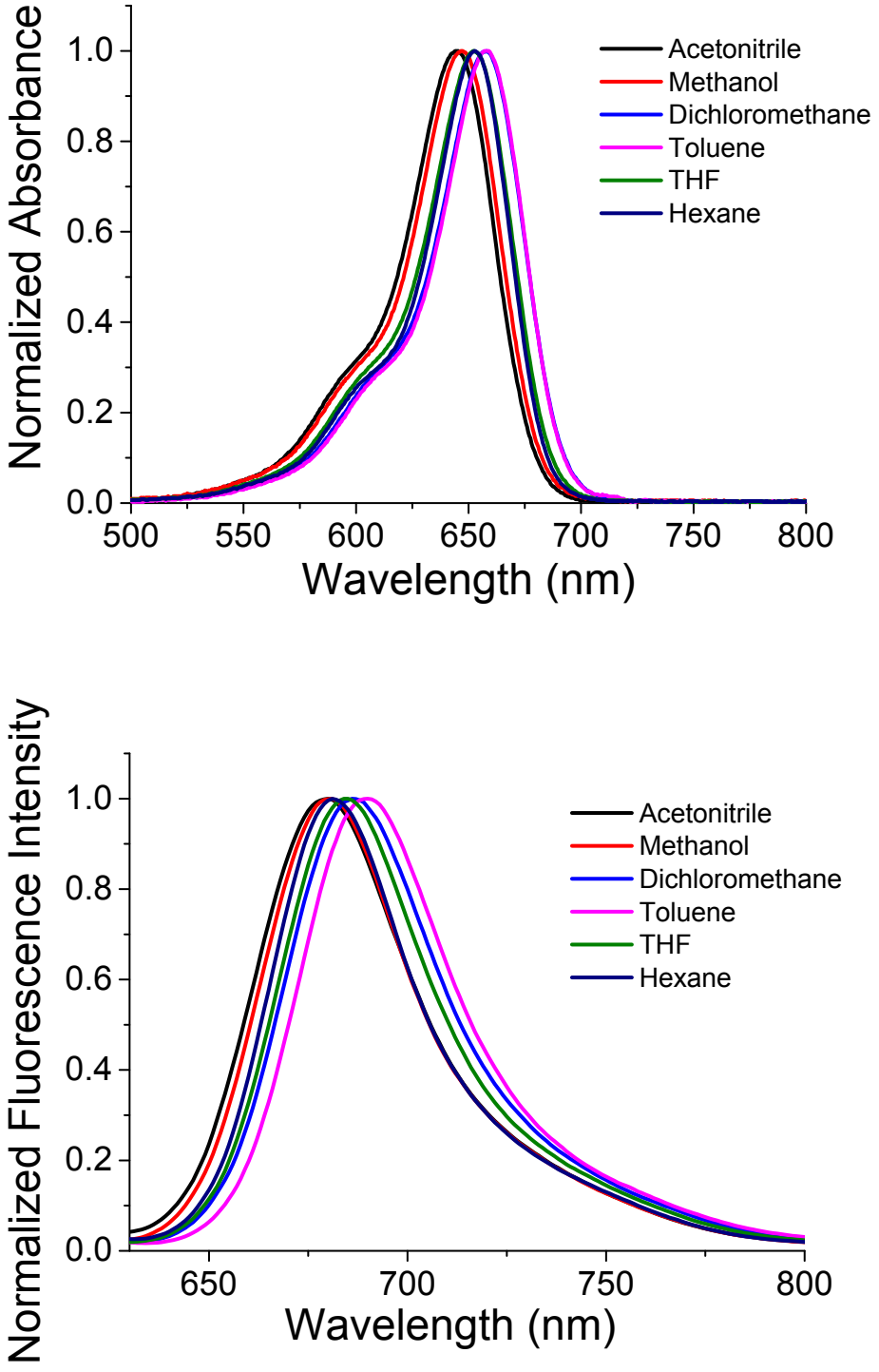


Figure S7. Absorption (top) and emission (bottom) spectra of compound **1a** recorded in different solvents. Excited at 620 nm.

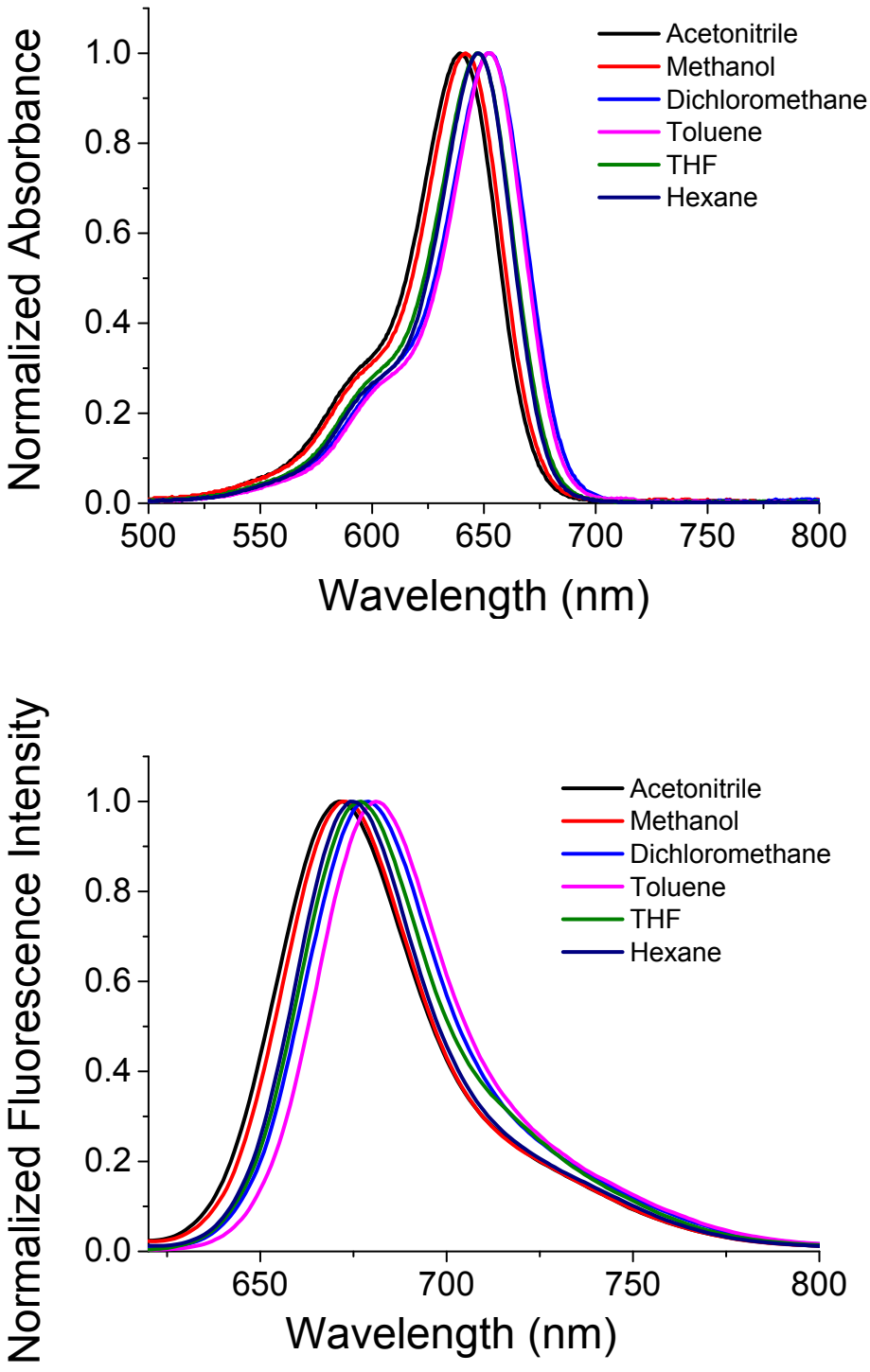


Figure S8. Absorption (top) and emission (bottom) spectra of compound **1b** recorded in different solvents. Excited at 610 nm.

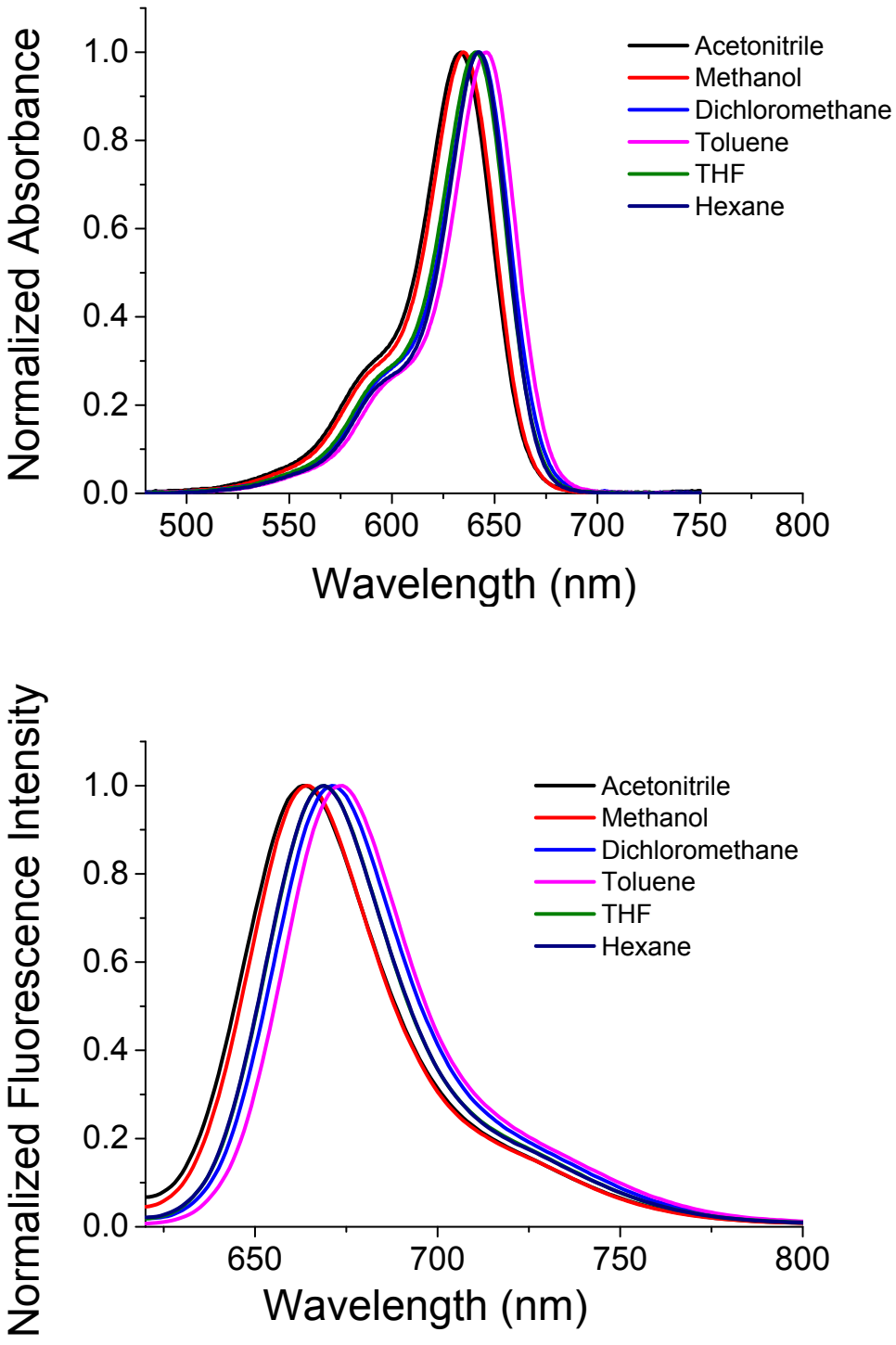


Figure S9. Absorption (top) and emission (bottom) spectra of compound **1c** recorded in different solvents. Excited at 610 nm.

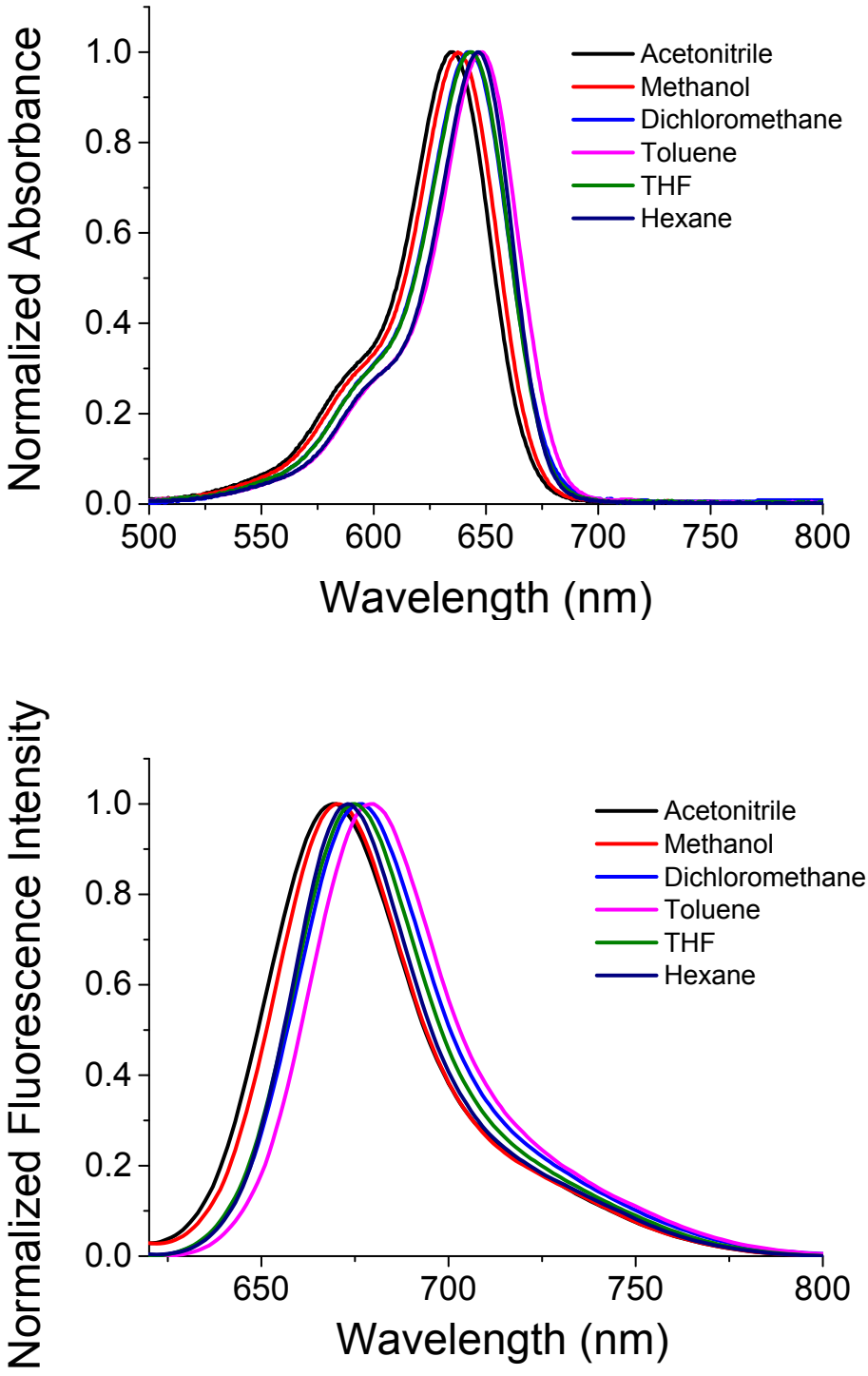


Figure S10. Absorption (top) and emission (bottom) spectra of compound **1d** recorded in different solvents. Excited at 610 nm.

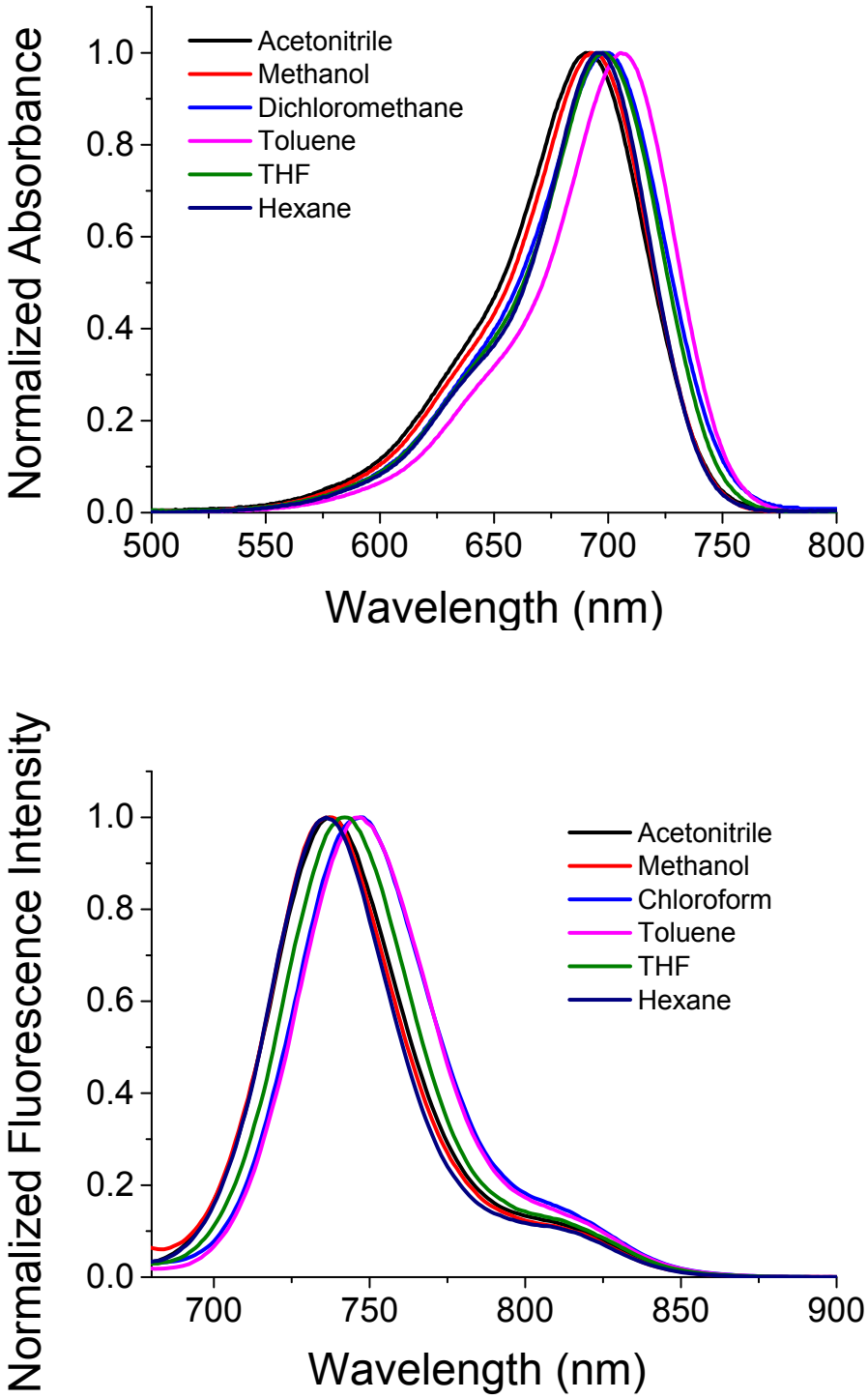


Figure S11. Absorption (top) and emission (bottom) spectra of compound **1e** recorded in different solvents. Excited at 660 nm.

