Electric Supporting Information

Asymmetrical benzo[a]-fused N_2O_2-boron-chelated BODIPYs as red to near-infrared absorbing chromophores; synthesis, characteristic and device applications for opto-electronics

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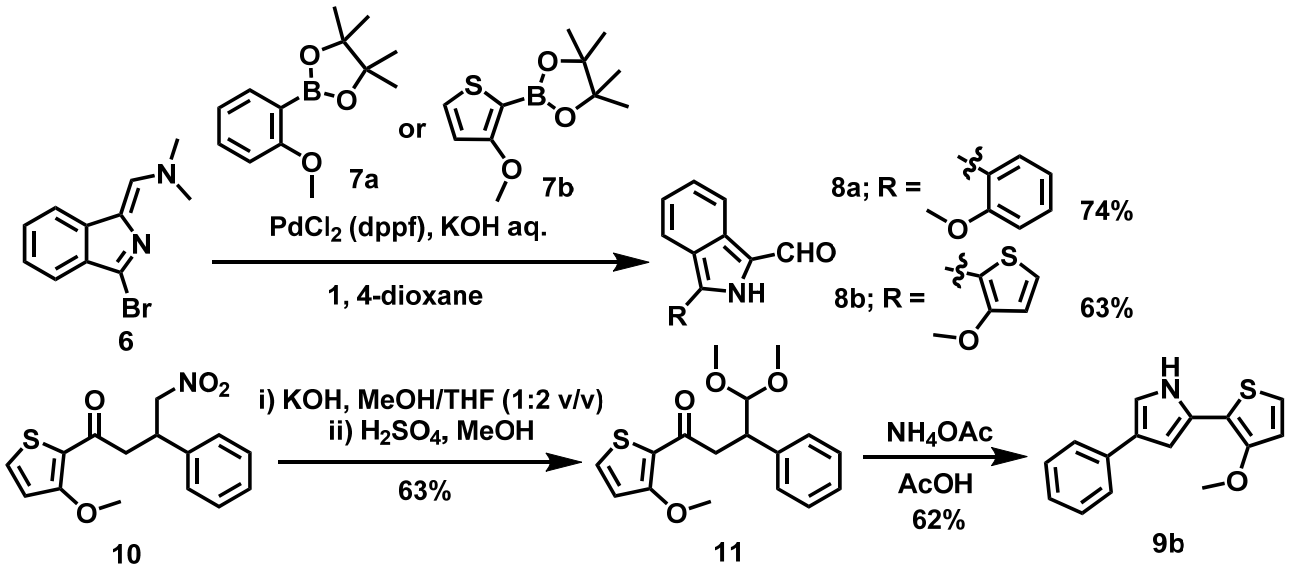
Synthesis



Scheme S1. Synthetic path of **8** and **9b**.

3-(2-Methoxyphenyl)-1-formylisoindole (8a): 1-(3-Bromo-1H-isoindol-1-ylidene)-*N*,*N*-dimethyl methanamine **6** (8.50 g, 33.9 mmol) and (2-methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (8.30 g, 35.5 mmol) were dissolved in 1,4-dioxane (500 mL) and the mixture was degassed by freeze-pump-thaw cycles 3 times. After adding $PdCl_2$ (dppf) (1.39 g, 1.70 mmol) and 4M KOH degassed by freeze-pump-thaw cycles, the resultant mixture was stirred overnight at 90 °C. After celite filtration, the reaction solution was evaporated and extracted with $CHCl_3$. The organic phase was chromatographed on silica gel (Wakogel C-300) using EtOAc:CH_2Cl_2 (1:1 v/v) as an eluent to afford 8.02 g of **8a** in 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 11.26 (1H, s), 9.94 (1H, s), 8.06 (1H, d, *J* = 8.60 Hz), 8.03 – 7.99 (2H, m), 7.44 – 7.38 (2H, m), 7.27 – 7.23 (1H, m), 7.16 (1H, t, *J* = 7.54 Hz), 7.11 (1H, d, *J* = 8.36 Hz), 4.02 (3H, s). FAB-MS: m/z = 251 [M^+] and 251 [M+1]$^+$.

3-(3-Methoxythiophen-2-yl)-1-formylisoindole (8b): Compound **8b** was synthesized in a similar manner as **8a** using 1-(3-bromo-1*H*-isoindol-1-ylidene)-*N*,*N*-dimethyl methanamine **6** (0.167 g, 0.666 mmol), 4,4,5,5-Tetramethyl-2-(3-methoxy-2-thienyl)-1,3,2-dioxaborolan (0.168 g, 0.698 mmol). 0.108 g of 8b was obtained in 63% yield. ^{1}H NMR (500MHz, $CDCl_3$) : δ (ppm) = 11.32 (1H, s), 9.88 (1H, s), 8.09 (1H, d, *J* = 8.60 Hz), 7.98 (1H, d, *J* = 8.40 Hz,), 7.40 (1H, t, *J* = 7.75 Hz), 7.38 (1H, d, *J* = 5.60 Hz), 7.27 – 7.24 (1H, m), 7.02 (1H, d, *J* = 5.45 Hz), 4.15 (s, 3H). FAB-MS: m/z = 257[$M]^+$, 258[M +H]$^+$.

4,4-Dimethoxy-1-(3-methoxythiophen-2-yl)-3-phenylbutan-1-one (11) To a solution of 1-(3-methoxythiophen-2-yl)-4-nitro-3-phenylbutan-1-one (4.95 g, 17.0 mmol) in MeOH (172mL) /THF (344 mL) was added KOH (4.84 g, 86.2 mmol) at room temperature and the resultant solution was stirred for 1 h. After adding 36N H_2SO_4 (32 mL) in MeOH (172 mL) under an icy condition, the mixture was then stirred for 1 h at room temperature. The resultant solution was poured into iced water, neutrlized with 4N NaOH aqueous solution, evaporated by half, and then

extracted with CH_2Cl_2. The organic layer was washed with water, dried with Na_2SO_4 and evaporated. The residue was then chromatographed on silica gel (Wakogel C300) using CH_2Cl_2 as an eluent to afford 3.44g of **11** in 63% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.45 (1H, d, *J* = 5.60 Hz), 7.32 (2H, dt, *J* = 8.25 and 1.57 Hz), 7.28 – 7.25 (2H, m), 7.17 (1H, tt, *J* = 7.11 and 1.67 Hz), 6.82 (1H, d, *J* = 5.52 Hz), 4.53 (1H, d, *J* = 6.20 Hz), 3.74 (1H, dt, J = 5.84 and 5.81 Hz), 3.42–3.31 (2H, m), 3.36 (s, 3H), 3.29 (s, 3H). FABMS: *m*/*z* = 289 $[M-OMe]^+$.

2-(3-Methoxythiophen-2-yl)-4-phenyl-1*H*-pyrrole (9b) The mixture of **11** (0.564 g, 1.76 mmol), NH_4OAc (0.686 g, 8.90 mmol) and AcOH (25 mL) was heated at 100°C for 1 h. After adding icy water, the solution was neutralized with 4M NaOH aq., extracted with CH_2Cl_2 and washed with water. The residue was chromatographed on silica gel (Wakogel C-300) using CH_2Cl_2 as an eluent (AcOEt/Hexane = 1/4 v/v) to afford 9b in 65% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 9.39 (1H, s), 7.55 (2H, dd, *J* = 8.35 and 1.18 Hz), 7.33 (2H, tt, *J* = 7.73 and 1.58 Hz), 7.17 (1H, tt, *J* = 7.35 and 1.23 Hz), 7.08 (1H, dd, *J* = 2.56 and 1.78 Hz), 7.00 (1H, d, *J* = 5.44 Hz), 6.86 (1H, d, *J* = 5.44 Hz), 6.59 (1H, dd, *J* = 2.64 and 1.70 Hz), 3.98 (3H, s) . FAB-MS: *m*/*z* = 255 $[M]^+$.

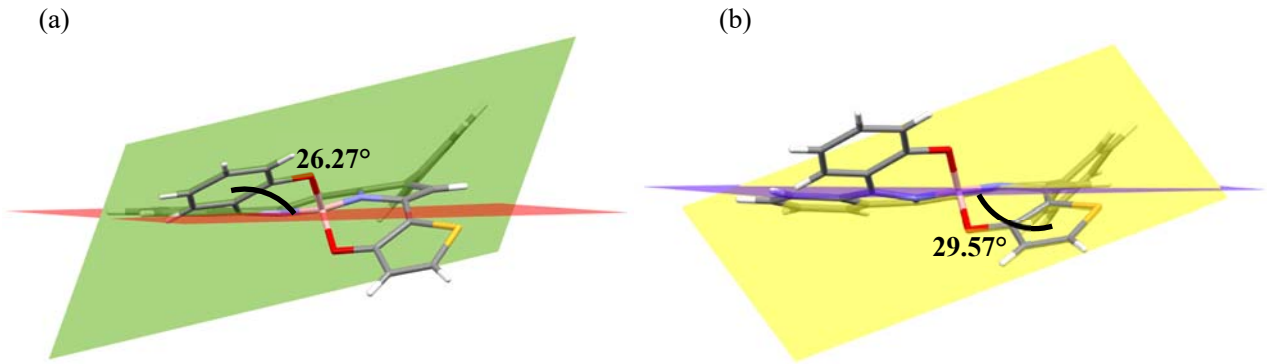


Fig. S1 Dihedral angles of 3-benzo[1,3,2]oxazaborinine (a) and 3- thieno[1,3,2]oxazaborinine units (b)

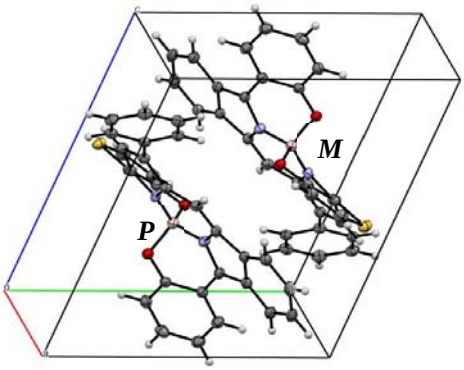


Fig. S2 A pair of the enantiomers of **2**.

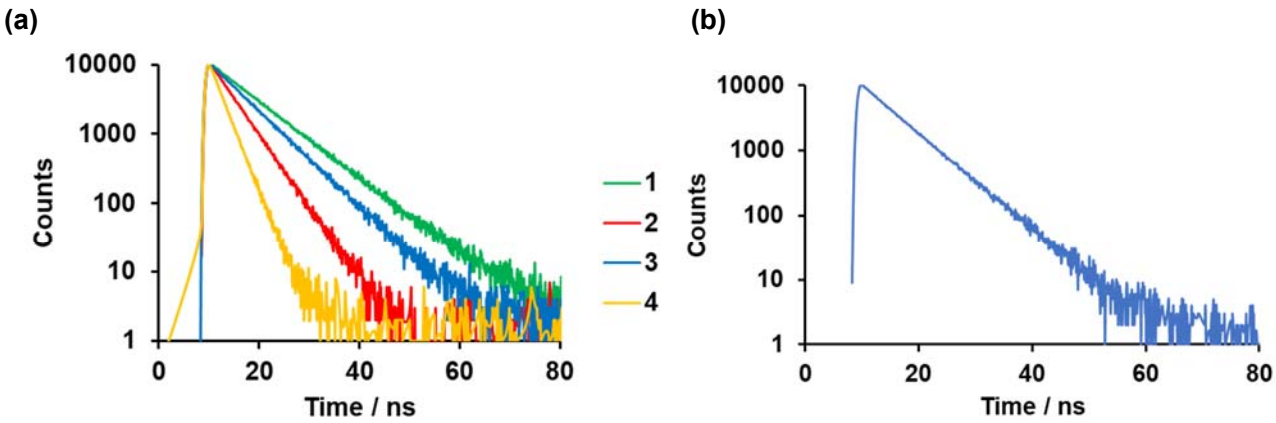


Fig. S3 (a) Fluorescence decay profiles of **1~4** (10 μM) in THF at 25.0°C. Excited with LED light at 630 nm. (b) Fluorescence decay profiles of **5** (10 μM) in THF at 25.0°C, which was monitored at 625 nm. Excited with LED light at 590 nm.

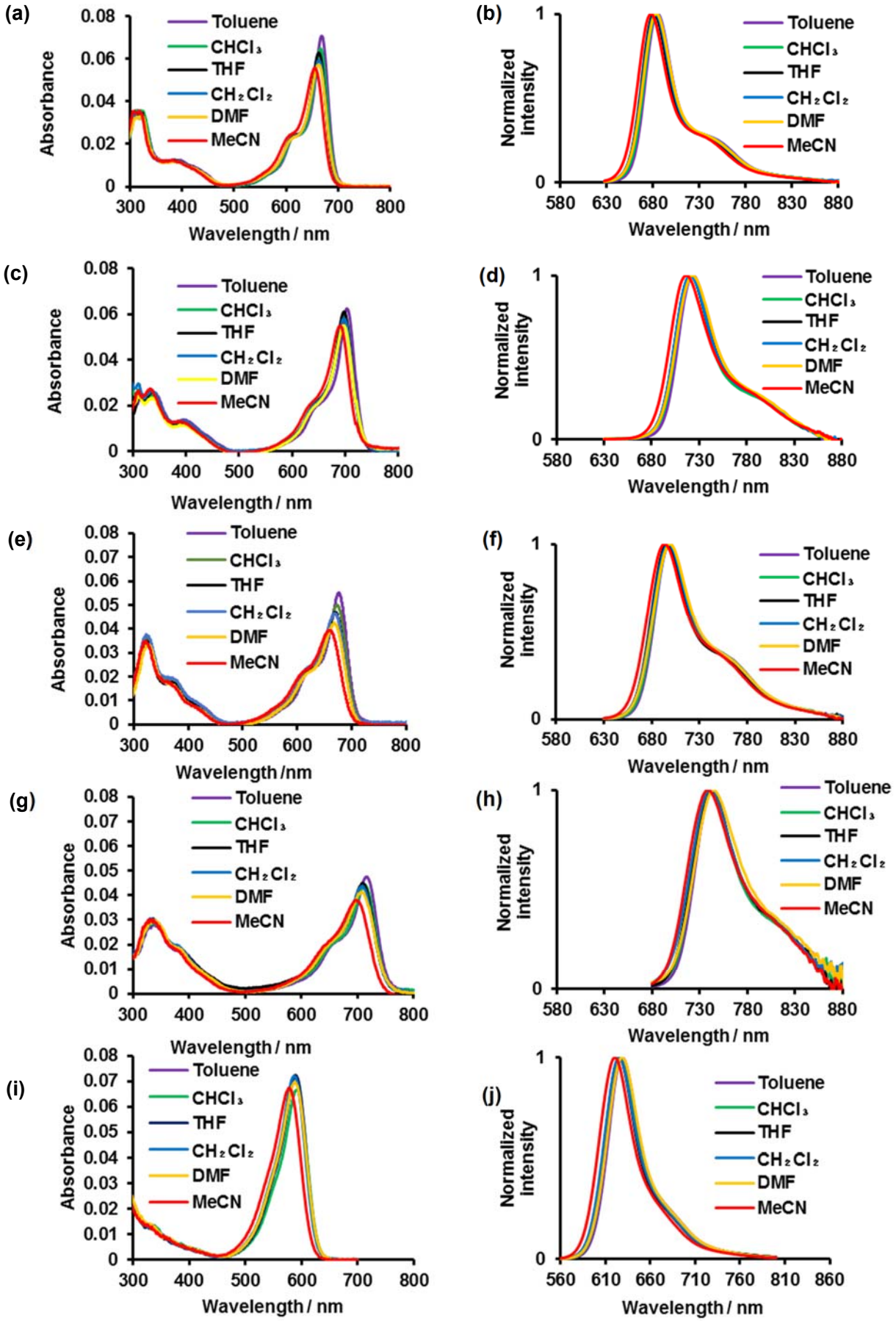
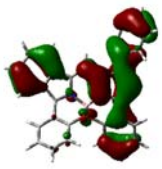

(a)
Absorbance
Wavelength / nm
(b)
Normalized Intensity
Wavelength / nm
(c)
Absorbance
Wavelength / nm
(d)
Normalized Intensity
Wavelength / nm
(e)
Absorbance
Wavelength /nm
(f)
Normalized Intensity
Wavelength / nm
(g)
Absorbance
Wavelength / nm
(h)
Normalized Intensity
Wavelength / nm
(i)
Absorbance
Wavelength / nm
(j)
Normalized Intensity
Wavelength / nm
Toluene
CHCl3
THF
CH2Cl2
DMF
MeCN

Fig. S4 Photophysical properties of the dyes (1 μM) in various solvents; absorption of **1** (a), fluorescence of **1** (b), absorption of **2** (c), fluorescence of **2** (d), absorption of **3** (e), fluorescence of **3** (f), absorption of **4** (g), fluorescence of **4** (h), absorption of **5** (i) and fluorescence of **5** (j).

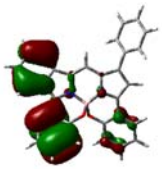
Table S1. Calculated values of excited wavelength (λ_{calcd}), oscillator strength (*f*) and molecular orbital (MO) transition assignment for selected transition energies for **1**. The reported transitions have oscillator strength (*f*) more than 0.1.

Dye	State	λ(calcd.) / nm	*f* / a.u.	MO transition assignment[a]
1	$S_0 \rightarrow S_1$	534	0.5030	HOMO → LUMO (97%)
	$S_0 \rightarrow S_2$	360	0.1216	HOMO−2 → LUMO (7%)
				HOMO−1 → LUMO (87%)
	$S_0 \rightarrow S_5$	309	0.1639	HOMO−6 → LUMO (7%)
				HOMO → LUMO+1 (87%)
	$S_0 \rightarrow S_7$	280	0.1835	HOMO−6 → LUMO (6%)
				HOMO−4 → LUMO (76%)
				HOMO−3 → LUMO (4%)
	$S_0 \rightarrow S_8$	266	0.1568	HOMO−8 → LUMO (3%)
				HOMO−7 → LUMO (83%)
	$S_0 \rightarrow S_9$	262	0.3642	HOMO−1 → LUMO+1 (3%)
				HOMO−1 → LUMO+2 (3%)
				HOMO → LUMO+2 (70%)
				HOMO → LUMO+3 (3%)
				HOMO → LUMO+5 (4%)

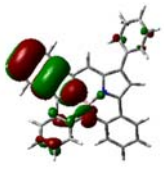
[a]Data given in parentheses are 2 × (CI coefficient)^2 × 100%; see the reference: M. Asgari, H. R. Memarian and H. Sabzyan, *J. Mol. Struct.*, 2020, **1207**, 127820.



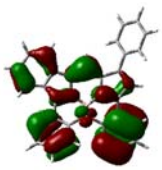
HOMO−8 : −8.89 eV



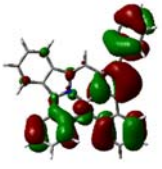
HOMO−7 : −8.53 eV



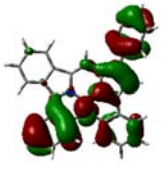
HOMO−6 : −8.42 eV



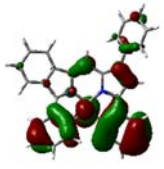
HOMO−4 : −8.01 eV



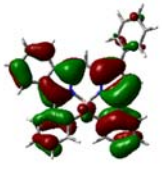
HOMO−3 : −7.68 eV



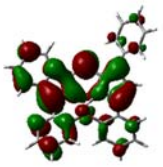
HOMO−2 : −7.56 eV



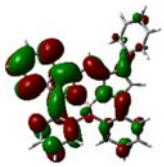
HOMO−1 : −7.16 eV



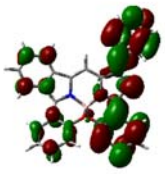
HOMO : −5.99 eV



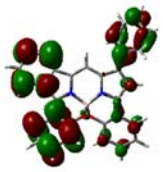
LUMO : −1.63 eV



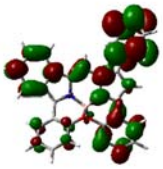
LUMO+1 : 0.16 eV



LUMO+2 : 0.91 eV



LUMO+3 : 1.00 eV



LUMO+5 : 1.26 eV

Fig. S5 The frontier molecular orbitals of the optimized structures of **1**.

Table S2. Calculated values of excited wavelength (λ_{calcd}), oscillator strength (*f*) and molecular orbital (MO) transition assignment for selected transition energies for **2**. The reported transitions have oscillator strength (*f*) more than 0.1.

Dye	State	λ(calcd.) / nm	*f* / a.u.	MO transition assignment[a]
2	$S_0 \rightarrow S_1$	558	0.4753	HOMO → LUMO (98%)
	$S_0 \rightarrow S_2$	357	0.1109	HOMO−2 → LUMO (5%)
				HOMO−1 → LUMO (87%)
				HOMO → LUMO+1 (3%)
	$S_0 \rightarrow S_4$	320	0.2329	HOMO−5 → LUMO (3%)
				HOMO−3 → LUMO (9%)
				HOMO−2 → LUMO (13%)
				HOMO → LUMO+1 (70%)
	$S_0 \rightarrow S_5$	314	0.1228	HOMO−3 → LUMO (37%)
				HOMO−2 → LUMO (33%)
				HOMO−1 → LUMO (4%)
				HOMO → LUMO+1 (19%)
	$S_0 \rightarrow S_8$	276	0.3838	HOMO−4 → LUMO (13%)
				HOMO → LUMO+2 (77%)
	$S_0 \rightarrow S_9$	265	0.1226	HOMO−8 → LUMO (2%)
				HOMO−7 → LUMO (81%)
				HOMO → LUMO+3 (3%)

[a]Data given in parentheses are 2 × (CI coefficient)^2 × 100%; see the reference: M. Asgari, H. R. Memarian and H. Sabzyan, *J. Mol. Struct.*, 2020, **1207**, 127820.

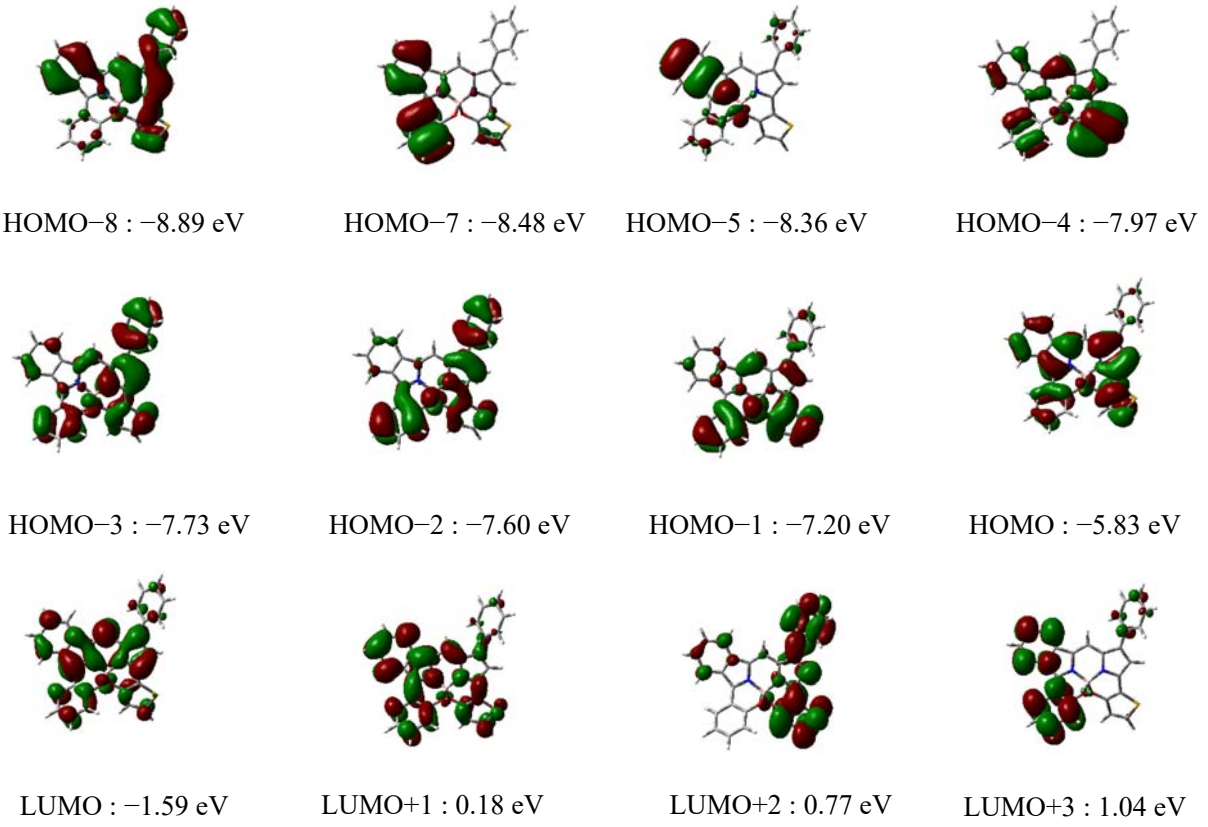


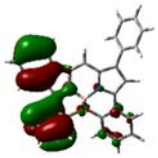
Fig. S6 The frontier molecular orbitals of the optimized structures of **2**.

Table S3. Calculated values of excited wavelength (λ_{calcd}), oscillator strength (*f*) and molecular orbital (MO) transition assignment for selected transition energies for **3**. The reported transitions have oscillator strength (*f*) more than 0.1.

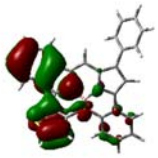
Dye	State	λ(calcd.) / nm	*f* / a.u.	MO transition assignment[a]
3	$S_0 \rightarrow S_1$	540	0.4609	HOMO → LUMO (97%)
	$S_0 \rightarrow S_2$	352	0.1108	HOMO−3 → LUMO (5%)
				HOMO−2 → LUMO (3%)
				HOMO−1 → LUMO (85%)
				HOMO → LUMO+1 (3%)
	$S_0 \rightarrow S_4$	319	0.2678	HOMO−2 → LUMO (2%)
				HOMO−1 → LUMO (2%)
				HOMO → LUMO+1 (89%)
	$S_0 \rightarrow S_6$	283	0.1111	HOMO−7 → LUMO (5%)
				HOMO−6 → LUMO (69%)
				HOMO−4 → LUMO (17%)
	$S_0 \rightarrow S_8$	269	0.3232	HOMO−7 → LUMO (45%)
				HOMO−6 → LUMO+1 (3%)

			HOMO−4 → LUMO (4%)
			HOMO → LUMO+2 (35%)
			HOMO → LUMO+3 (3%)
$S_0 \rightarrow S_9$	264	0.2639	HOMO−7 → LUMO (19%)
			HOMO−4 → LUMO (3%)
			HOMO−3 → LUMO (3%)
			HOMO → LUMO+2 (4%)
			HOMO → LUMO+3 (54%)

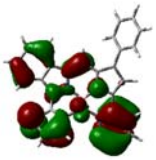
[a]Data given in parentheses are 2 × (CI coefficient)^2 × 100%; see the reference: M. Asgari, H. R. Memarian and H. Sabzyan, *J. Mol. Struct.*, 2020, **1207**, 127820.



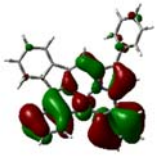
HOMO−7 : −8.52 eV



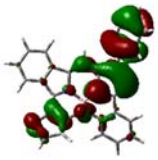
HOMO−6 : −8.46 eV



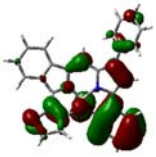
HOMO−4 : −8.06 eV



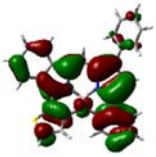
HOMO−3 : −7.69 eV



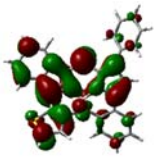
HOMO−2 : −7.55 eV



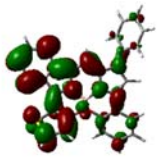
HOMO−1 : −7.14 eV



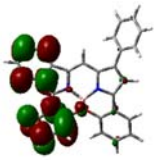
HOMO : −5.87 eV



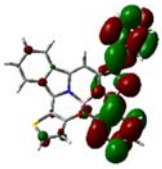
LUMO : −1.54 eV



LUMO+1 : 0.09 eV



LUMO+2 : 0.79 eV



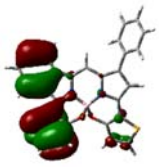
LUMO+3 : 1.00 eV

Fig. S7 The frontier molecular orbitals of the optimized structures of **3**.

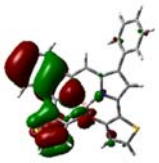
Table S4. Calculated values of excited wavelength (λ_{calcd}), oscillator strength (*f*) and molecular orbital (MO) transition assignment for selected transition energies for **4**. The reported transitions have oscillator strength (*f*) more than 0.1.

Dye	State	λ(calcd.) / nm	*f* / a.u.	MO transition assignment[a]
4	$S_0 \rightarrow S_1$	567	0.4368	HOMO → LUMO (98%)
	$S_0 \rightarrow S_3$	354	0.3575	HOMO−1 → LUMO (12%)
				HOMO → LUMO+1 (81%)
	$S_0 \rightarrow S_5$	322	0.1140	HOMO−6 → LUMO (4%)
				HOMO−4 → LUMO (17%)
				HOMO−3 → LUMO (70%)
				HOMO−2 → LUMO (2%)
				HOMO−1 → LUMO (3%)
	$S_0 \rightarrow S_7$	280	0.1885	HOMO−6 → LUMO (17%)
				HOMO → LUMO+2 (64%)
				HOMO → LUMO+3 (7%)
	$S_0 \rightarrow S_8$	276	0.2701	HOMO−4 → LUMO (49%)
				HOMO−3 → LUMO (17%)
				HOMO → LUMO+3 (21%)
	$S_0 \rightarrow S_9$	271	0.1221	HOMO−7 → LUMO (23%)
				HOMO−4 → LUMO (8%)
				HOMO → LUMO+2 (13%)
				HOMO → LUMO+3 (45%)

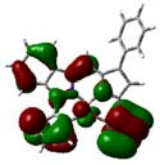
[a]Data given in parentheses are 2 × (CI coefficient)^2 × 100%; see the reference: M. Asgari, H. R. Memarian and H. Sabzyan, *J. Mol. Struct.*, 2020, **1207**, 127820.



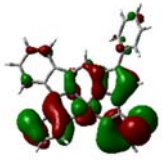
HOMO−7 : −8.48 eV



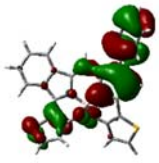
HOMO−6 : −8.42 eV



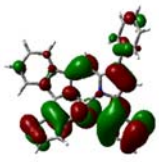
HOMO−4 : −7.98 eV



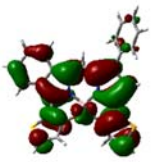
HOMO−3 : −7.77 eV



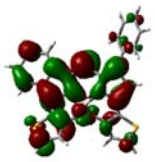
HOMO−2 : −7.59 eV



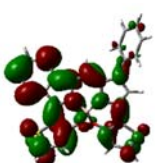
HOMO−1 : −7.16 eV



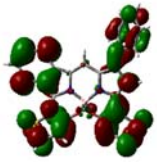
HOMO : −5.72 eV



LUMO : −1.52 eV



LUMO+1 : 0.10 eV



LUMO+2 : 0.80 eV

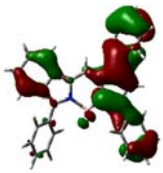
LUMO+3 : 0.88 eV

Fig. S8 The frontier molecular orbitals of the optimized structures of **4**.

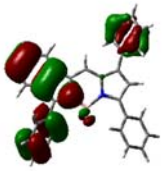
Table S5. Calculated values of excited wavelength (λ_{calcd}), oscillator strength (*f*) and molecular orbital (MO) transition assignment for selected transition energies for **5**. The reported transitions have oscillator strength (*f*) more than 0.1.

Dye	State	λ(calcd.) / nm	*f* / a.u.	MO transition assignment[a]
5	$S_0 \rightarrow S_1$	482	0.8209	HOMO → LUMO (98%)
	$S_0 \rightarrow S_2$	332	0.1025	HOMO−9 → LUMO (2%)
				HOMO−5 → LUMO (2%)
				HOMO−2 → LUMO (5%)
				HOMO−1 → LUMO (86%)
	$S_0 \rightarrow S_4$	283	0.3431	HOMO−2 → LUMO (63%)
				HOMO−1 → LUMO (4%)
				HOMO → LUMO+1 (20%)
	$S_0 \rightarrow S_5$	282	0.1173	HOMO−5 → LUMO (27%)
				HOMO−2 → LUMO (19%)
				HOMO → LUMO+1 (45%)

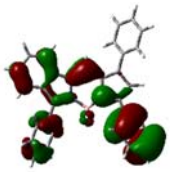
[a]Data given in parentheses are 2 × (CI coefficient)^2 × 100%; see the reference: M. Asgari, H. R. Memarian and H. Sabzyan, *J. Mol. Struct.*, 2020, **1207**, 127820.



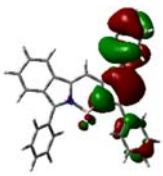
HOMO−9 : −9.12 eV



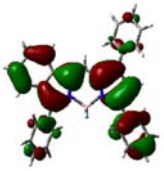
HOMO−5 : −8.41 eV



HOMO−2 : −7.96 eV

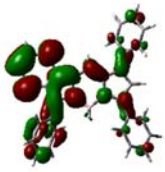


HOMO−1 : −7.64 eV



HOMO : −6.21 eV

LUMO : −1.65 eV



LUMO+1 : 0.30 eV

Fig. S9 The frontier molecular orbitals of the optimized structures of **5**.

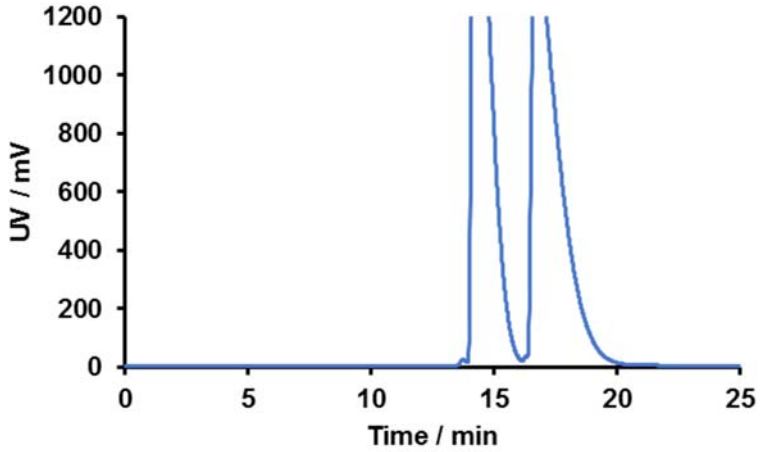


Fig. S10 Chromatogram of the enantiomeric separation of **2**. CHIRALPACK-IE was used, where the flow rate and solvent were 1.9 mL min^{-1} and CH_2Cl_2:hexane (2:1 v/v), respectively.

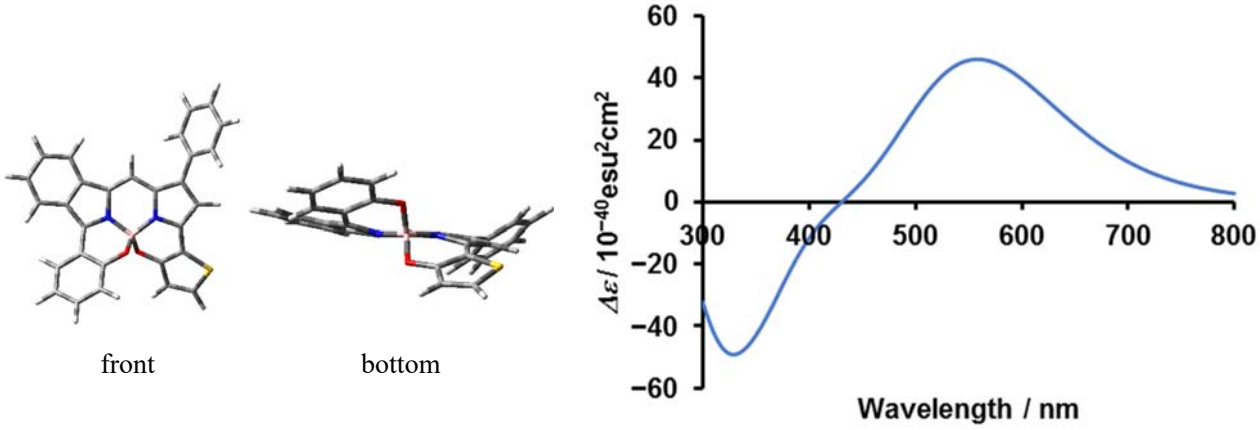


Fig. S11 Calculated CD spectrum of *P*-isomer of **2**, being conducted by DFT and TDDFT method at CAM-B3LYP/6-31G(d,p).

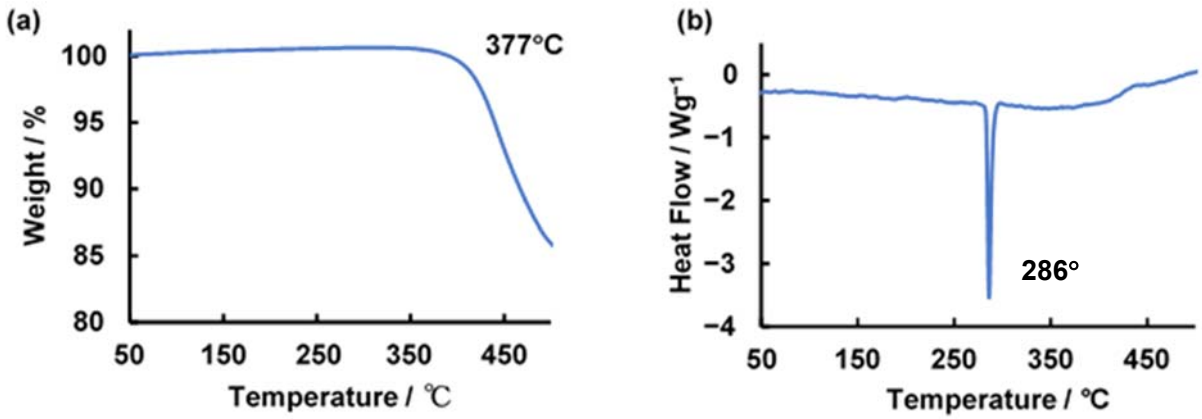


Fig. S12 DSC (a) and TGA (b) plots of **2**.

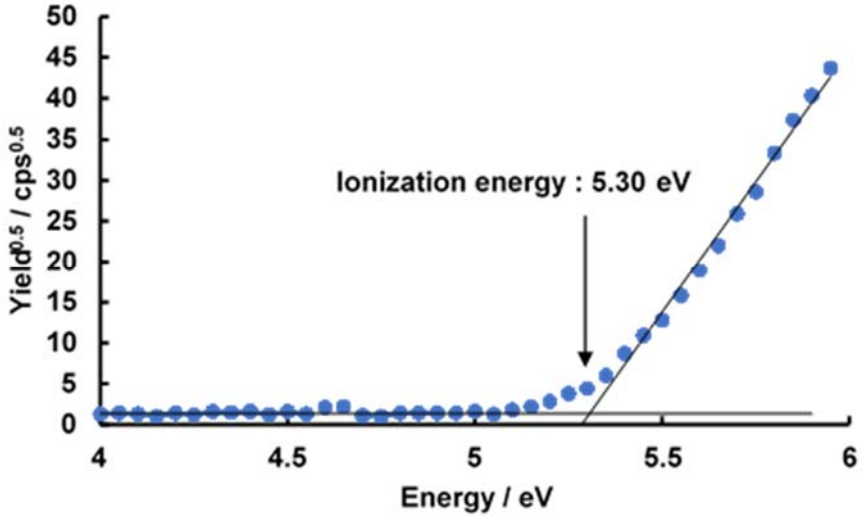
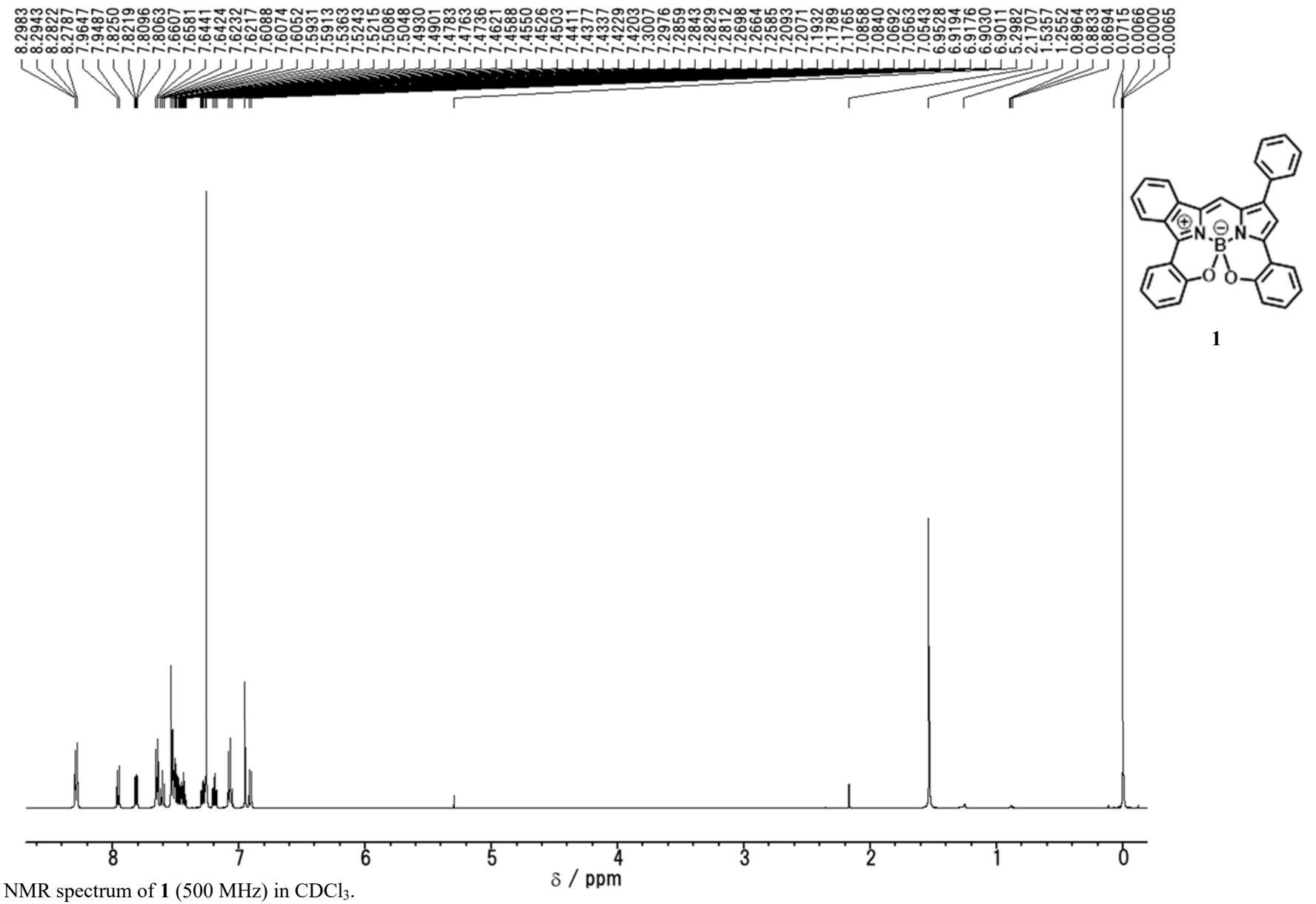
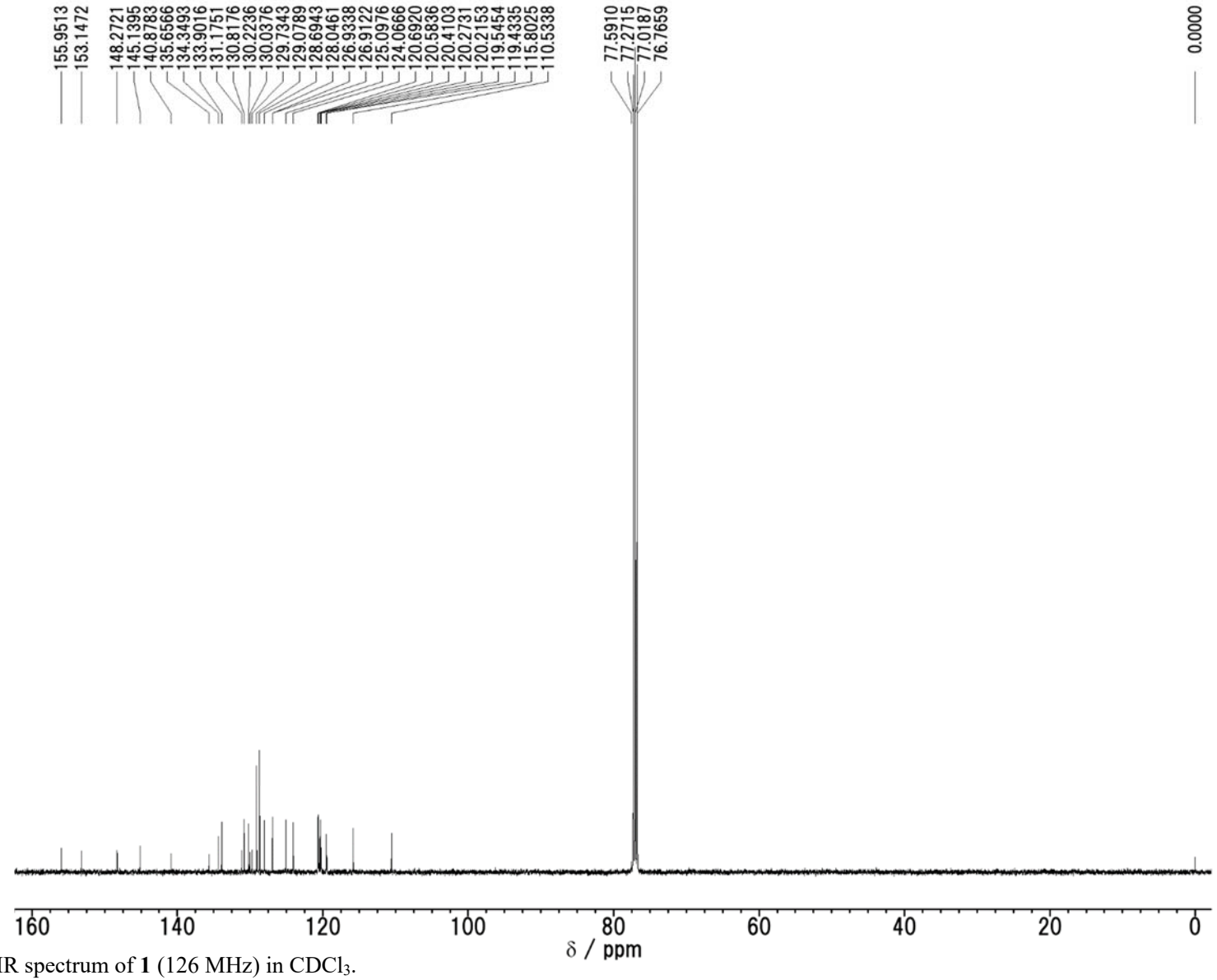


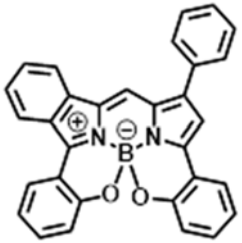
Fig. S13 Photoelectron spectroscopic analysis of film **2**.



1

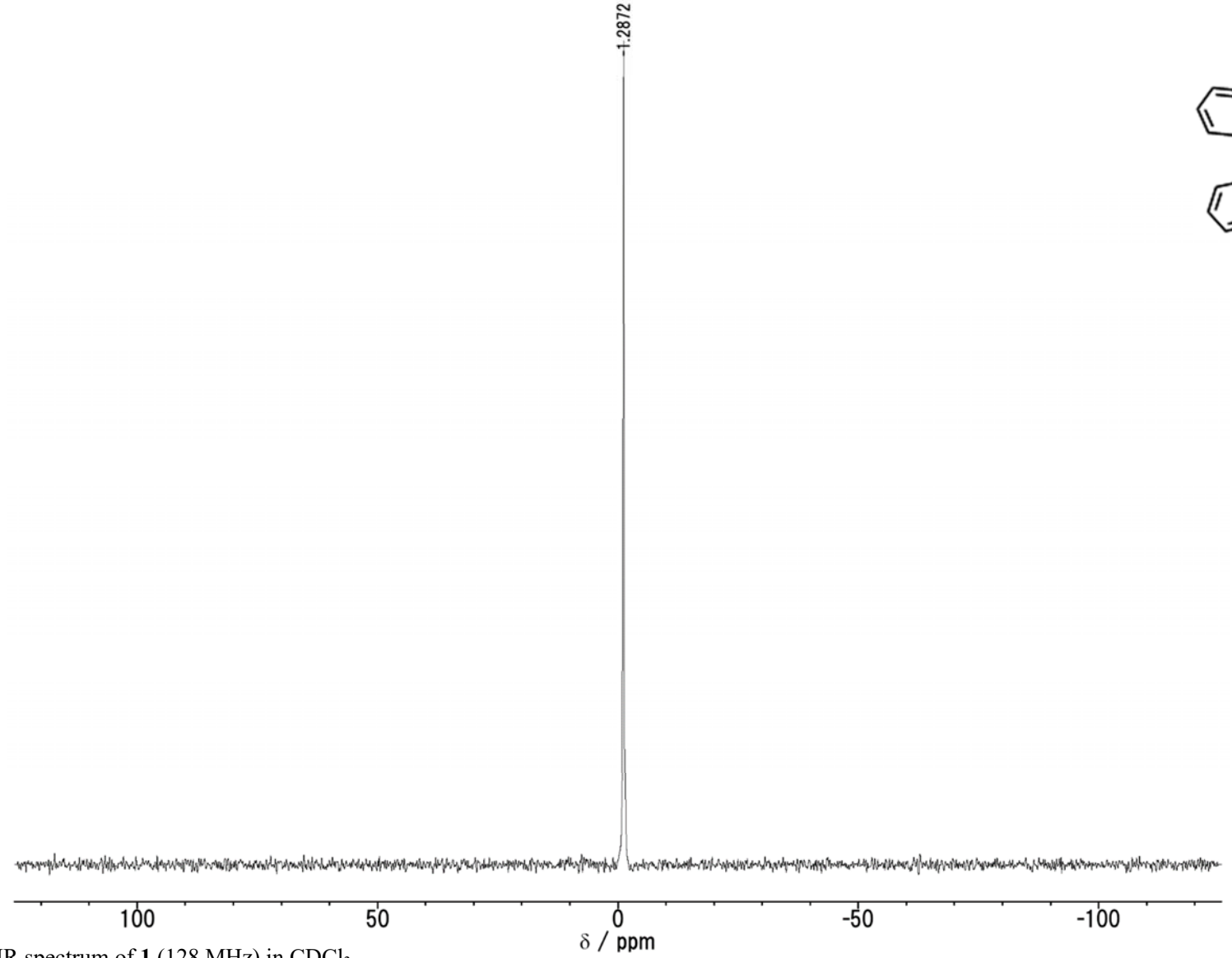
Fig. S14 ^{1}H NMR spectrum of **1** (500 MHz) in $CDCl_3$.

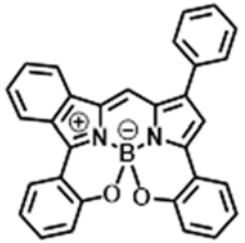




1

Fig. S15 ^{13}C NMR spectrum of **1** (126 MHz) in $CDCl_3$.

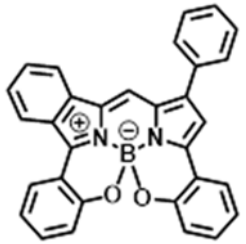




1

Fig. S16 ^{11}B NMR spectrum of **1** (128 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 20181205-nozawaEXP48-001 Date : 05-Dec-2018 17:13
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (5,10)
BP : m/z 136 Int. : 3.47 (36348)
Output m/z range : 50 to 540 Cut Level : 0.00 %



1

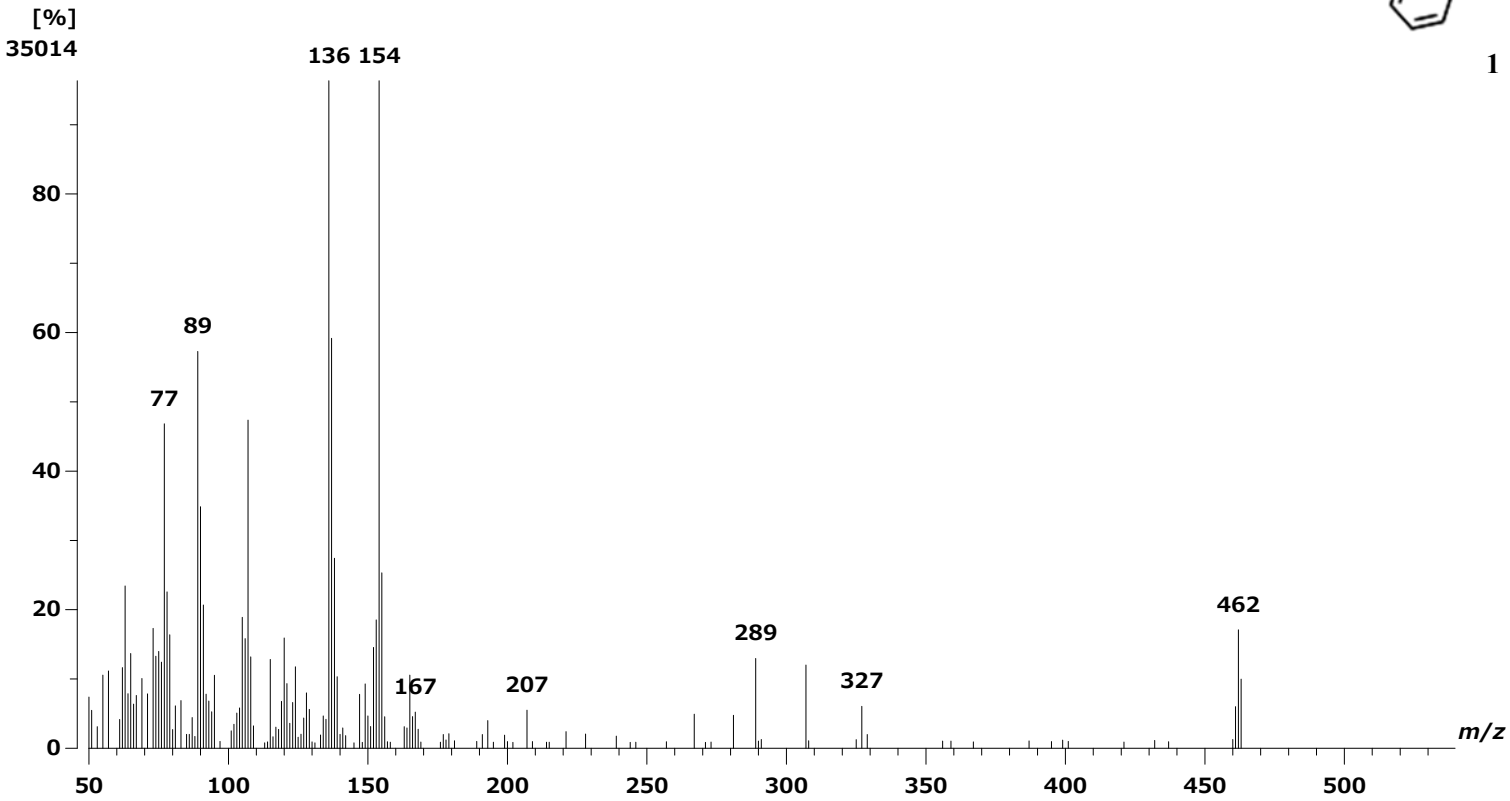


Fig. S17 FAB mass spectrum (positive mode) of **1**.

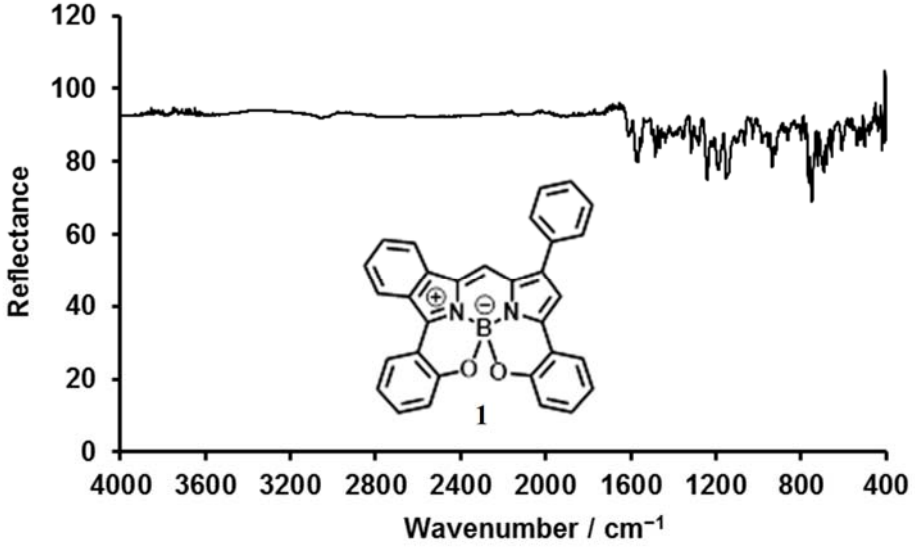


Fig. S18 ATR-FT-IR spectrum of **1**.

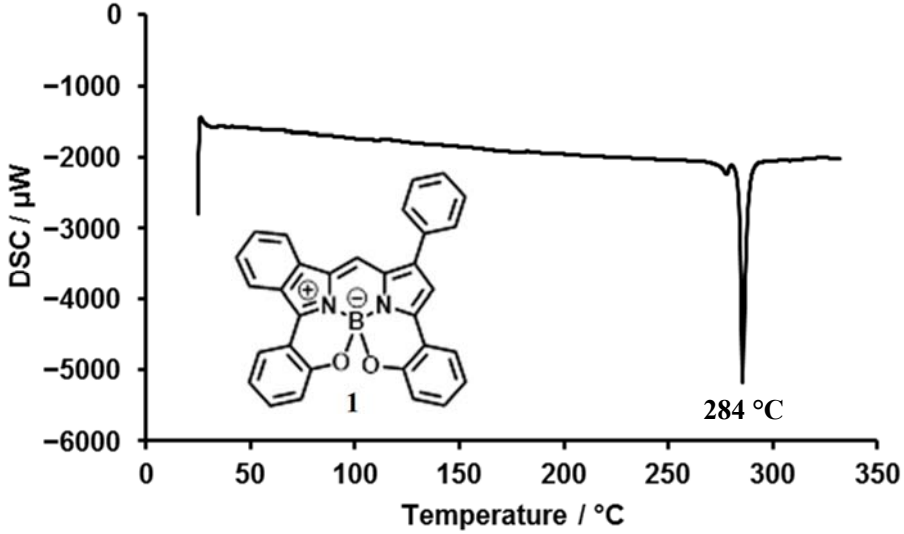
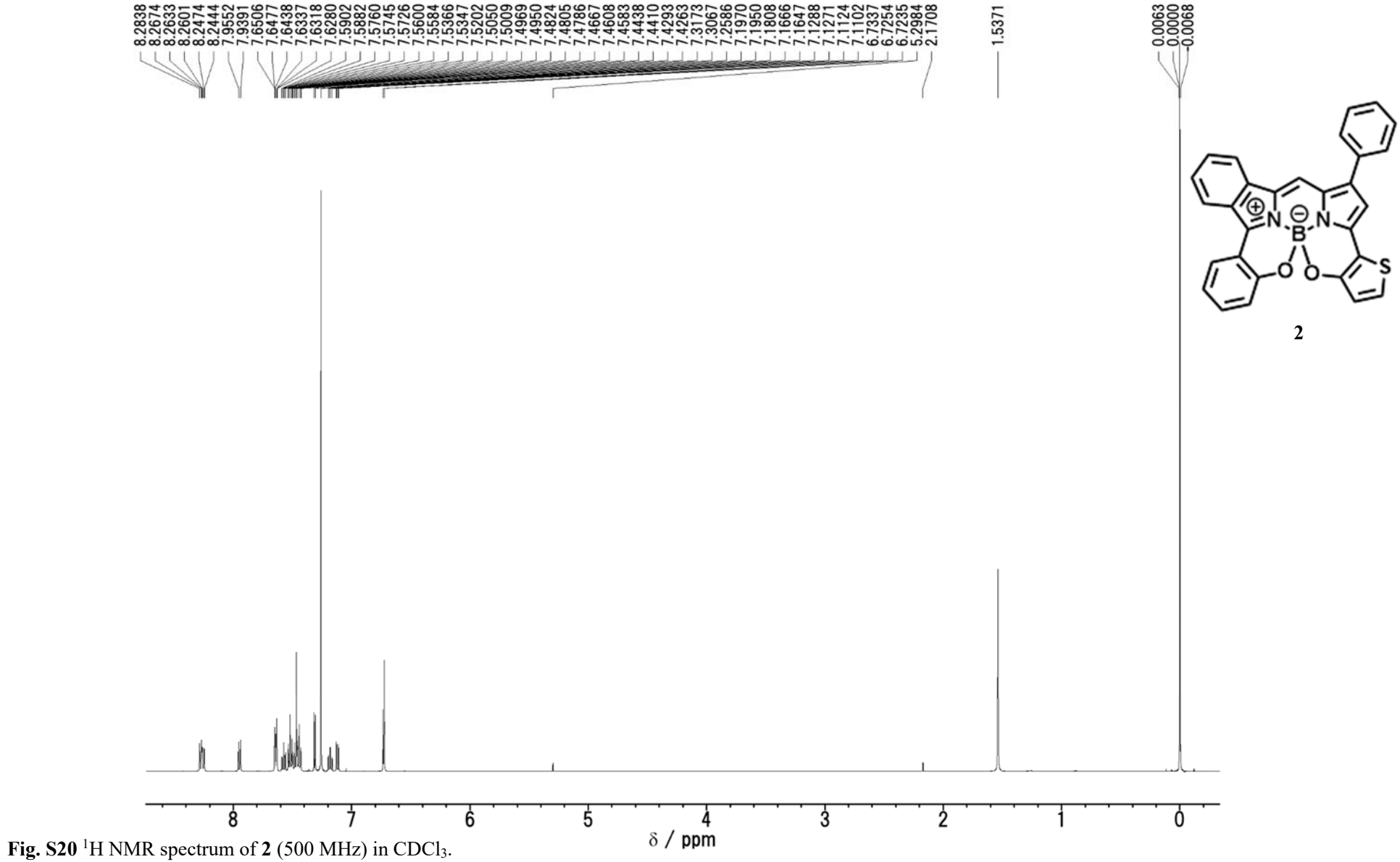
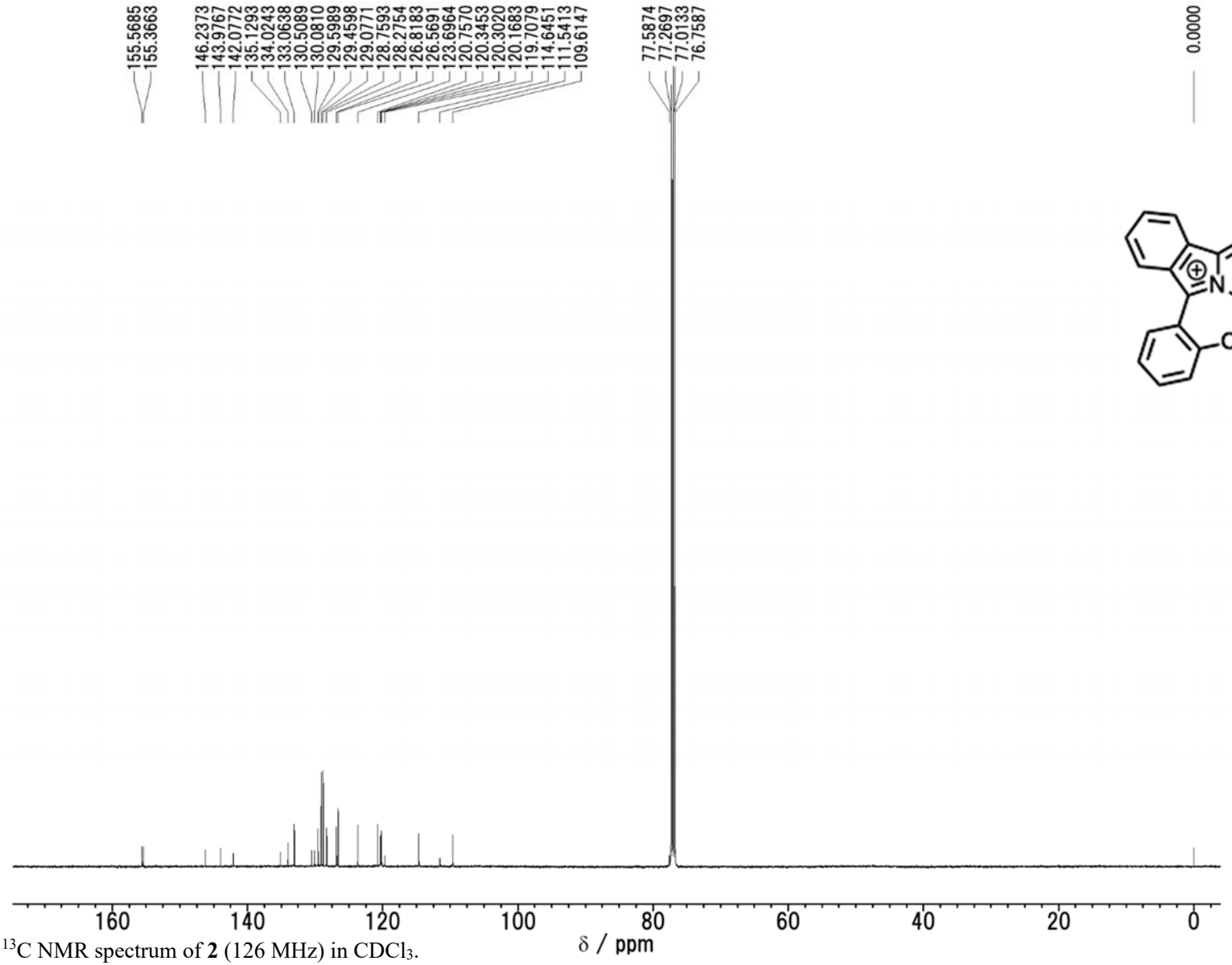


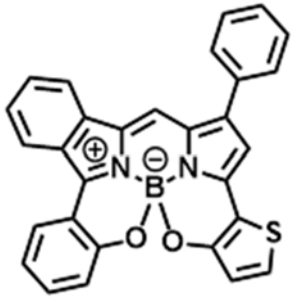
Fig. S19 DSC plots of **1**.



2

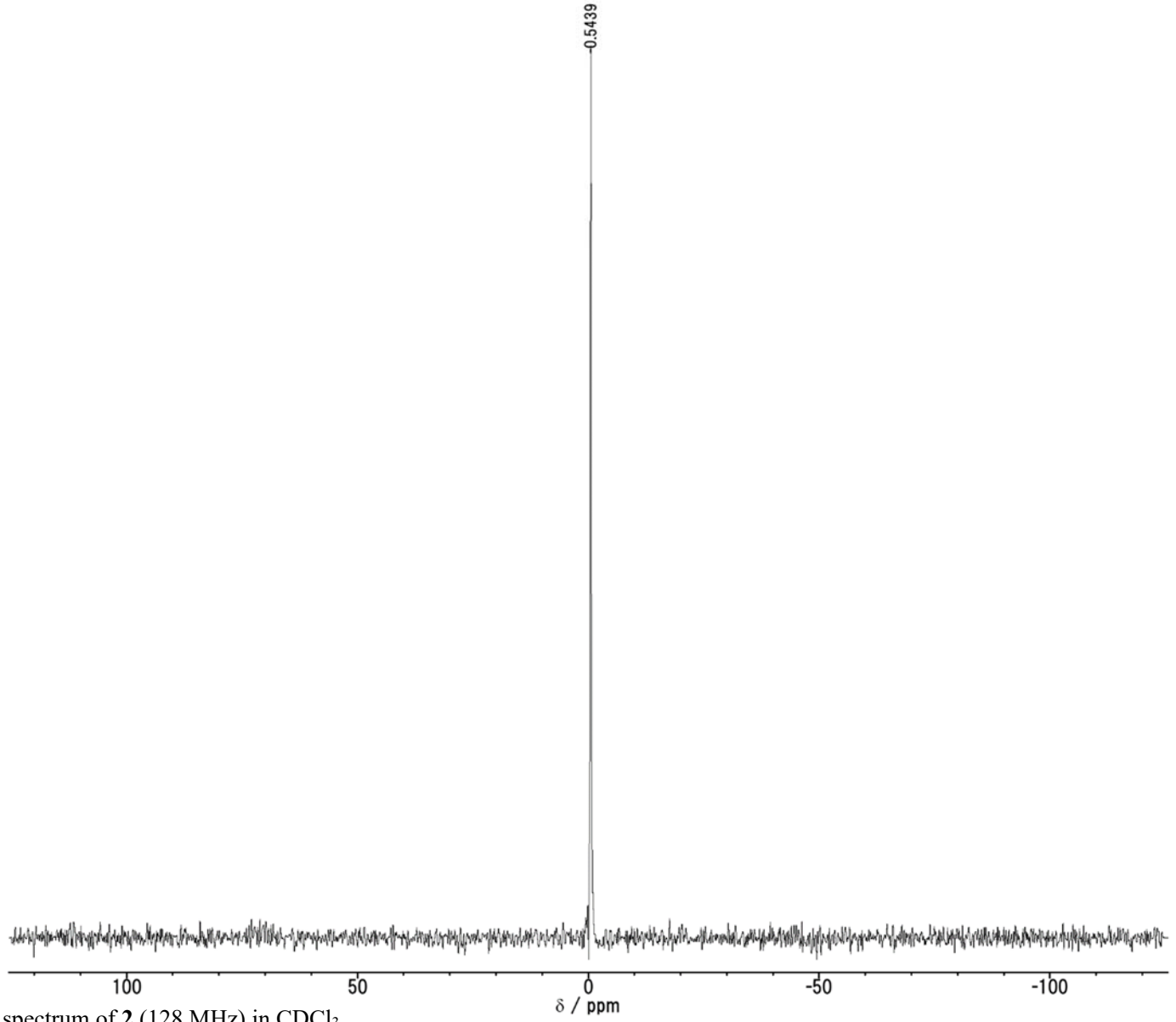
Fig. S20 ^{1}H NMR spectrum of **2** (500 MHz) in $CDCl_3$.

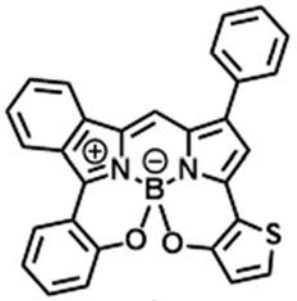




2

Fig. S21 ^{13}C NMR spectrum of **2** (126 MHz) in $CDCl_3$.

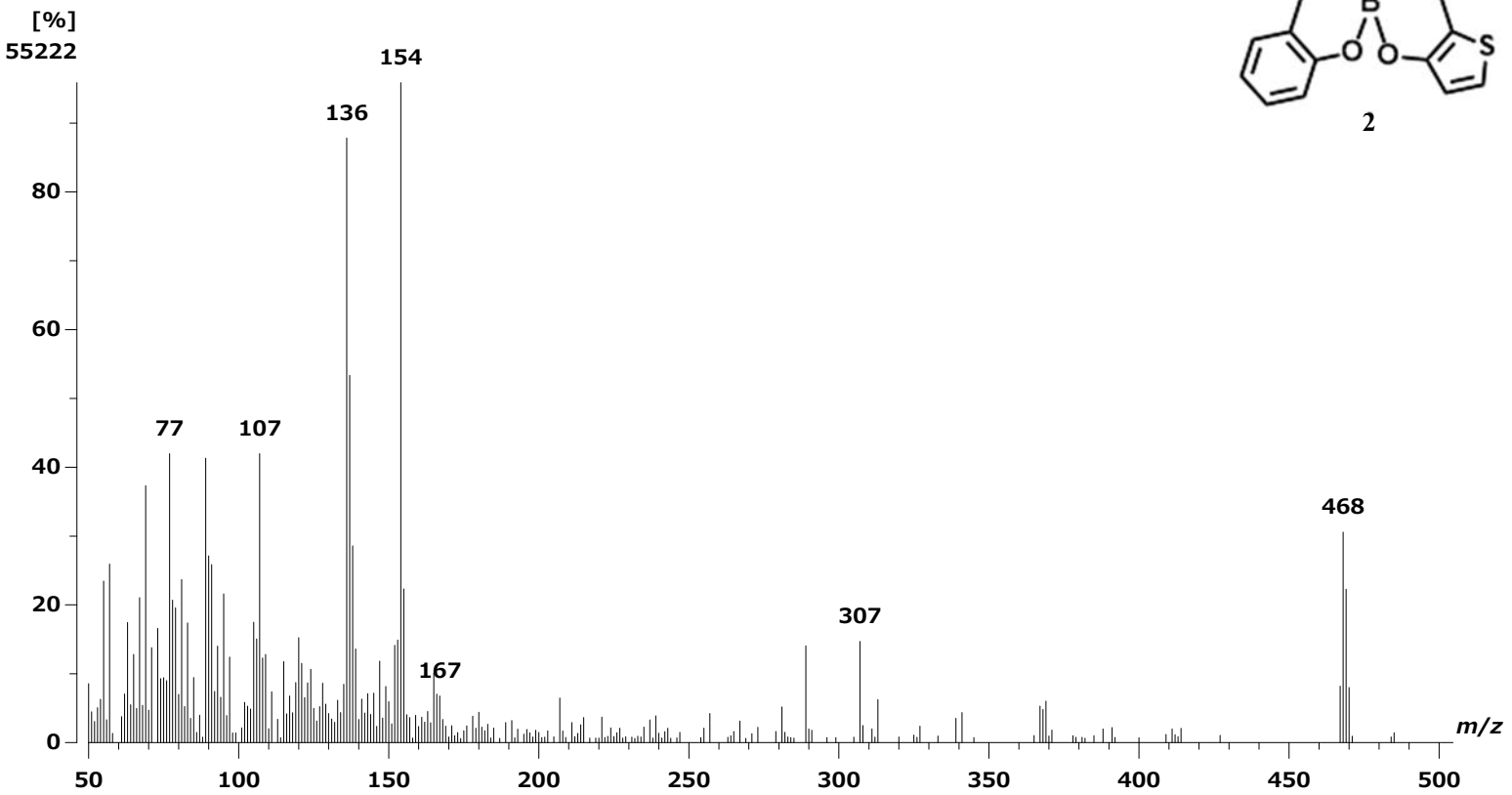


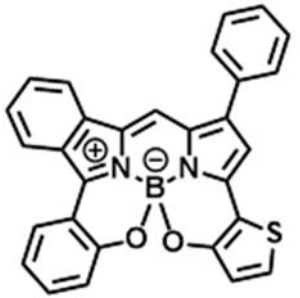


2

Fig. S22 ^{11}B NMR spectrum of **2** (128 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 181127- EXP185-001 Date : 27-Nov-2018 19:40
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,6)
BP : m/z 154 Int. : 5.49 (57595)
Output m/z range : 50 to 505 Cut Level : 0.00 %





2

Fig. S23 FAB mass spectrum (positive mode) of **2**.