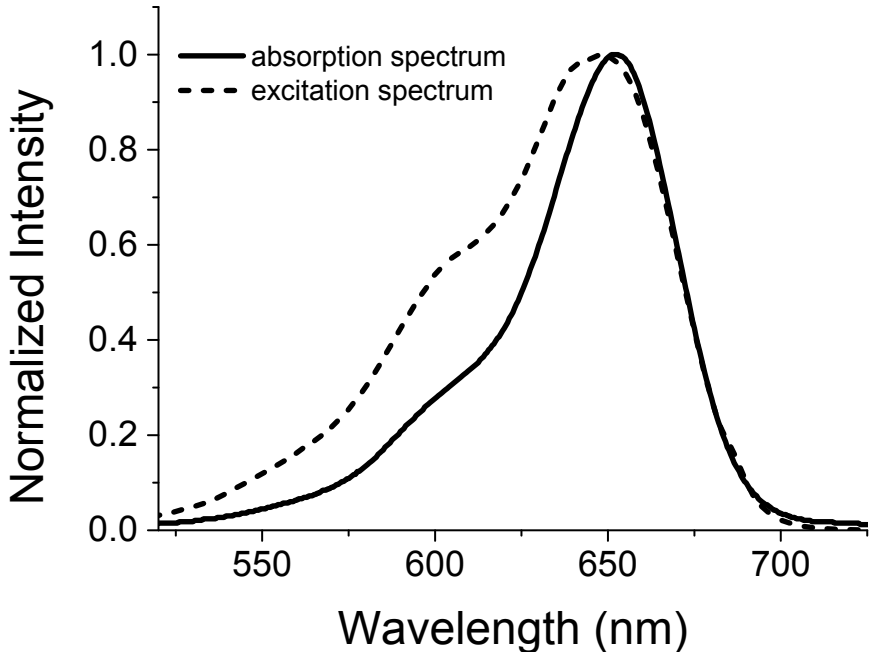


Figure S12. Excitation spectrum (dash line) and absorption spectrum (solid line) of **1a** in dichloromethane.

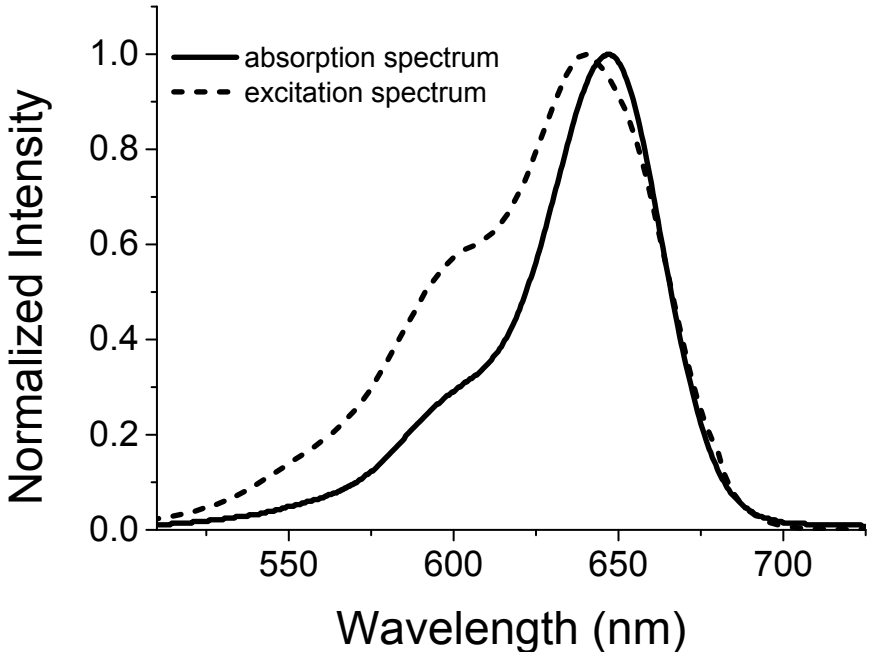


Figure S13. Excitation spectrum (dash line) and absorption spectrum (solid line) of **1b** in dichloromethane.

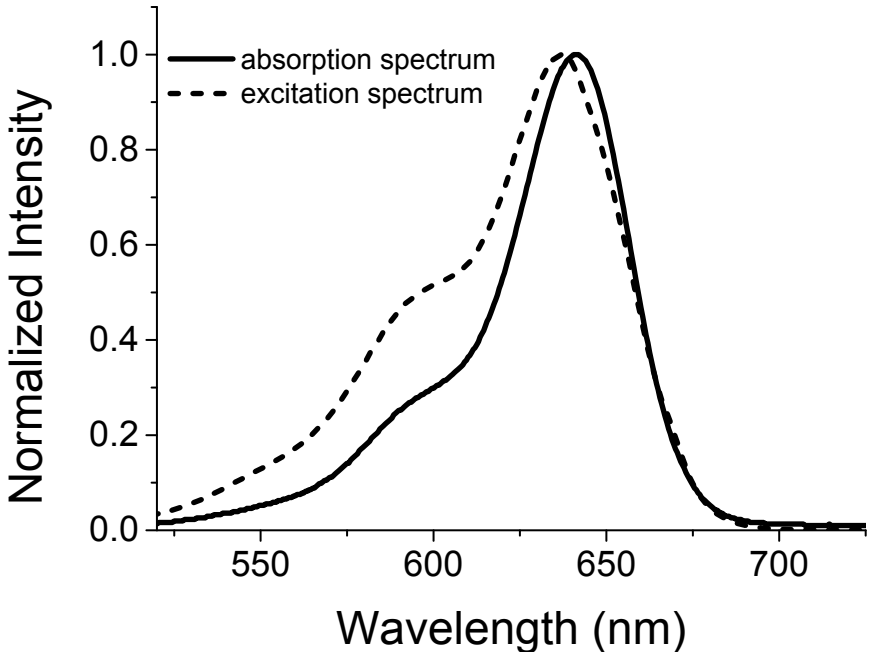


Figure S14. Excitation spectrum (dash line) and absorption spectrum (solid line) of **1c** in dichloromethane.

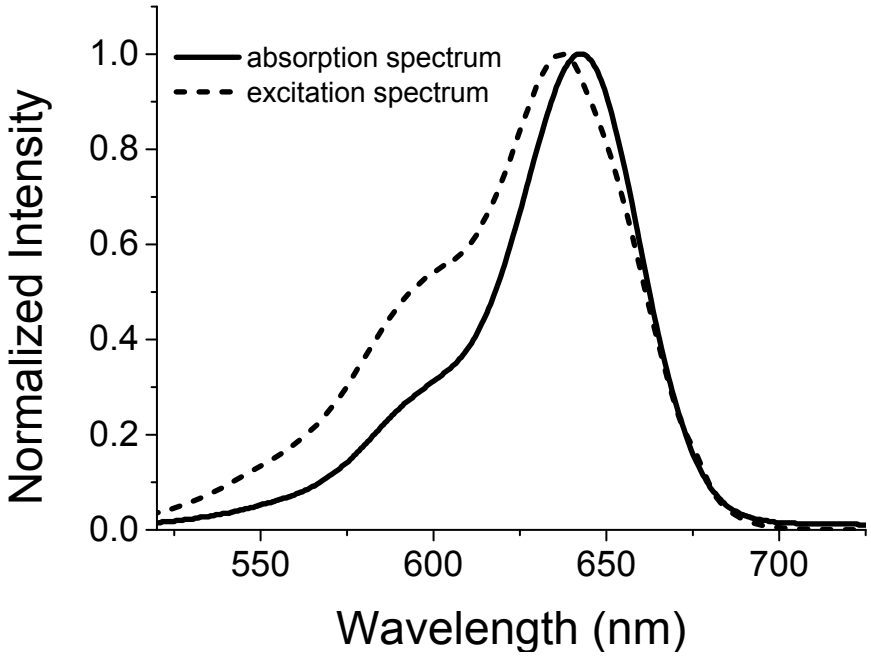


Figure S15. Excitation spectrum (dash line) and absorption spectrum (solid line) of **1d** in dichloromethane.

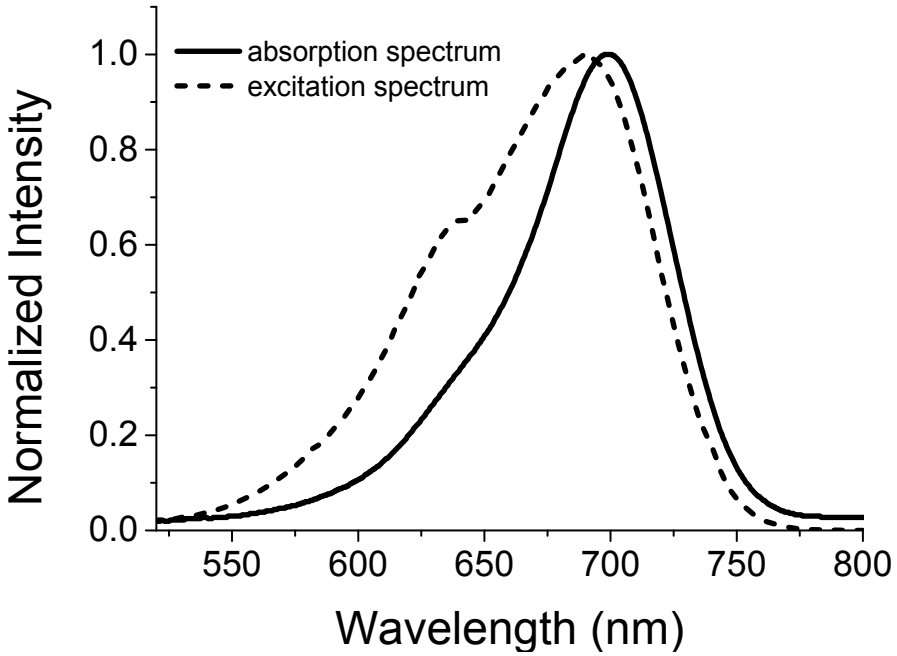
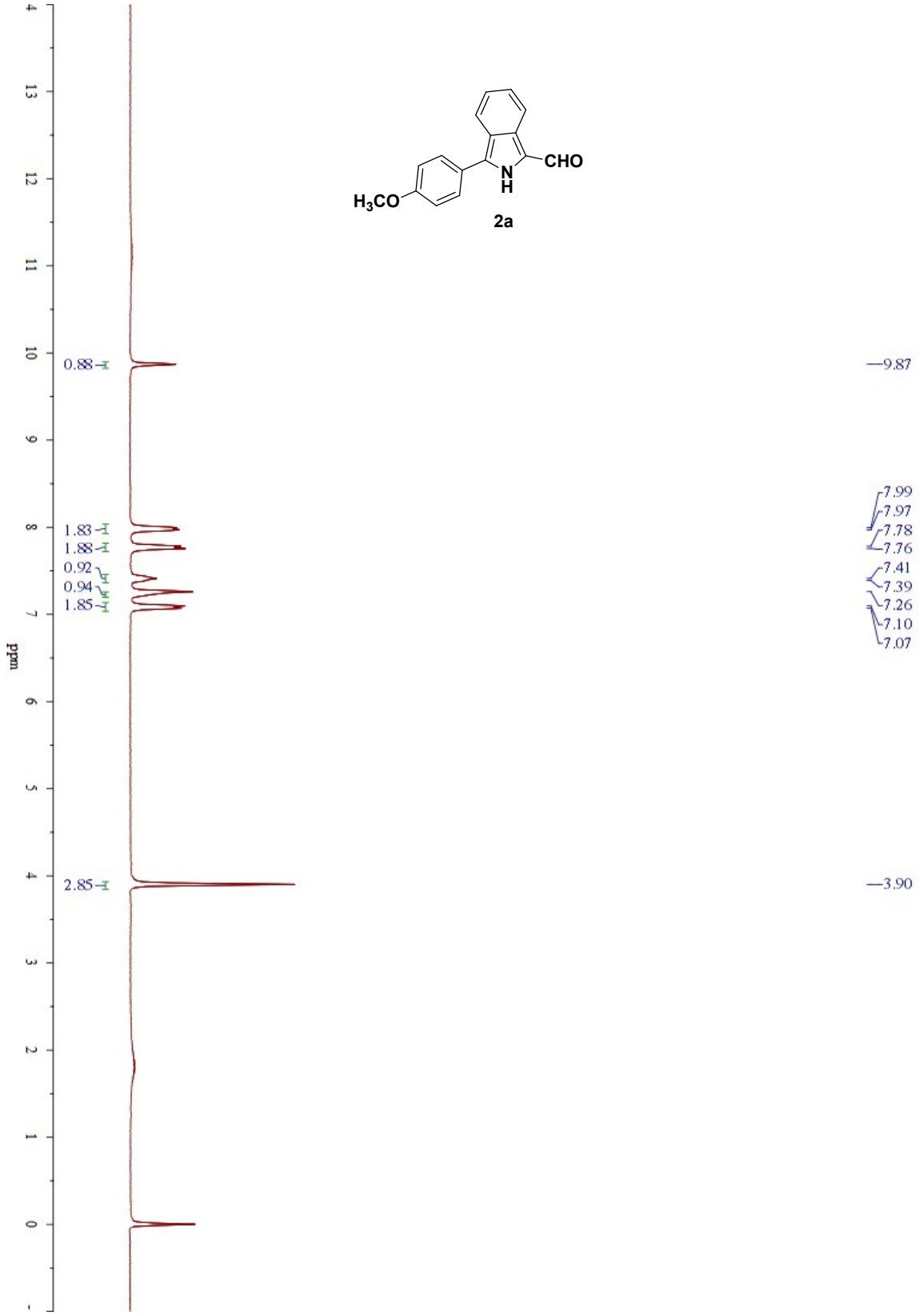
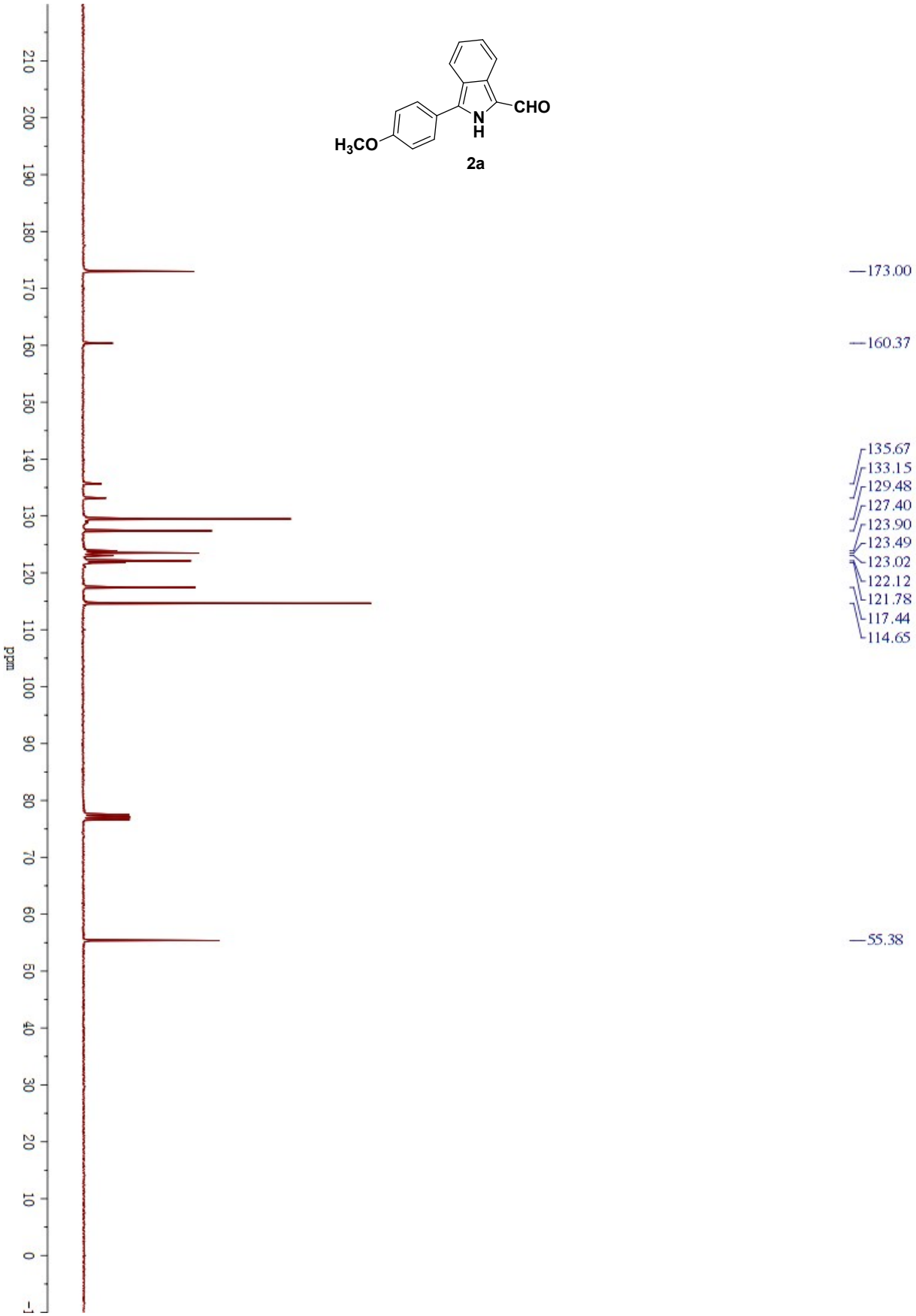


Figure S16. Excitation spectrum (dash line) and absorption spectrum (solid line) of **1e** in dichloromethane.