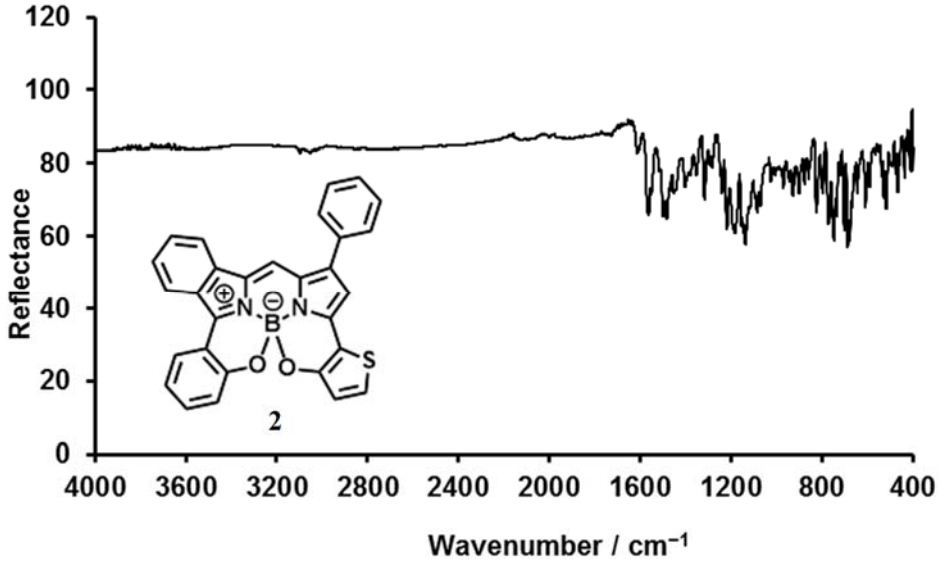
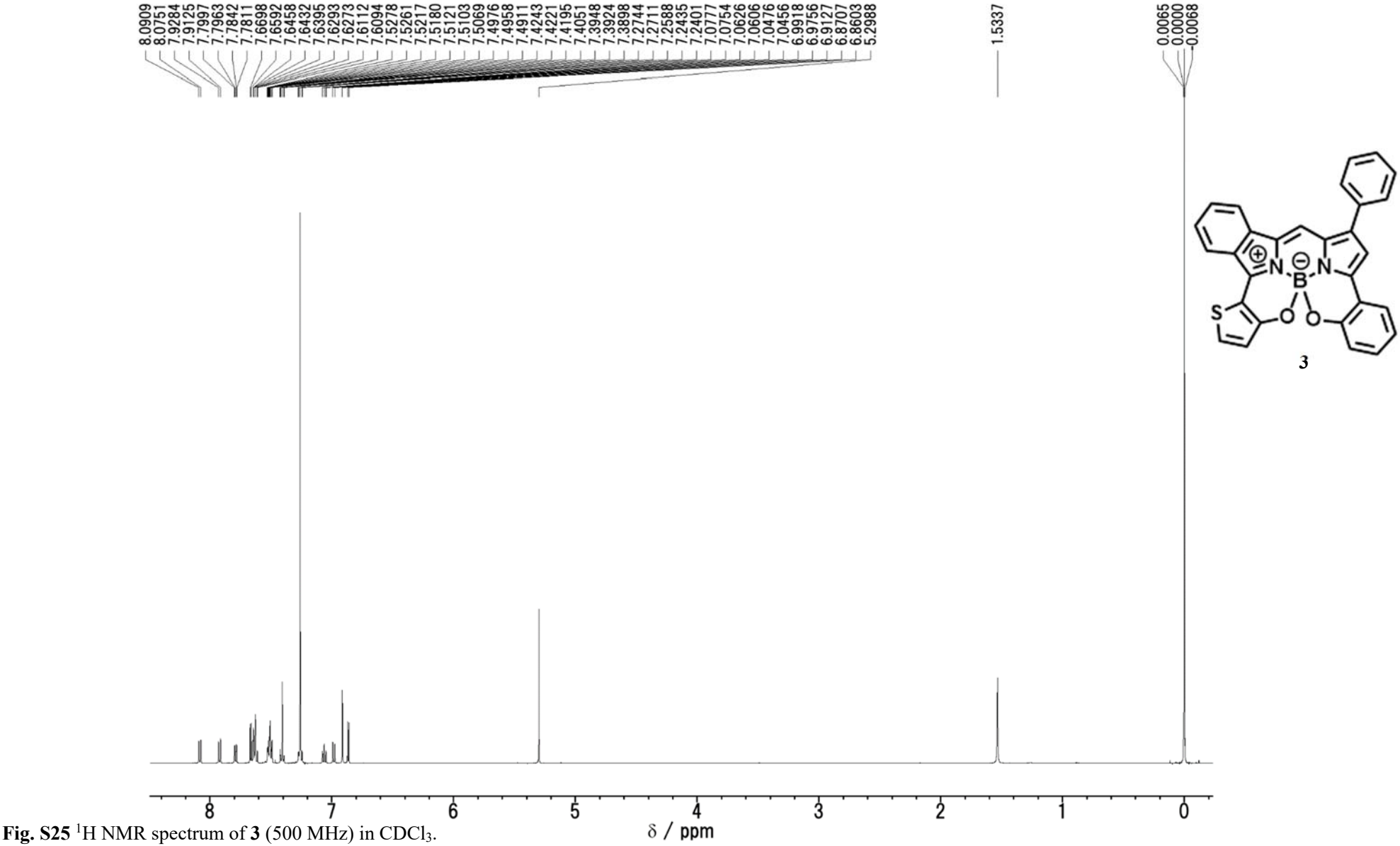
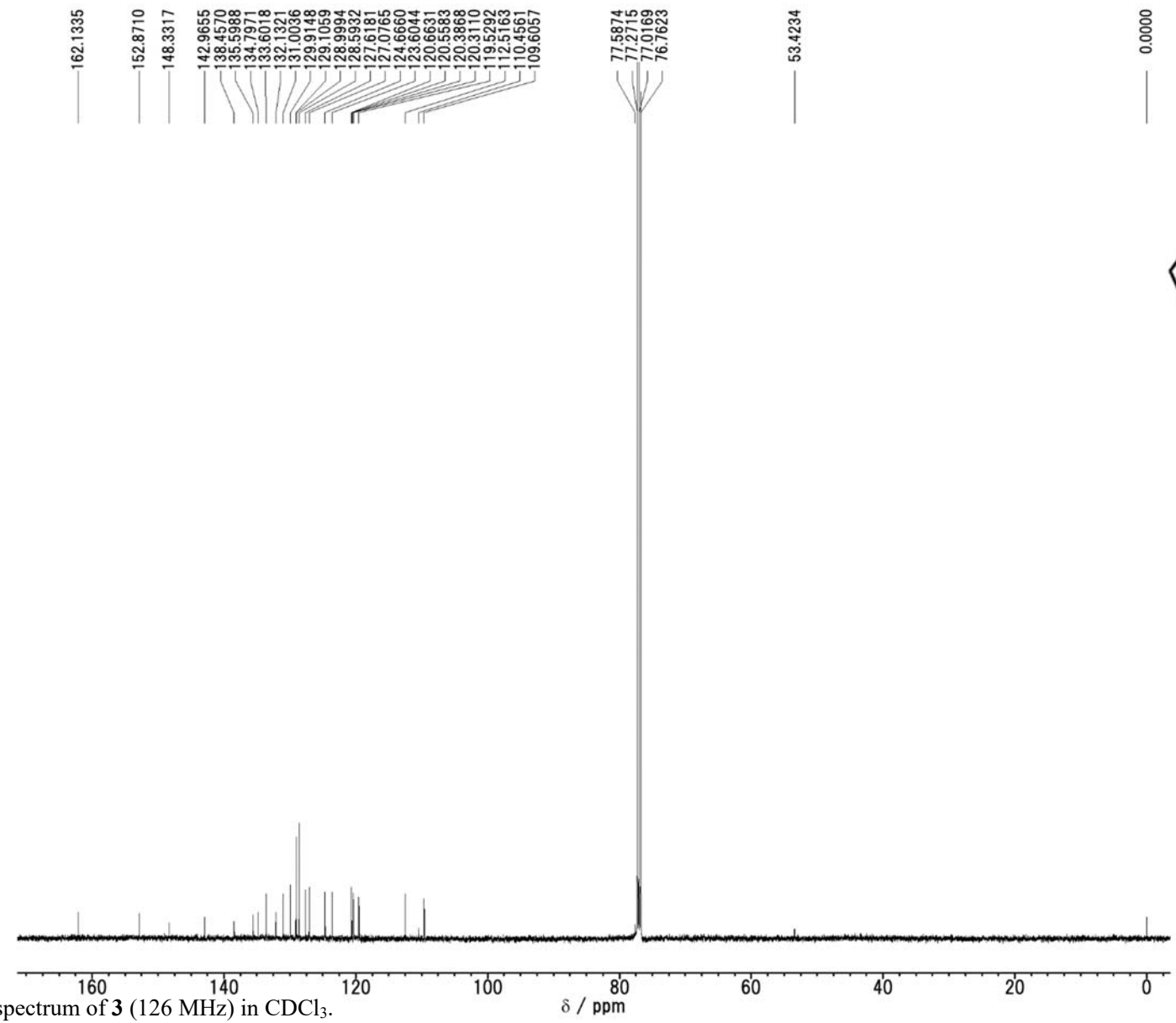


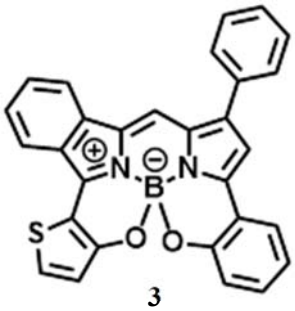
Fig. S24 ATR-FT-IR spectrum of **2**.



3

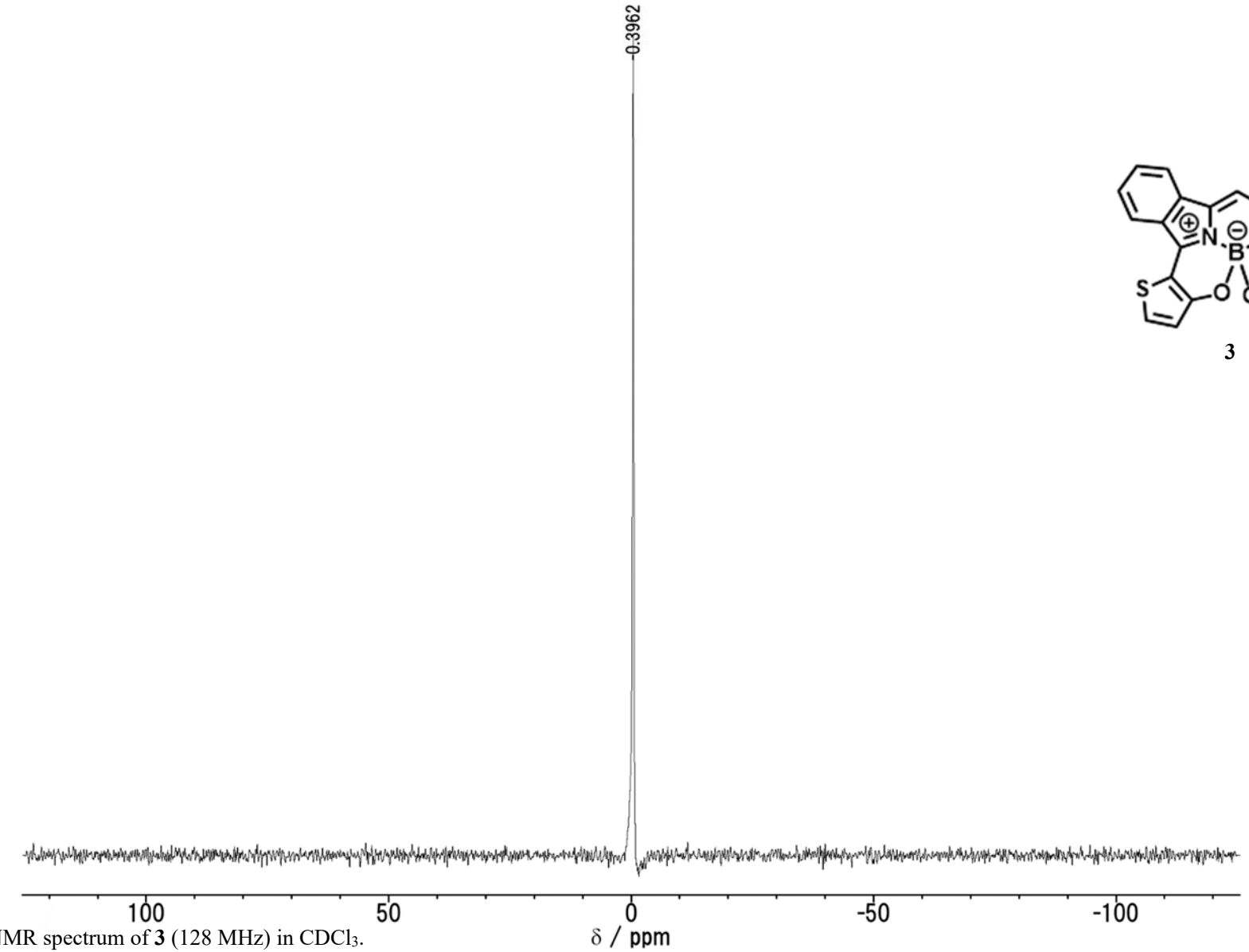
Fig. S25 ^{1}H NMR spectrum of **3** (500 MHz) in $CDCl_3$.





3

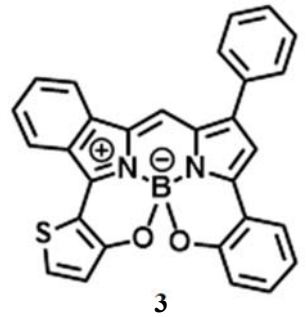
Fig. S26 ^{13}C NMR spectrum of **3** (126 MHz) in $CDCl_3$.



3

Fig. S27 ^{11}B NMR spectrum of **3** (128 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 190111- nozawa EXP56-001 Date : 11-Jan-2019 10:31
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,3)
BP : m/z 468 Int. : 4.94 (51807)
Output m/z range : 50 to 502 Cut Level : 0.00 %



3

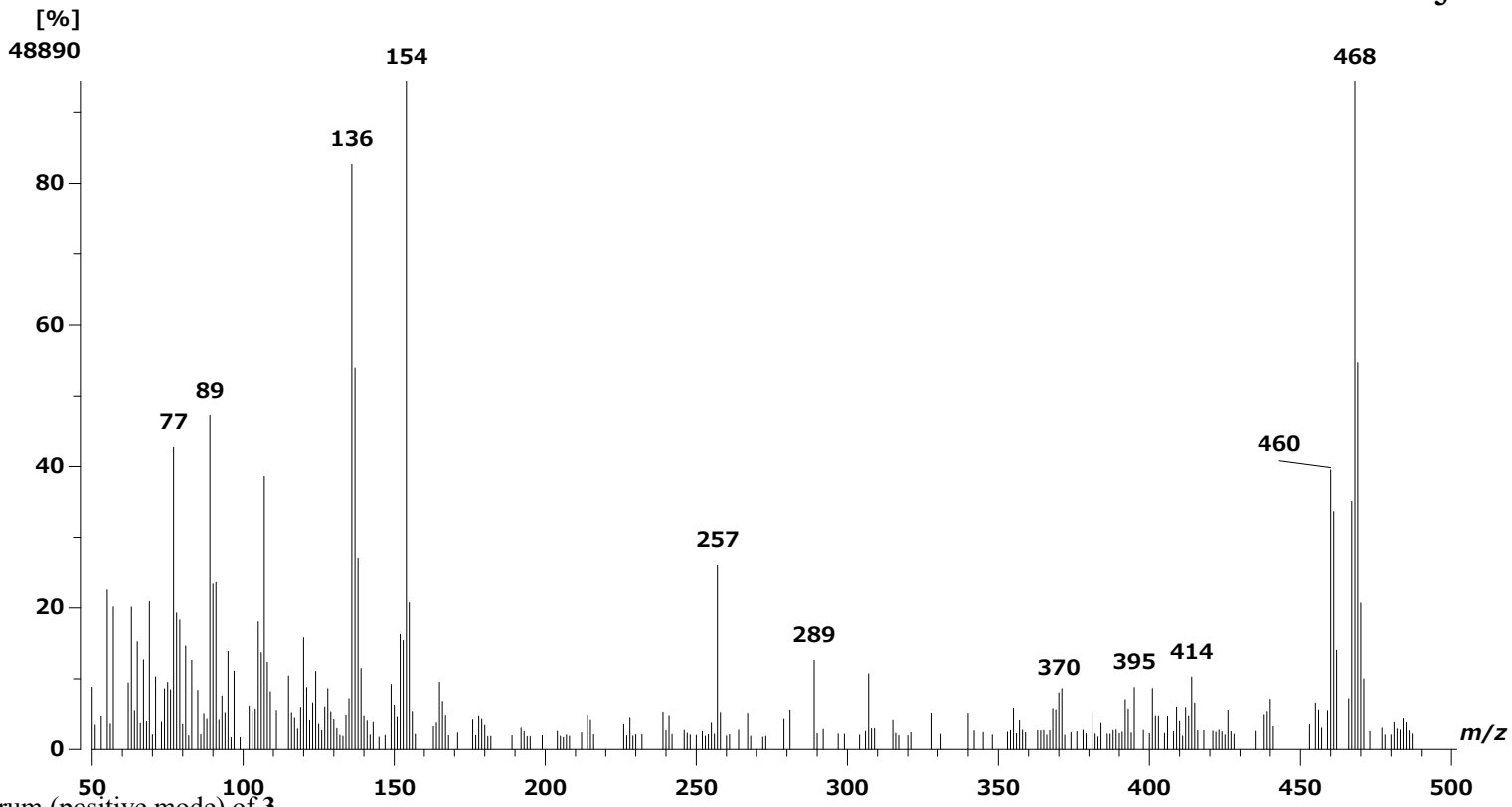


Fig. S28 FAB mass spectrum (positive mode) of **3**.

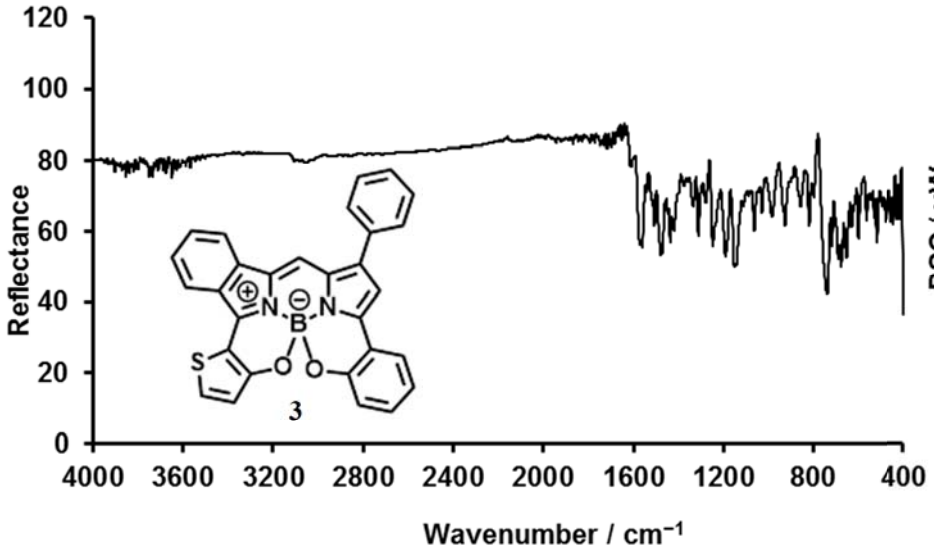


Fig. S29 ATR-FT-IR spectrum of **3**.

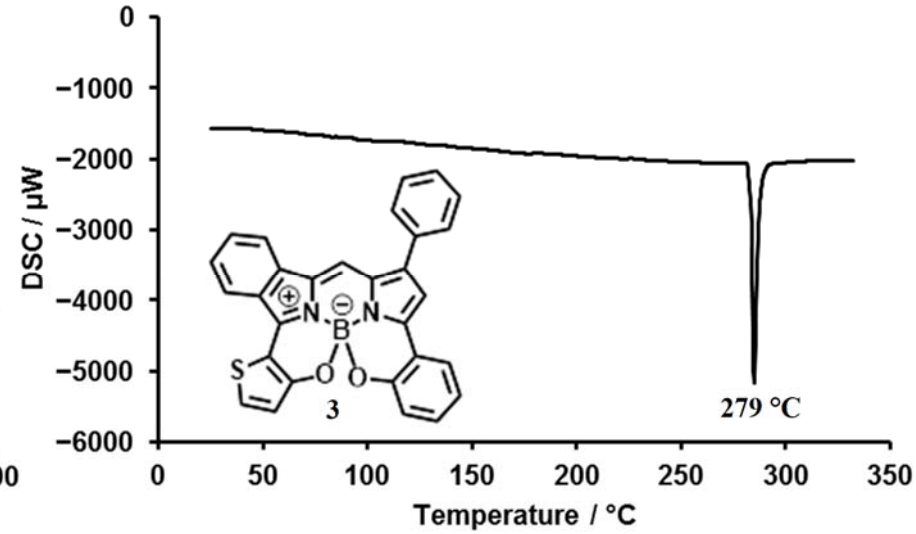


Fig. S30 DSC plots of **3**.

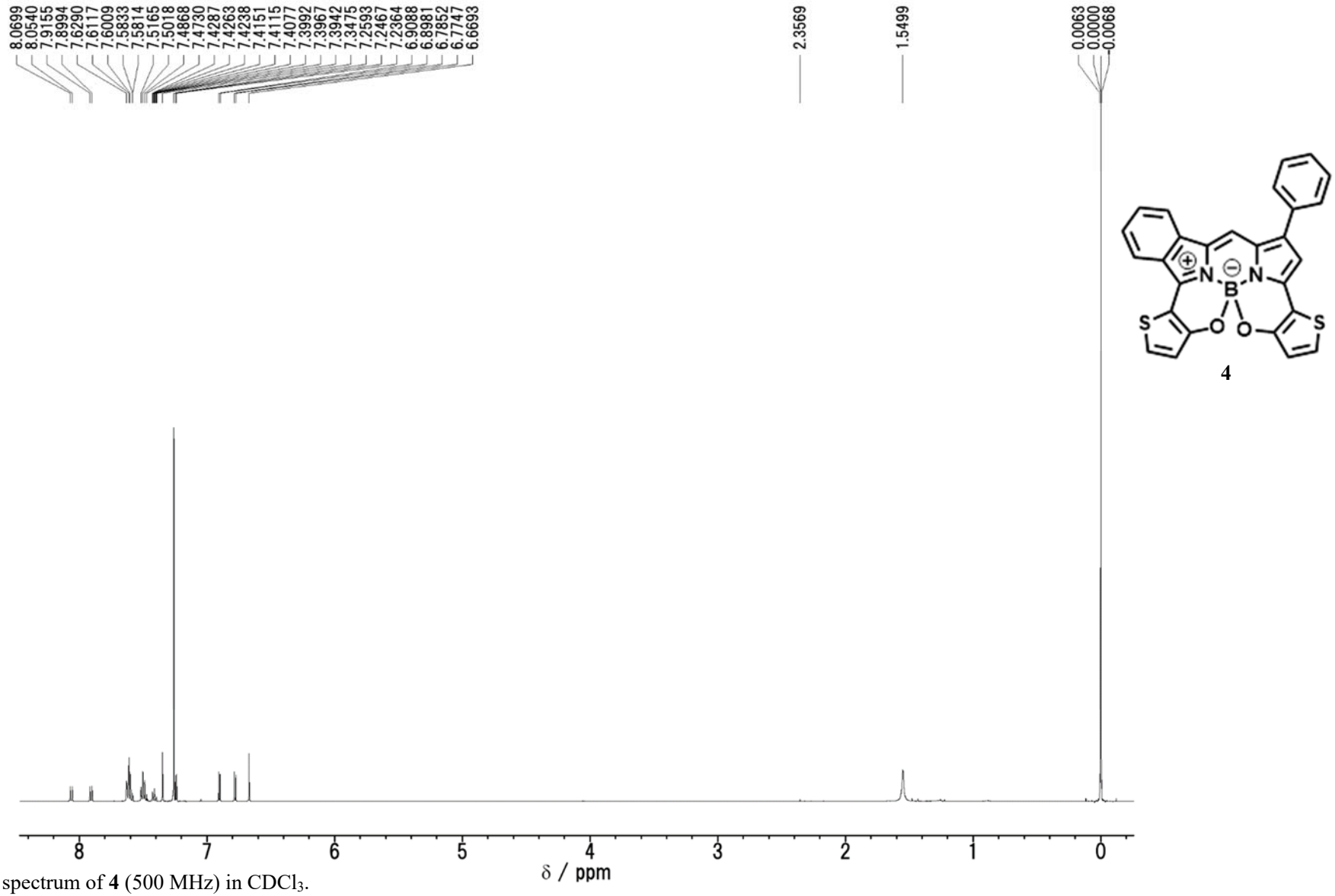
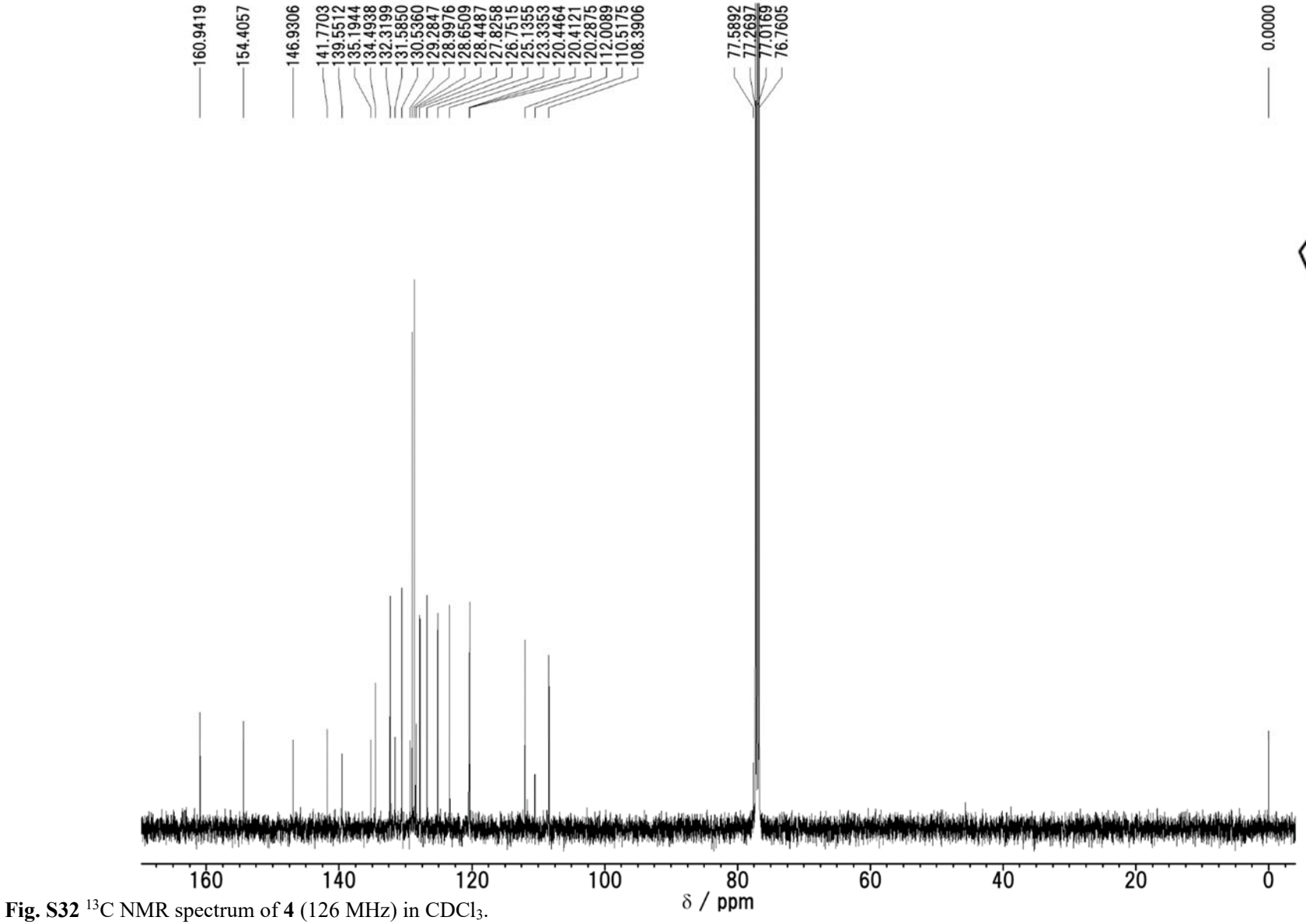
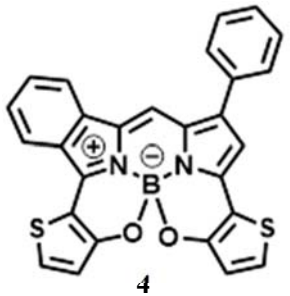


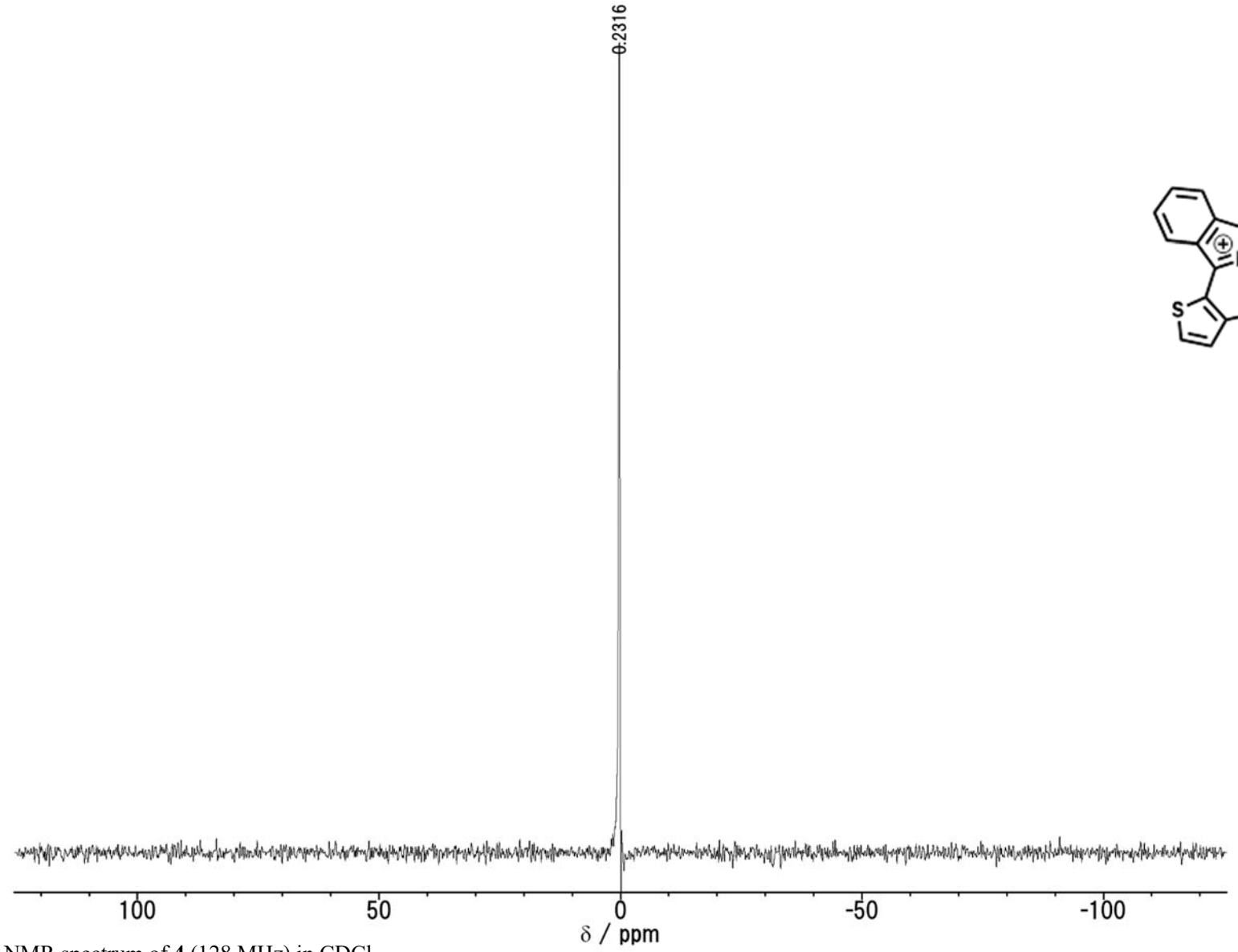
Fig. S31 ^{1}H NMR spectrum of **4** (500 MHz) in $CDCl_3$.

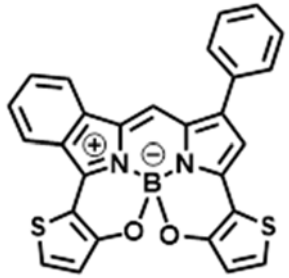




4

Fig. S32 ^{13}C NMR spectrum of **4** (126 MHz) in $CDCl_3$.

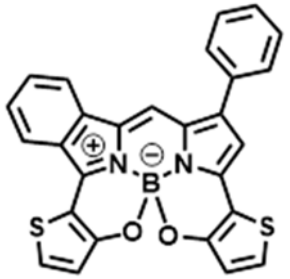




4

Fig. S33 ^{11}B NMR spectrum of **4** (128 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 190612-Nozawa EXP85 after hexane wash-002 Date : 19-Jun-2019 17:20
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (3,8)
BP : m/z 154 Int. : 96.56 (1012546)
Output m/z range : 50 to 522 Cut Level : 0.00 %



4

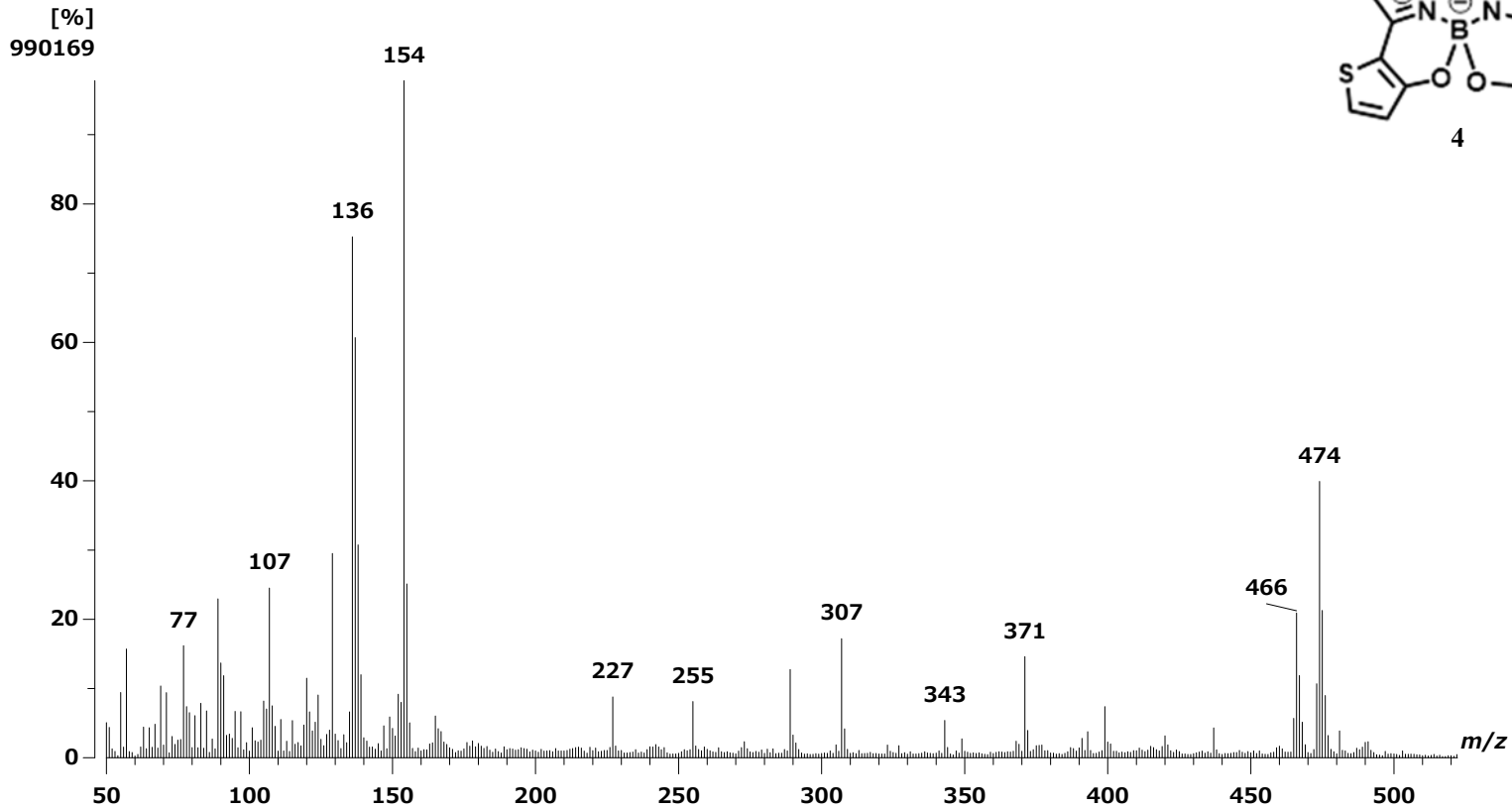


Fig. S34 FAB mass spectrum (positive mode) of **4**.

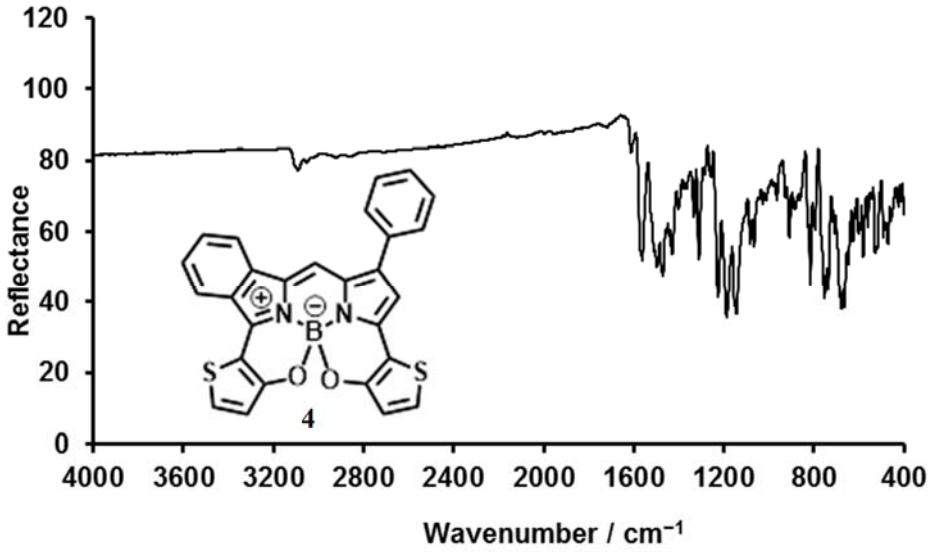


Fig. S35 ATR-FT-IR spectrum of **4**.

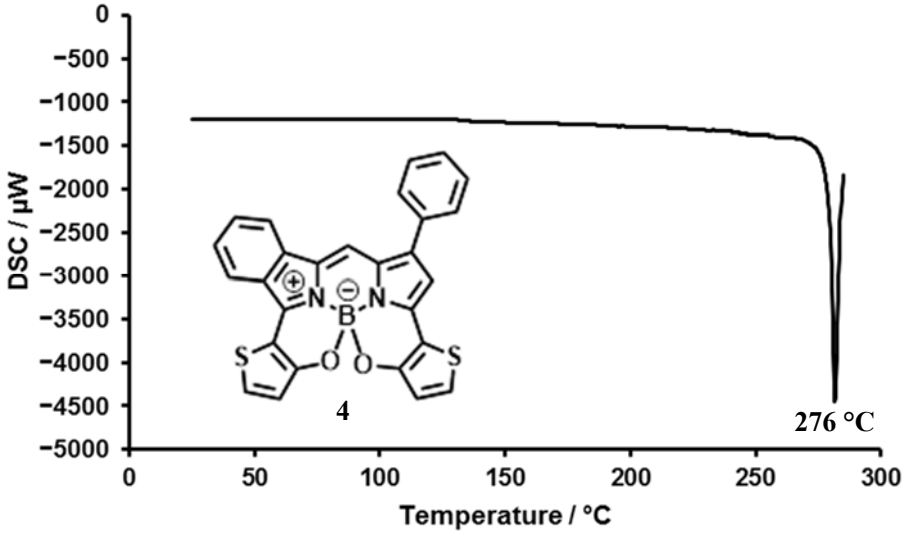


Fig. S36 DSC plots of **4**.