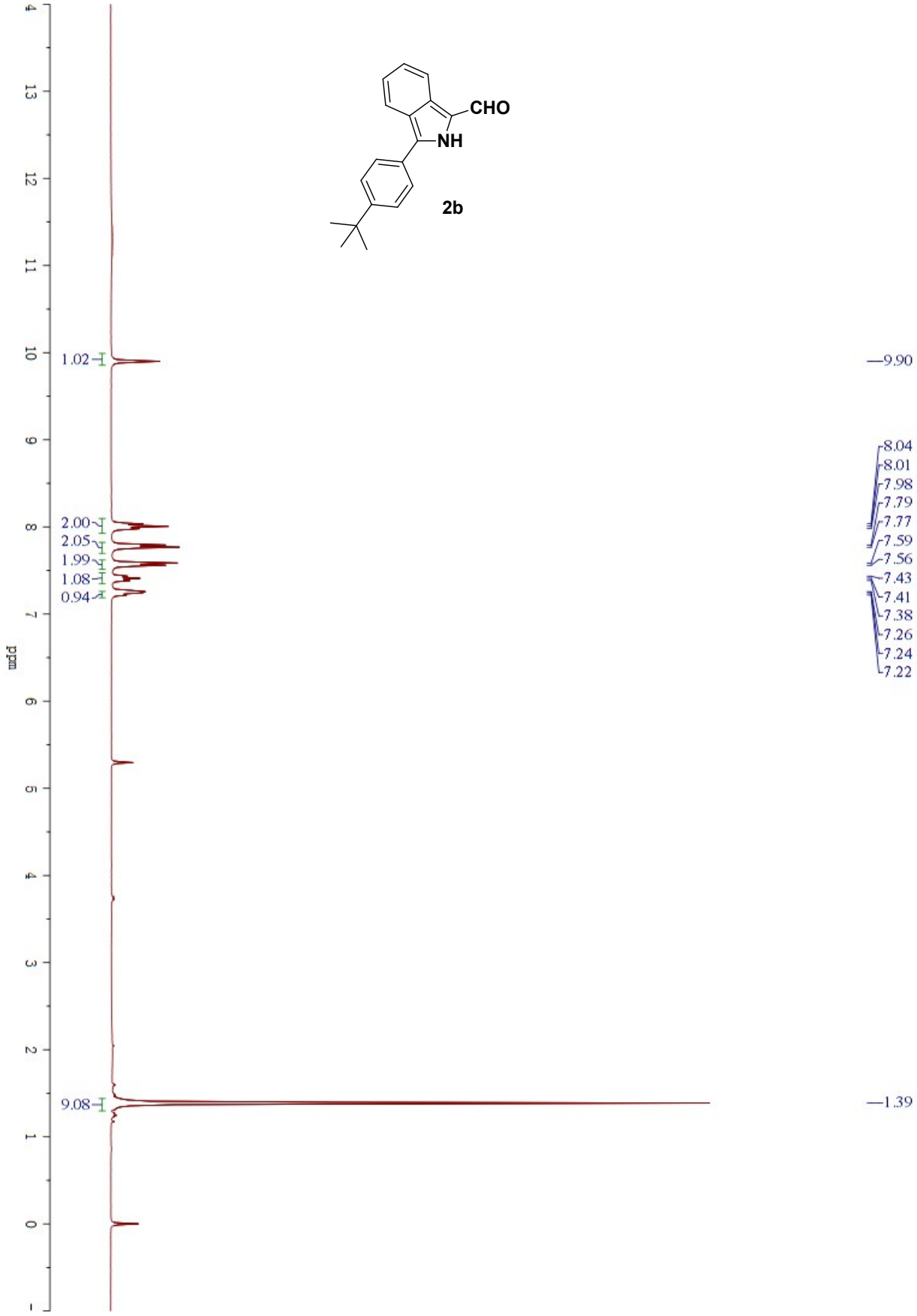
5. Copies of ^{1}H and ^{13}C NMR spectra



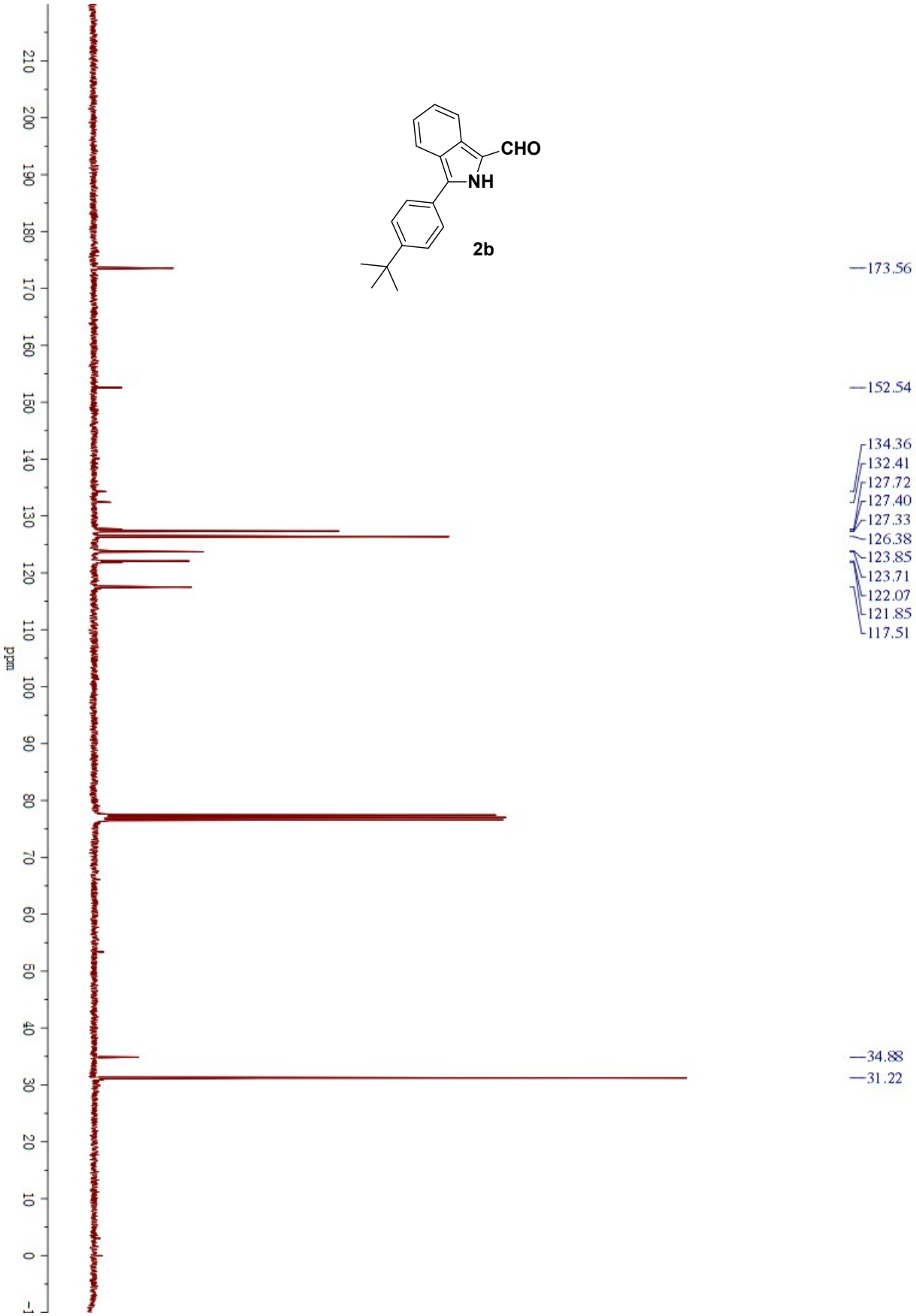
^{1}H NMR spectrum of **2a** in $CDCl_3$



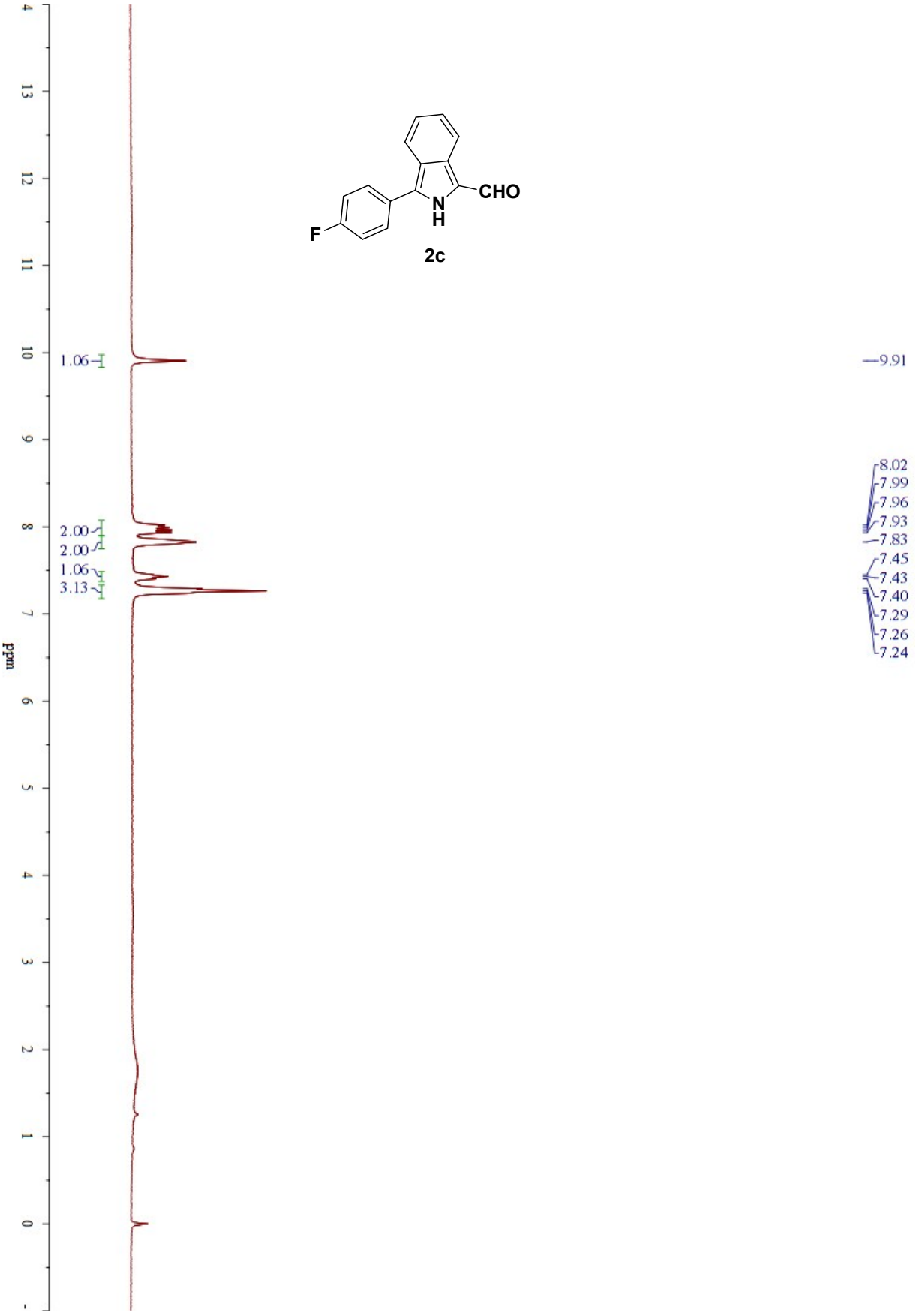
^{13}C NMR spectrum of **2a** in $CDCl_3$



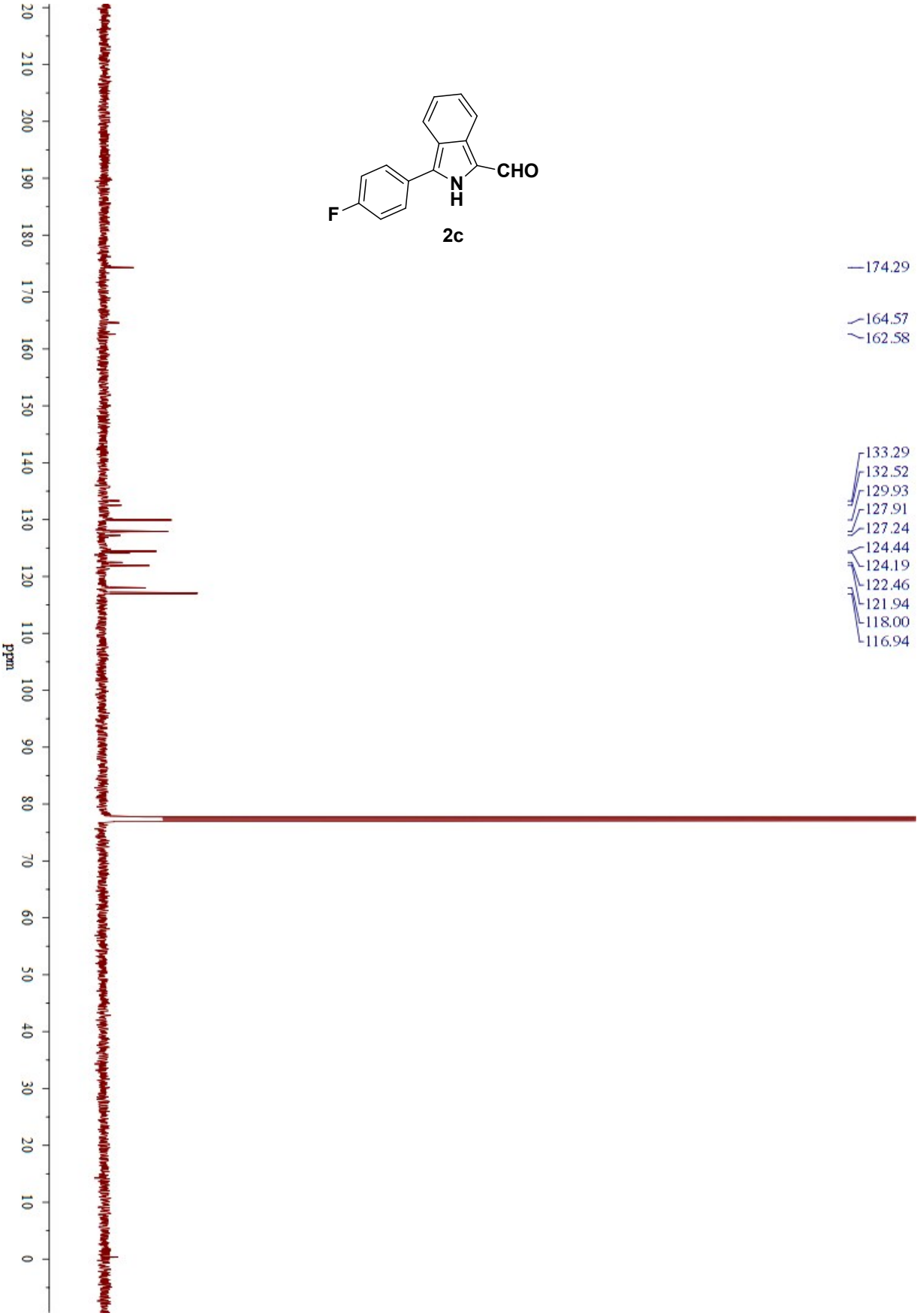
^{1}H NMR spectrum of **2b** in $CDCl_3$