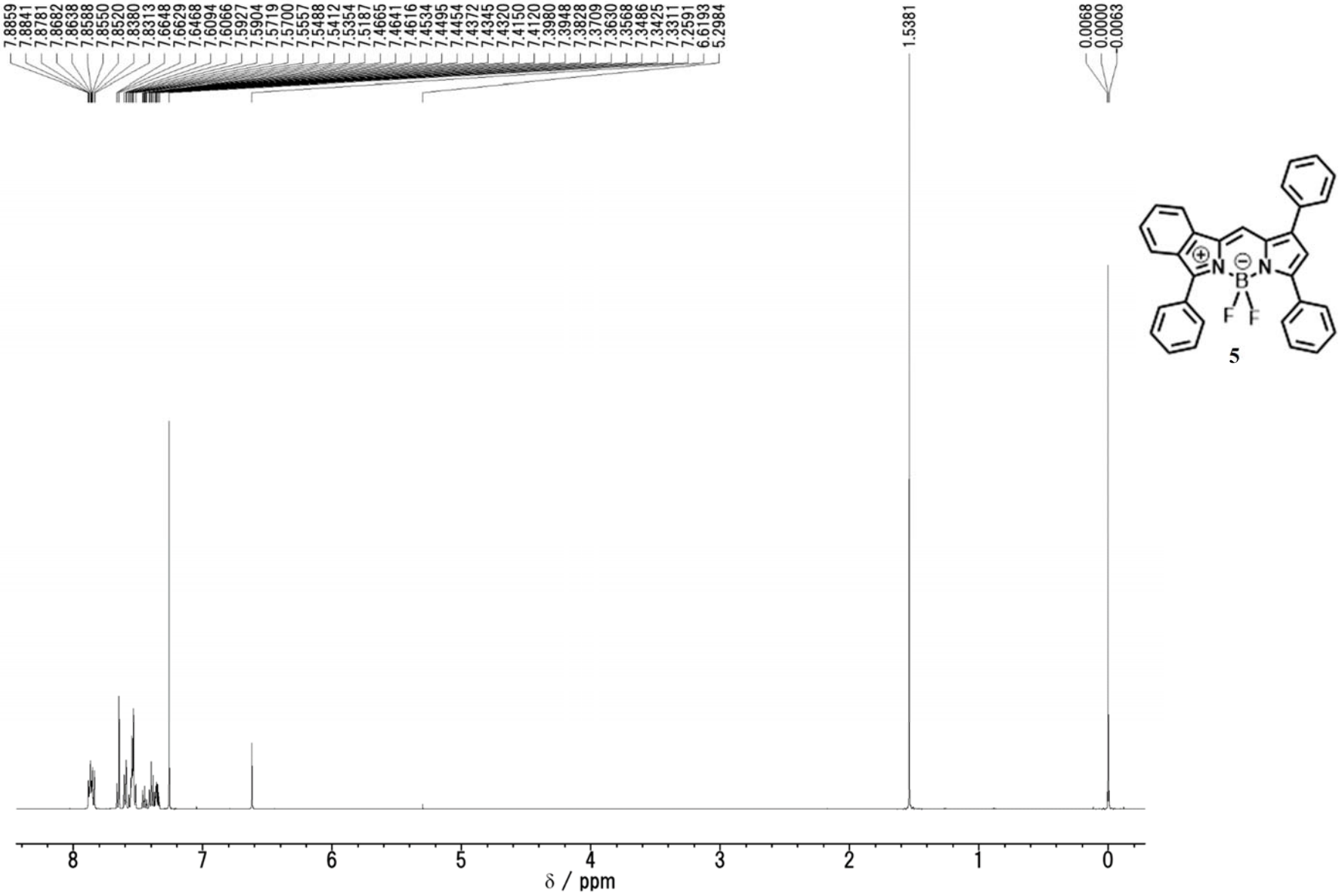
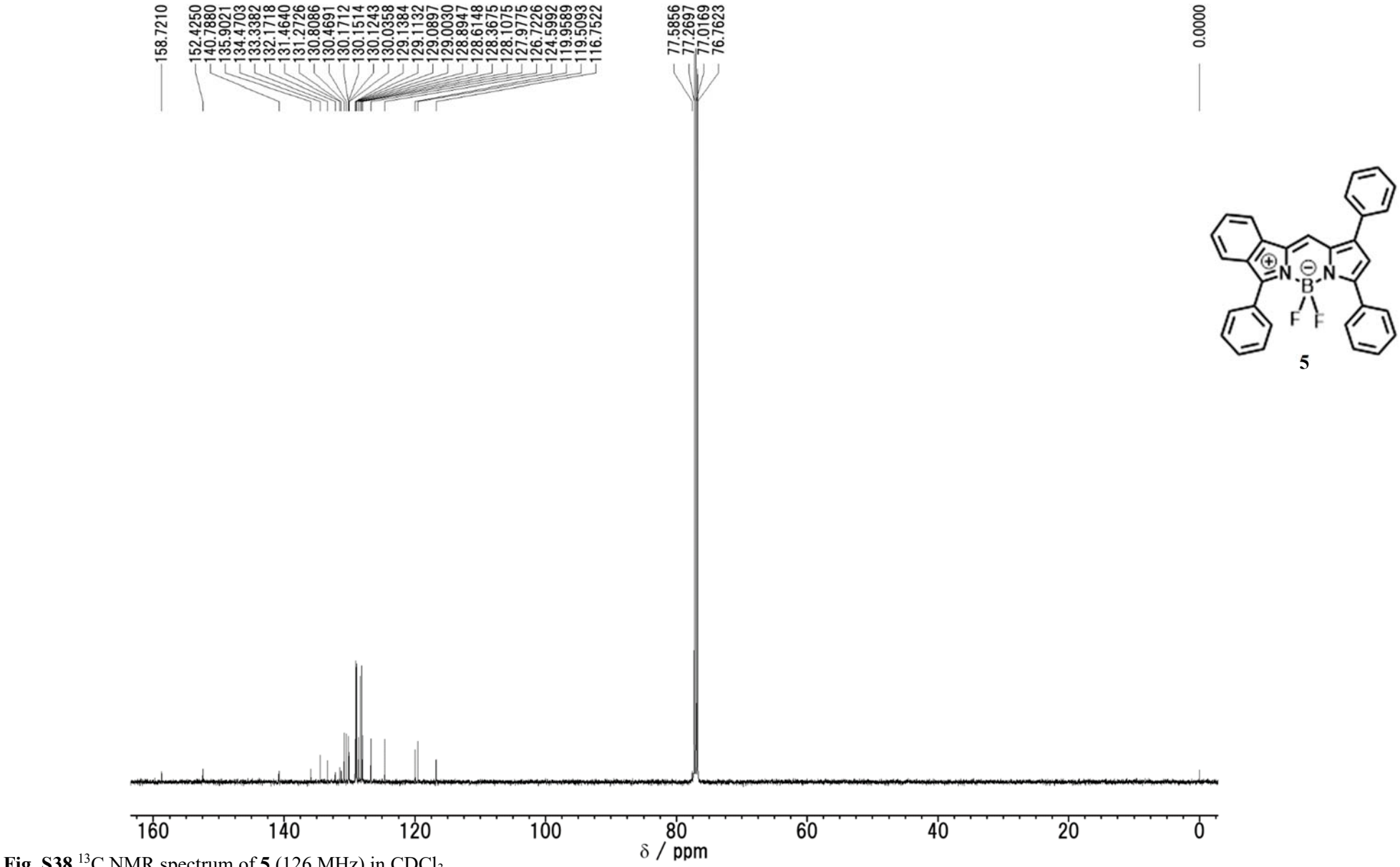
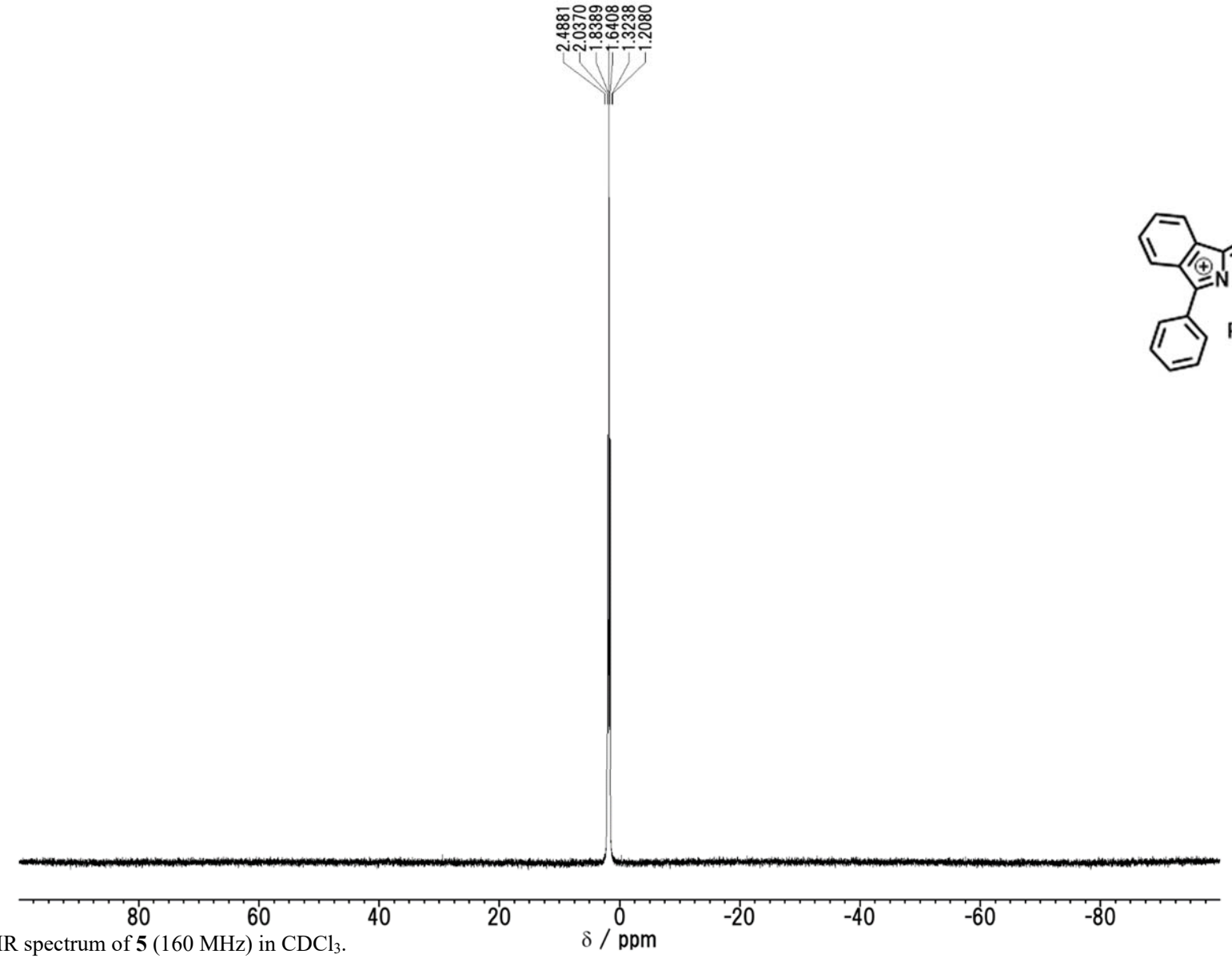


Fig. S37 ^{1}H NMR spectrum of **5** (500 MHz) in $CDCl_3$.



5

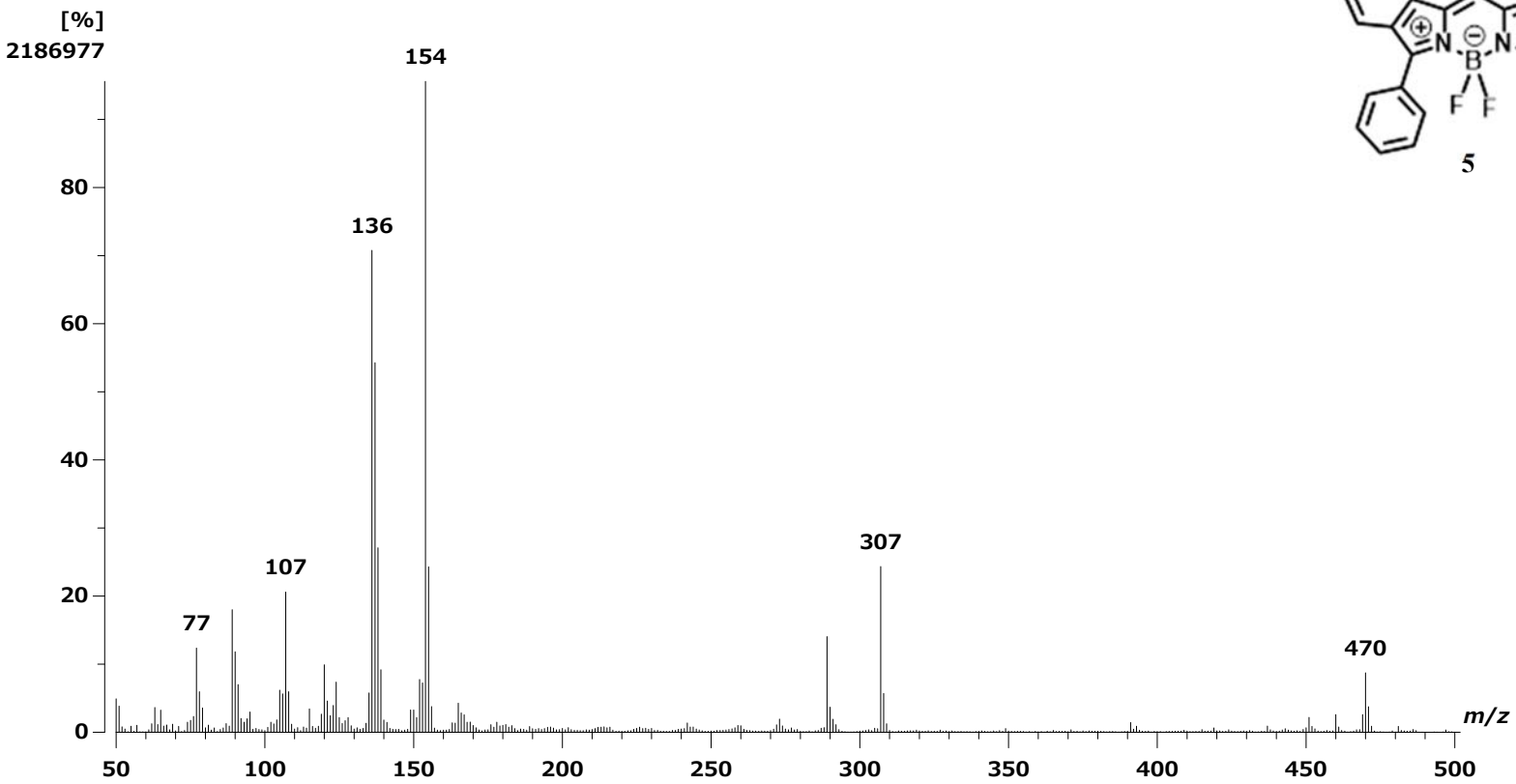
Fig. S38 ^{13}C NMR spectrum of **5** (126 MHz) in $CDCl_3$.

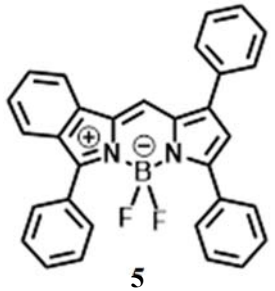


5

Fig. S39 ^{11}B NMR spectrum of **5** (160 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 190718-Nozawa EXP93-001 Date : 18-Jul-2019 19:48
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (3,8)
BP : m/z 154 Int. : 218.19 (2287872)
Output m/z range : 50 to 502 Cut Level : 0.00 %





5

Fig. S40 FAB mass spectrum (positive mode) of **5**.

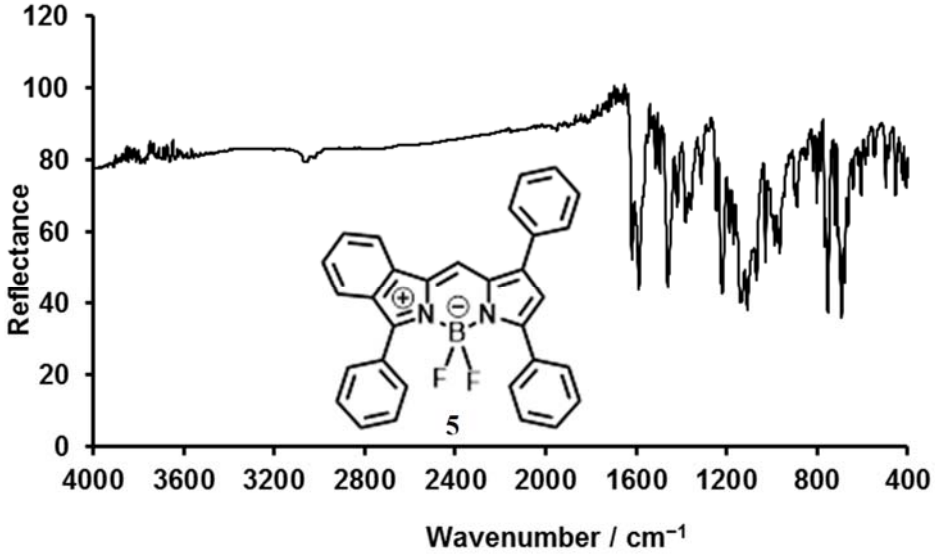


Fig. S41 ATR-FT-IR spectrum of **5**.

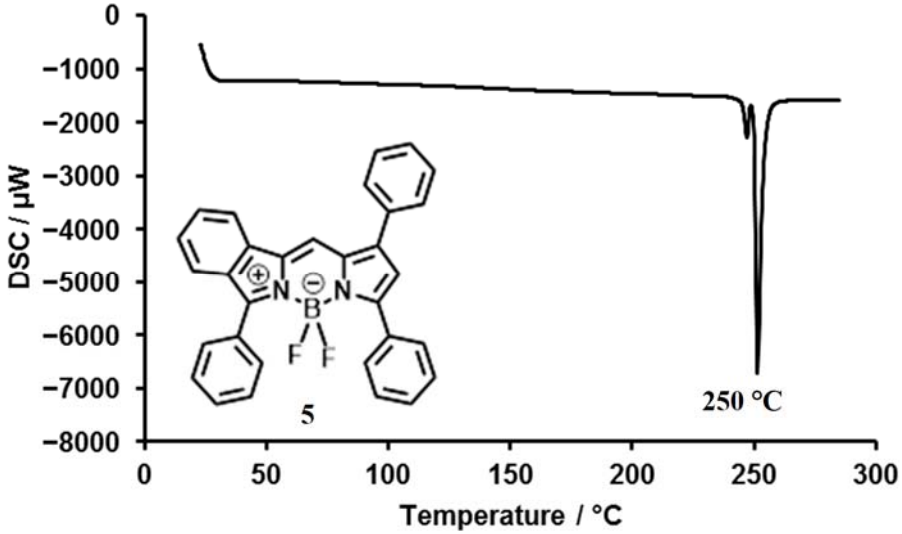
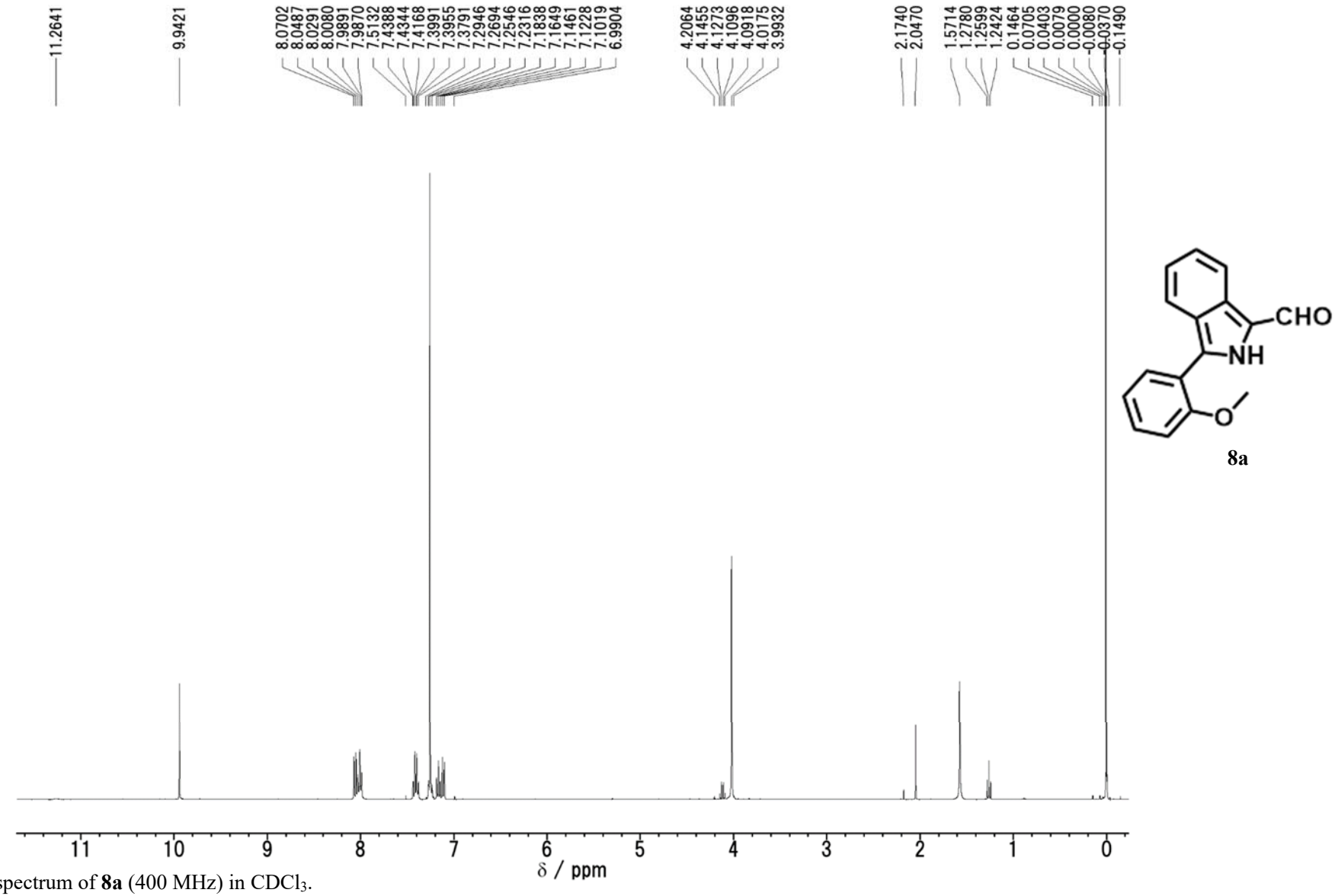


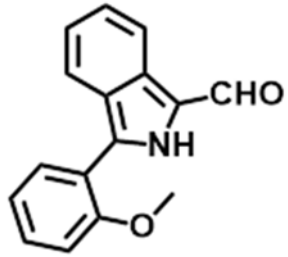
Fig. S42 DSC plots of **5**.



8a

Fig. S43 ^{1}H NMR spectrum of **8a** (400 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 180825- nozawaEXP28 -001 Date : 25-Aug-2018 17:43
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,5)
BP : m/z 251 Int. : 12.02 (126041)
Output m/z range : 50 to 277 Cut Level : 0.00 %



8a

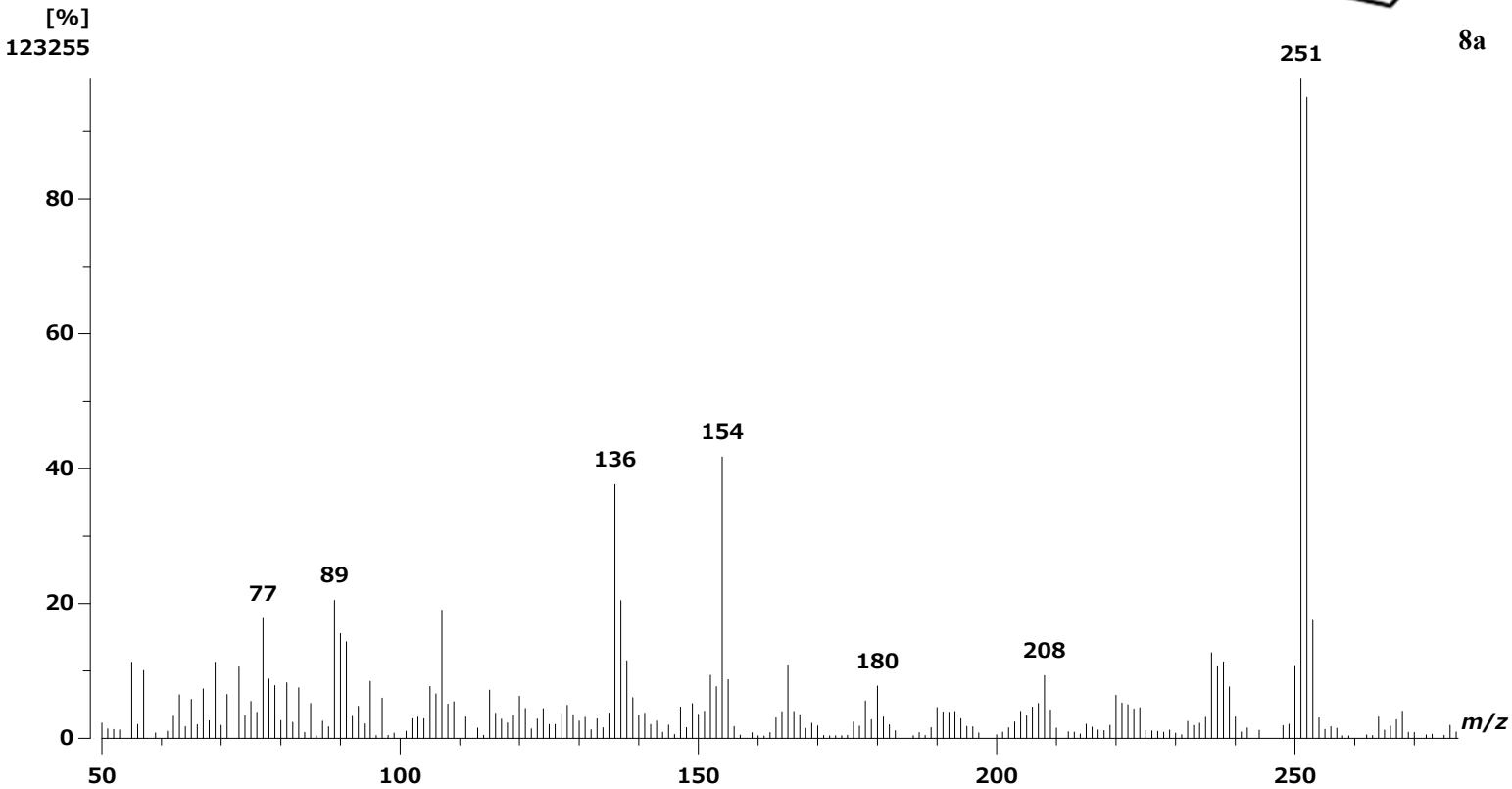


Fig. S44 FAB mass spectrum (positive mode) of **8a**.

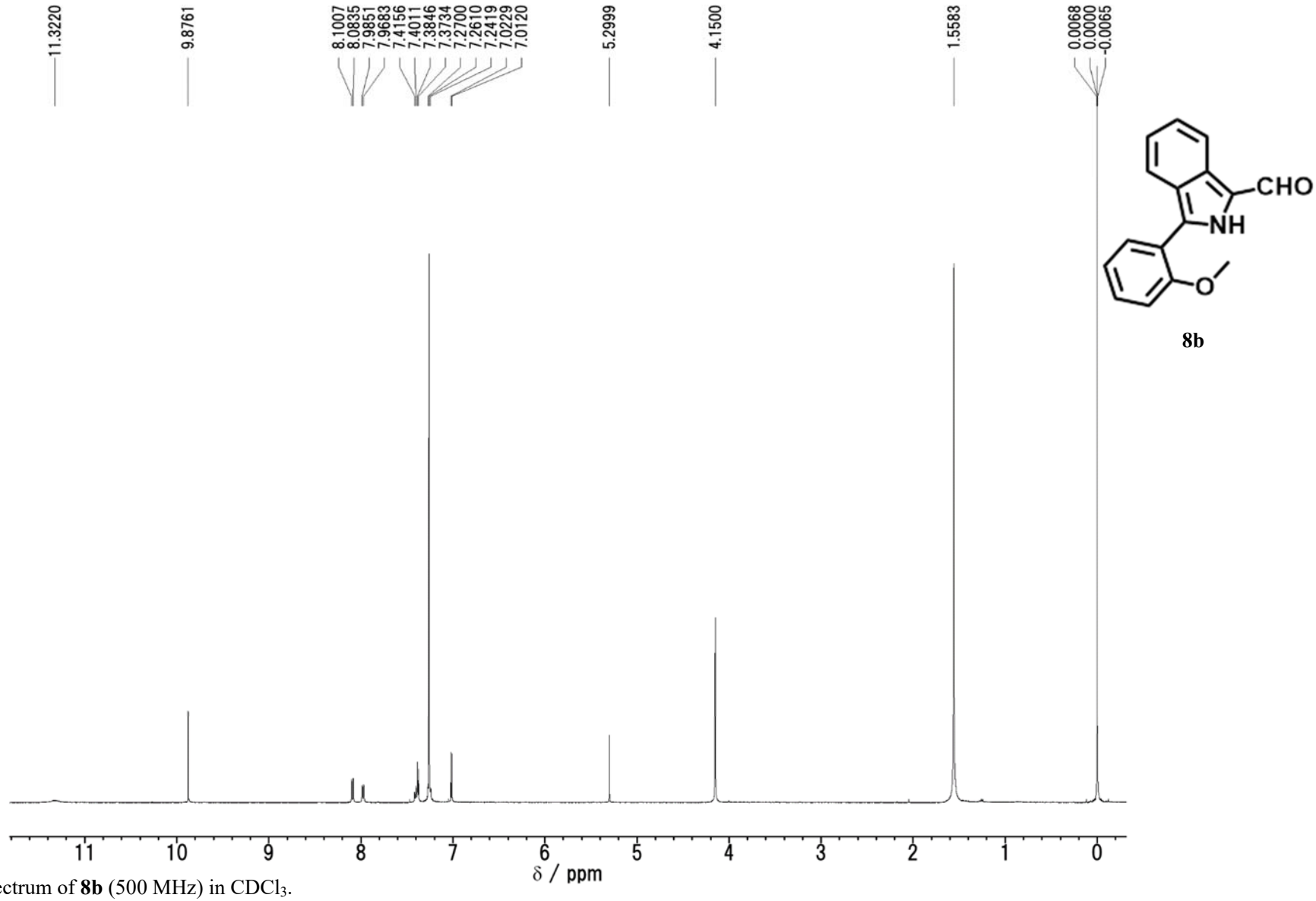
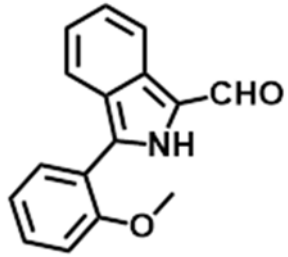


Fig. S45 ^{1}H NMR spectrum of **8b** (500 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 20180719-nozawaEXP20_Frc3-001 Date : 19-Jul-2018 15:46
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (4,8)
BP : m/z 69 Int. : 1.39 (14565)
Output m/z range : 50 to 286 Cut Level : 0.00 %



8b

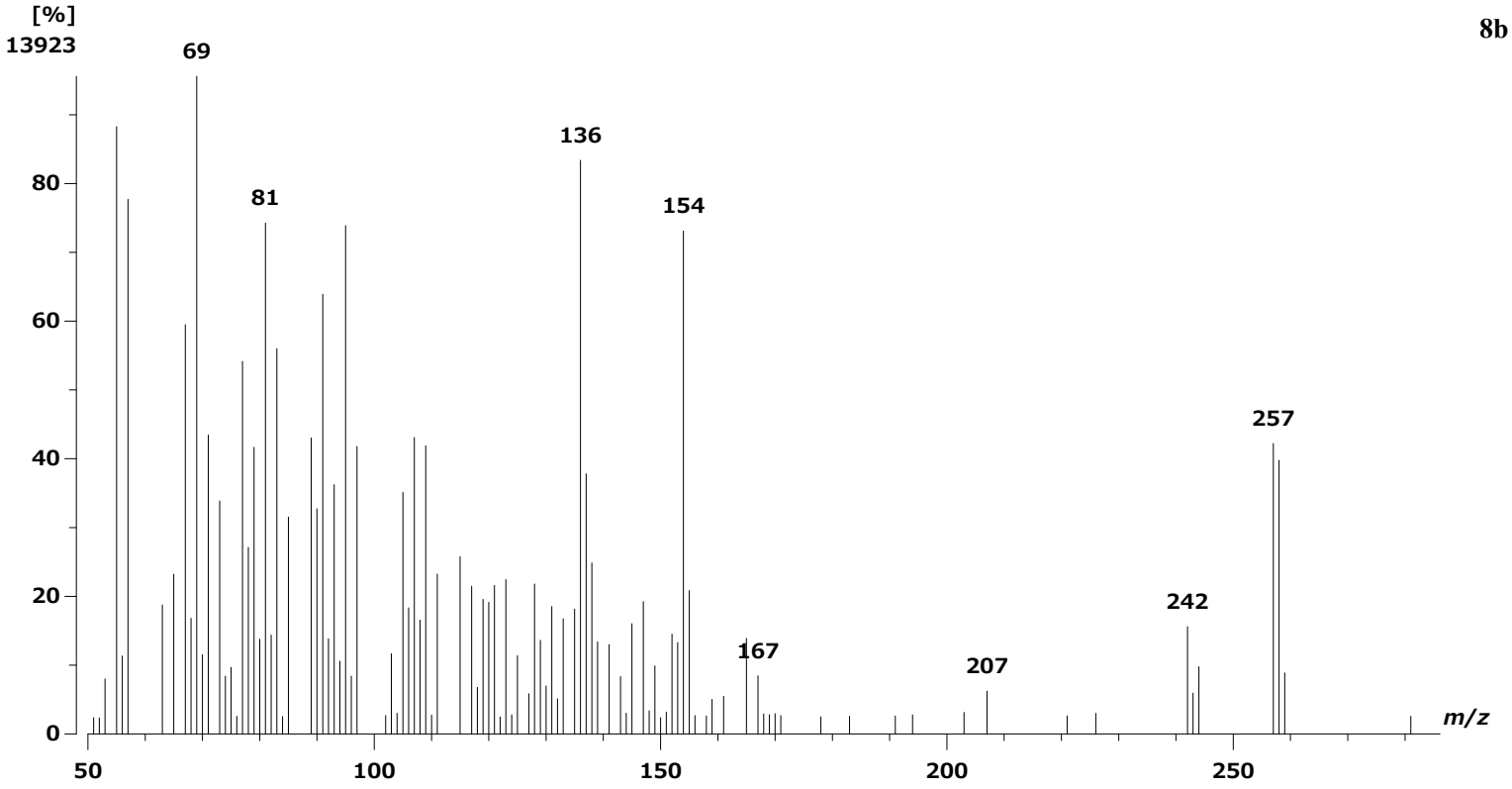
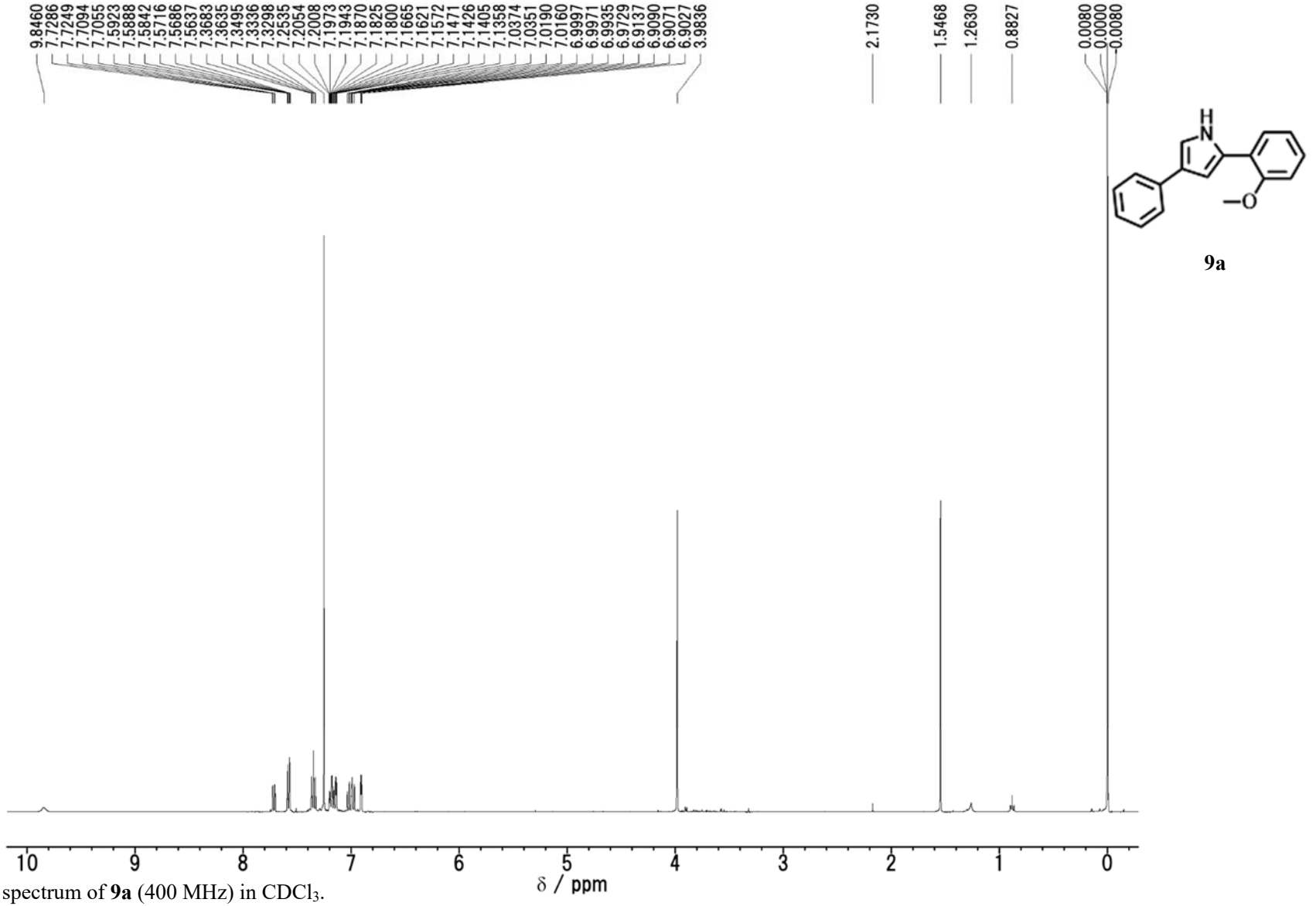


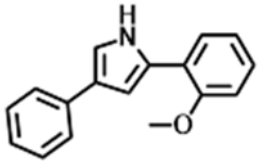
Fig. S46 FAB mass spectrum (positive mode) of **8b**.



9a

Fig. S47 ^{1}H NMR spectrum of **9a** (400 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 20181124-nozawaEXP43-001 Date : 25-Nov-2018 02:50
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,4)
BP : m/z 249 Int. : 109.69 (1150165)
Output m/z range : 50 to 371 Cut Level : 0.00 %



9a

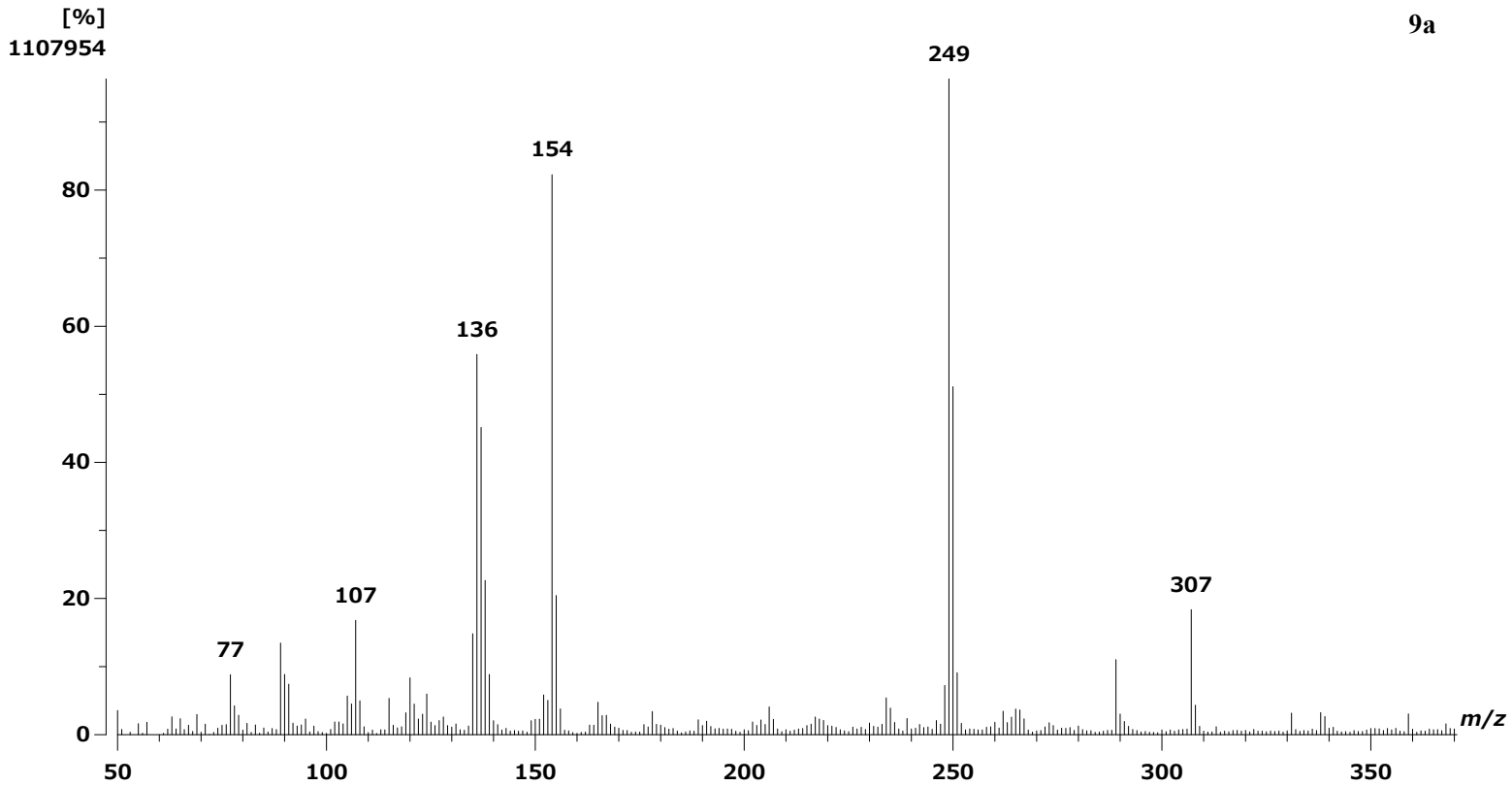


Fig. S48 FAB mass spectrum (positive mode) of **9a**.