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



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



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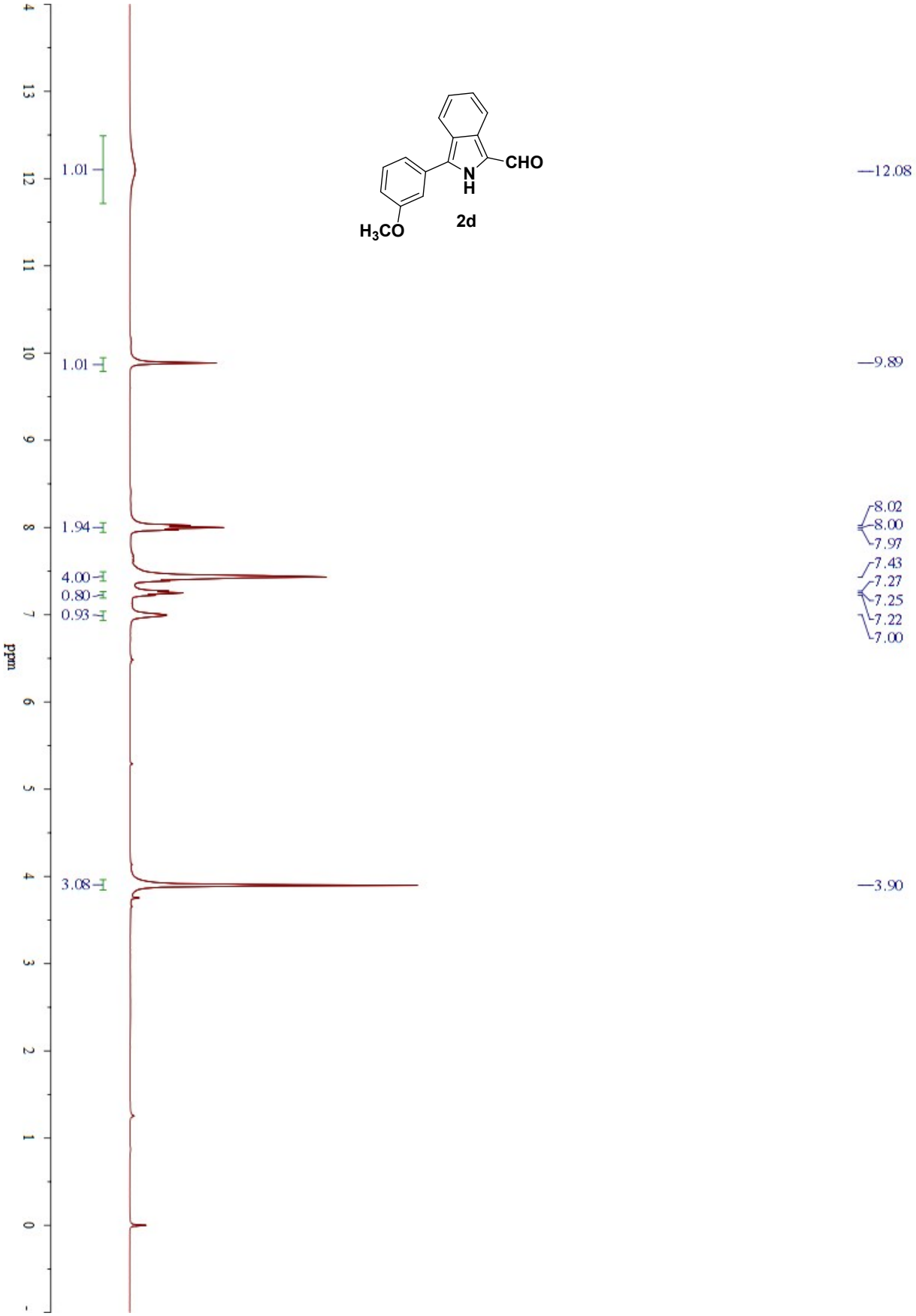
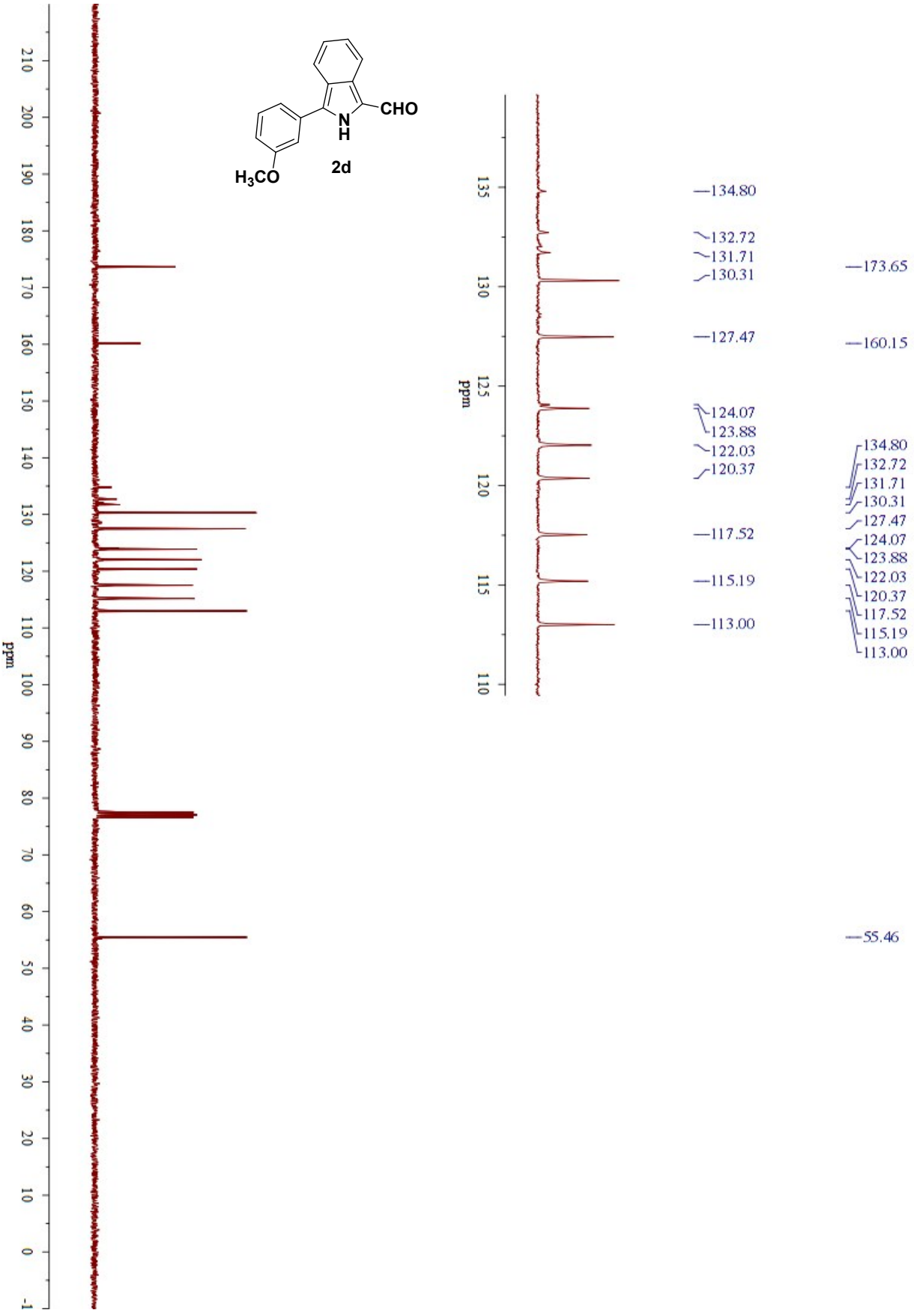


^{1}H NMR spectrum of **2d** in $CDCl_3$



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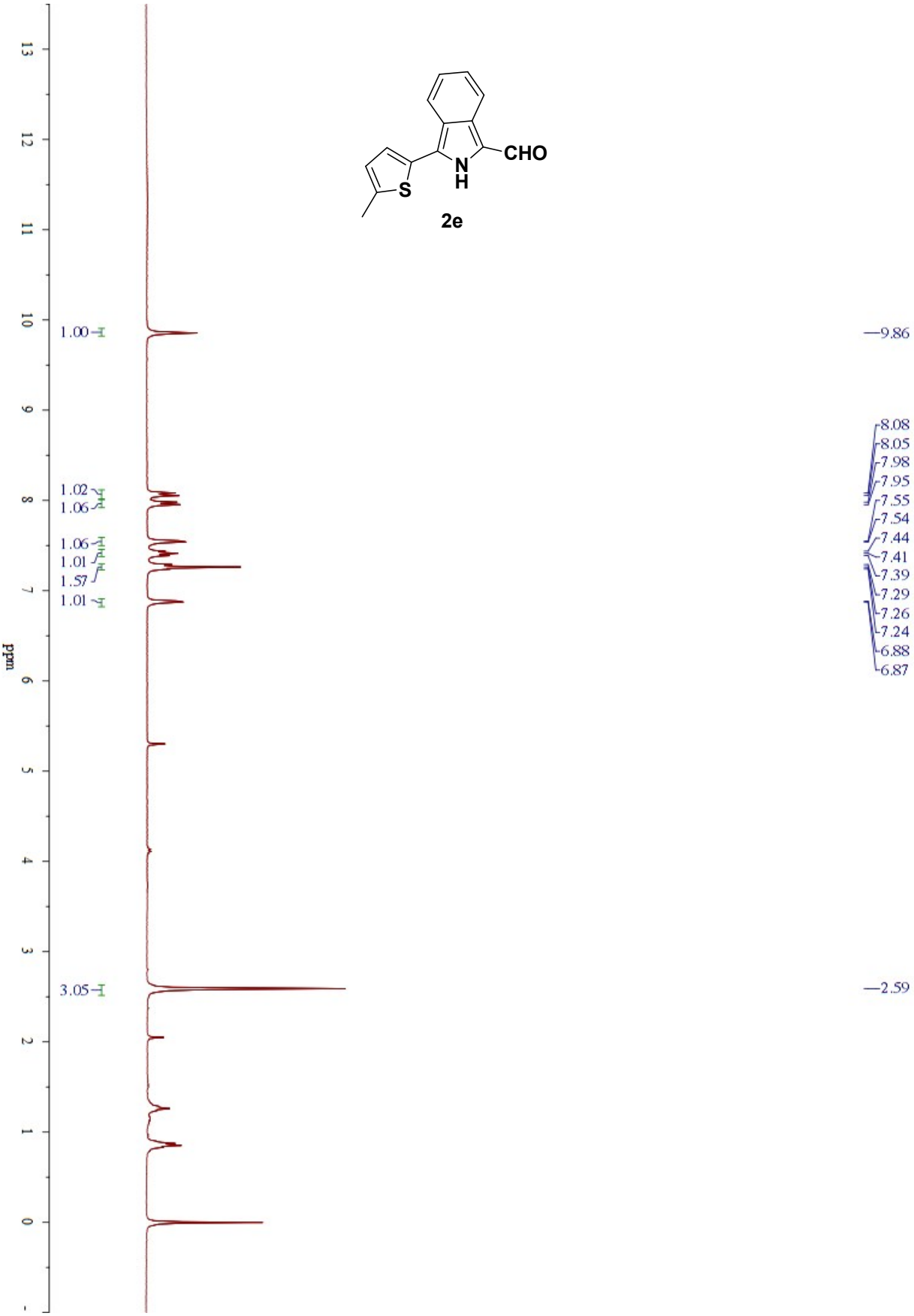

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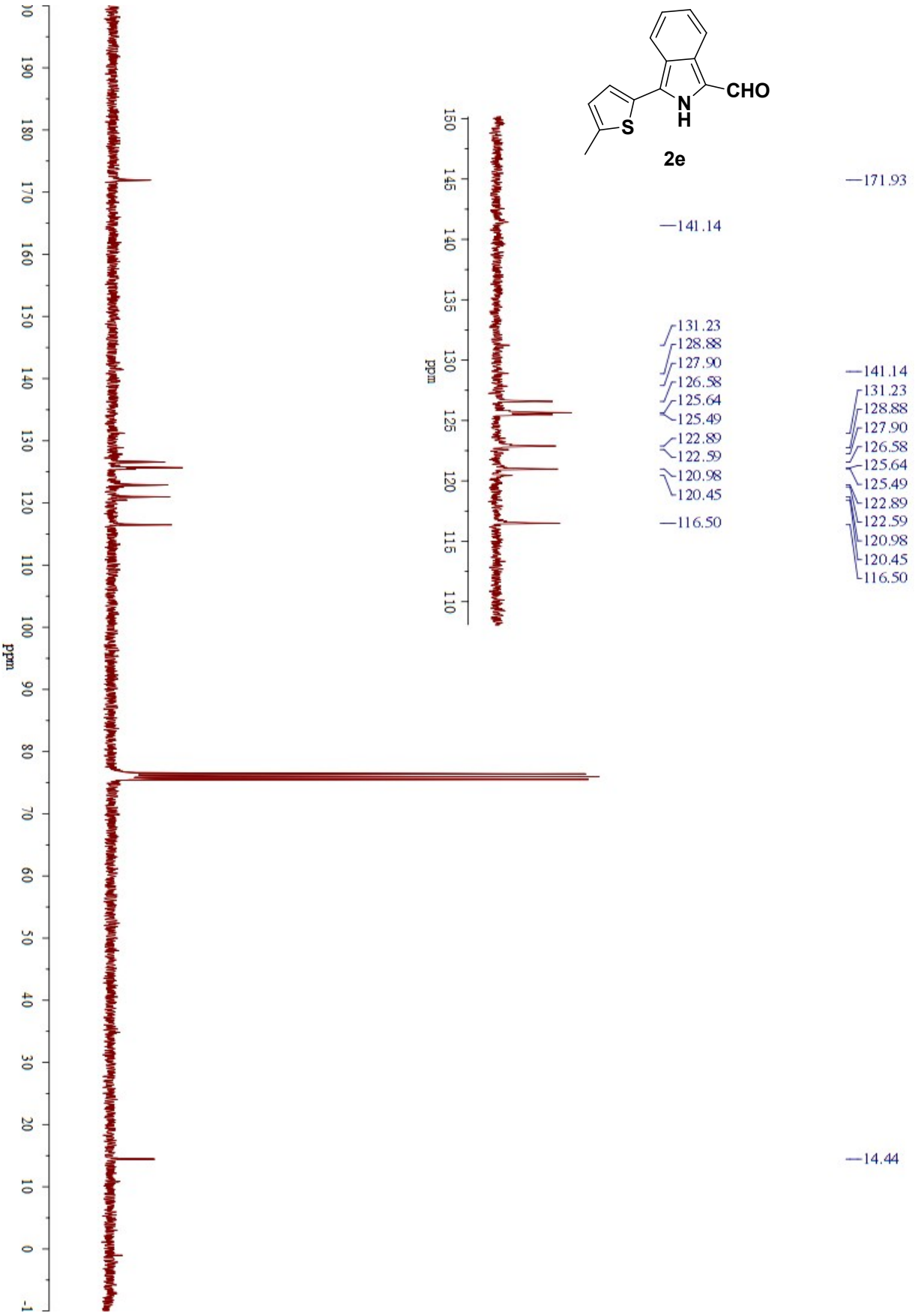

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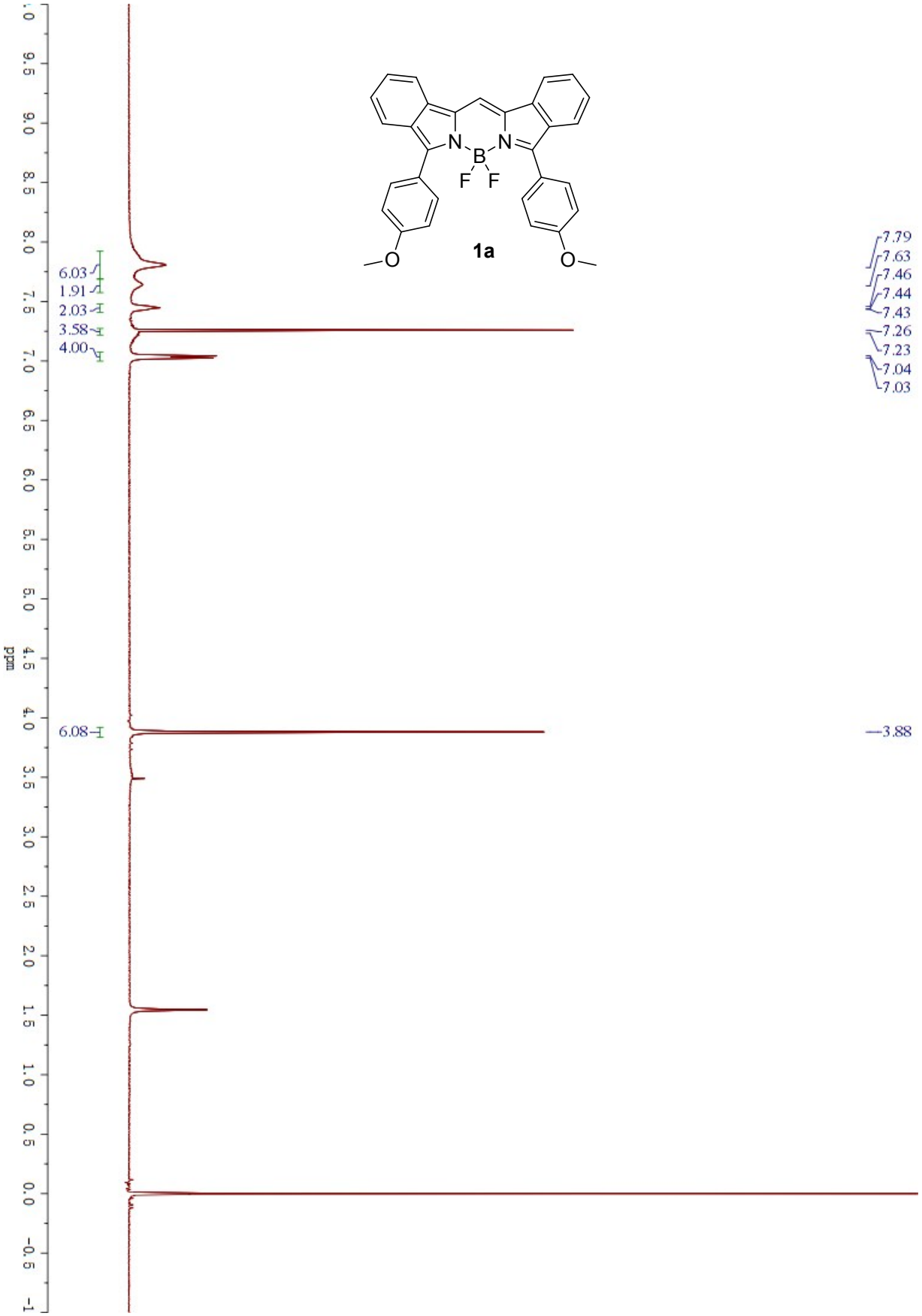