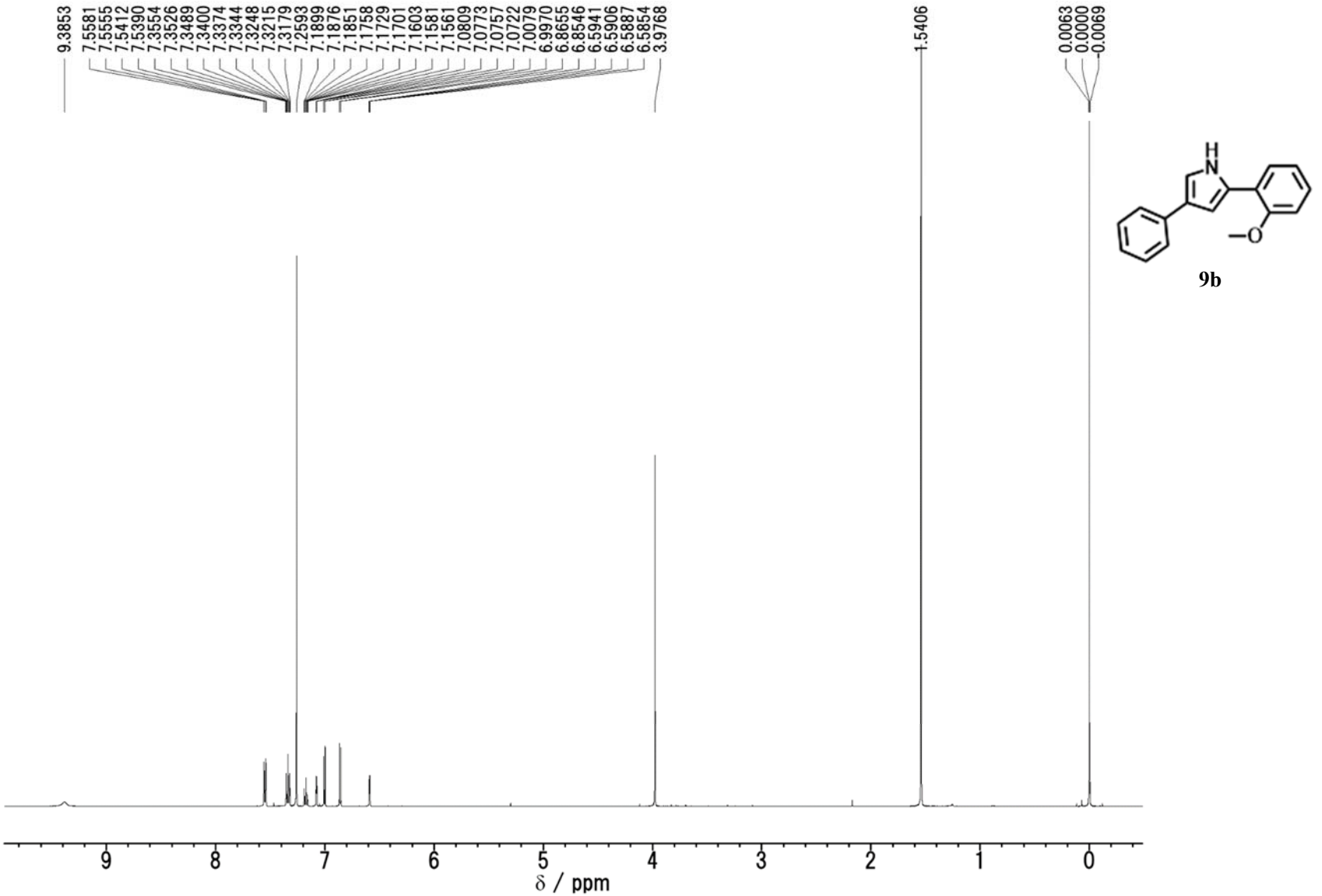
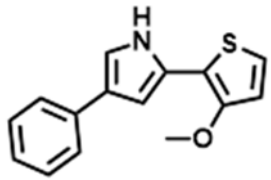


Fig. S49 ^{1}H NMR spectrum of **9b** (500 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 180603- EXP137 -001 Date : 03-Jun-2018 16:48
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,3)
BP : m/z 255 Int. : 87.14 (913704)
Output m/z range : 50 to 269 Cut Level : 0.00 %



9b

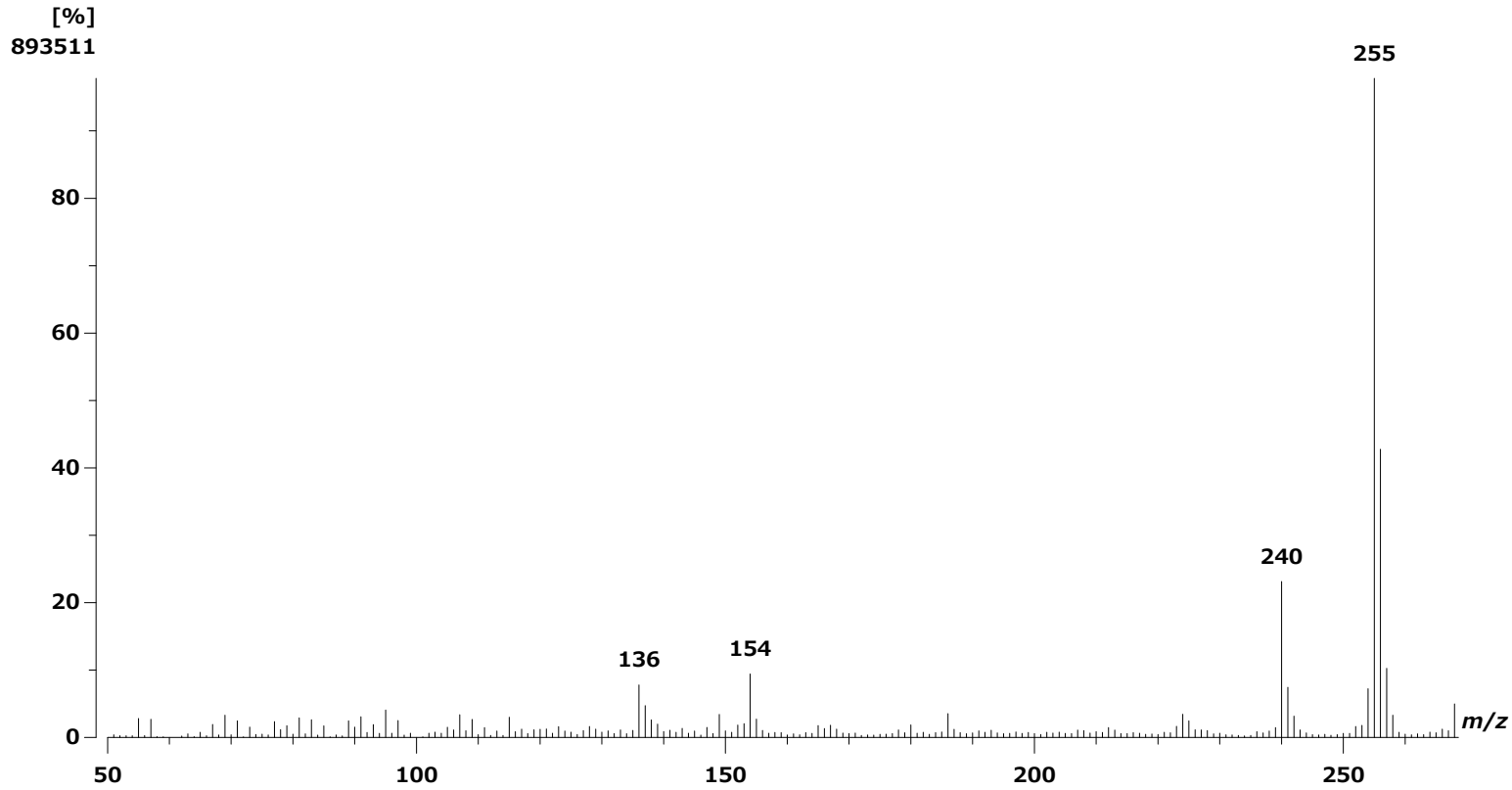


Fig. S50 FAB mass spectrum (positive mode) of **9b**.

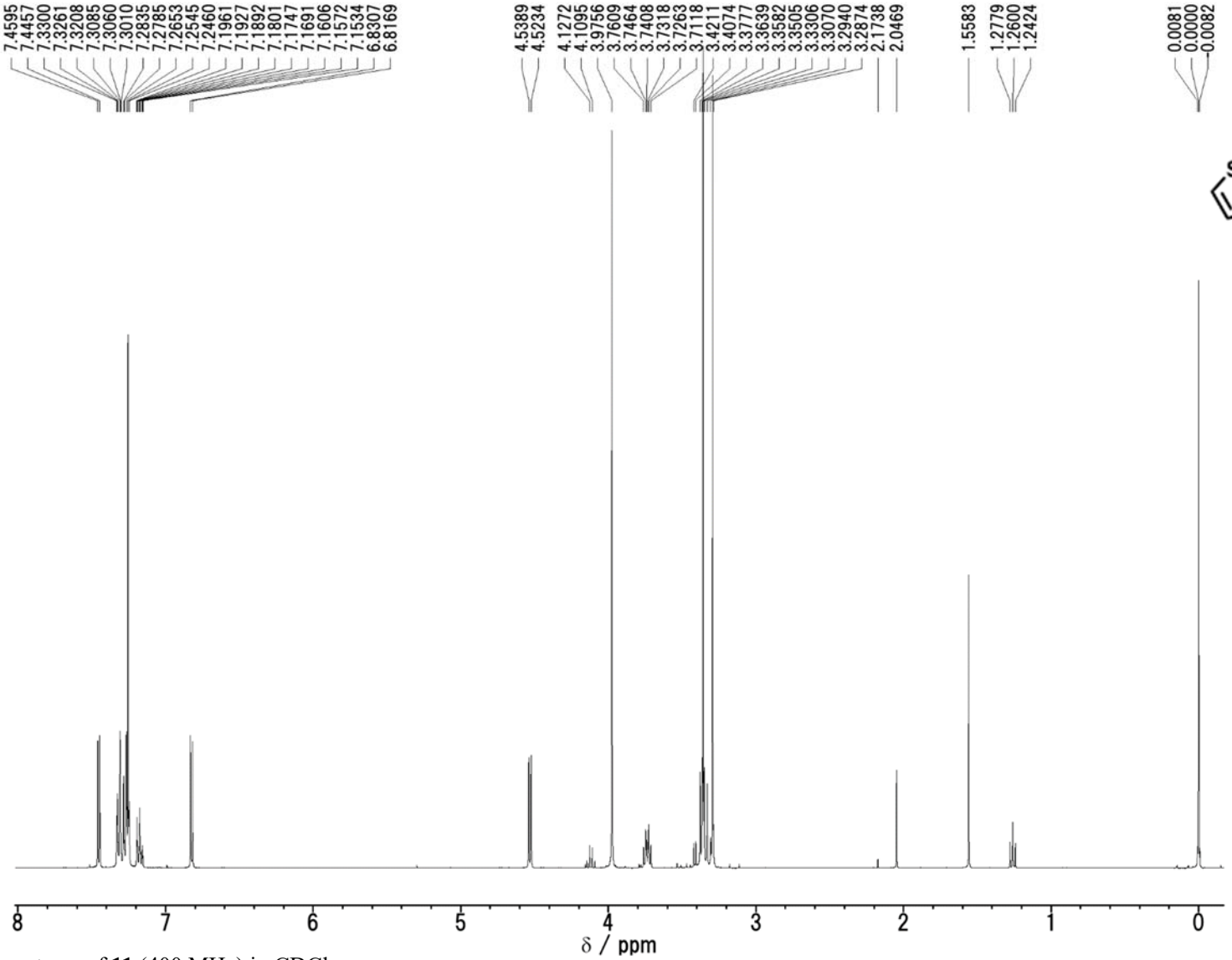
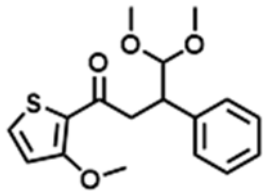


Fig. S51 ^{1}H NMR spectrum of **11** (400 MHz) in $CDCl_3$.

[Mass Spectrum]
Data : 20180531_shimada_EXP84-001 Date : 31-May-2018 15:32
Instrument : MStation
Sample : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
Scan# : (2,3)
BP : m/z 289 Int. : 70.63 (740568)
Output m/z range : 50 to 315 Cut Level : 0.00 %



11

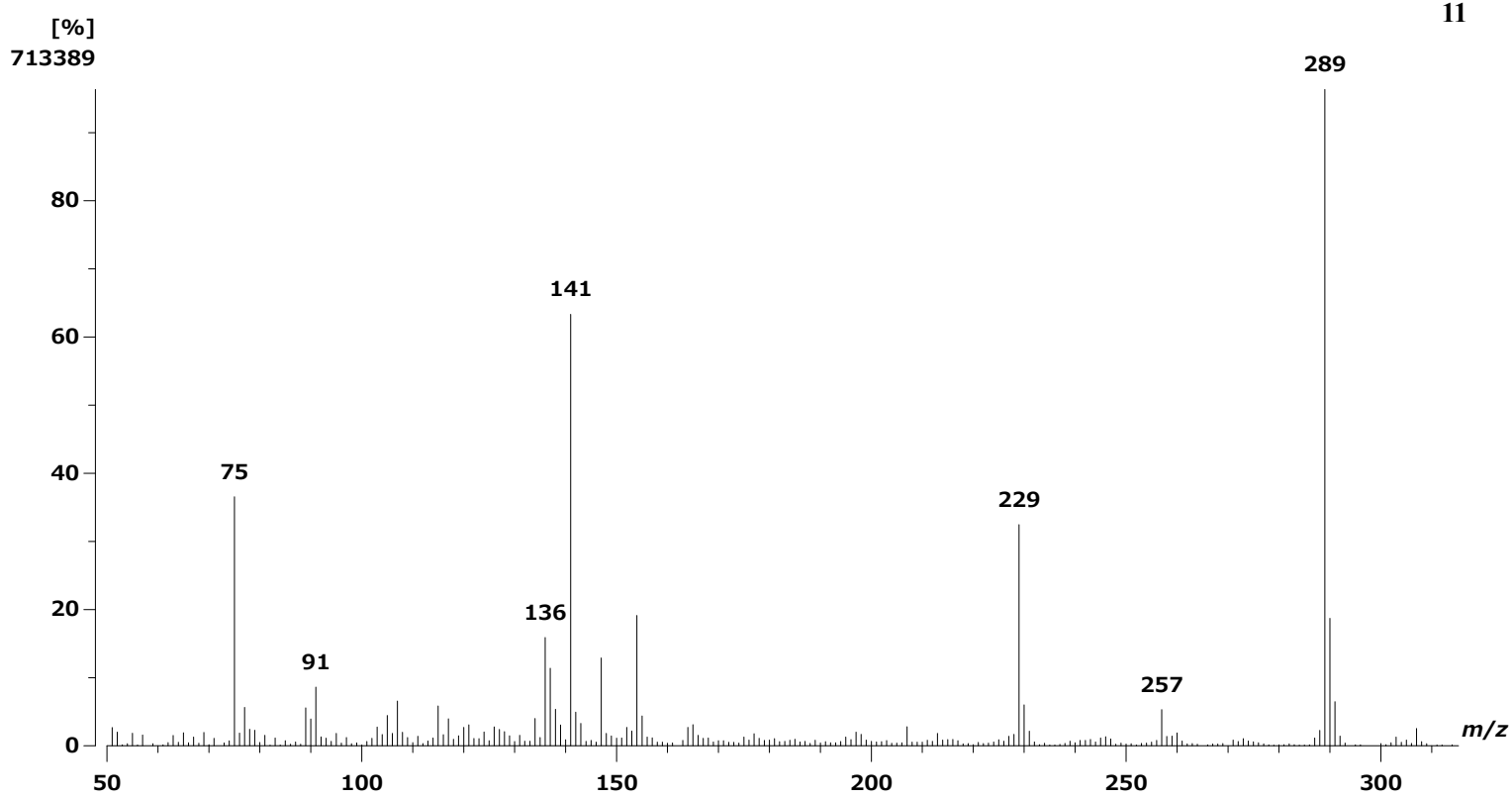
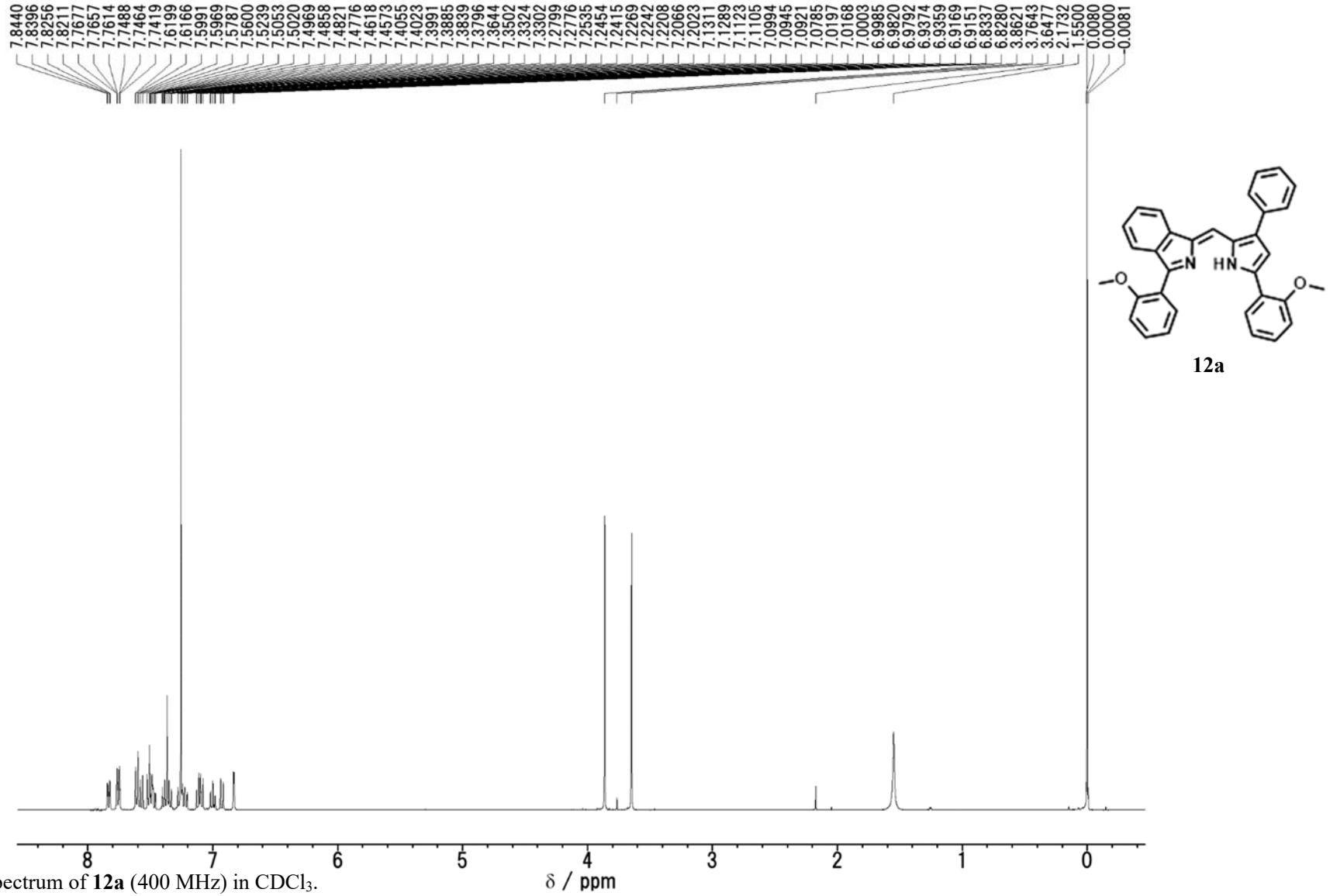
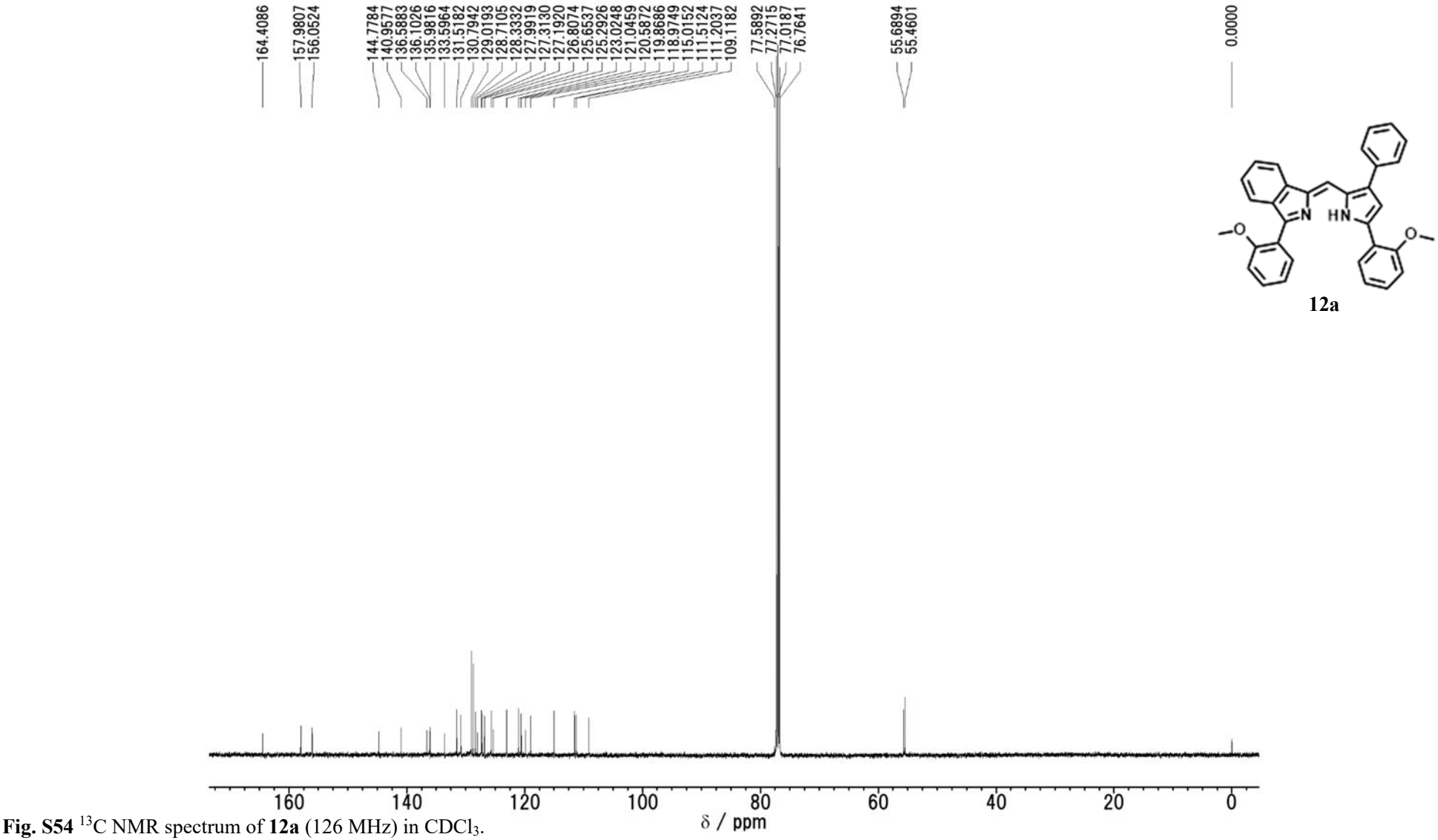


Fig. S52 FAB mass spectrum (positive mode) of **11**.



12a

Fig. S53 ^{1}H NMR spectrum of **12a** (400 MHz) in $CDCl_3$.



12a

Fig. S54 ^{13}C NMR spectrum of **12a** (126 MHz) in $CDCl_3$.

Generic Display Report

Analysis Info

Analysis Name	D:\Data\syn1\kubo20201219\#1_Exp44_1.d	Acquisition Date	12/20/2020 1:52:48 AM
Method	APCI_pos_DIP.m	Operator	BDAL@DE
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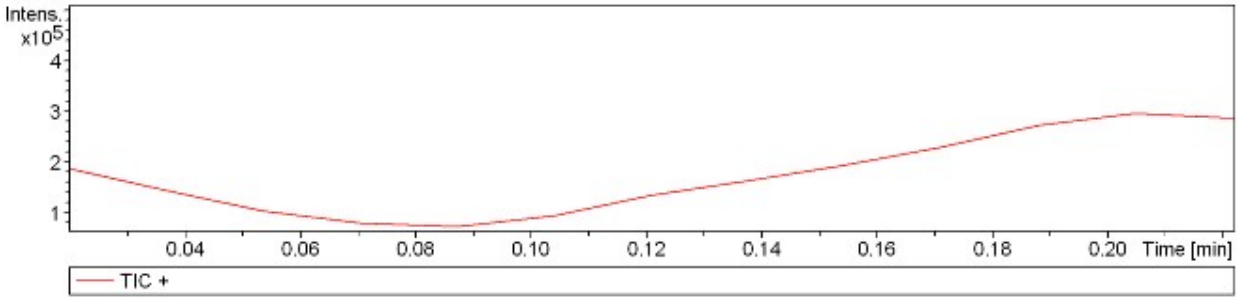
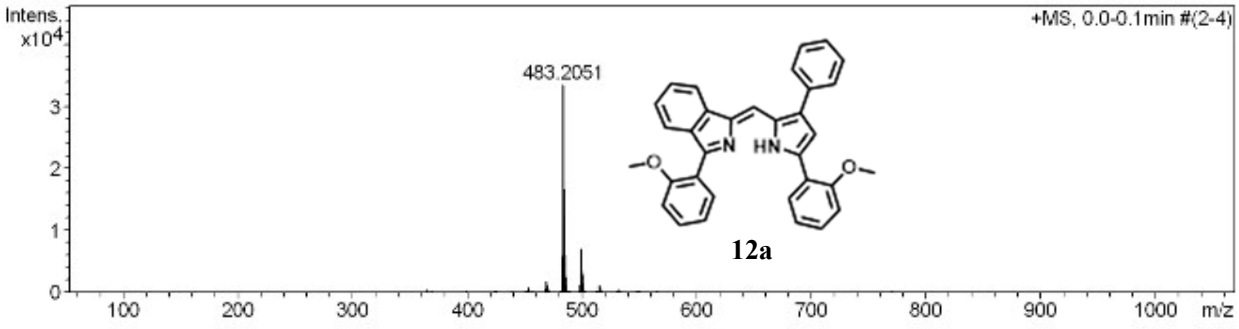
Comment	Cap 150 Hex 400		





12a

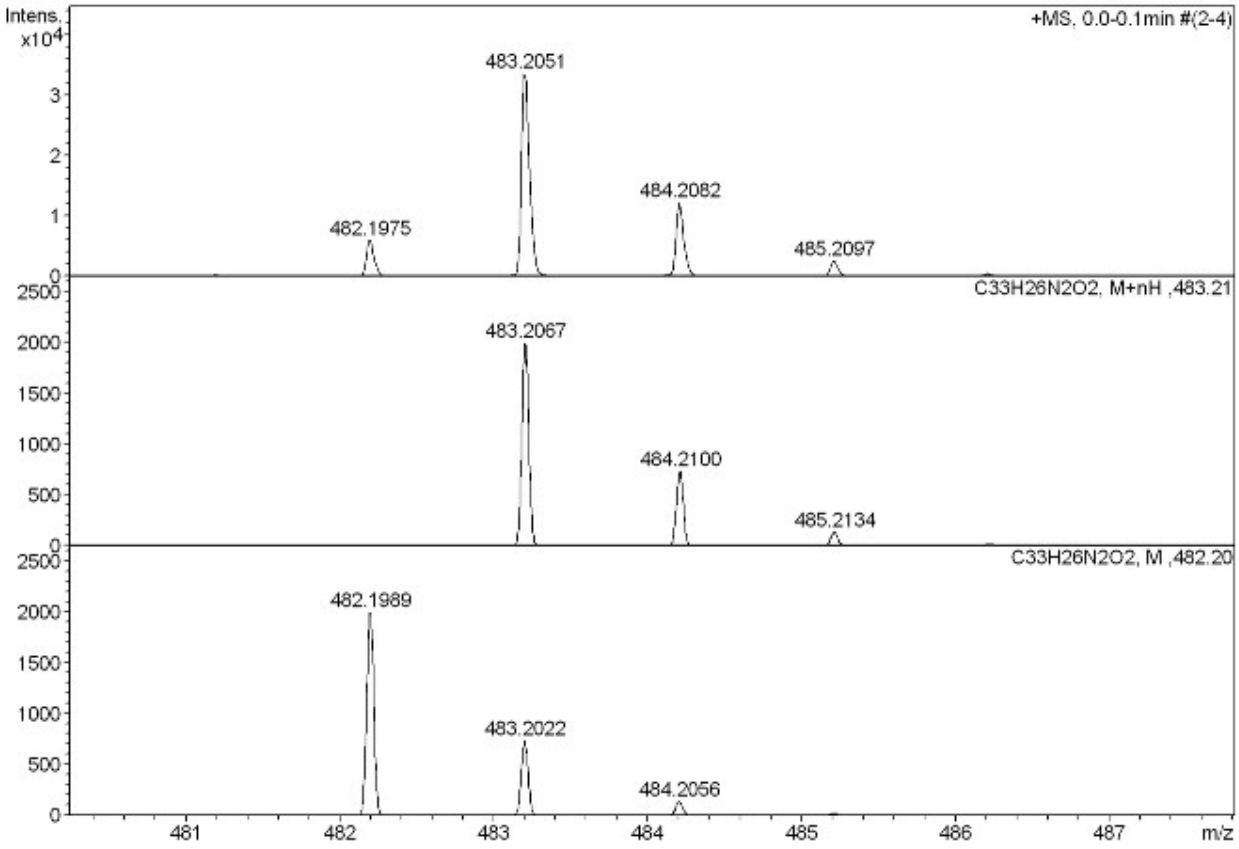


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Fig. S55 High resolution of APCI mass spectrum (positive mode) of **12a**.

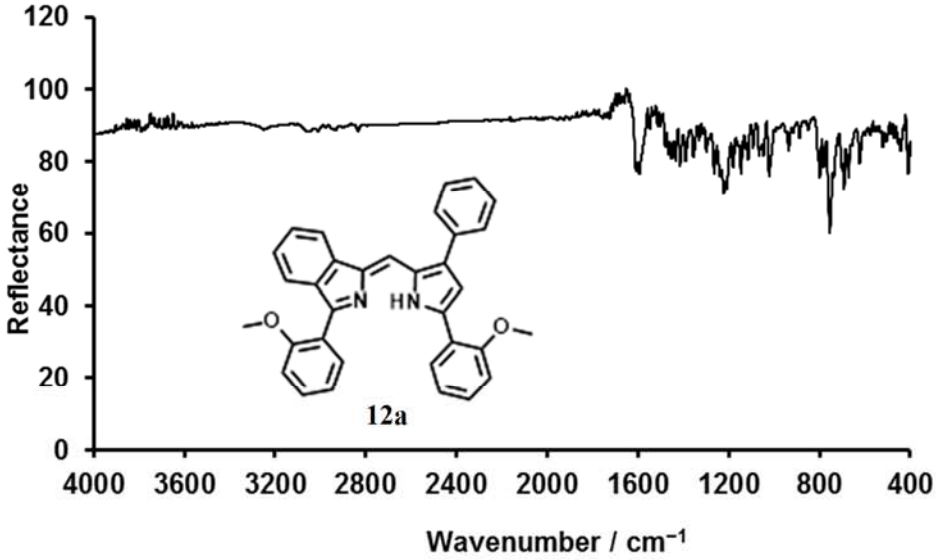


Fig. S56 ATR-FT-IR spectrum of **12a**.

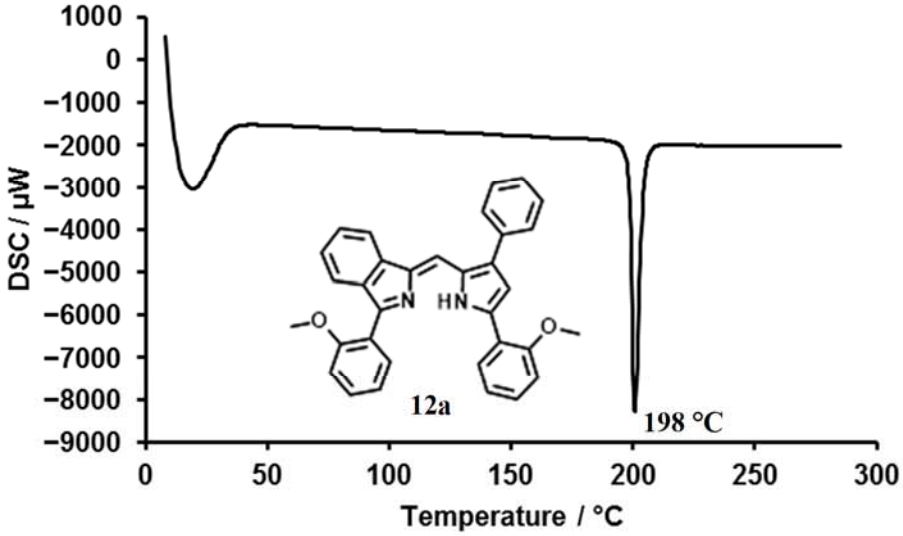


Fig. S57 DSC plots of **12a**.

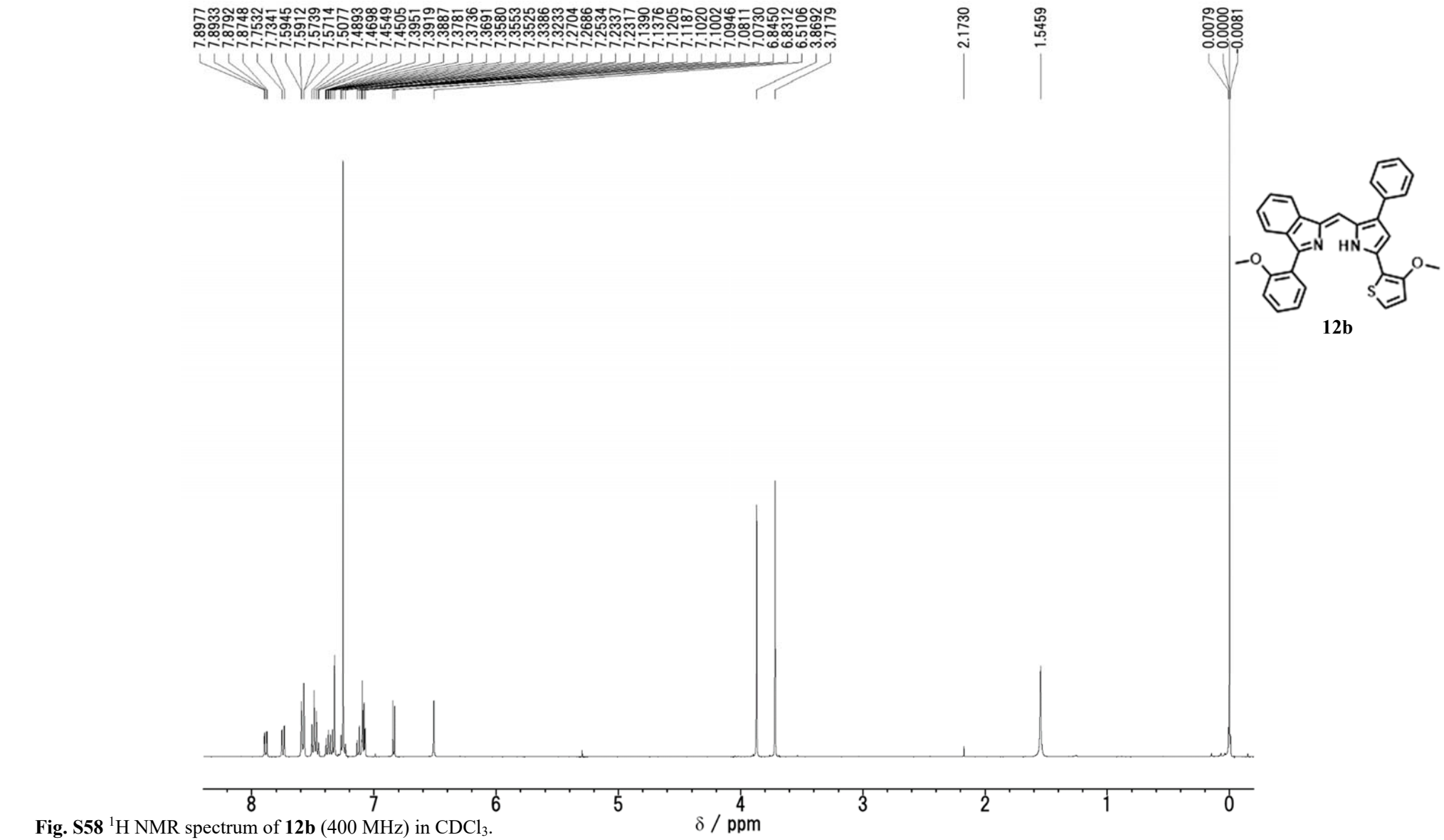
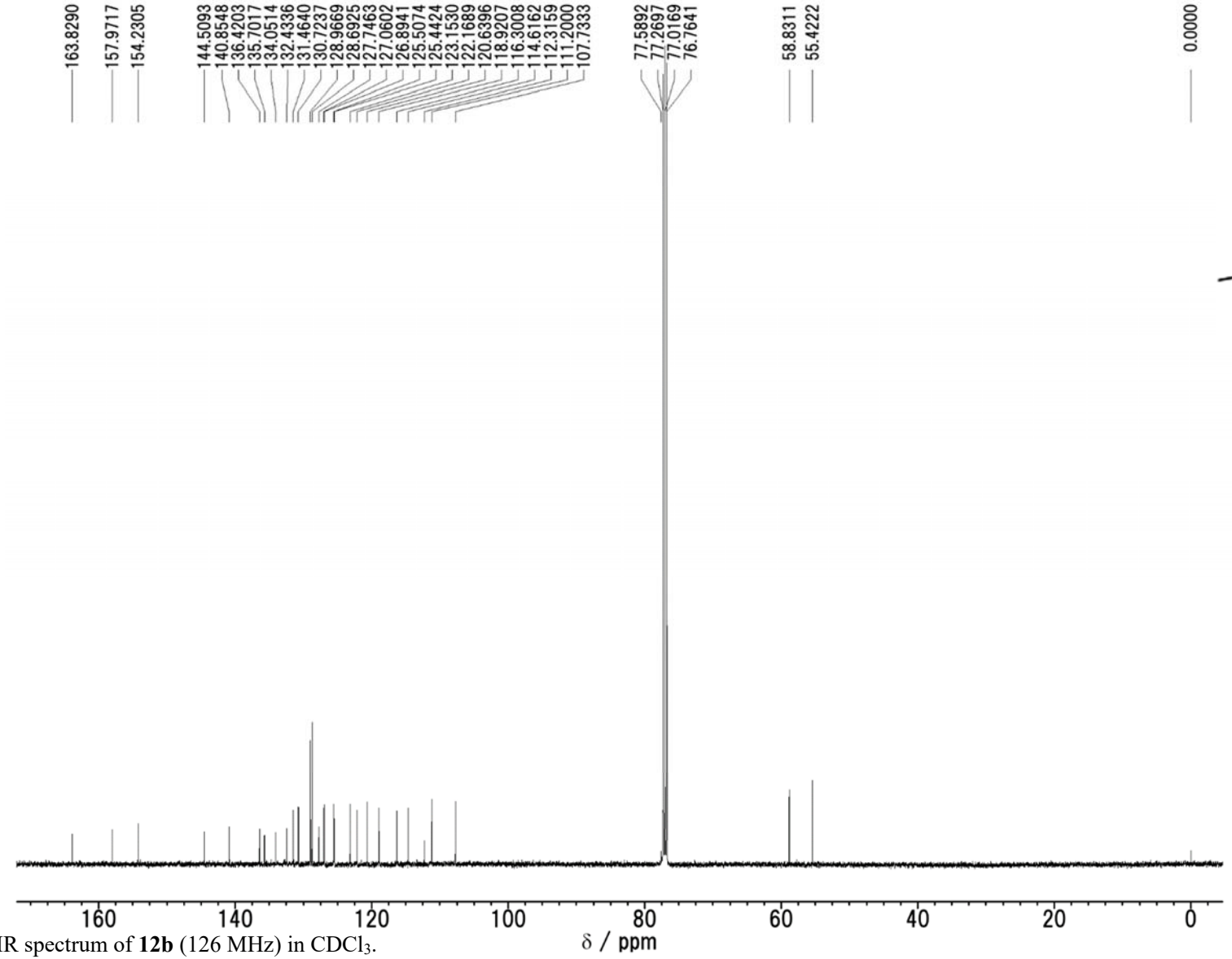
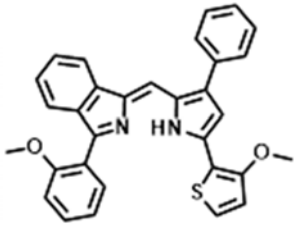


Fig. S58 ^{1}H NMR spectrum of **12b** (400 MHz) in $CDCl_3$.