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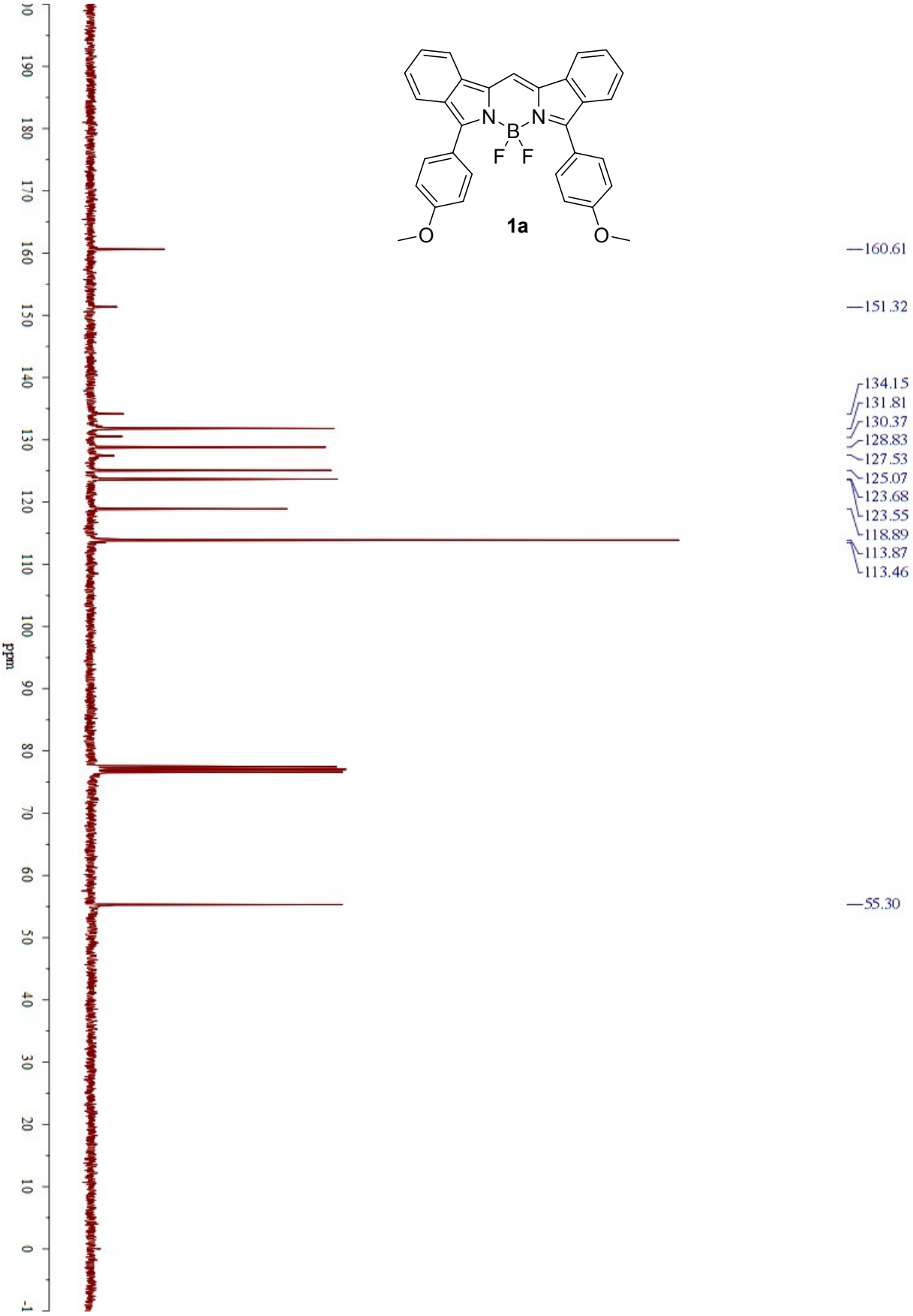
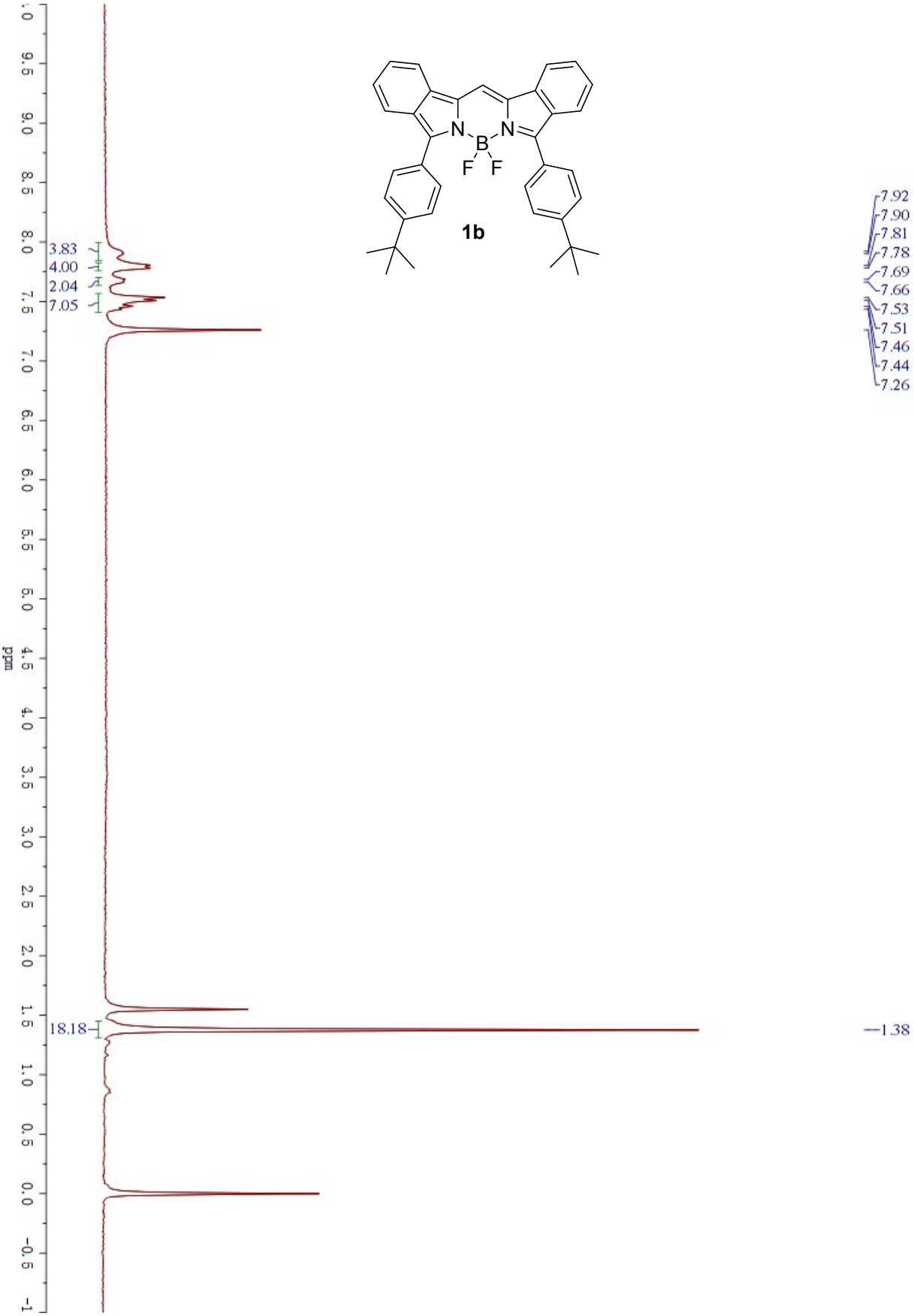
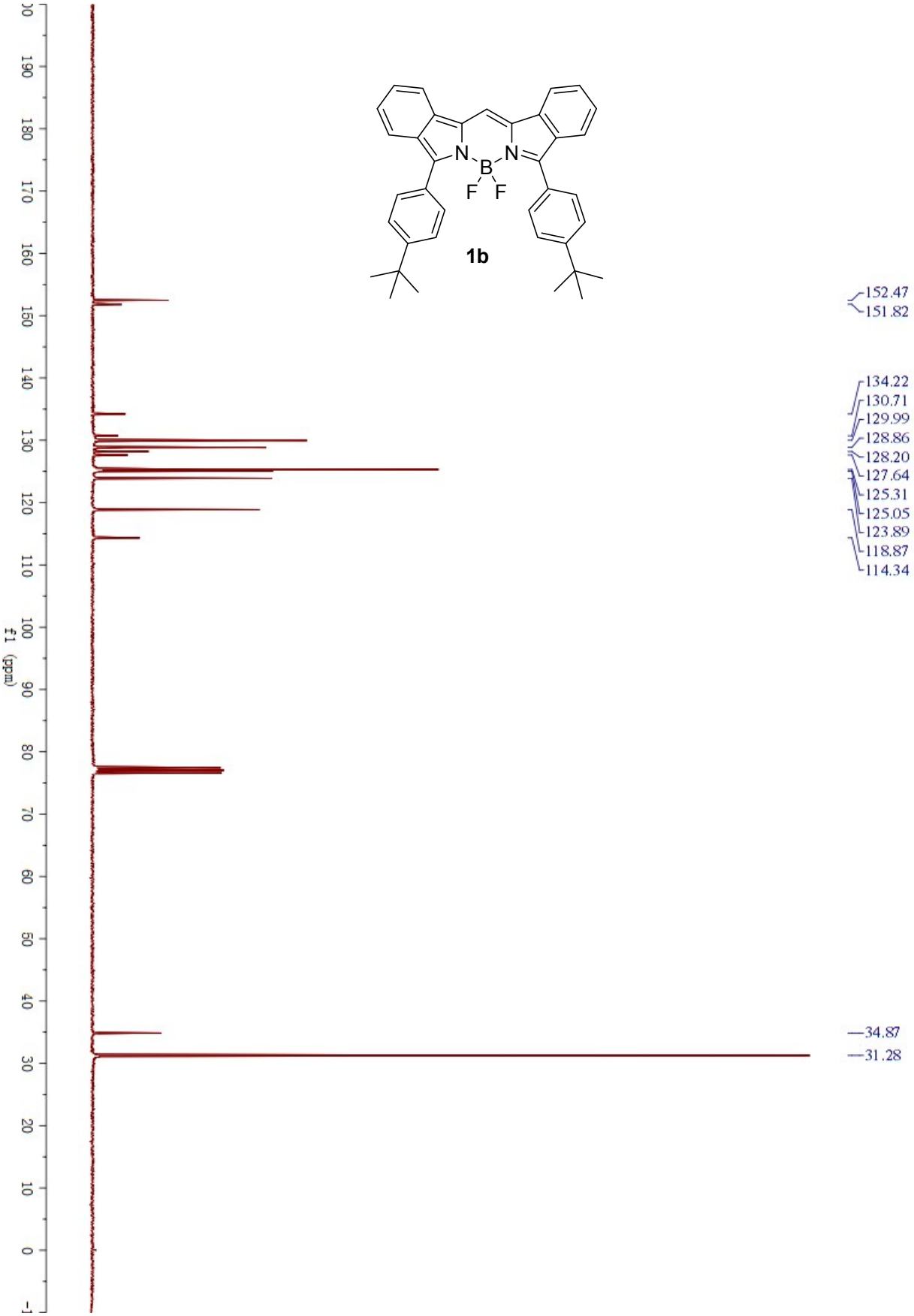


^{13}C NMR spectrum of **1a** in $CDCl_3$



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



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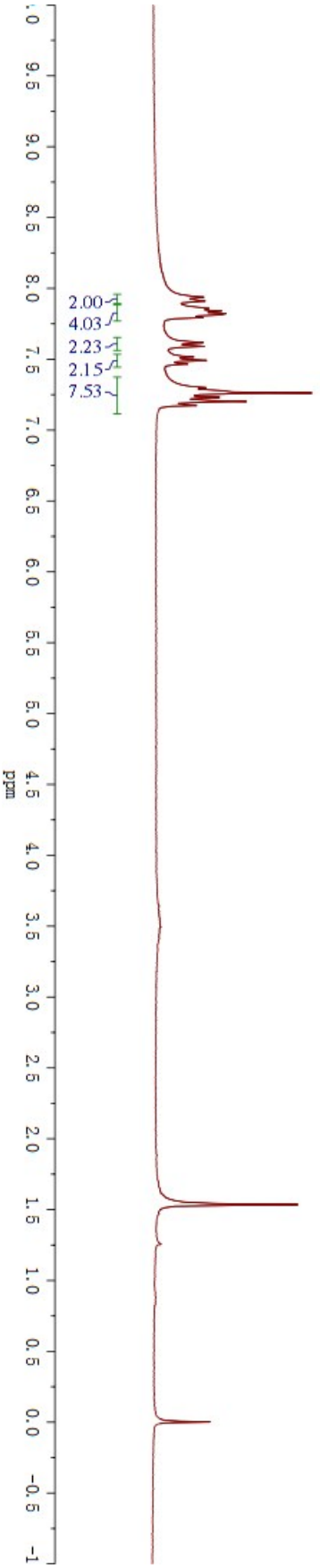
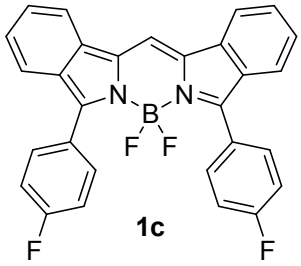
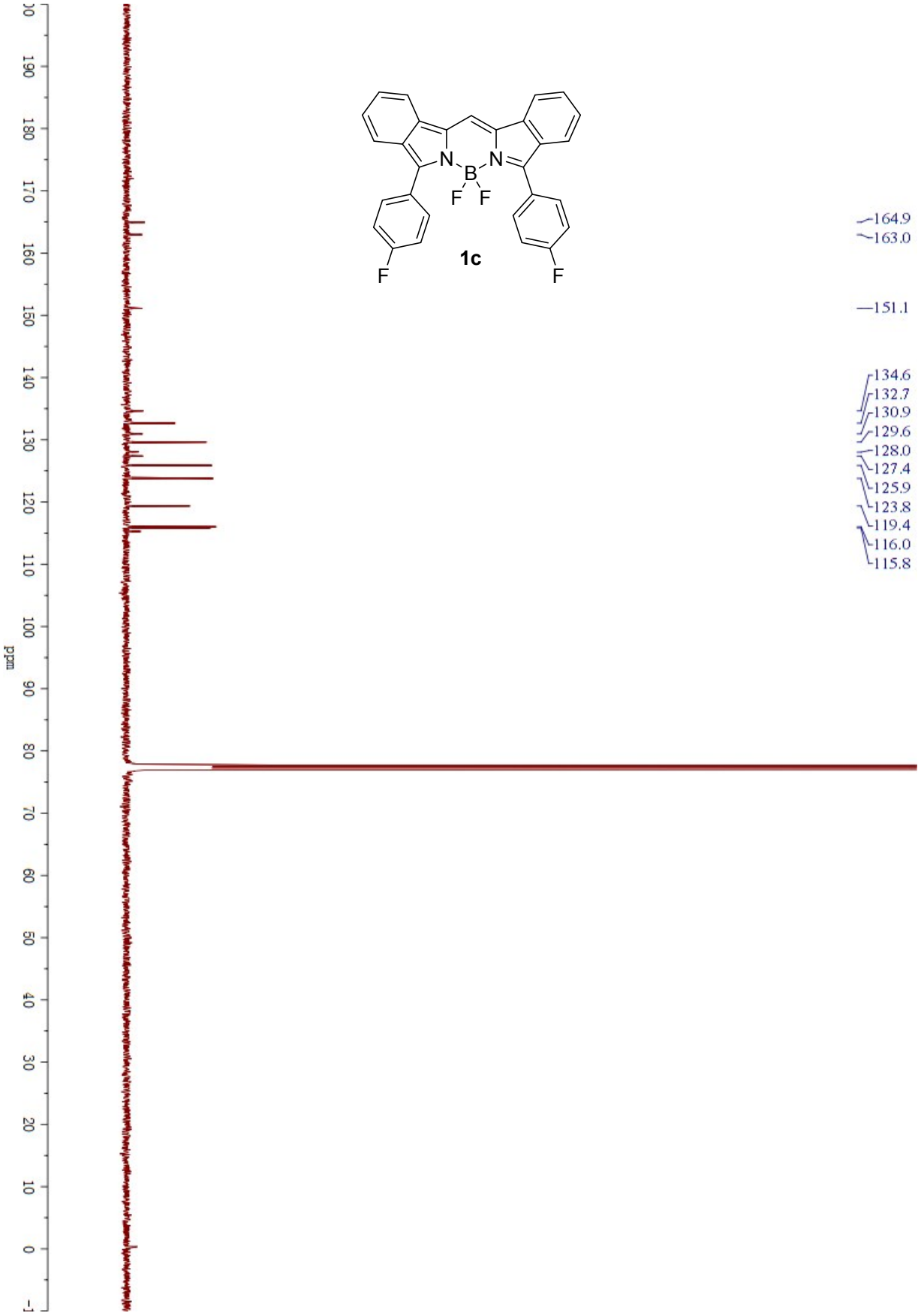