12b

Fig. S59 ^{13}C NMR spectrum of **12b** (126 MHz) in $CDCl_3$.

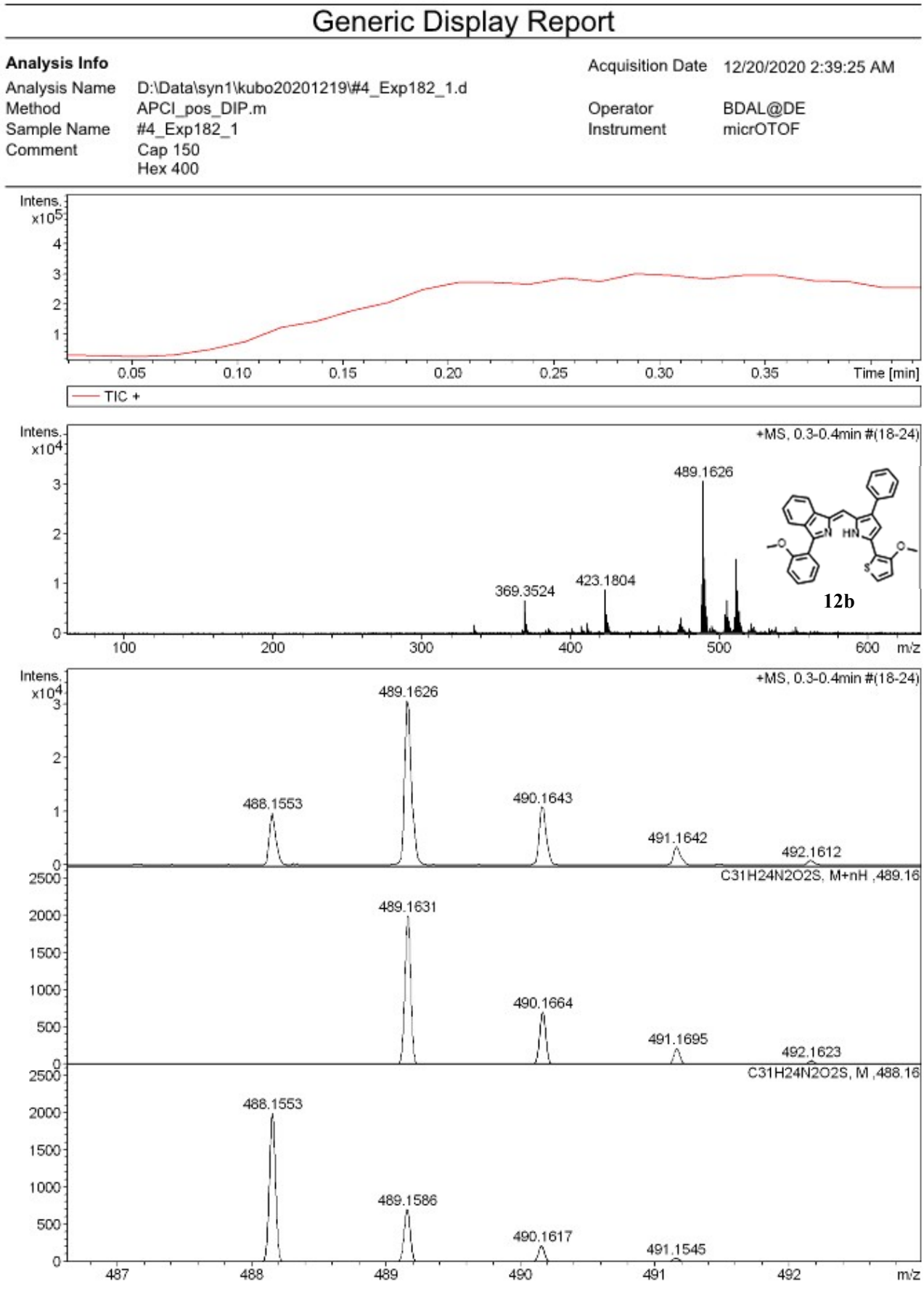


Fig. S60 High resolution of APCI mass spectrum (positive mode) of **12b**.

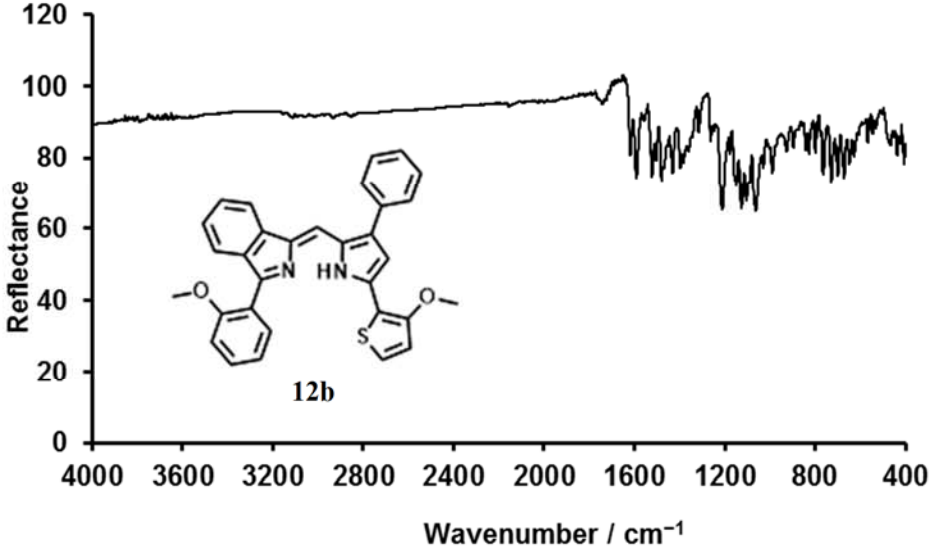


Fig. S61 ATR-FT-IR spectrum of **12b**.

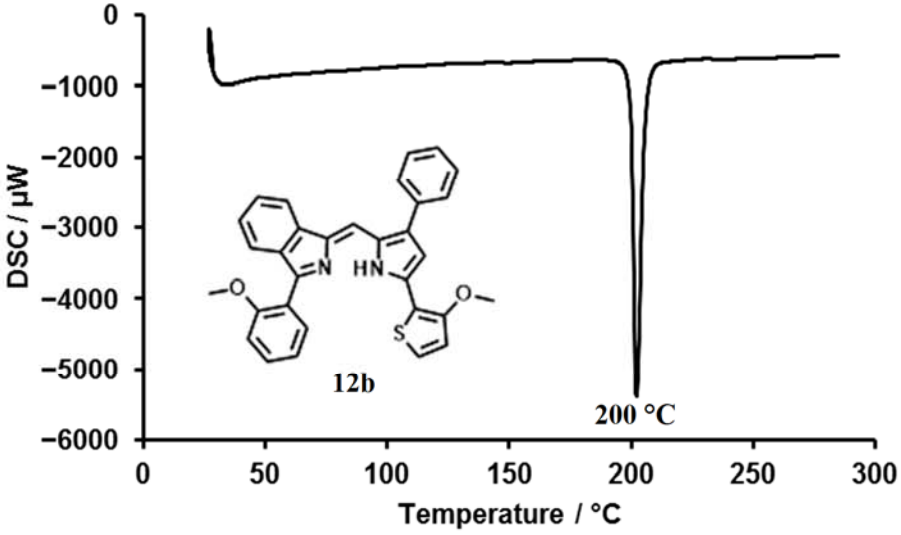


Fig. S62 DSC plots of **12b**.

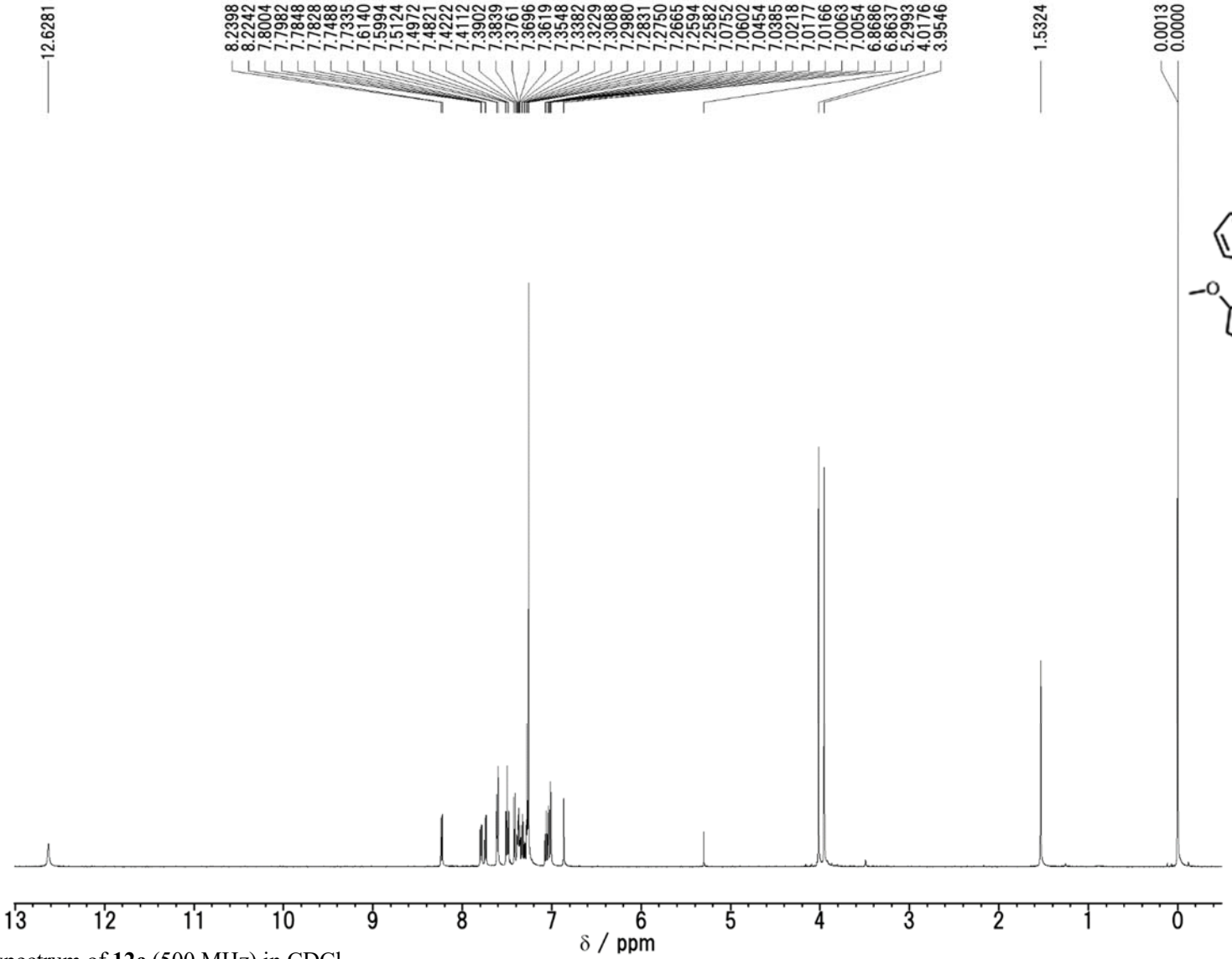


Fig. S63 ^{1}H NMR spectrum of **12c** (500 MHz) in $CDCl_3$.

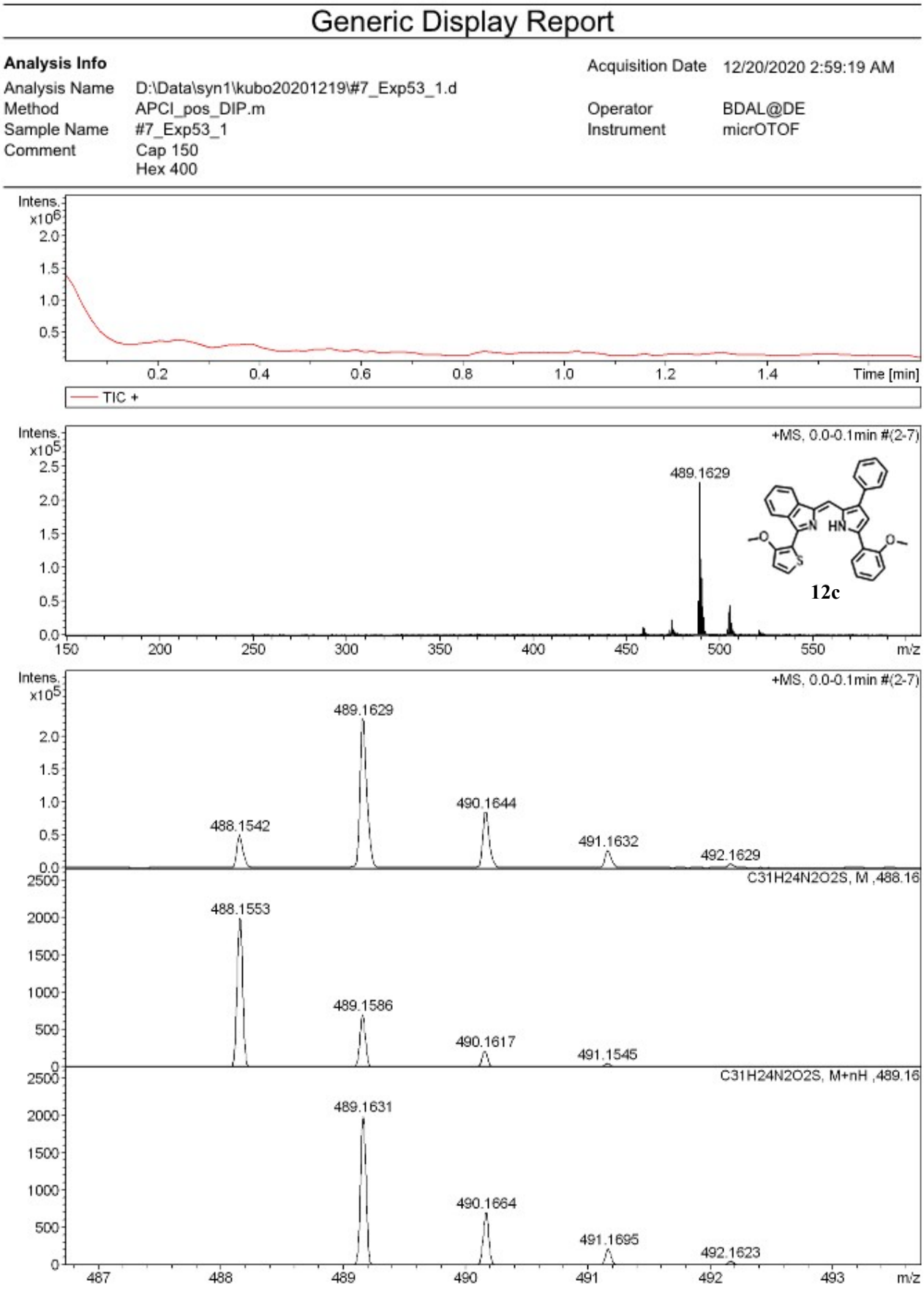


Fig. S64 High resolution of APCI mass spectrum (positive mode) of **12c**.

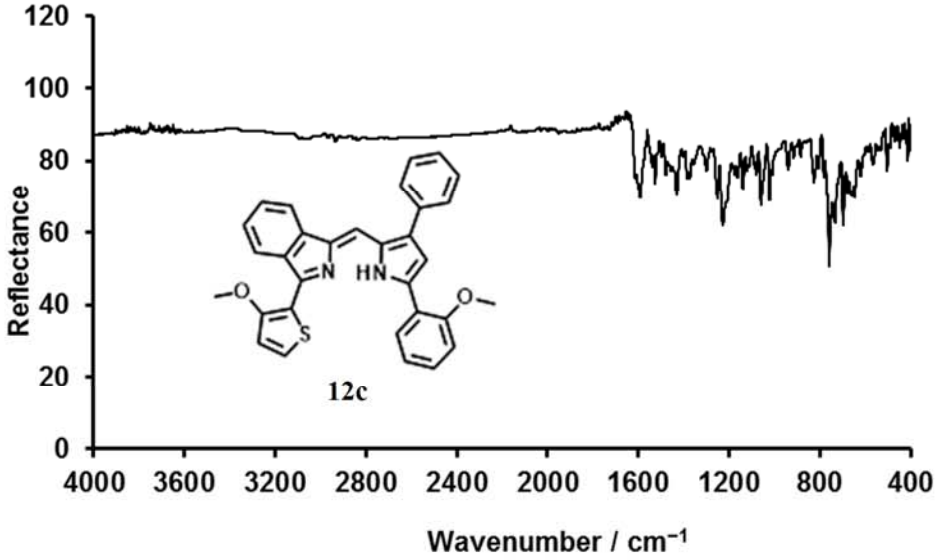


Fig. S65 ATR-FT-IR spectrum of **12c**.

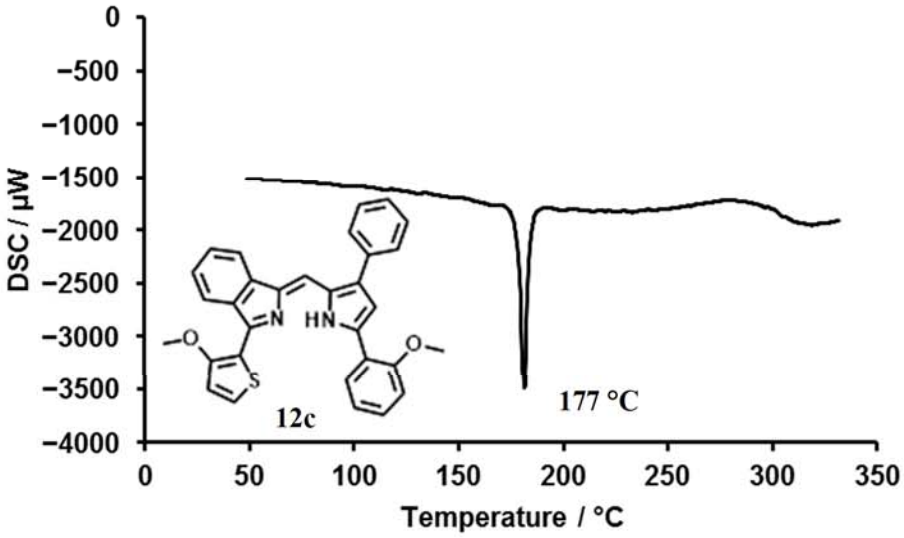
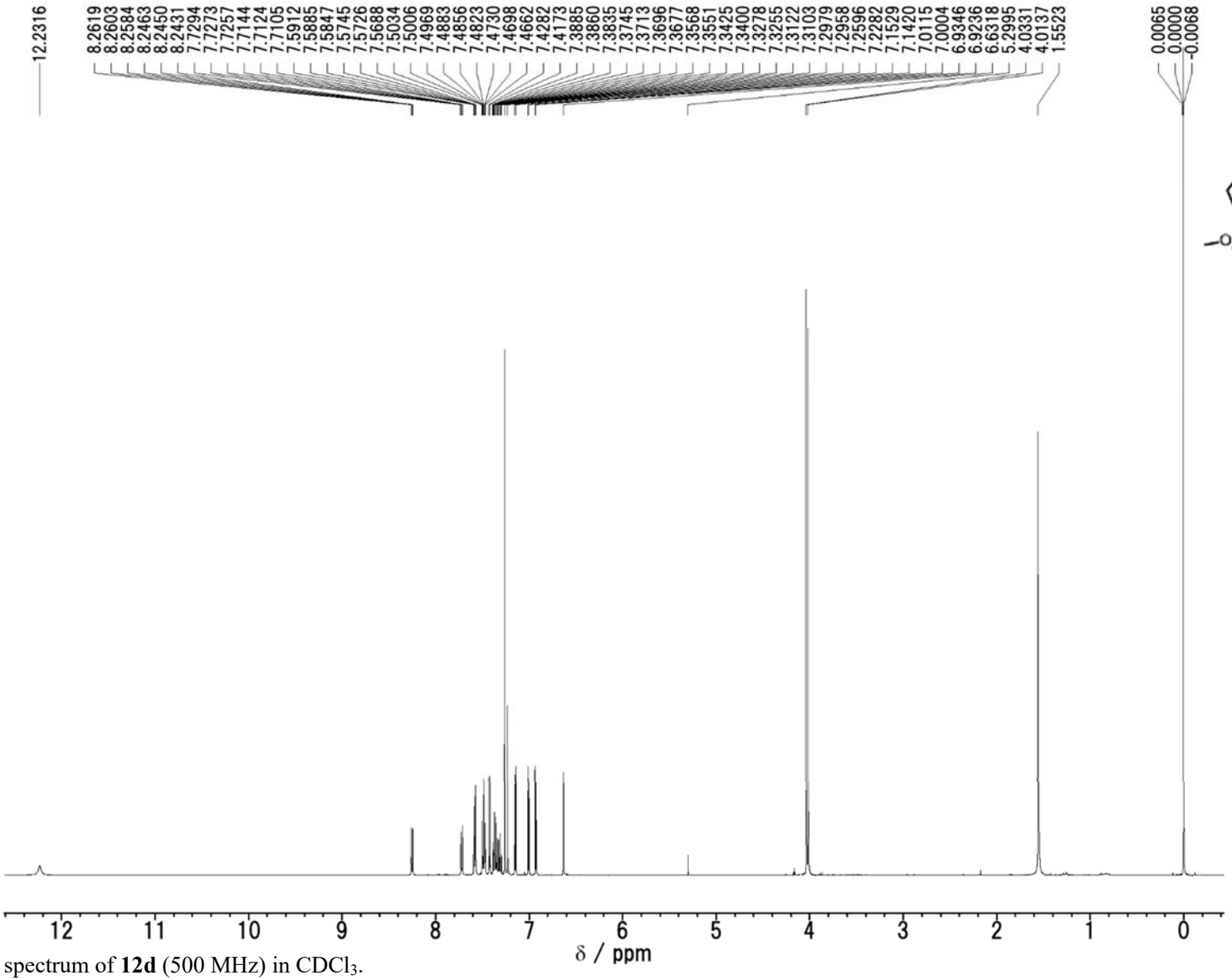
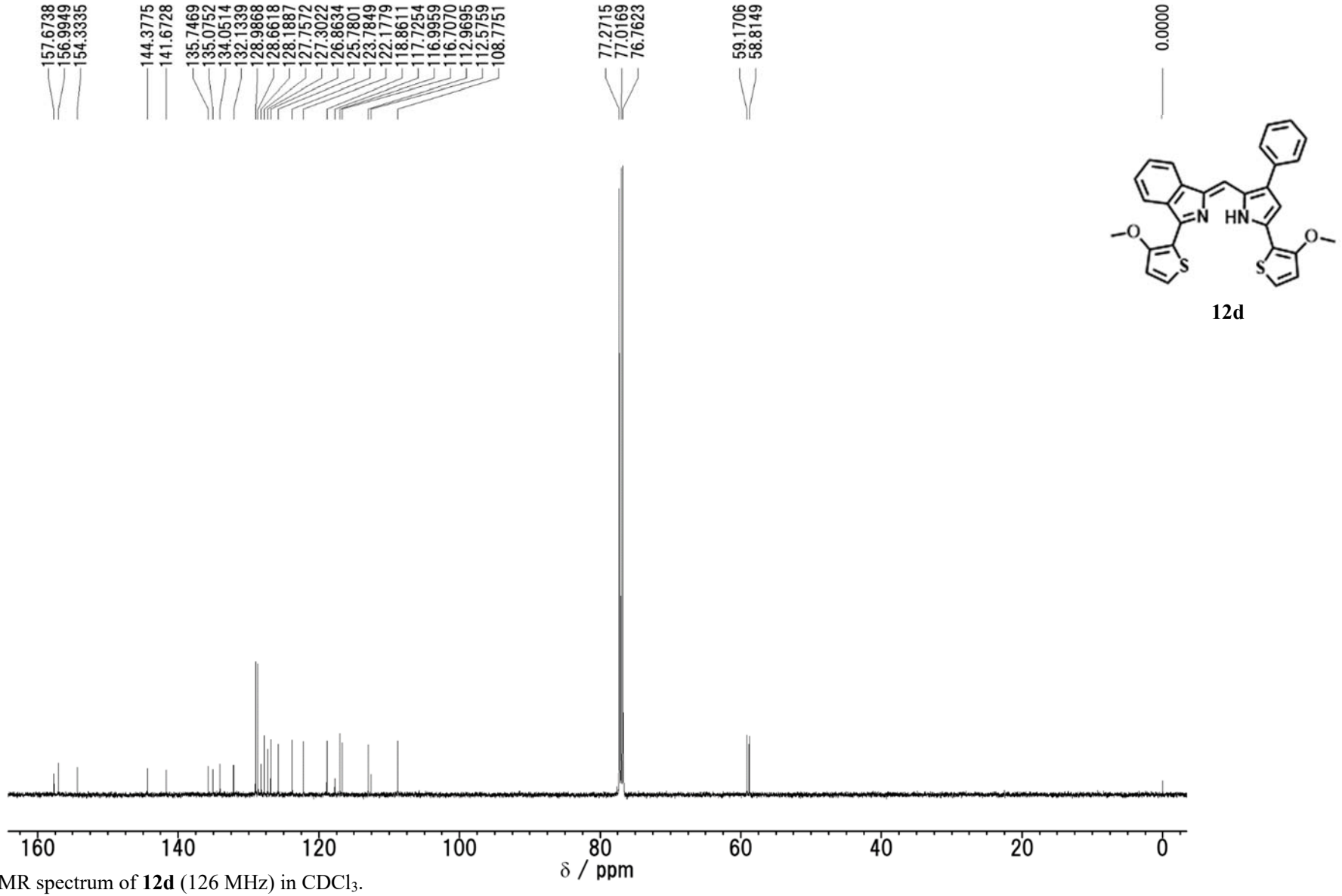


Fig. S66 *DSC* plots of **12c**.



12d

Fig. S67 ^{1}H NMR spectrum of **12d** (500 MHz) in $CDCl_3$.



12d

Fig. S68 ^{13}C NMR spectrum of **12d** (126 MHz) in $CDCl_3$.

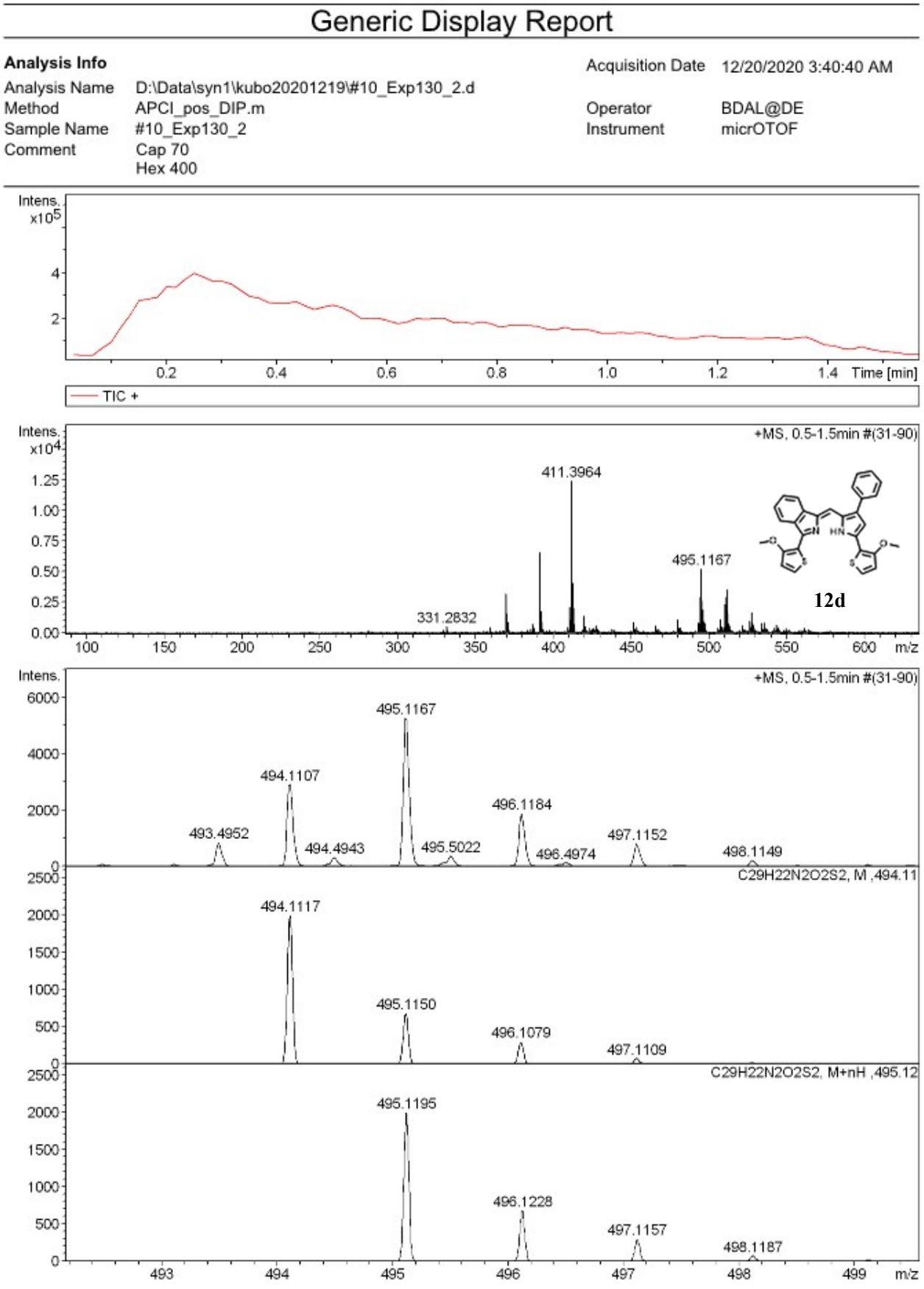


Fig. S69 High resolution of APCI mass spectrum (positive mode) of **12d**.

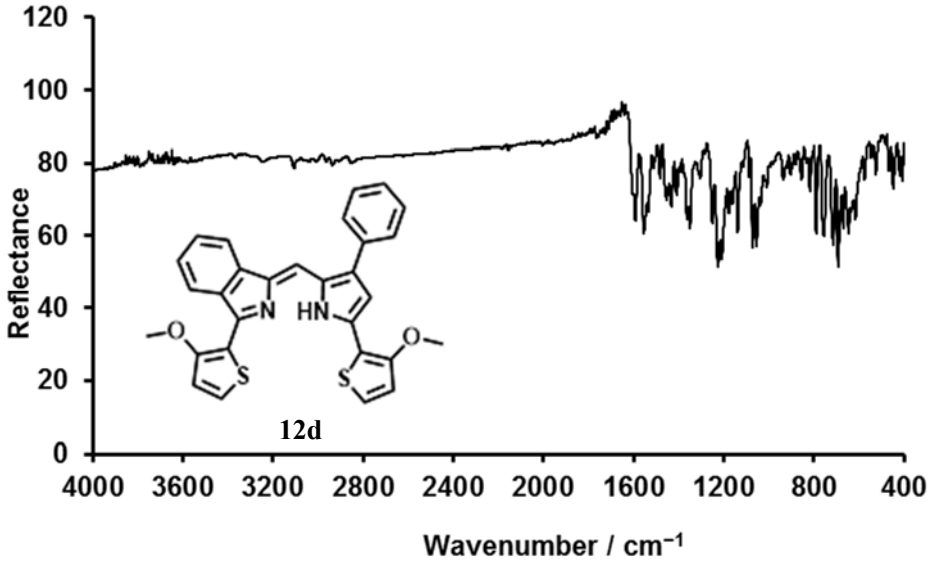


Fig. S70 ATR-FT-IR spectrum of **12d**.

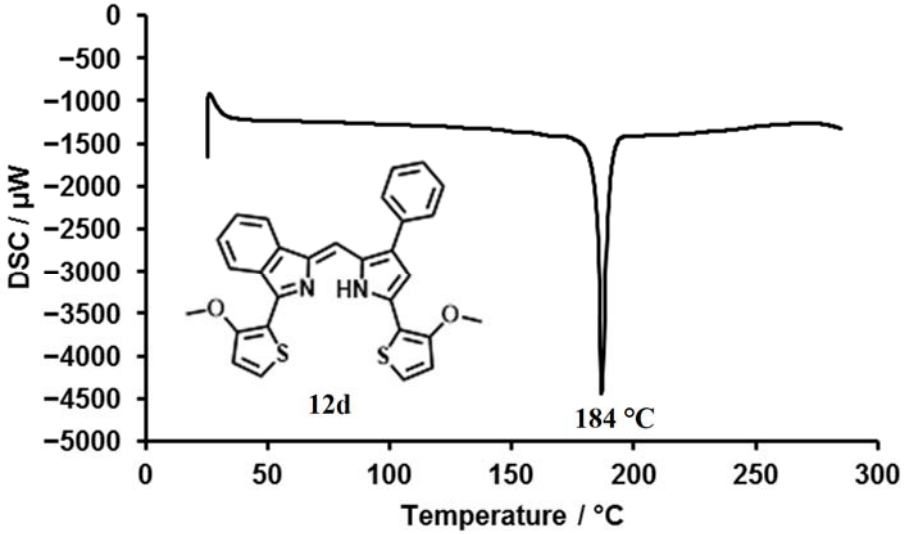
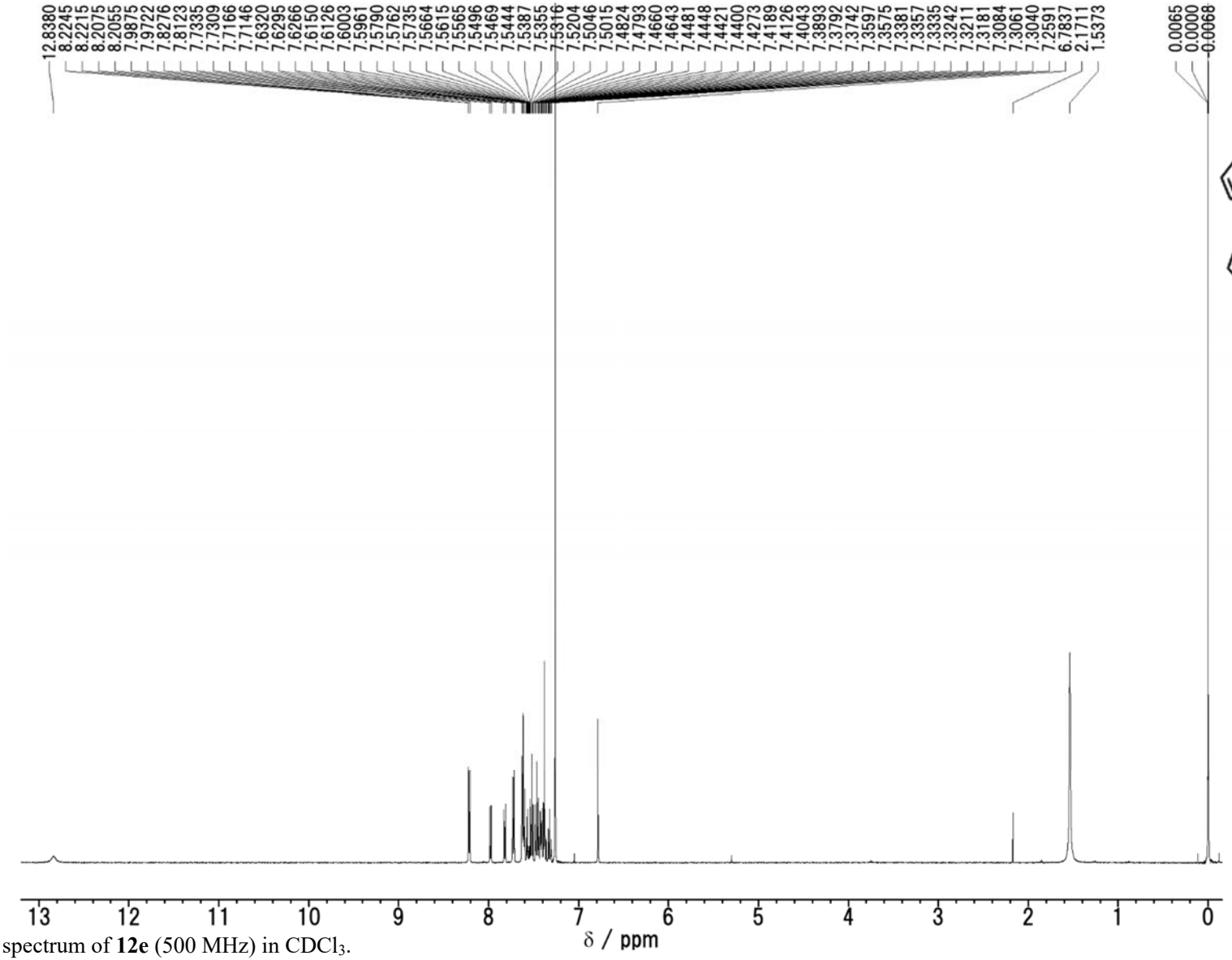
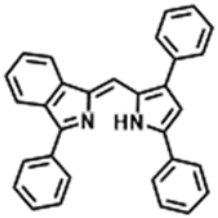


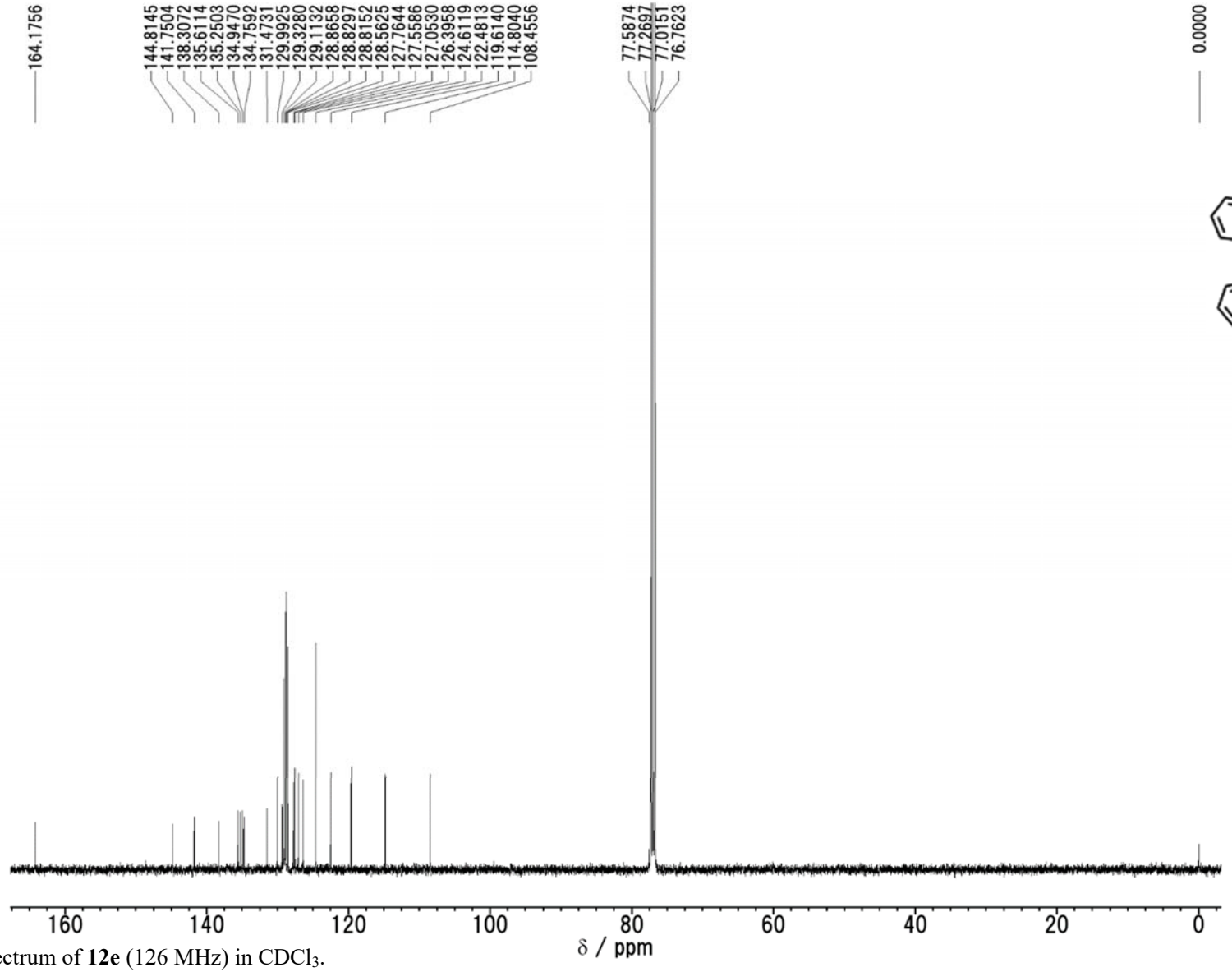
Fig. S71 DSC plots of **12d**.