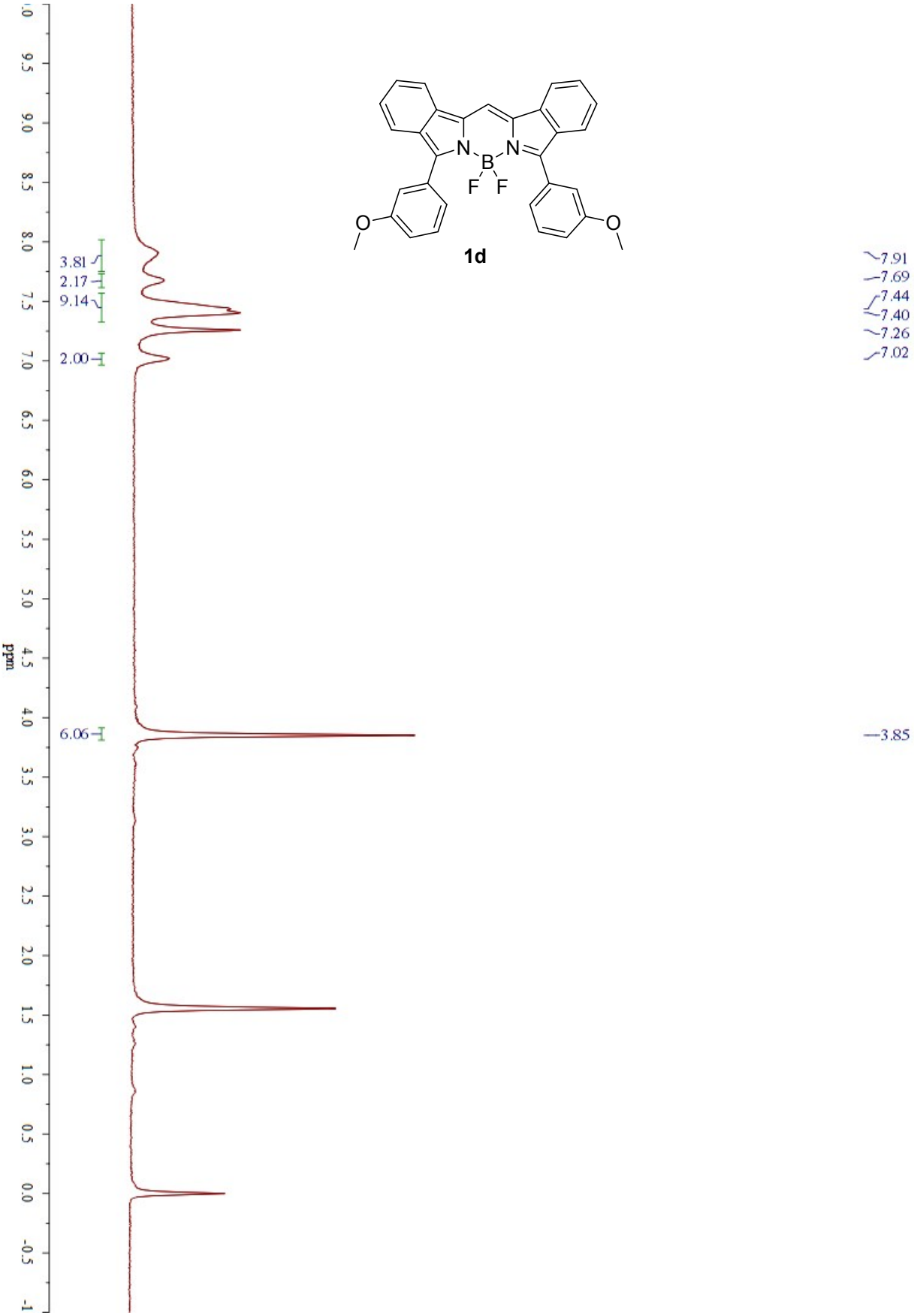


1c

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



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



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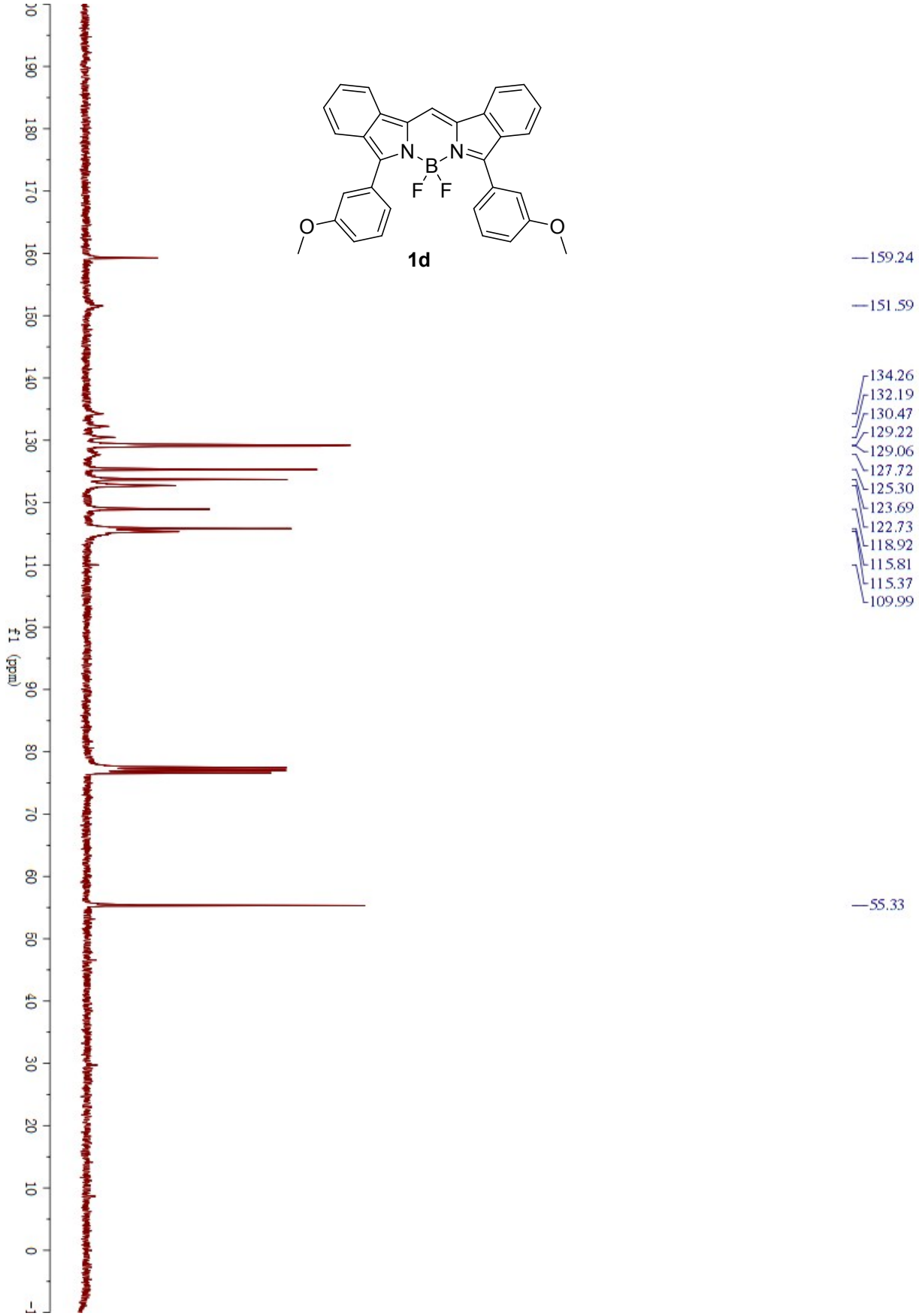

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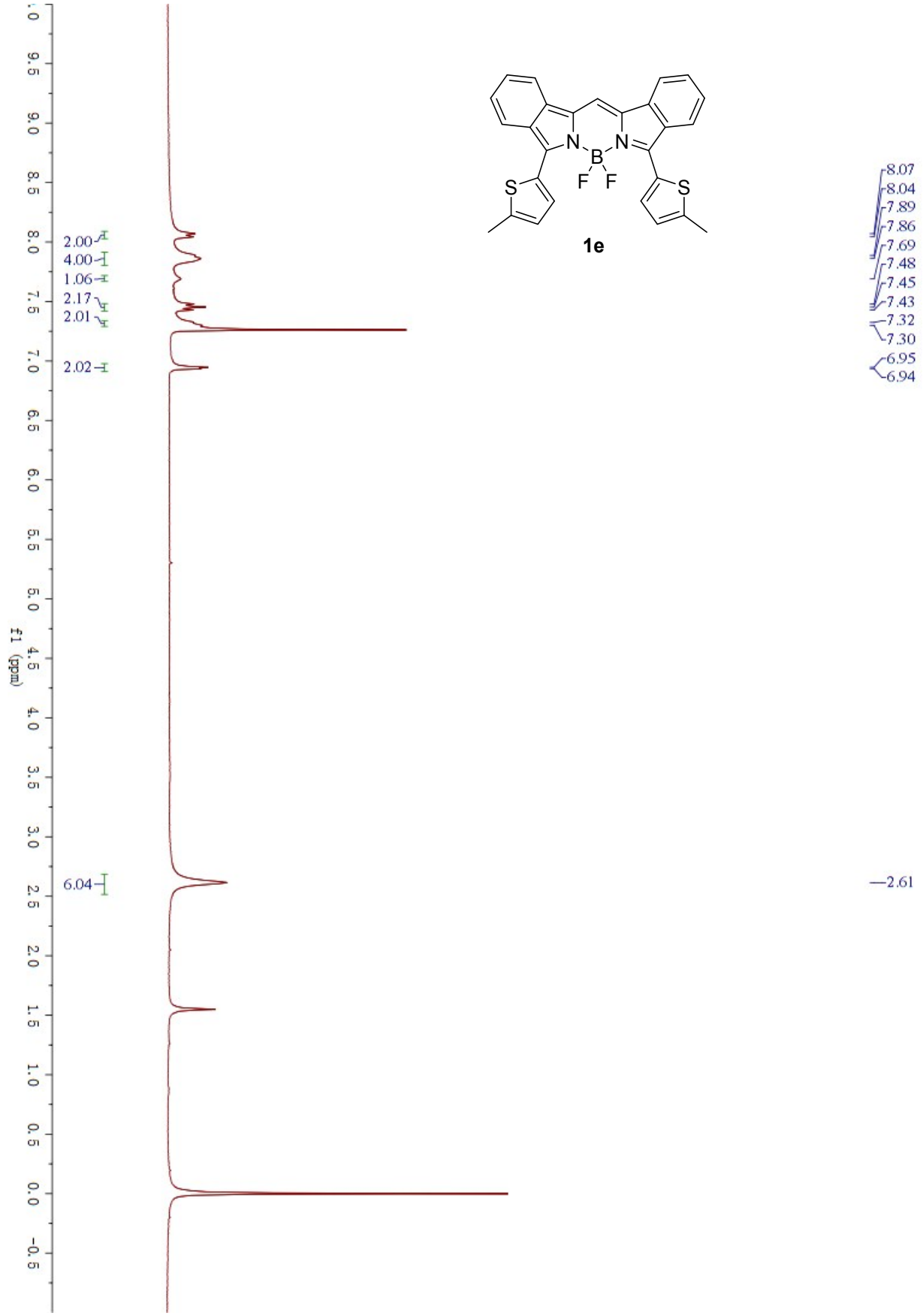
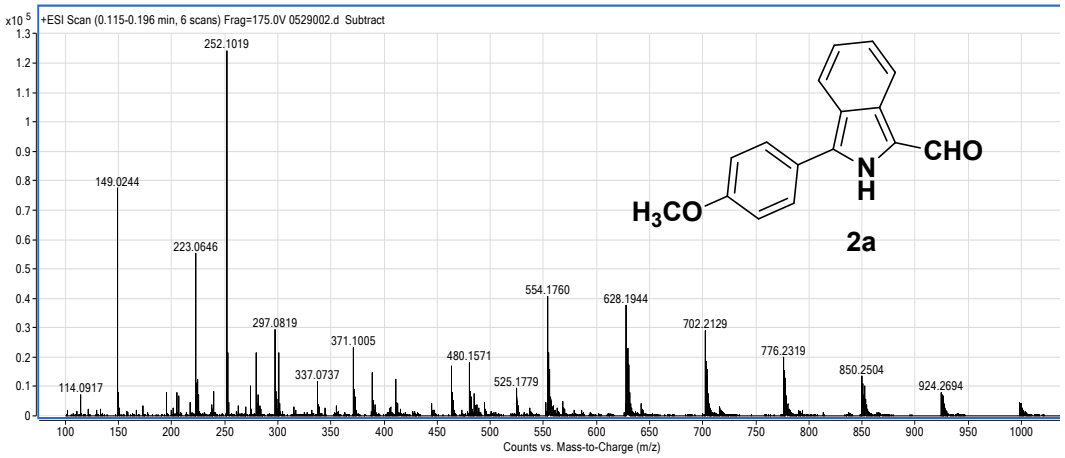
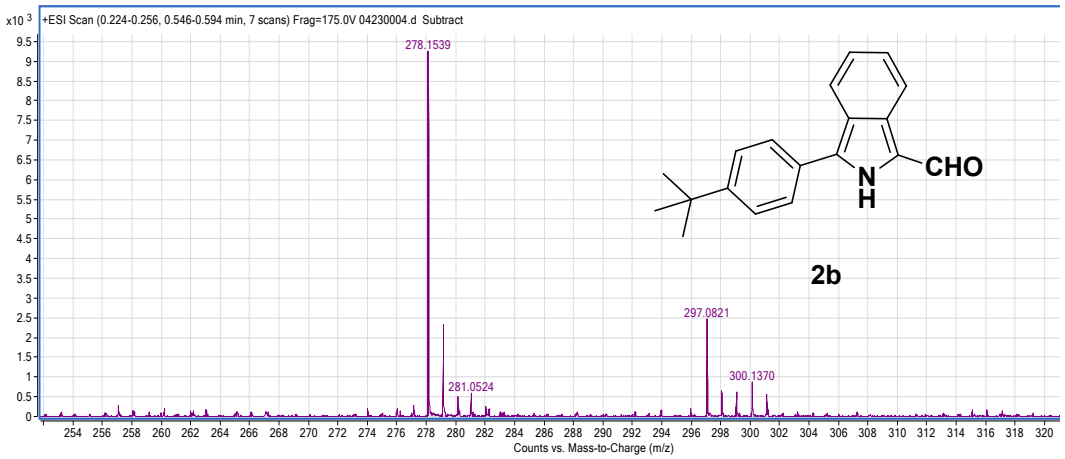


^{1}H NMR spectrum of **1e** in $CDCl_3$

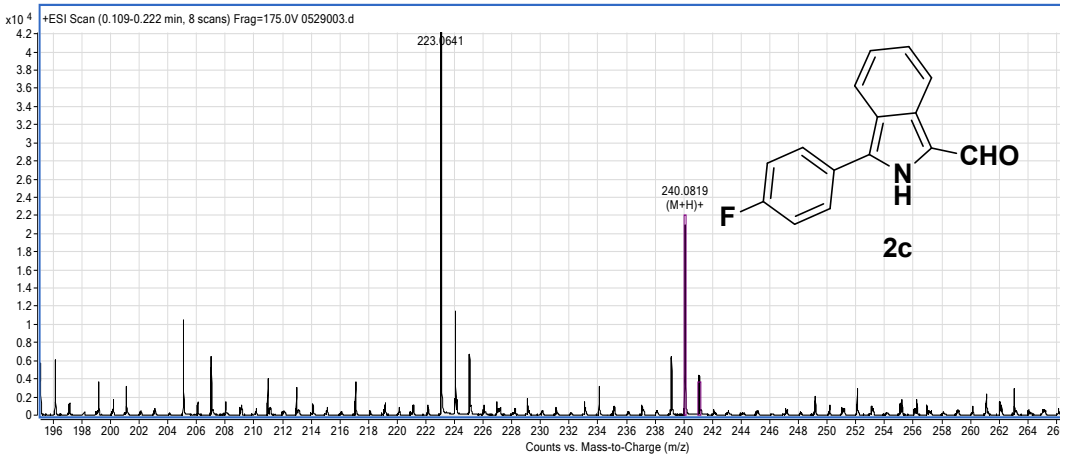
6. Copies of HRMS



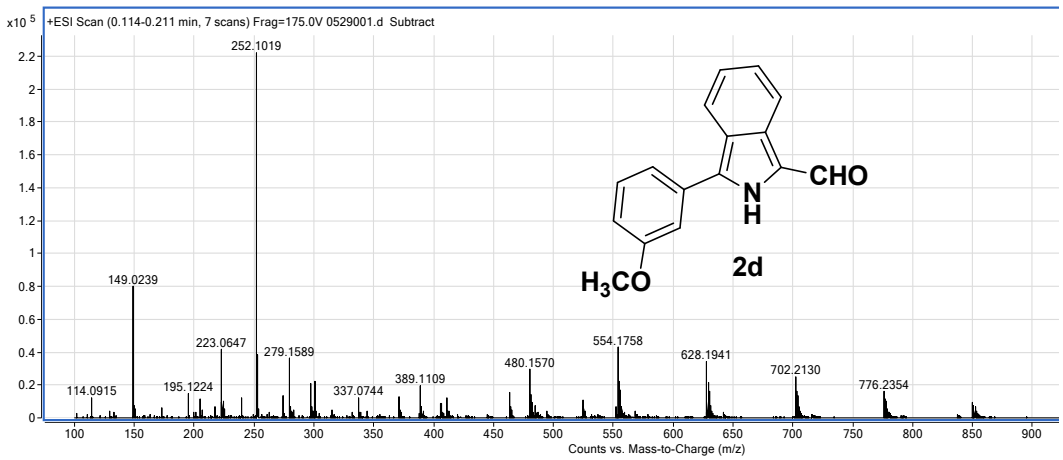
HRMS (ESI) calcd. for $C_{16}H_{14}O_2N$ $[M+H]^+$: 252.1025, found 252.1019.