12e

Fig. S72 ^{1}H NMR spectrum of **12e** (500 MHz) in $CDCl_3$.



12e

Fig. S73 ^{13}C NMR spectrum of **12e** (126 MHz) in $CDCl_3$.

Generic Display Report

Analysis Info

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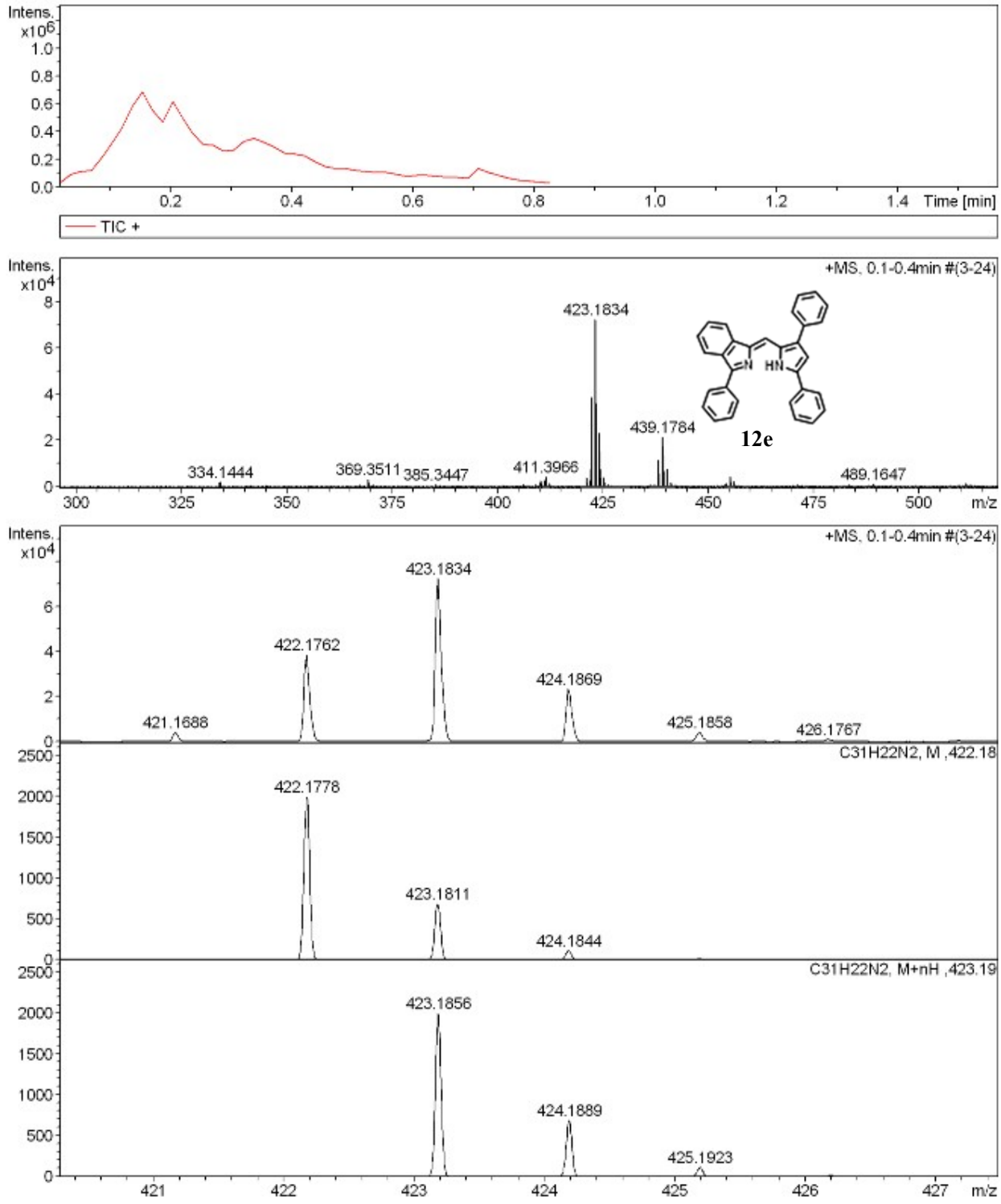


Bruker Compass DataAnalysis 4.0 printed: 12/19/2020 7:07:41 PM Page 1 of 1

Fig. S74 High resolution of APCI mass spectrum (positive mode) of **12e**.

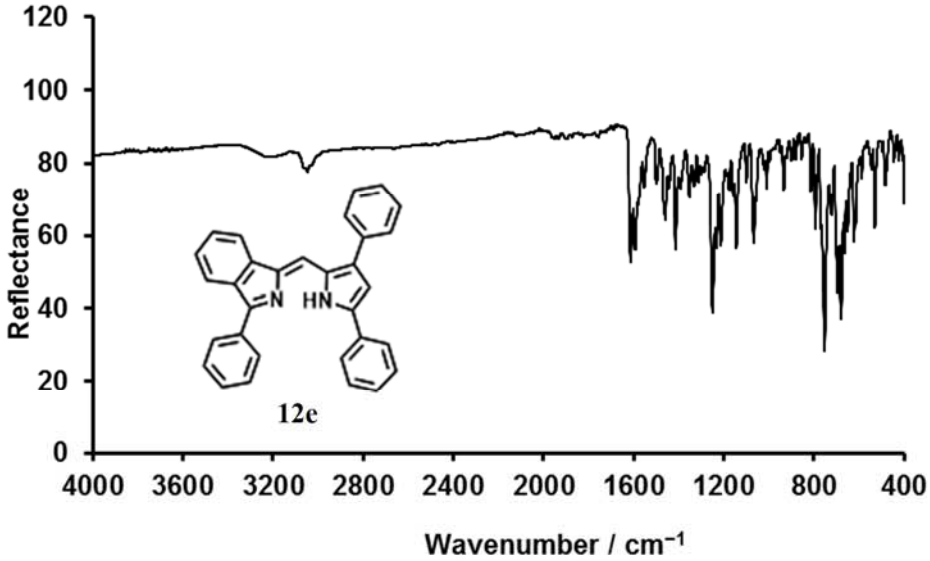


Fig. S75 ATR-FT-IR spectrum of **12e**.

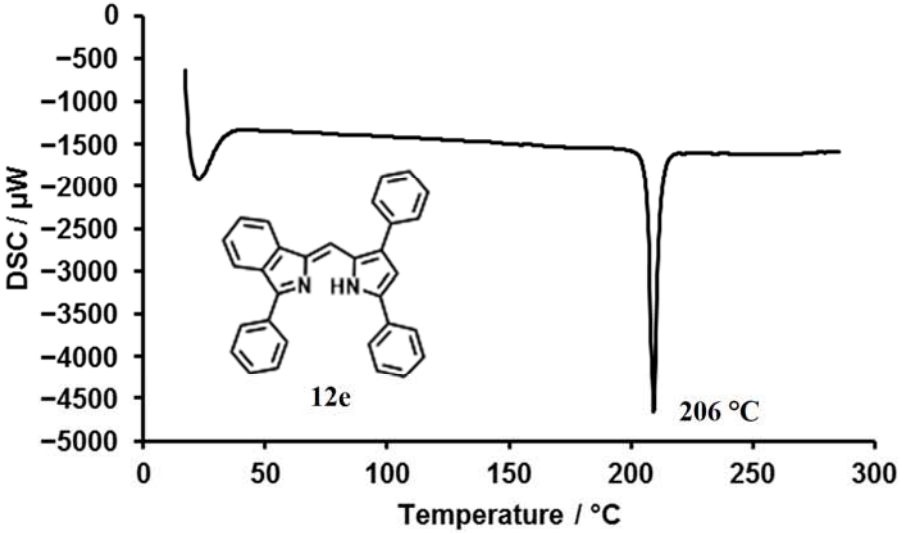
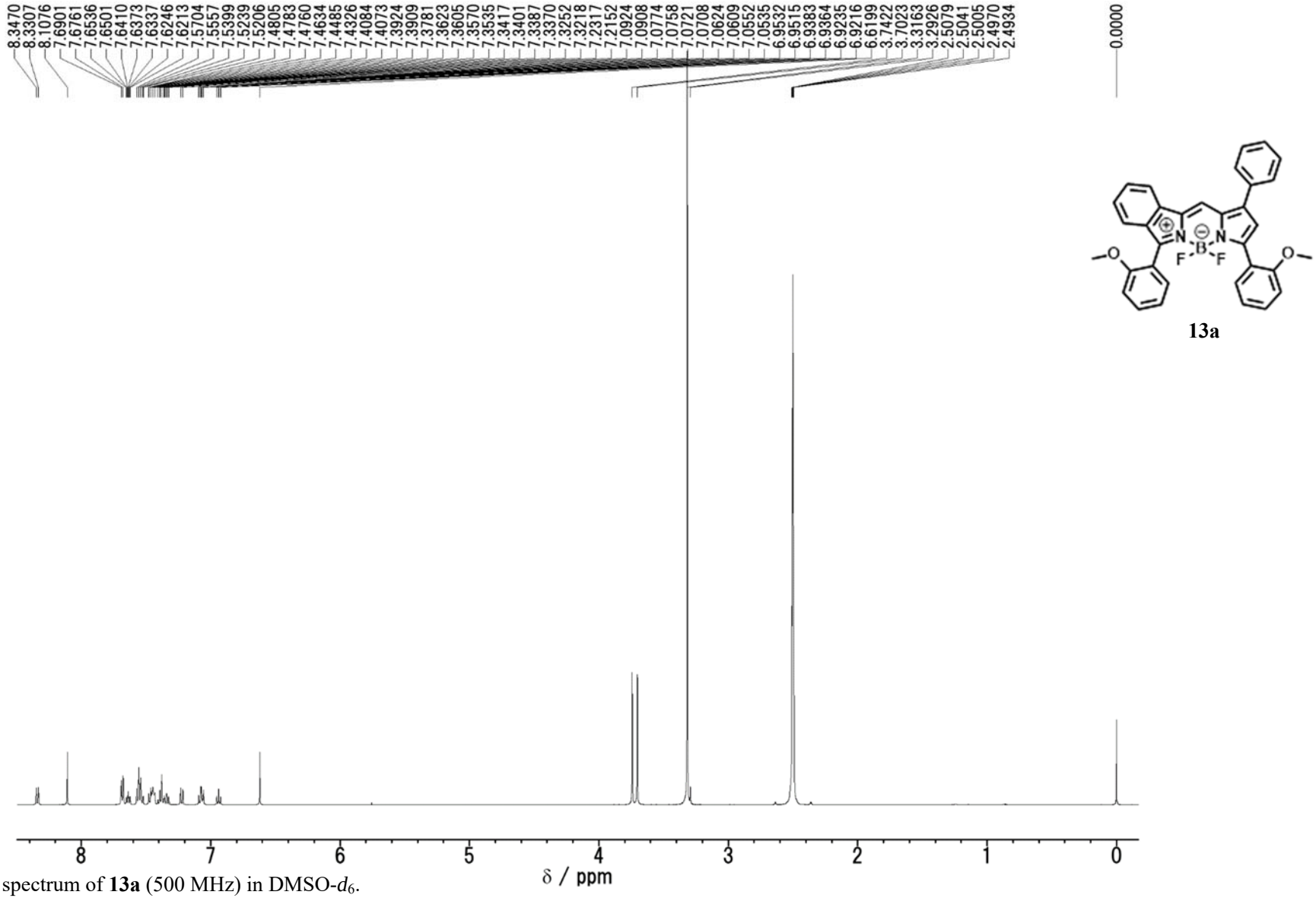
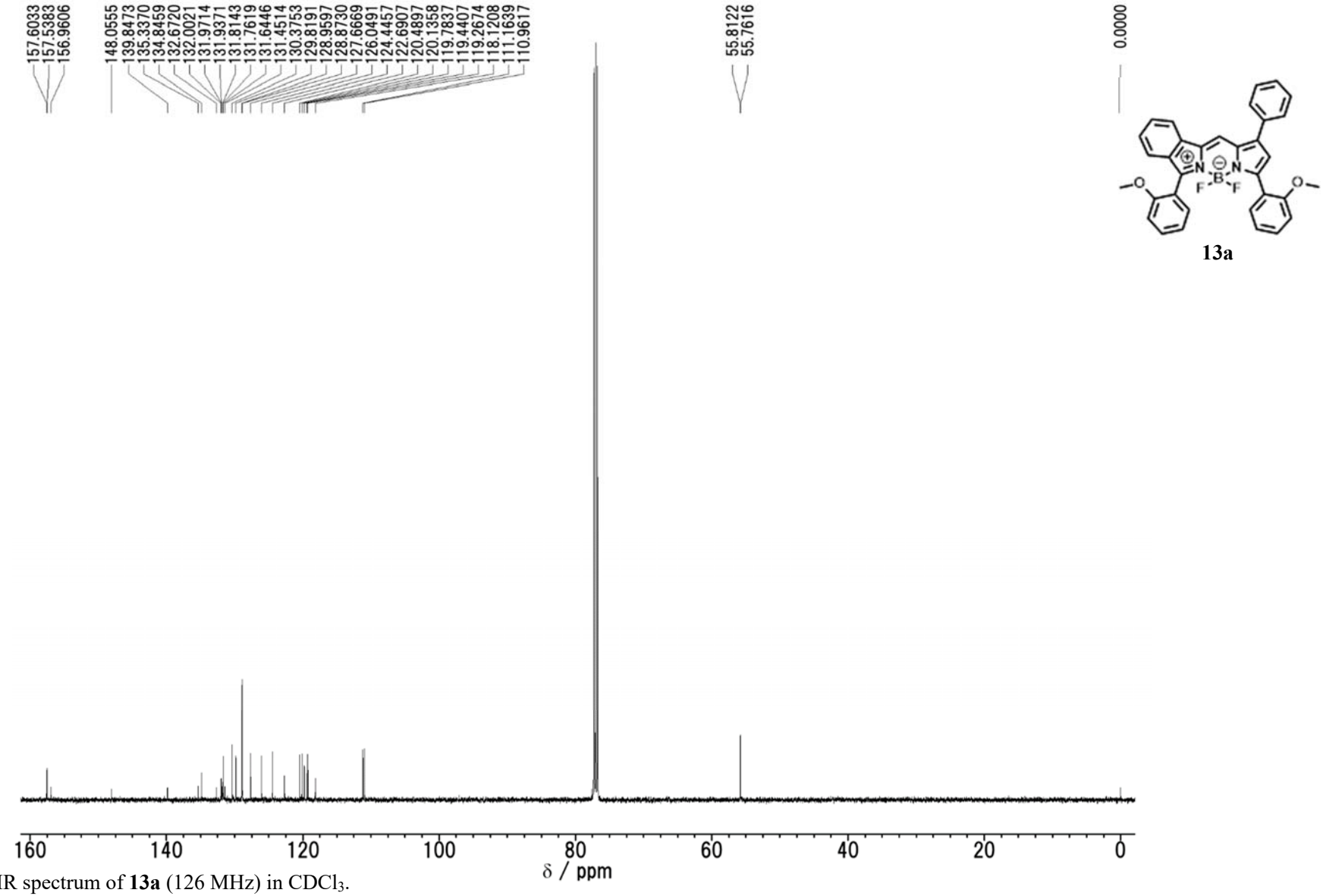


Fig. S76 *DSC plots of* **12e**.



13a

Fig. S77 ^{1}H NMR spectrum of **13a** (500 MHz) in DMSO-d_6.



13a

Fig. S78 ^{13}C NMR spectrum of **13a** (126 MHz) in $CDCl_3$.

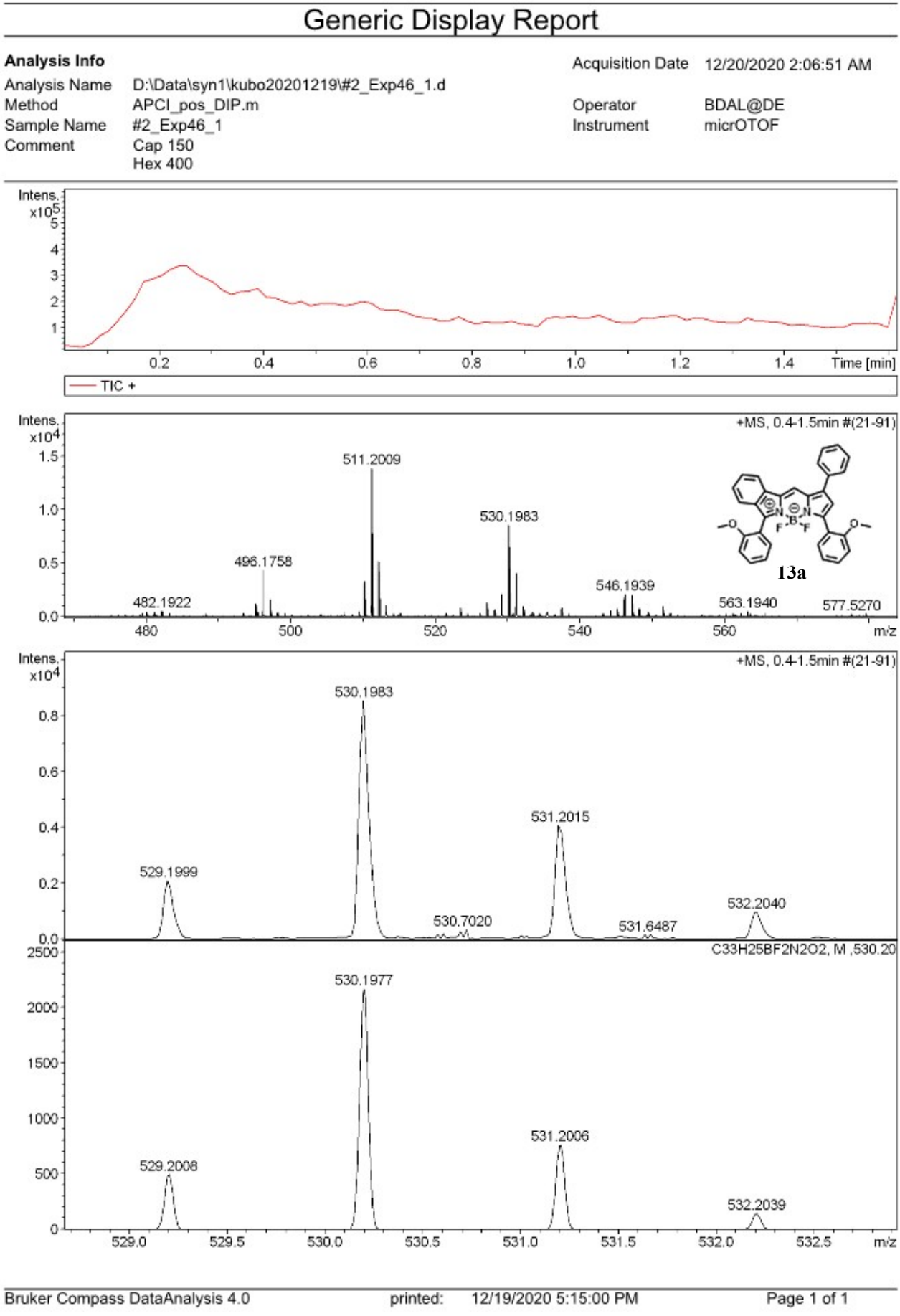


Fig. S79 High resolution of APCI mass spectrum (positive mode) of **13a**.

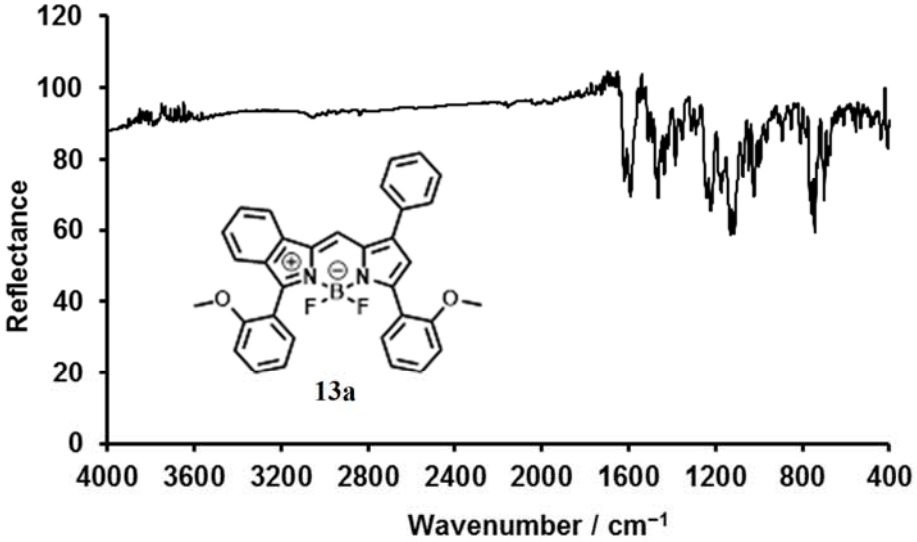


Fig. S80 ATR-FT-IR spectrum of **13a**.

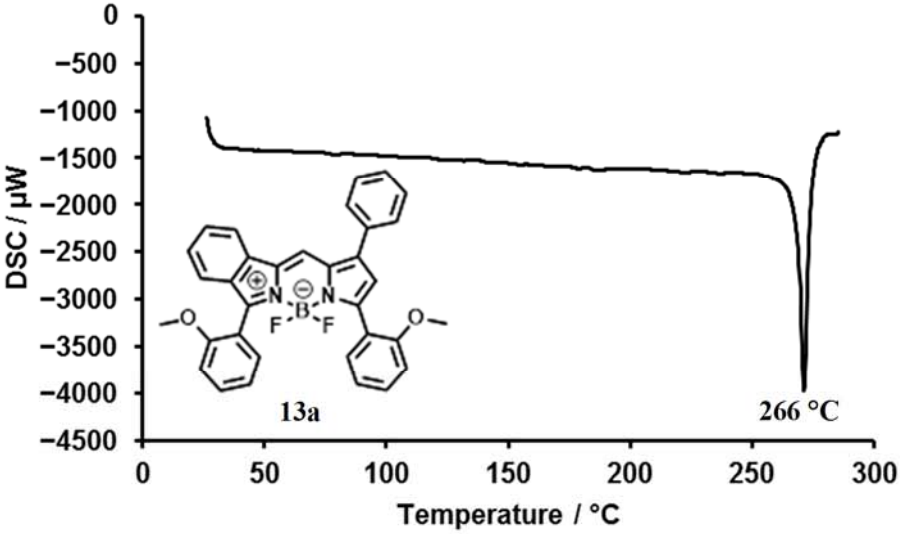
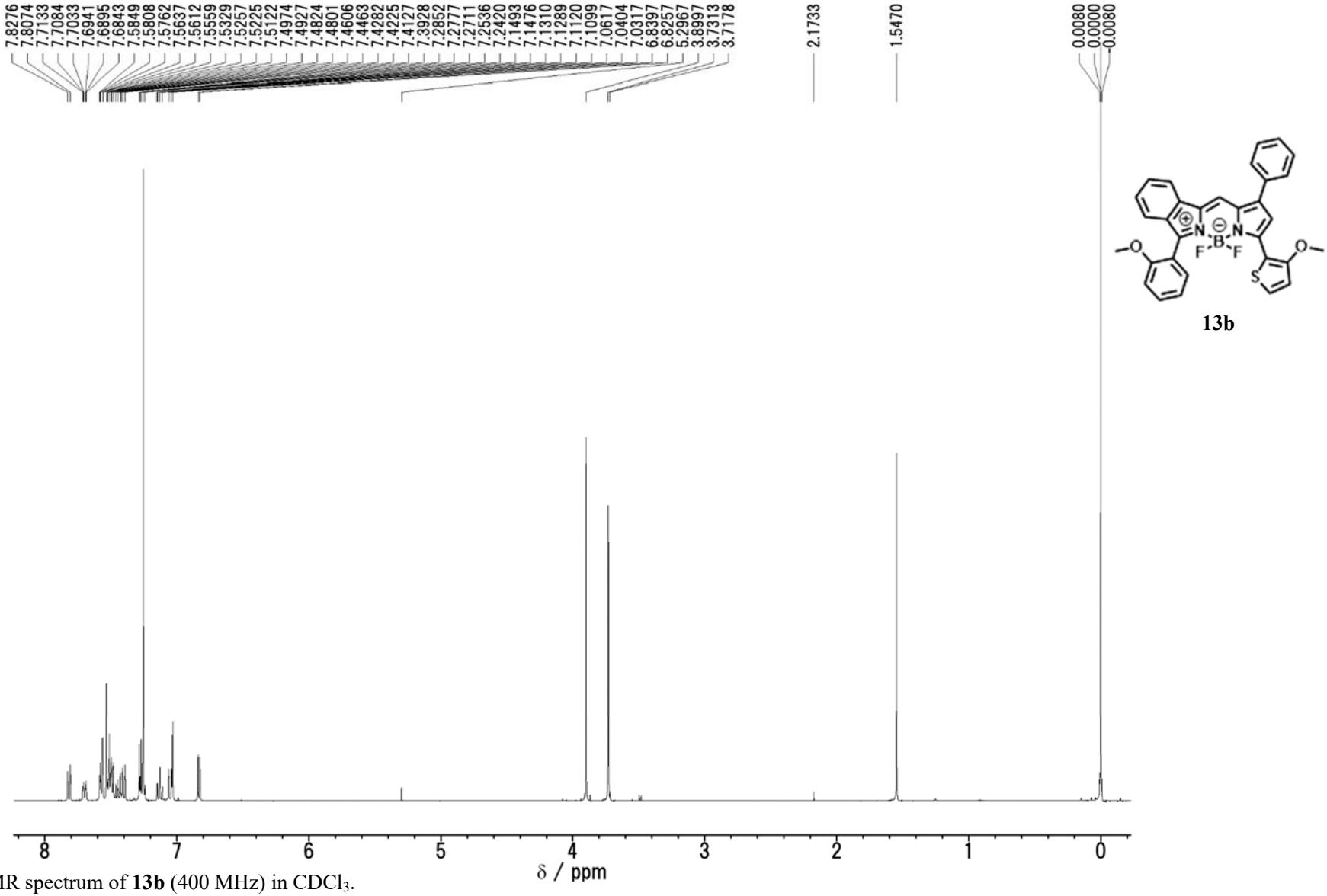
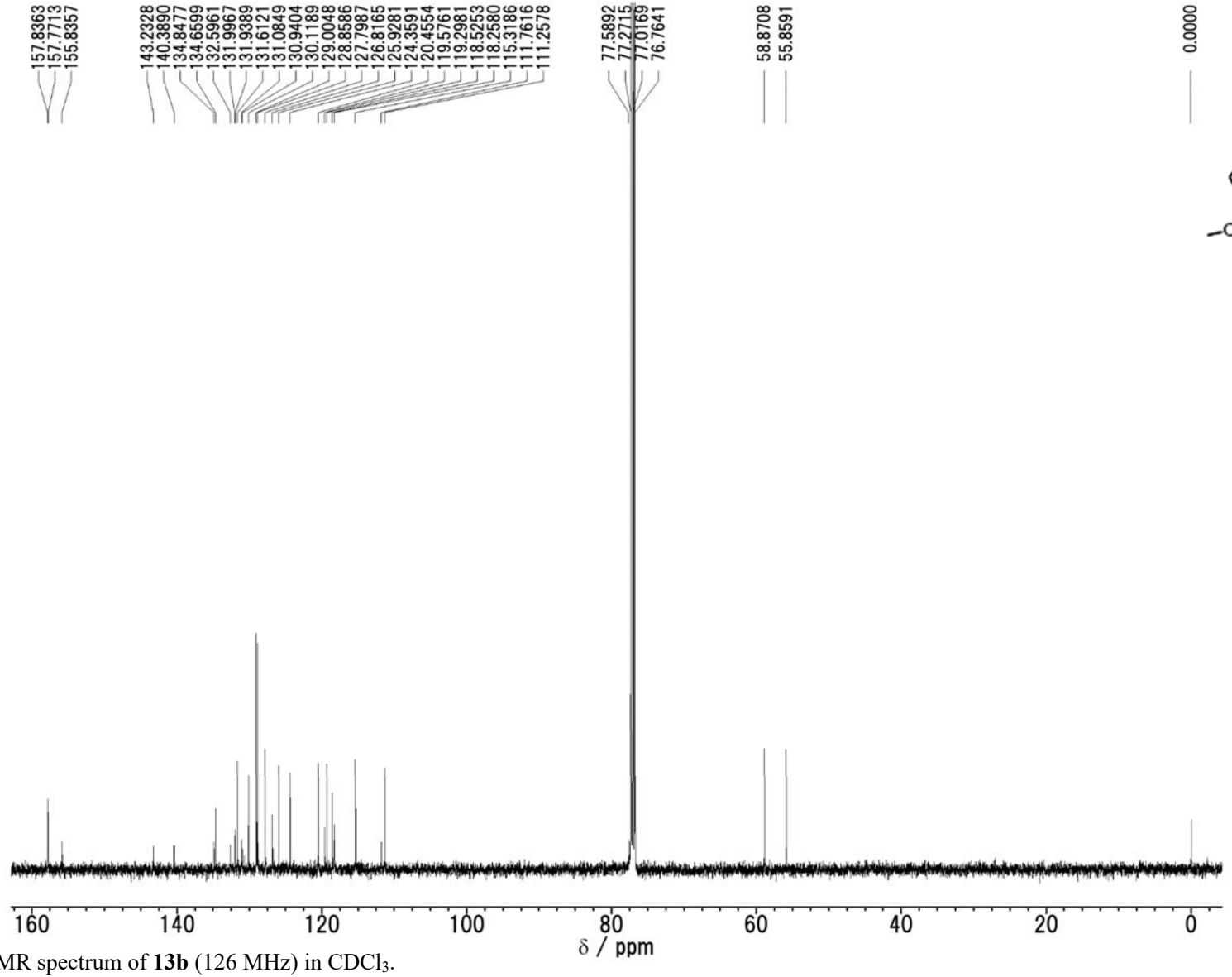


Fig. S81 DSC plots of **13a**.



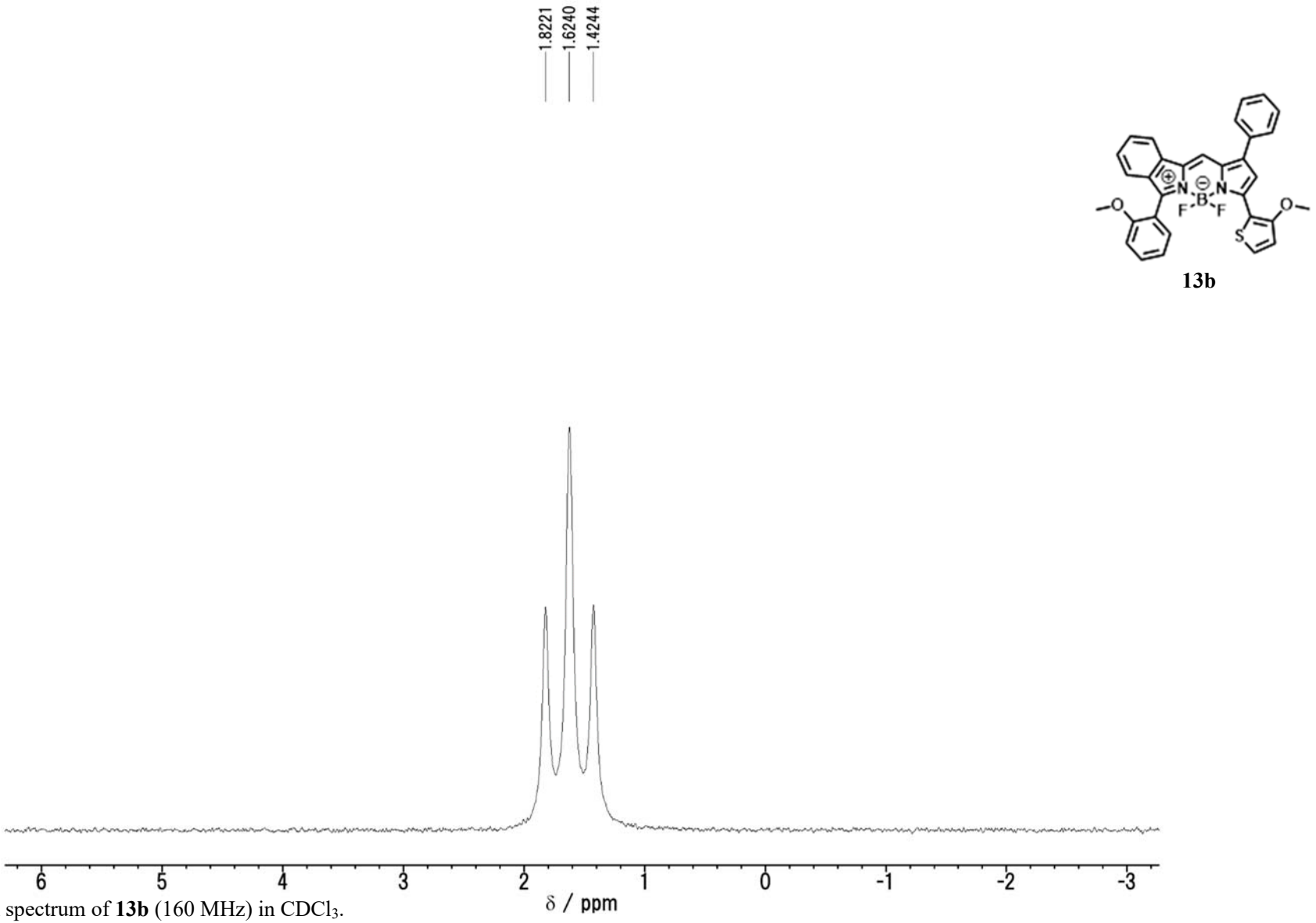
13b

Fig. S82 ^{1}H NMR spectrum of **13b** (400 MHz) in $CDCl_3$.



13b

Fig. S83 ^{13}C NMR spectrum of **13b** (126 MHz) in $CDCl_3$.



13b

Fig. S84 ^{11}B NMR spectrum of **13b** (160 MHz) in $CDCl_3$.

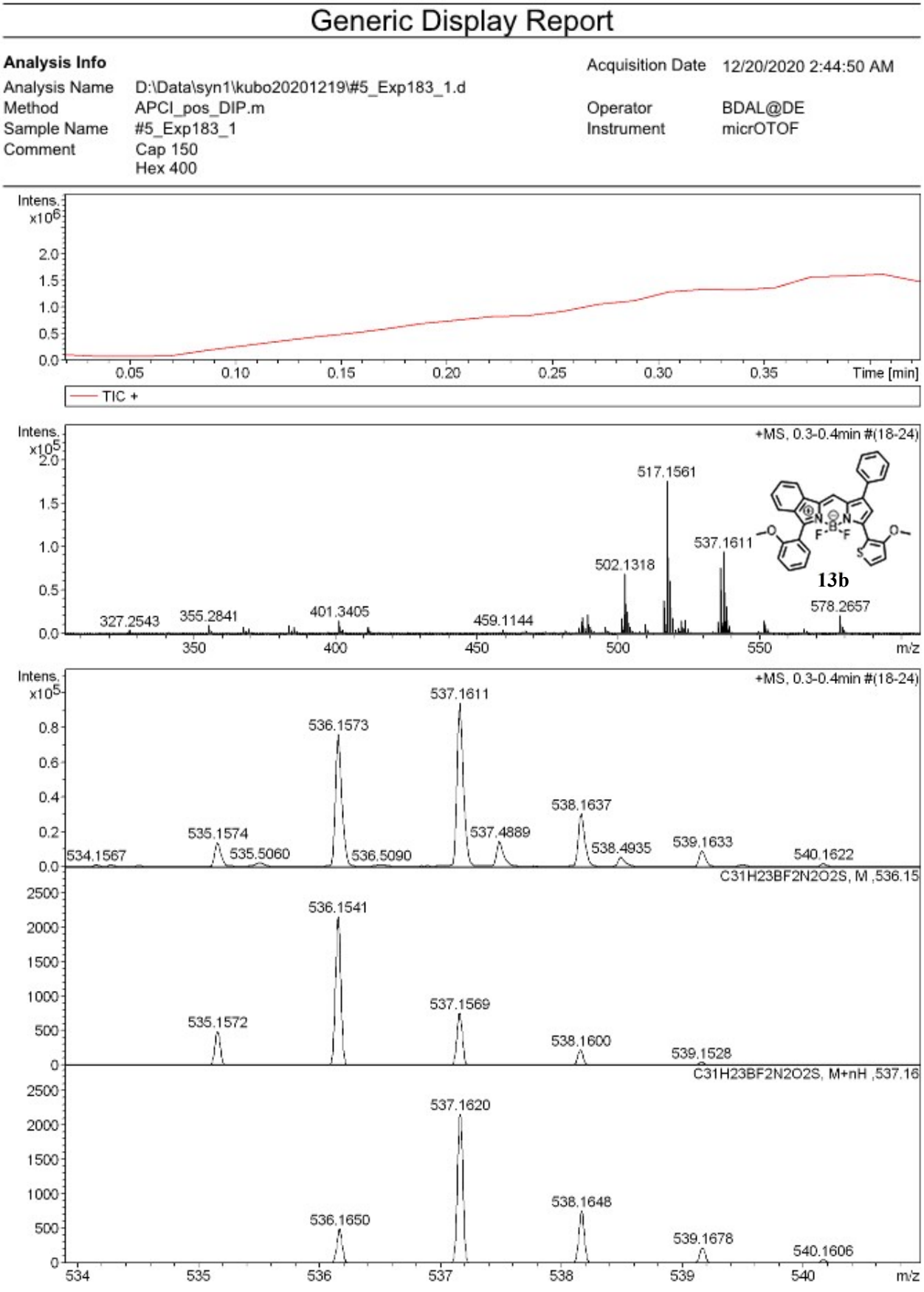


Fig. S85 High resolution of APCI mass spectrum (positive mode) of **13b**.