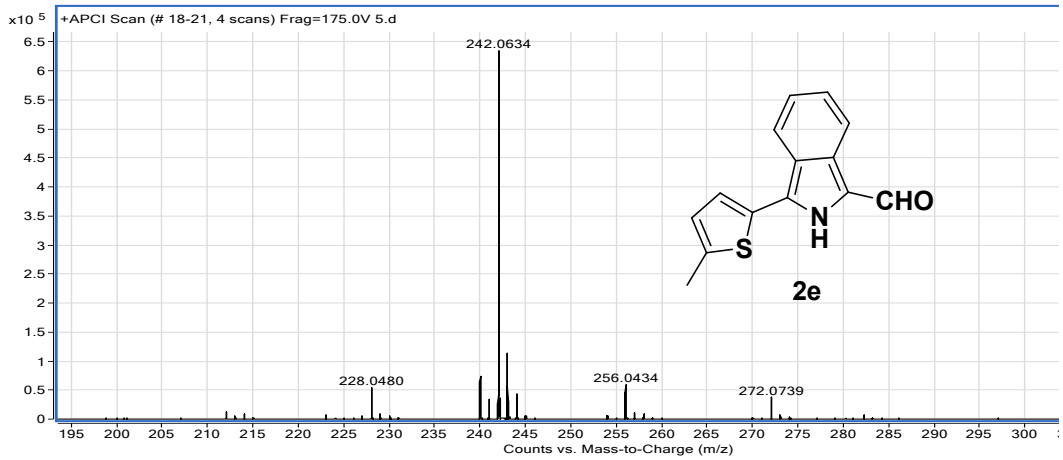
HRMS (ESI) calcd. for $C_{19}H_{20}ON$ $[M+H]^+$: 278.1545, found 278.1539



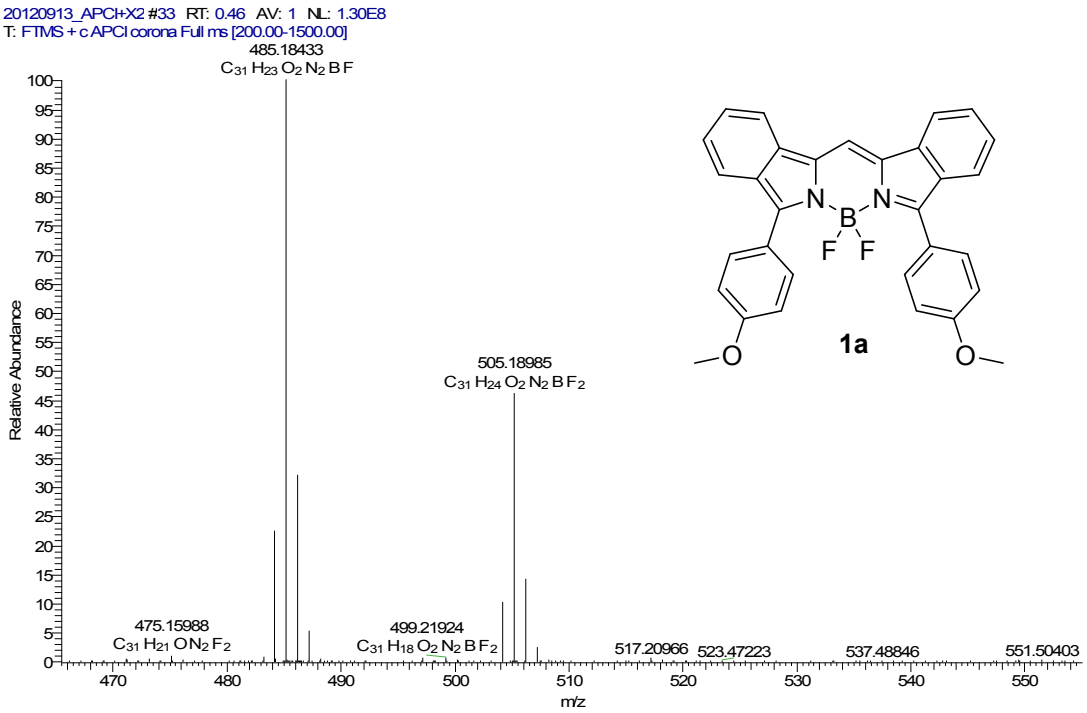
HRMS (ESI) calcd. for $C_{19}H_{20}ON$ $[M+H]+$: 240.0825, found 240.0819



HRMS (ESI) calcd. for $C_{16}H_{14}O_2N$ $[M+H]^+$: 252.1025, found 252.1019.

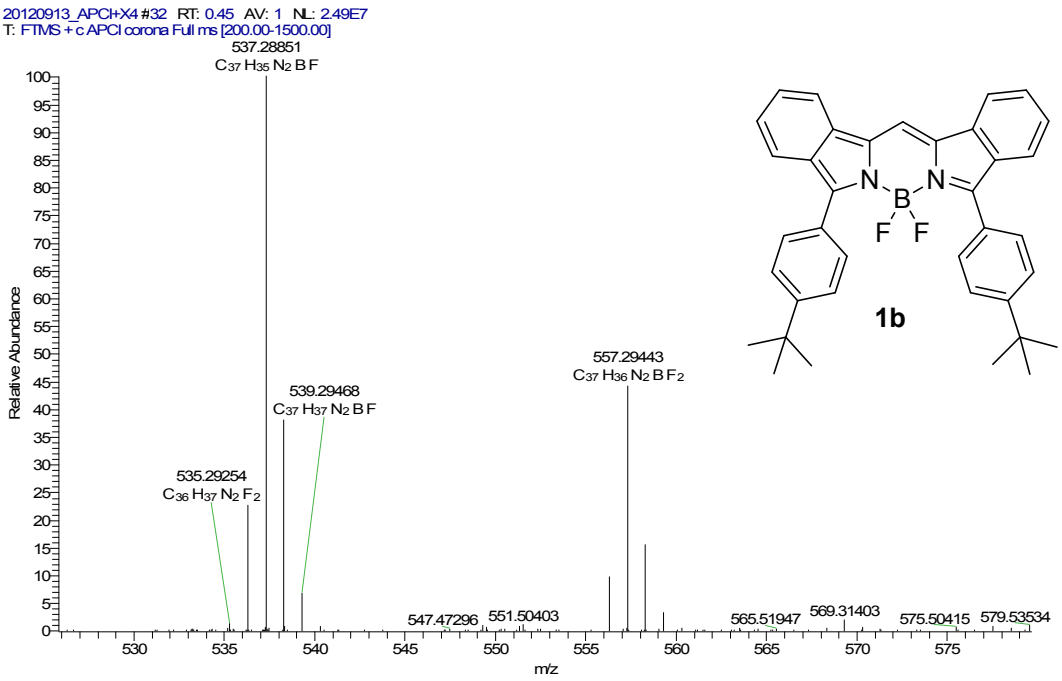


HRMS(ACPI) calcd. for $C_{14}H_{12}NOS$ $[M+H]^+$: 242.0640, found 242.0634.



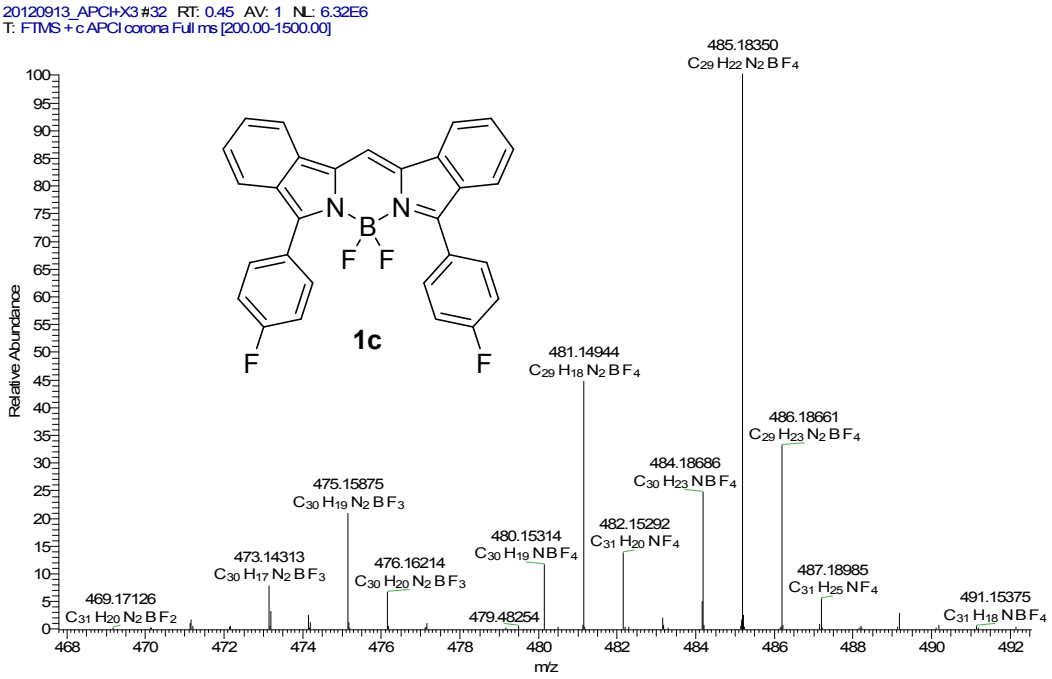
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
484.188	29109278	22.46	484.196	-7.88	18	C30 H26 O2 N2 F2
485.184	1.3E+08	100	485.183	1.21	21	C31 H23 O2 N2 B F
486.187	41444232	31.98	486.191	-3.8	20.5	C31 H24 O2 N2 B F
504.193	13141613	10.14	504.182	11.63	20.5	C31 H23 O2 N2 B F2
505.19	59830828	46.17	505.189	0.51	20	C31 H24 O2 N2 B F2

HRMS (ACPI) calcd. for $C_{31}H_{24}O_2N_2BF_2$ $[M+H]^+$: 505.1899, found 505.1898;



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
509.296	12046101	48.29	509.295	0.65	20.5	C37 H37 N2
510.299	4770769	19.13	510.301	-2.1	15.5	C33 H37 N2 B F2
511.303	900611.1	3.61	511.305	-1.96	16	C35 H39 N F2
536.292	5646697	22.64	536.3	-7.95	18	C36 H38 N2 F2
537.289	24943784	100	537.287	1.33	21	C37 H35 N2 B F
538.291	9461482	37.93	538.295	-3.69	20.5	C37 H36 N2 B F
539.295	1686477	6.76	539.303	-8.16	20	C37 H37 N2 B F
556.298	2412247	9.67	556.286	11.96	20.5	C37 H35 N2 B F2
557.294	11010414	44.14	557.293	1.02	20	C37 H36 N2 B F2
558.297	3858148	15.47	558.301	-4.06	19.5	C37 H37 N2 B F2

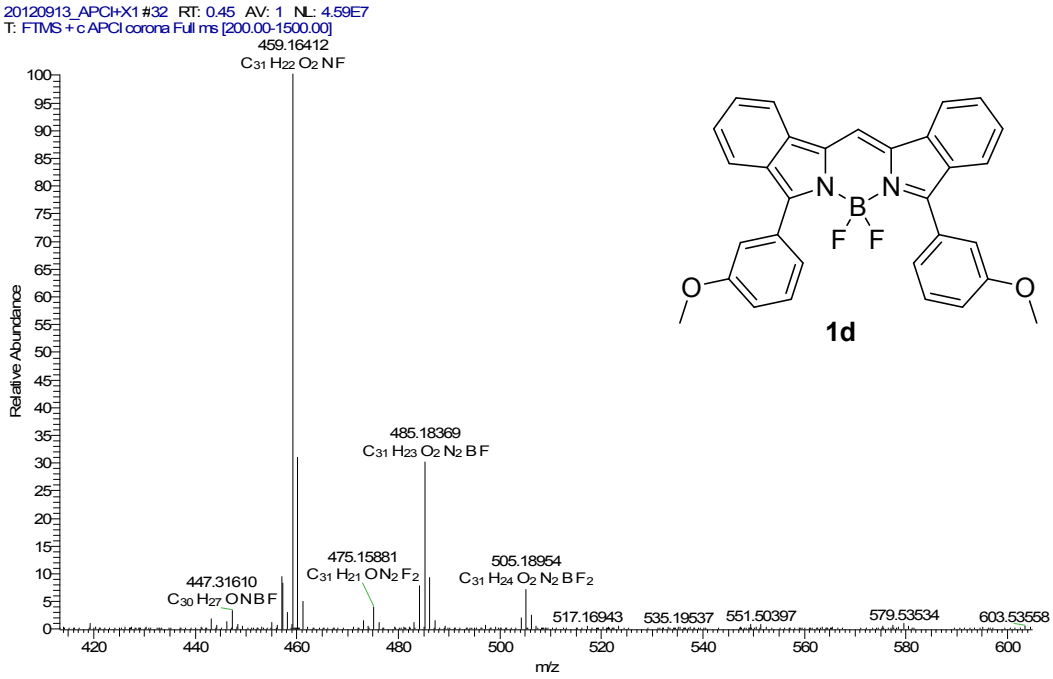
HRMS (ACPI) calcd. for $C_{37}H_{36}N_2BF_2$ $[M+H]^+$: 557.2940, found 557.2944;



m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
473.143	487544	7.71	473.143	-0.01	22	C30 H17 N2 B F3
475.159	1309349	20.7	475.159	-0.04	21	C30 H19 N2 B F3
476.162	415903.3	6.58	476.167	-4.48	20.5	C30 H20 N2 B F3
480.153	728624	11.52	480.154	-0.98	20	C30 H19 N B F4
481.149	2822913	44.64	481.149	0.08	20	C29 H18 N2 B F4
482.153	868623.7	13.74	482.153	0.28	20.5	C31 H20 N F4
484.187	1558229	24.64	484.185	1.44	18	C30 H23 N B F4
485.184	6323982	100	485.181	2.83	18	C29 H22 N2 B F4
486.187	2090009	33.05	486.188	-1.88	17.5	C29 H23 N2 B F4
487.19	343277.4	5.43	487.192	-1.91	18	C31 H25 N F4

HRMS (ACPI) calcd. for $C_{29}H_{18}N_2BF_4$ $[M+H]^+$: 481.1499, found 481.1494;

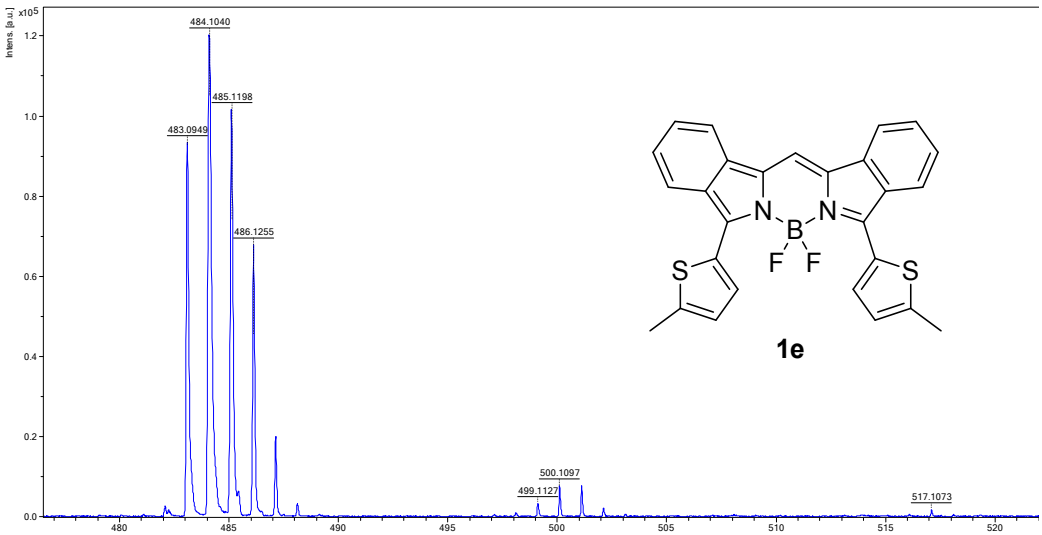
.



1d

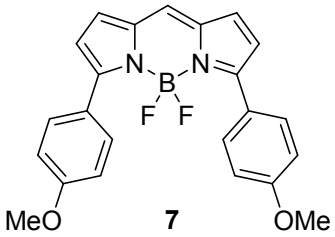
m/z	Intensity	Relative	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
457.149	4315139	9.4	457.151	-1.82	22.5	C31 H19 N2 F2
457.192	3725417	8.12	457.191	0.69	20.5	C31 H25 O2 N2
459.164	45884960	100	459.163	1.21	21	C31 H22 O2 N F
460.167	14156451	30.85	460.168	-0.49	20	C30 H21 O N B F2
461.171	2252479	4.91	461.166	4.58	20.5	C30 H22 O2 N2 F
475.159	1768956	3.86	475.162	-2.83	21.5	C31 H21 O N2 F2
484.187	3520584	7.67	484.196	-8.52	18	C30 H26 O2 N2 F2
485.184	13793157	30.06	485.183	0.57	21	C31 H23 O2 N2 B F
486.187	4192357	9.14	486.191	-4.32	20.5	C31 H24 O2 N2 B F
505.19	3253841	7.09	505.189	0.2	20	C31 H24 O2 N2 B F2

HRMS (ACPI) calcd. for $C_{31}H_{24}O_2N_2BF_2$ [M+H]+: 505.1899, found 505.1895;



HRMS (MALDI-TOF) calcd. for $C_{27}H_{20}N_2S_2BF_2$ [M+H]+: 485.1129, found 485.1198;

7. DFT calculation



7

Chart S1. Chemical Structure of BODIPY **7**.

Table S4. Selected electronic excitation energies (eV) and oscillator strengths (f), configurations of the low-lying excited states of the BODIPY **1a-e** calculated by TD-B3LYP/6-31+G(d,p) // B3LYP/6-31G(d) based on the optimized ground state geometries. The TDDFT of all the molecules in dichloromethane were using the Self-Consistent Reaction Field (SCRF) method and the Polarizable Continuum Model (PCM).

	Electronic transition	**TD-B3LYP/6-31+G(d,p)//B3LYP/6-31G(d)**				
		Energy/ eV [a]		f **[b]**	**Composition [c]**	**CI [d]**
1a	S0→S1	2.0433 eV	606.79 nm	0.9165	HOMO → LUMO	0.7092
1b	S0→S1	2.0834 eV	595.12 nm	0.9277	HOMO → LUMO	0.7095
1c	S0→S1	2.0989 eV	590.71 nm	0.8952	HOMO → LUMO	0.7104
					HOMO ← LUMO	0.1016
1d	S0→S1	2.0897 eV	593.30 nm	0.8824	HOMO → LUMO	0.7097
1e	S0→S1	1.8786 eV	659.99 nm	0.8795	HOMO → LUMO	0.7169
					HOMO ← LUMO	0.1073

[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values.

DFT optimized coordinates

Compound **1a**

B	-0.05420300	-0.17649200	0.02740500
C	-4.10456500	5.73761400	-0.41939300
H	-3.04475400	5.90727400	-0.18964200
H	-4.68209900	6.61899600	-0.13500000
H	-4.21681300	5.56223900	-1.49727500
F	-0.16491600	0.58616400	1.17824800
N	-1.36988200	-1.05271000	-0.09076100
O	-4.63648000	4.66304100	0.34134900
C	-4.08614100	3.42683700	0.18567600
F	0.11714200	0.59372300	-1.11324900
N	1.18927300	-1.15434300	0.12489200
O	4.73839100	4.38176400	0.20940700
C	-3.03493700	3.12434100	-0.68846300
H	-2.58951700	3.89077000	-1.31215900
C	-2.54501000	1.82216200	-0.76806000
H	-1.72693900	1.60719700	-1.44215200
C	-3.08951200	0.78994200	0.01202100
C	-4.15104300	1.11487800	0.88503500
H	-4.57265000	0.34421600	1.52259200
C	-4.63884000	2.40843600	0.97722200
H	-5.44229600	2.65947000	1.66250700
C	-2.65124200	-0.60827900	-0.07611700
C	-3.52781700	-1.74579800	-0.13714900
C	-4.92977600	-1.86238700	-0.22041300
H	-5.56016700	-0.97912900	-0.23727500
C	-5.48545300	-3.12841400	-0.29507800
H	-6.56405500	-3.24055600	-0.35993400
C	-4.66831600	-4.28374400	-0.29772700
H	-5.13555000	-5.26314000	-0.35674000
C	-3.28730800	-4.18738000	-0.24056600
H	-2.67028200	-5.08189600	-0.25953800
C	-2.70860700	-2.90860200	-0.16807200
C	-1.35623600	-2.44913300	-0.12370400
C	-0.16683200	-3.15691500	-0.05008500
H	-0.20660700	-4.24122600	-0.08431400
C	1.07205600	-2.54471700	0.06746300
C	2.38575300	-3.10538500	0.08529200
C	2.86829300	-4.42567500	0.07634700
H	2.18688200	-5.27160700	0.03749000
C	4.23794600	-4.62742700	0.12767000
H	4.63120700	-5.64050900	0.12388200
C	5.13863900	-3.53783600	0.19899000

H	6.20564200	-3.73384800	0.25653300
C	4.67856300	-2.23218000	0.20615400
H	5.37178100	-1.40010300	0.27886100
C	3.28926300	-2.00683100	0.13083600
C	2.50023600	-0.80669700	0.14201500
C	3.04150700	0.55886400	0.14337100
C	2.58877500	1.57305500	1.01267500
H	1.76859900	1.37093600	1.68779700
C	3.17783500	2.82703600	1.00829800
H	2.83432200	3.60629600	1.68136700
C	4.23530400	3.11779000	0.13291100
C	4.69773100	2.12643200	-0.74086400
H	5.50356700	2.32409200	-1.43843500
C	4.10519600	0.86441300	-0.72243200
H	4.45734200	0.11088000	-1.42005300
C	5.80628300	4.73570600	-0.65560700
H	6.69274600	4.11260800	-0.47808600
H	6.04486800	5.77572000	-0.42596700
H	5.51425600	4.65507700	-1.71090600

Compound **1b**

B	0.00007900	-0.76026900	0.00022900
F	-0.14117400	0.00406800	1.14605700
N	-1.27976200	-1.69094300	-0.10983700
C	-4.17406300	2.71912600	-0.00081900
F	0.14128100	0.00447400	-1.14533500
N	1.27995000	-1.69090000	0.10997800
C	-3.13759700	2.38381100	-0.88245800
C	-2.58793800	1.10308300	-0.92424500
C	-3.06415100	0.09170000	-0.07701000
C	-4.10922700	0.41731100	0.80922800
C	-4.64173700	1.70003300	0.84715300
C	-2.57531100	-1.29464200	-0.11465400
C	-3.41045200	-2.46262500	-0.13893600
C	-4.80751600	-2.63042600	-0.21563600
C	-5.31769800	-3.91701400	-0.24919600
C	-4.45979400	-5.04218500	-0.21630100
C	-3.08302300	-4.89583500	-0.16213900
C	-2.54976600	-3.59579200	-0.13041000
C	-1.21506900	-3.08596900	-0.09659900
C	0.00015100	-3.74655900	0.00005700
C	1.21535100	-3.08592700	0.09670400
C	2.55008700	-3.59565400	0.13039600
C	3.08341300	-4.89567000	0.16204500

C	4.46019600	-5.04194900	0.21606700
C	5.31803300	-3.91672400	0.24889500
C	4.80777900	-2.63016200	0.21540300
C	3.41069800	-2.46242800	0.13885000
C	2.57546900	-1.29450100	0.11466100
C	3.06419500	0.09187700	0.07704200
C	2.58801600	1.10316900	0.92440200
C	3.13754900	2.38395200	0.88260900
C	4.17383500	2.71942300	0.00082200
C	4.64151700	1.70040400	-0.84724100
C	4.10914400	0.41762900	-0.80930300
H	-2.73810800	3.12836100	-1.56197700
H	-1.78280400	0.88891700	-1.61420300
H	-4.48300600	-0.33693600	1.49508600
H	-5.43531600	1.90923000	1.55925000
H	-5.46763100	-1.76987500	-0.25705000
H	-6.39162100	-4.06974400	-0.30824500
H	-4.89210800	-6.03882800	-0.24389700
H	-2.43519100	-5.76847100	-0.15189500
H	0.00016500	-4.83216700	0.00005900
H	2.43561400	-5.76833200	0.15183700
H	4.89257700	-6.03856400	0.24360200
H	6.39197200	-4.06938300	0.30783700
H	5.46786500	-1.76958900	0.25675600
H	1.78299600	0.88889200	1.61446200
H	2.73810800	3.12841300	1.56225200
H	5.43500300	1.90970300	-1.55940900
H	4.48292800	-0.33655500	-1.49522400
C	-4.79528400	4.12460900	0.07092900
C	-4.15906700	5.09973300	-0.93745200
H	-4.63293000	6.08374100	-0.84728800
H	-3.08650400	5.23180300	-0.75610400
H	-4.29277100	4.76247400	-1.97158200
C	-6.30935800	4.03405800	-0.23556800
H	-6.83261700	3.38857100	0.47764100
H	-6.76911200	5.02874000	-0.18416000
H	-6.48258600	3.63156800	-1.24019900
C	-4.59390900	4.70214900	1.49256500
H	-3.52822700	4.78537400	1.73391800
H	-5.03869700	5.70233100	1.56362200
H	-5.06143900	4.07420800	2.25817500
C	4.79485100	4.12498700	-0.07101900
C	4.59303100	4.70250800	-1.49260800
H	5.03748100	5.70283700	-1.56373100

H	5.06063200	4.07473100	-2.25830800
H	3.52727900	4.78539000	-1.73376700
C	4.15875400	5.09998600	0.93755500
H	3.08612800	5.23193700	0.75648600
H	4.29275700	4.76268600	1.97163100
H	4.63247000	6.08405700	0.84731500
C	6.30900800	4.03467300	0.23511000
H	6.76862300	5.02940600	0.18344200
H	6.48253200	3.63236000	1.23976100
H	6.83218400	3.38914100	-0.47812000

Compound **1c**

B	0.00000400	0.17678000	-0.00037900
C	-2.57549500	-0.35544700	-0.09208300
C	-3.41173300	-1.52190800	-0.10863600
C	-4.80979500	-1.68881600	-0.17248900
C	-5.32084700	-2.97499400	-0.19968100
C	-4.46331900	-4.10069400	-0.17315800
C	-3.08604800	-3.95542100	-0.13206500
C	-2.55162900	-2.65577000	-0.10677200
C	-1.21617600	-2.14715300	-0.08571200
C	-0.00011500	-2.80799700	-0.00015600
C	1.21602200	-2.14729800	0.08538800
C	2.55147100	-2.65588300	0.10685200
C	3.08593600	-3.95551500	0.13225100
C	4.46320900	-4.10073000	0.17355200
C	5.32070600	-2.97500700	0.20012300
C	4.80961300	-1.68884500	0.17280800
C	3.41156000	-1.52200200	0.10883000
C	2.57530500	-0.35556900	0.09203400
C	-3.06038600	1.03279900	-0.04860200
C	-2.58238200	2.03918500	-0.90812900
C	-3.11765300	3.32330700	-0.86658400
C	-4.13325300	3.60365000	0.04022400
C	-4.62995600	2.63797800	0.90804200
C	-4.09297800	1.35488800	0.85401500
C	3.06028500	1.03267500	0.04858100
C	4.09273700	1.35472600	-0.85419600
C	4.62990600	2.63774400	-0.90812500
C	4.13353900	3.60333400	-0.04002300
C	3.11810600	3.32300600	0.86697200
C	2.58264300	2.03895300	0.90841700
F	0.13135800	0.94332000	-1.14695100
F	-0.13121100	0.94387500	1.14581600

F	-4.65156900	4.84746500	0.08073400
F	4.65205900	4.84707600	-0.08041300
N	-1.28002000	-0.75218500	-0.09866800
N	1.27985800	-0.75231200	0.09829500
H	-5.47065000	-0.82858100	-0.21009300
H	-6.39525400	-3.12713200	-0.24899600
H	-4.89663000	-5.09693600	-0.19548300
H	-2.43890500	-4.82851800	-0.12678300
H	-0.00021500	-3.89355100	-0.00012100
H	2.43883200	-4.82863900	0.12685400
H	4.89654700	-5.09696000	0.19595000
H	6.39511100	-3.12711400	0.24954100
H	5.47041200	-0.82856000	0.21038600
H	-1.78550000	1.81466400	-1.60379500
H	-2.75883400	4.10488900	-1.52804600
H	-5.41399800	2.89745800	1.61162800
H	-4.45753300	0.59786100	1.54081800
H	4.45706300	0.59771000	-1.54114000
H	5.41384200	2.89723100	-1.61182500
H	2.75957200	4.10453500	1.52864800
H	1.78588600	1.81441900	1.60421500

Compound **1d**

B	-0.25898100	-0.01142100	0.22870100
C	-2.88797600	0.07400000	0.01726800
C	-3.89647000	1.07699000	-0.17798200
C	-5.29875500	1.00380700	-0.29773900
C	-6.00504600	2.17490700	-0.51288800
C	-5.33870000	3.41892300	-0.61969600
C	-3.95902300	3.50658600	-0.52587700
C	-3.22792200	2.32576200	-0.31079000
C	-1.83100600	2.04885600	-0.18880300
C	-0.74435300	2.90871900	-0.15482500
C	0.55725300	2.47761900	0.05357800
C	1.78936100	3.20130400	0.04794200
C	2.10442800	4.56531200	-0.07818400
C	3.43674200	4.94120200	-0.02106700
C	4.46333800	3.98507500	0.16788900
C	4.16945300	2.63810000	0.29154100
C	2.82092300	2.23533900	0.21697800
C	2.18679500	0.95316800	0.32742400
C	-3.14729500	-1.35732600	0.23830200
C	-2.43369300	-2.35361600	-0.45049700
C	-2.72075100	-3.70137000	-0.22741400

C	-3.73951600	-4.06757600	0.66518700
C	-4.45037400	-3.08053800	1.33787500
C	-4.16647900	-1.72939000	1.13143900
C	-0.97842700	-4.40874900	-1.69853900
C	2.89346000	-0.33114800	0.47644700
C	3.98578000	-0.58078900	-0.36548000
C	4.73347900	-1.75793400	-0.24272200
C	4.39974700	-2.69560300	0.74023400
C	3.31264600	-2.43926100	1.58184200
C	2.55861500	-1.27790100	1.46398500
C	6.55113700	-3.06986000	-1.07063100
F	0.05800100	-0.86727500	-0.81876900
F	-0.31521100	-0.65607700	1.45044000
N	-1.67110400	0.67147400	-0.01658200
N	0.84547000	1.12537500	0.24790800
O	-2.06261900	-4.72933900	-0.83446300
O	5.76339500	-1.89211300	-1.13075600
H	-5.81083400	0.04929100	-0.23162000
H	-7.08665500	2.14214000	-0.60832300
H	-5.92262300	4.31971600	-0.78858400
H	-3.45871000	4.46639000	-0.62478400
H	-0.92120200	3.97042000	-0.29627100
H	1.32528100	5.31134800	-0.21083600
H	3.70178900	5.99094700	-0.11447300
H	5.49578600	4.31858700	0.22145100
H	4.95751100	1.90863900	0.44872400
H	-1.65302600	-2.05974100	-1.13437800
H	-3.94530700	-5.12232800	0.81828300
H	-5.22949200	-3.36519700	2.03984500
H	-4.70278600	-0.96837000	1.68803300
H	-1.32434300	-3.87200500	-2.59181800
H	-0.54527000	-5.36489500	-1.99801300
H	-0.22156600	-3.80111900	-1.18824600
H	4.25558800	0.11778800	-1.14999100
H	4.96693100	-3.61198700	0.85678300
H	3.05501600	-3.16655600	2.34702800
H	1.71658000	-1.10096500	2.11809900
H	7.06162200	-3.16720100	-0.10302500
H	7.29658000	-2.97193800	-1.86200900
H	5.94791500	-3.96968500	-1.25074100

Compound **1e**

B	-0.00004000	0.27664600	-0.00029000
C	-4.39045100	3.22134200	0.24727300

C	-3.23977200	3.43626500	-0.46898500
C	-2.47519600	2.26481800	-0.70580000
C	-3.03783500	1.12227800	-0.17417700
C	-2.58130600	-0.25256200	-0.19778600
C	-3.40994900	-1.42993100	-0.26009000
C	-4.80005700	-1.62098400	-0.39693900
C	-5.29077400	-2.91493700	-0.44951200
C	-4.42339600	-4.02943700	-0.37807100
C	-3.05289000	-3.86211500	-0.26758500
C	-2.54068000	-2.55490500	-0.21534300
C	-1.21138900	-2.03858100	-0.12979300
C	-0.00002900	-2.70077900	-0.00035100
C	1.21126800	-2.03854500	0.12940700
C	2.54056500	-2.55492700	0.21493000
C	3.40984100	-1.42997400	0.26010500
C	2.58123400	-0.25255900	0.19780400
C	-5.41954200	4.22248600	0.67893900
C	3.05274600	-3.86212100	0.26741700
F	-0.15851600	1.04449800	1.14403100
F	0.15839600	1.04391000	-1.14488400
N	-1.27888200	-0.64770300	-0.13745400
N	1.27879100	-0.64768300	0.13737400
H	-2.94779800	4.41999300	-0.82309200
H	-1.54284000	2.24951400	-1.25152300
H	-5.47624800	-0.77668400	-0.47263500
H	-6.35937100	-3.07903800	-0.55534200
H	-4.84100800	-5.03167000	-0.42181700
H	-2.39180800	-4.72387600	-0.22913400
H	0.00003000	-3.78598800	-0.00048300
H	-6.41042200	3.99620200	0.26613500
H	-5.13156000	5.22027100	0.33369300
H	-5.52088000	4.26093700	1.77052800
H	2.39167500	-4.72388500	0.22877700
C	4.79990000	-1.62104200	0.39744100
H	5.47606800	-0.77673000	0.47316300
C	4.42320900	-4.02946600	0.37842400
H	4.84078800	-5.03170800	0.42230400
C	5.29059000	-2.91500000	0.45014600
H	6.35914400	-3.07914500	0.55633500
S	-4.54941900	1.53284500	0.64484300
C	2.47501700	2.26497500	0.70539400
C	3.23989700	3.43628000	0.46882100
H	1.54242900	2.24986400	1.25072600
C	4.39081500	3.22112200	-0.24697400

H	2.94791100	4.42007000	0.82273800
C	3.03773800	1.12227300	0.17424100
C	5.41969100	4.22228400	-0.67912500
H	5.51632100	4.26479700	-1.77101800
H	5.13478300	5.21918300	-0.32880700
H	6.41197600	3.99283900	-0.27154900
S	4.54987200	1.53254900	-0.64410400