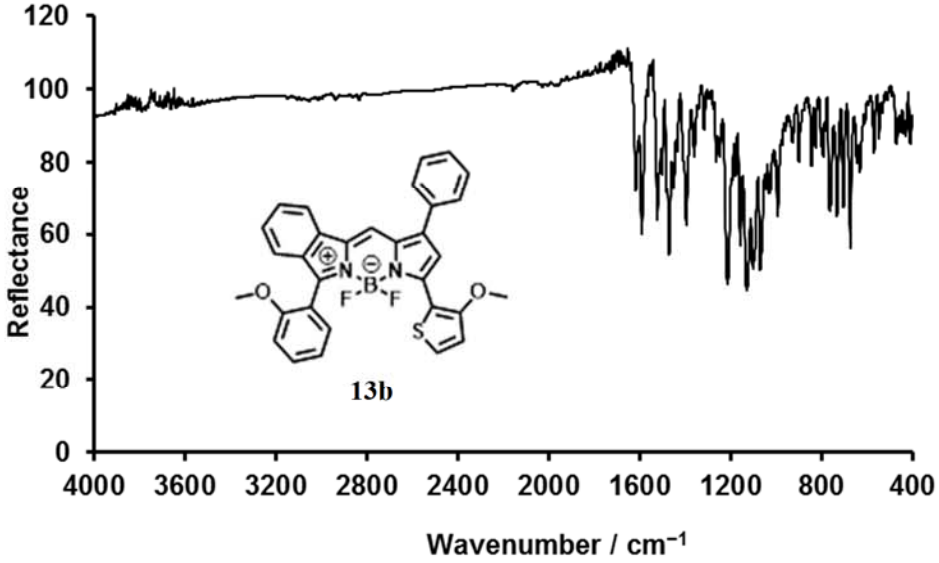


Fig. S86 ATR-FT-IR spectrum of **13b**.

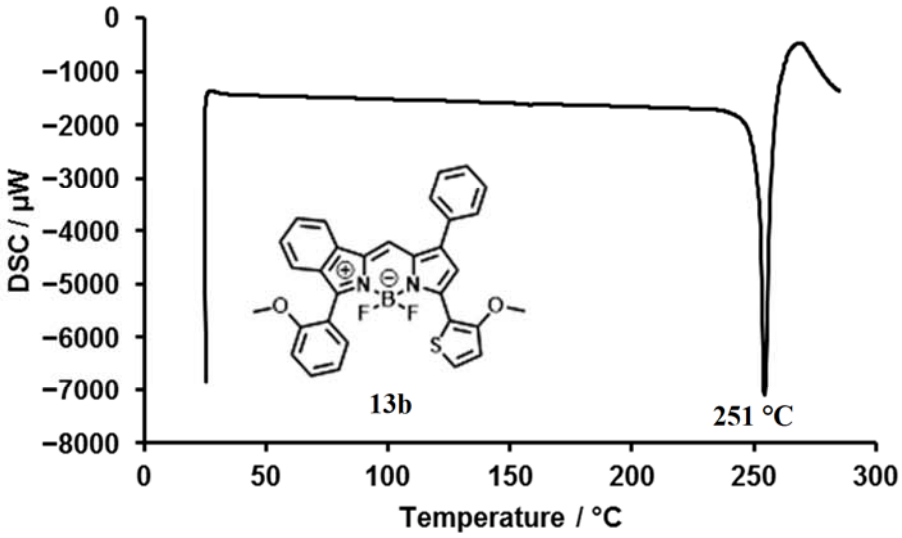
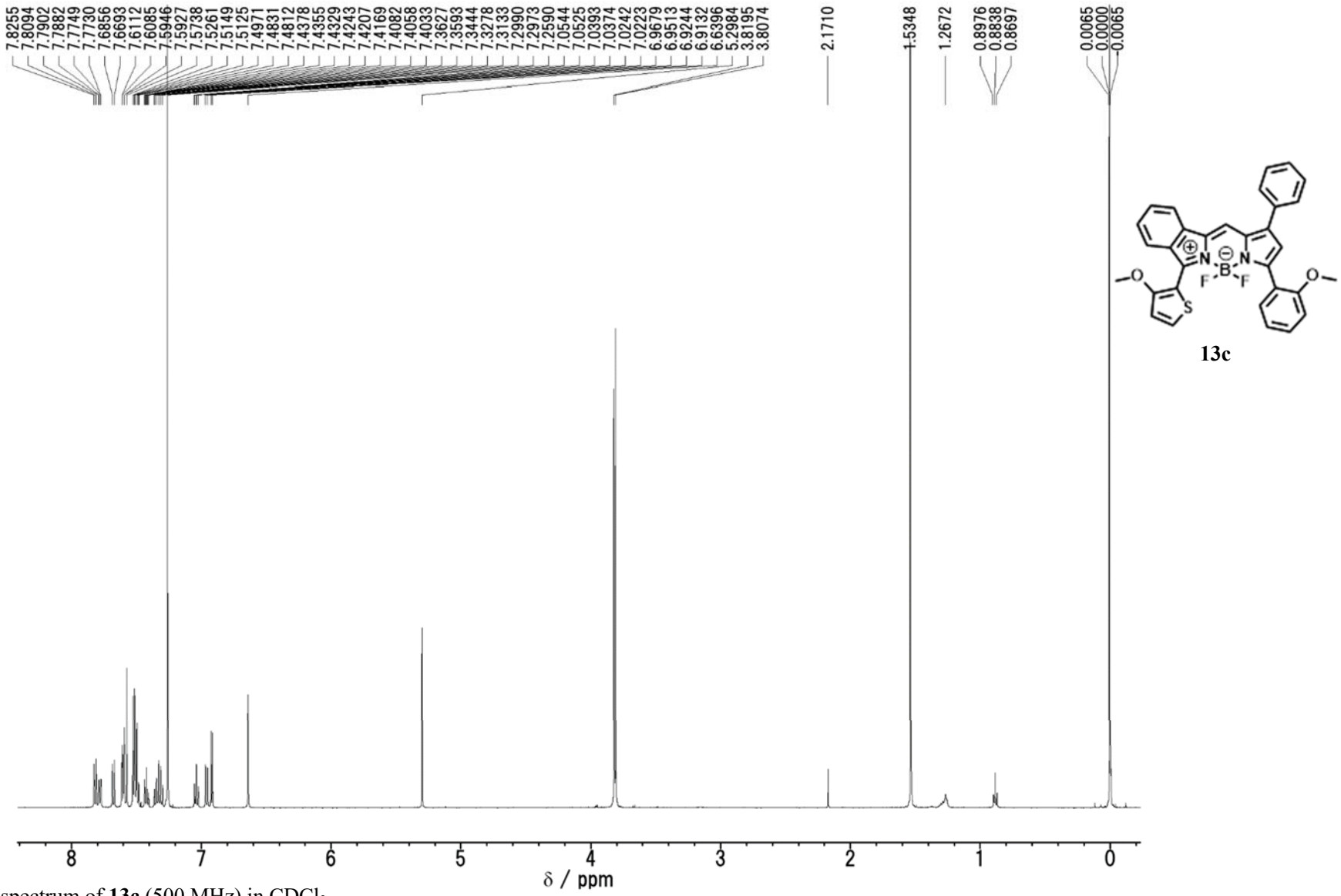
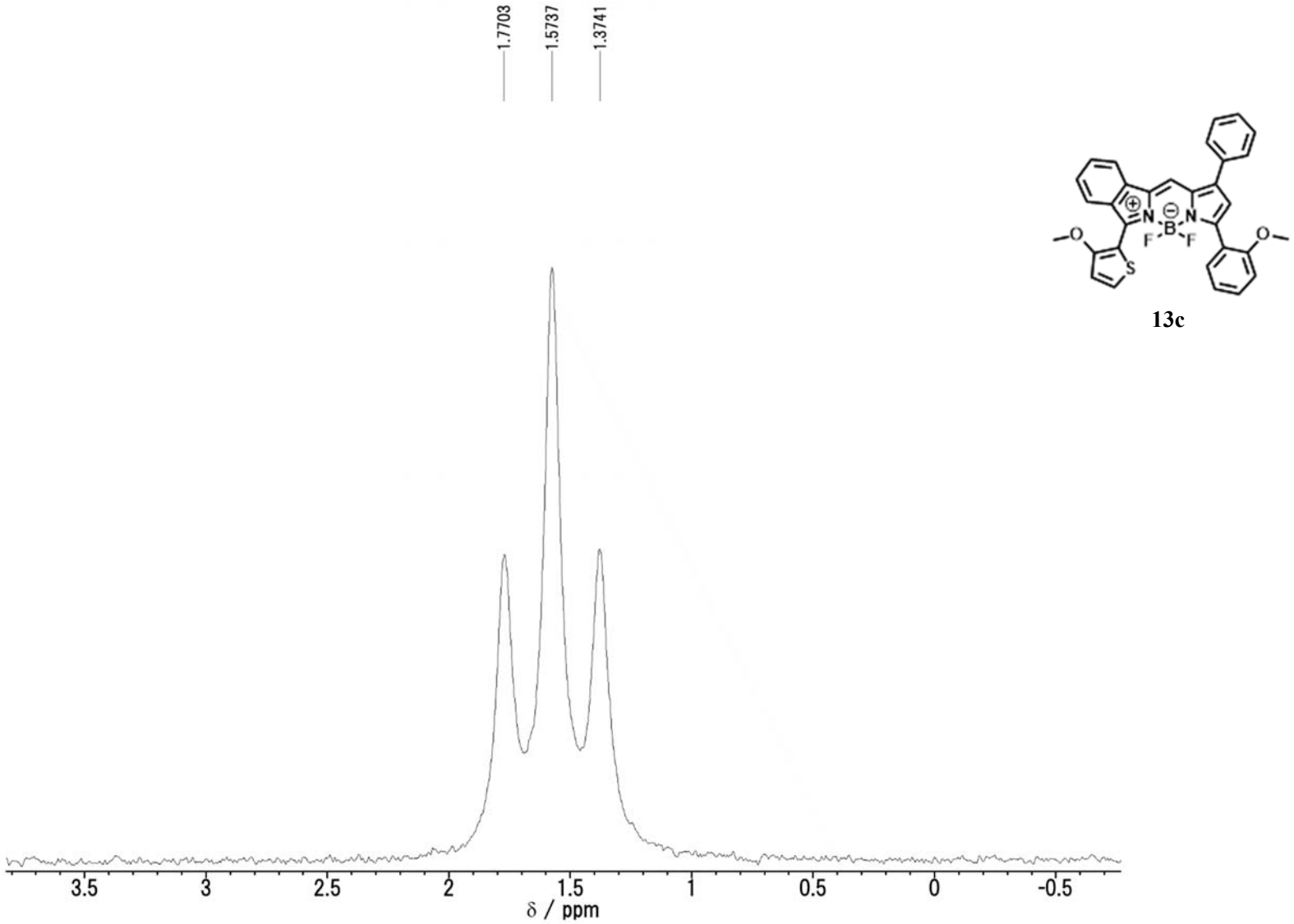


Fig. S87 DSC plots of **13b**.



13c

Fig. S88 ^{1}H NMR spectrum of **13c** (500 MHz) in $CDCl_3$.



13c

Fig. S89 ^{11}B NMR spectrum of **13c** (160 MHz) in $CDCl_3$.

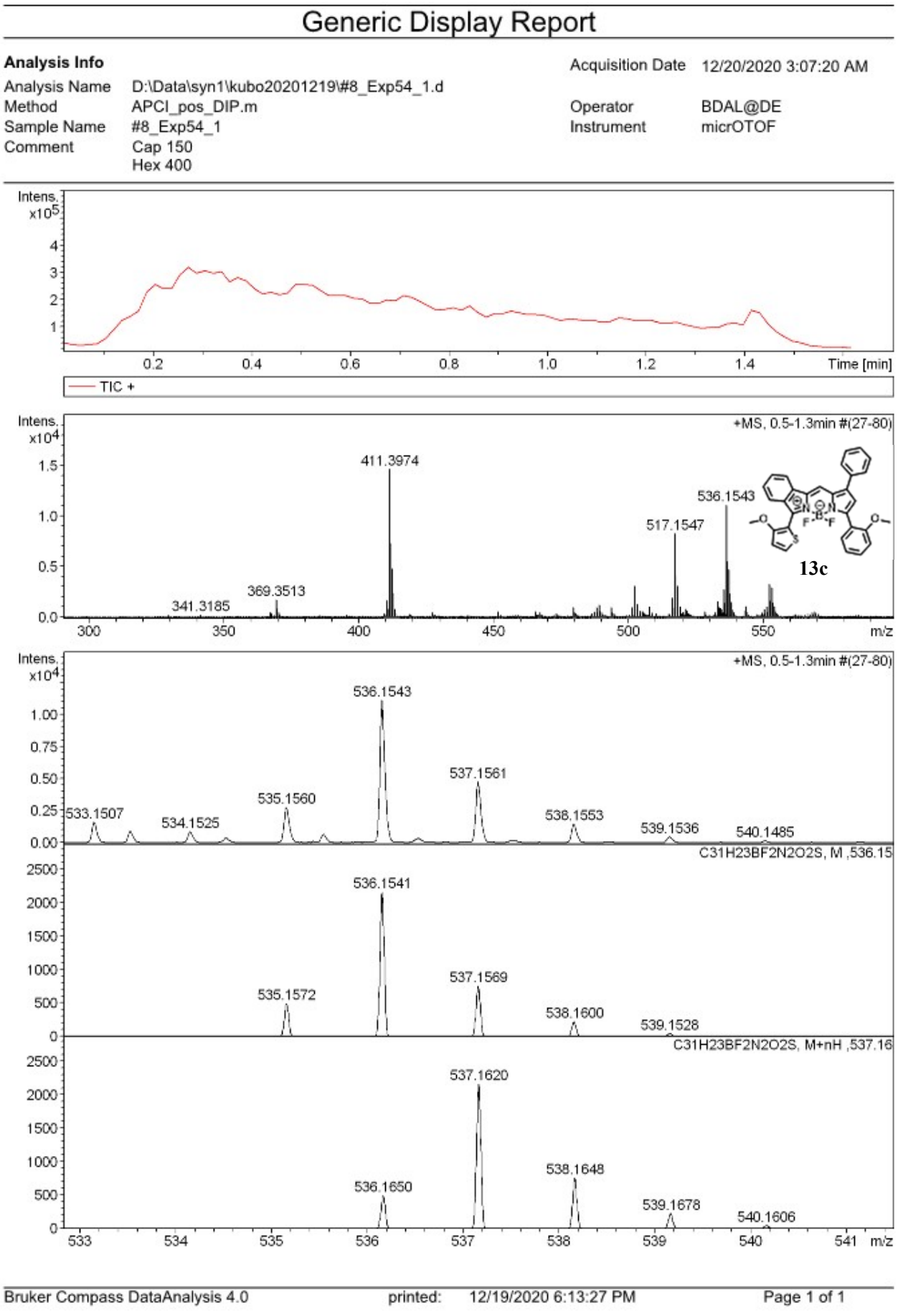


Fig. S90 High resolution of APCI mass spectrum (positive mode) of **13c**.

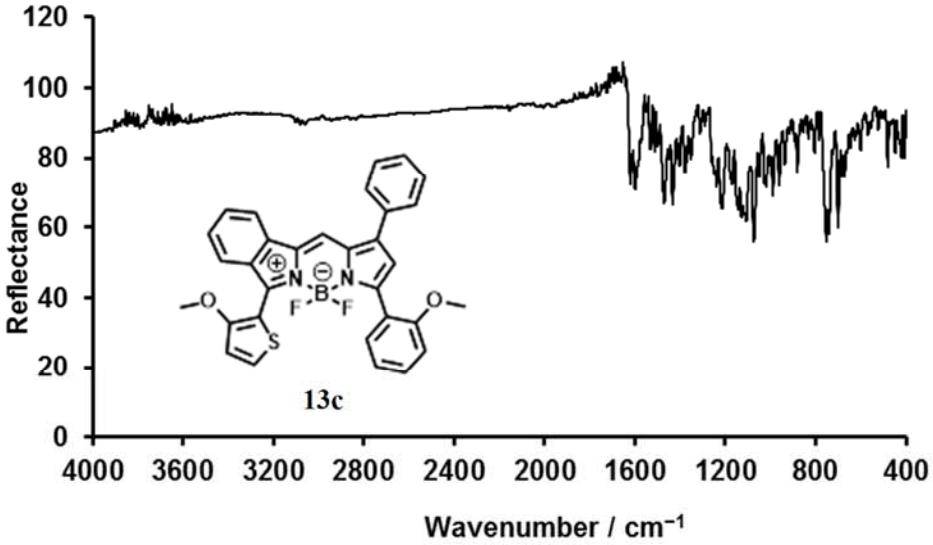


Fig. S91 ATR-FT-IR spectrum of **13c**.

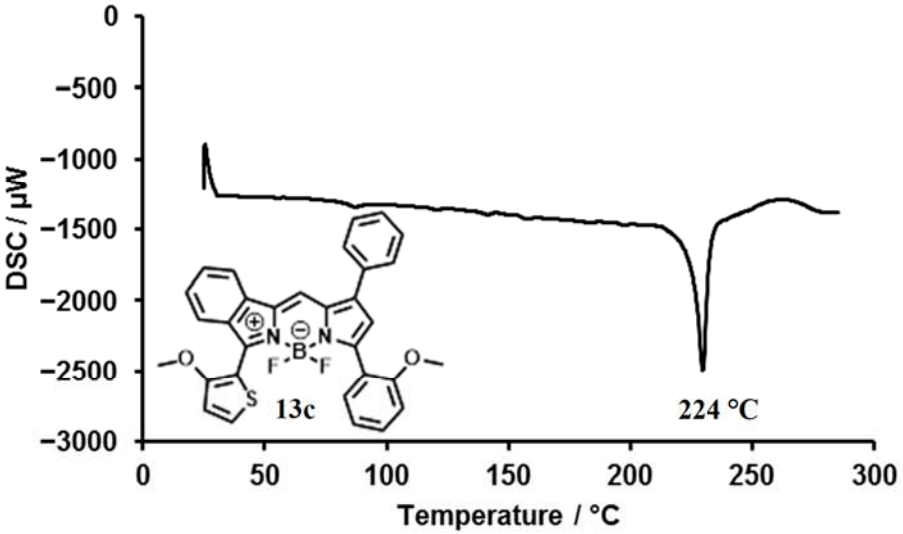


Fig. S92 DSC plots of **13c**.

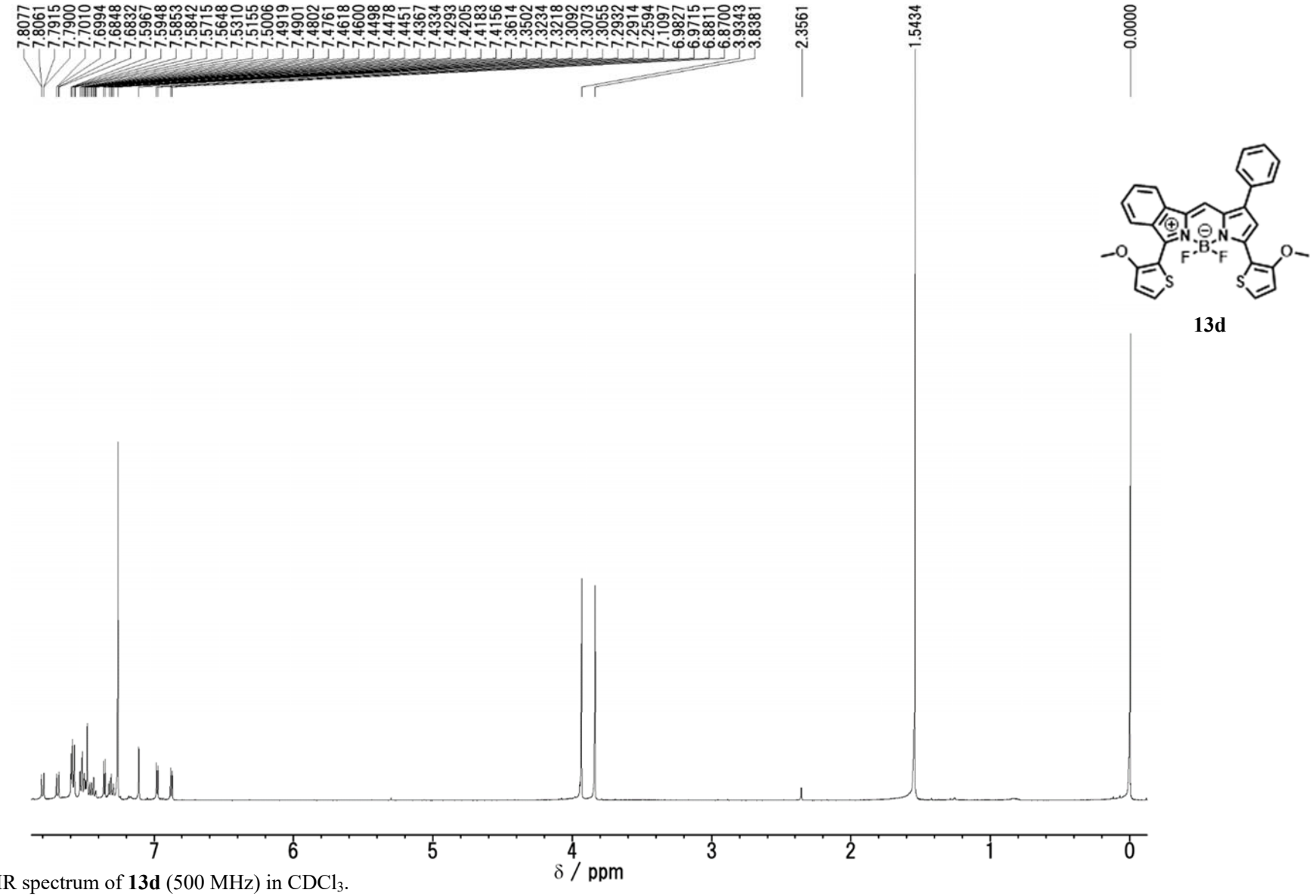


Fig. S93 ^{1}H NMR spectrum of **13d** (500 MHz) in $CDCl_3$.

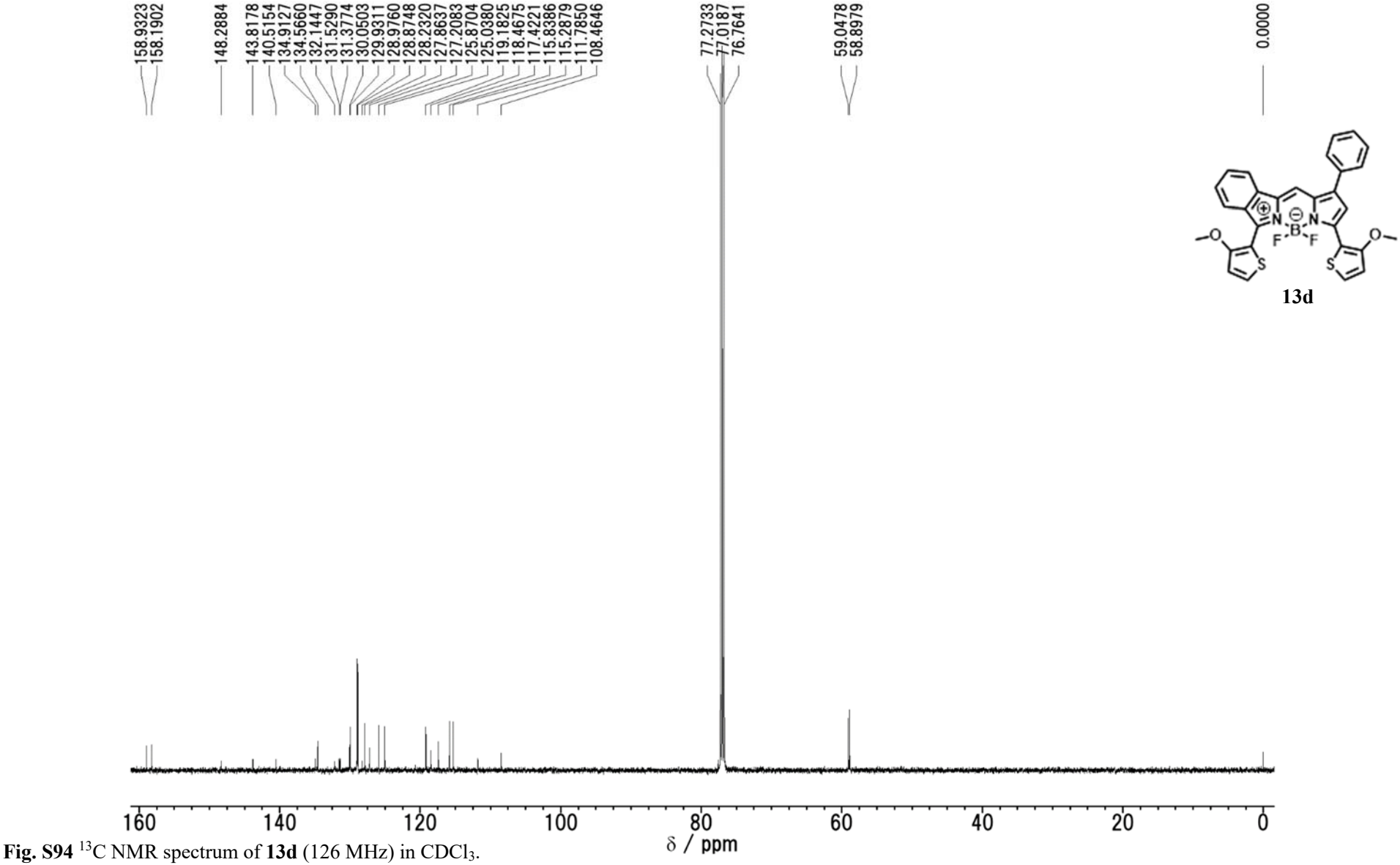


Fig. S94 ^{13}C NMR spectrum of **13d** (126 MHz) in $CDCl_3$.

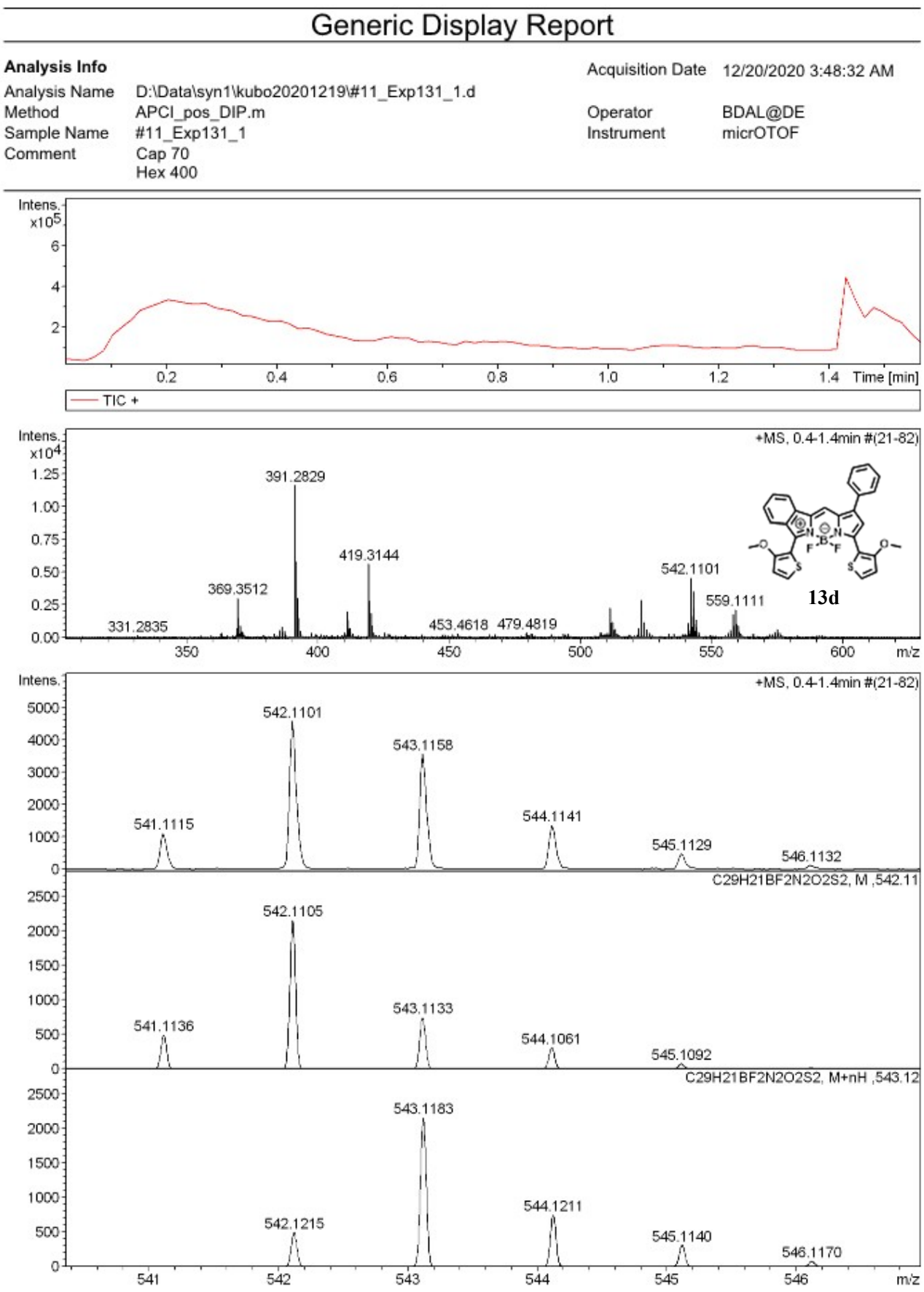


Fig. S95 High resolution of APCI mass spectrum (positive mode) of **13d**.

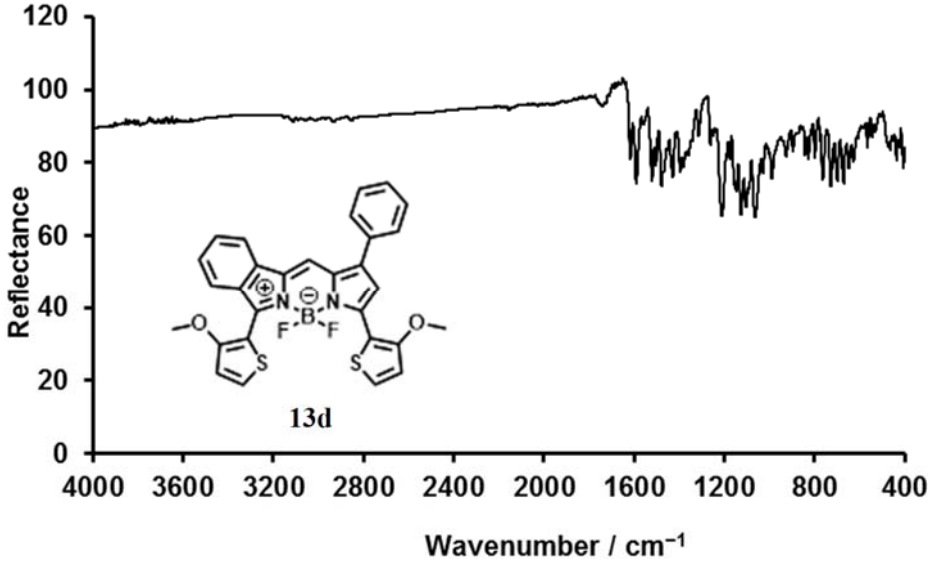


Fig. S96 ATR-FT-IR spectrum of **13d**.

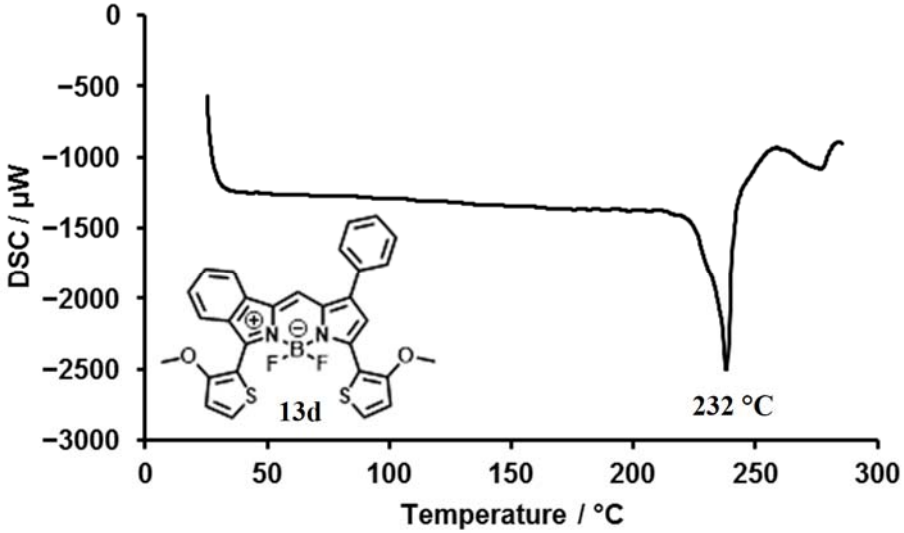


Fig. S97 DSC plots of **13d**.

Single crystal X-ray diffraction study for **2**
(CCDC No. 2024003)

Data Collection

A green platelet crystal of $C_{29}H_{17}BN_2O_2S$ having approximate dimensions of 0.450 × 0.190 × 0.080 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using graphite monochromated Mo-Ka radiation.

The crystal-to-detector distance was 50.03 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	=	10.254(7) Å	α	=	65.218(16)°
b	=	10.429(6) Å	β	=	86.33(2)°
c	=	11.673(7) Å	γ	=	77.330(19)°
V	=	1105.2(12) Å^3			

For Z = 2 and F.W. = 468.34, the calculated density is 1.407 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -173 ± 1°C to a maximum 2q value of 54.9°. A total of 540 oscillation images were collected. A sweep of data was done using w scans from -60.0 to 120.0° in 1.00° step, at c=54.0° and f = 0.0°. The exposure rate was 16.0 [sec./°]. The detector swing angle was 29.87°. A second sweep was performed using w scans from -60.0 to 120.0° in 1.00° step, at c=54.0° and f = 120.0°. The exposure rate was 16.0 [sec./°]. The detector swing angle was 29.87°. Another sweep was performed using w scans from -60.0 to 120.0° in 1.00° step, at c=54.0° and f = 240.0°. The exposure rate was 16.0 [sec./°]. The detector swing angle was 29.87°. The crystal-to-detector distance was 50.03 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 11623 reflections were collected, where 4988 were unique (R_{int} = 0.0319); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). [1]

The linear absorption coefficient, m, for Mo-Ka radiation is 1.785 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.909 to 0.986. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 4983 observed reflections and 316 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum ||Fo| - |Fc|| / \sum |Fo| = 0.0525$$

$$wR2 = [\sum (w (Fo^2 - Fc^2)^2)/ \sum w(Fo^2)^2]^{1/2} = 0.1928$$

The goodness of fit[4] was 1.32. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.39 and -0.86 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Df' and Df'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL Version 2014/7[10].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_V)]^{1/2}$$

where: N_o = number of observations
N_V = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.3: Crystal Structure Analysis Package, Rigaku Corporation (2000-2018). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

A. Crystal Data

Empirical Formula	$C_{29}H_{17}BN_2O_2S$
Formula Weight	468.34
Crystal Color, Habit	green, platelet
Crystal Dimensions	0.450 × 0.190 × 0.080 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.254(7) Å b = 10.429(6) Å c = 11.673(7) Å α = 65.218(16) ° β = 86.33(2) ° γ = 77.330(19) ° V = 1105.2(12) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.407 g/cm^3
F_{000}	484.00
μ(MoKa)	1.785 cm^{-1}

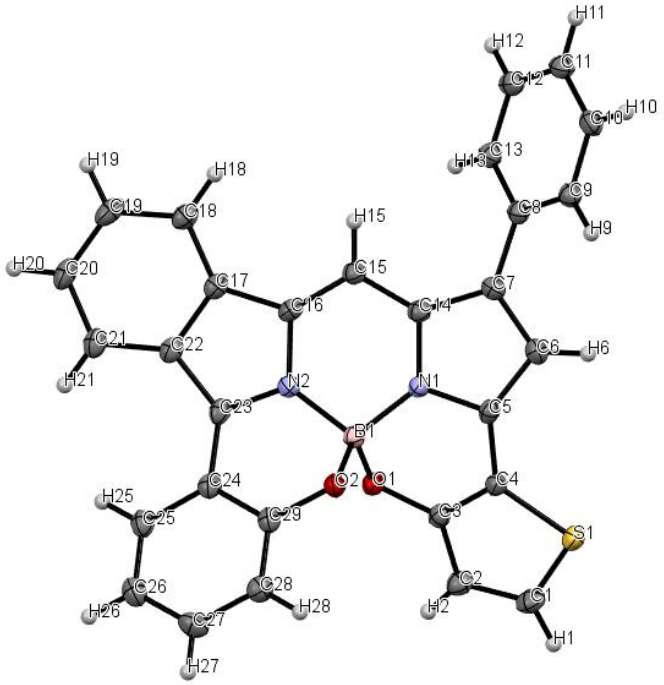
B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKa (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-173.0°C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0°
Exposure Rate	16.0 sec./°
Detector Swing Angle	29.87°
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0°
Exposure Rate	16.0 sec./°
Detector Swing Angle	29.87°
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0°
Exposure Rate	16.0 sec./°
Detector Swing Angle	29.87°
Detector Position	50.03 mm
Pixel Size	0.073 mm
$2q_{max}$	54.9°
No. of Reflections Measured	Total: 11623 Unique: 4988 (R_{int} = 0.0319)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.909 - 0.986)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2(Fo^2) + (0.1000 \cdot P)^2 + 0.0000 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4983
No. Variables	316
Reflection/Parameter Ratio	15.77
Residuals: R1 (I>2.00σ(I))	0.0525
Residuals: R (All reflections)	0.0673
Residuals: wR2 (All reflections)	0.1928
Goodness of Fit Indicator	1.321
Max Shift/Error in Final Cycle	0.014
Maximum peak in Final Diff. Map	0.39 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.86 $e^-/Å^3$

Atom numbering of **2**.



Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
S1	0.83348(6)	0.94948(6)	0.43263(5)	1.941(16)
O1	0.74590(15)	0.57441(16)	0.63216(14)	1.65(3)
O2	0.61354(15)	0.65199(16)	0.77550(13)	1.56(3)
N1	0.53260(18)	0.73970(19)	0.54970(17)	1.44(3)
N2	0.52586(18)	0.4978(2)	0.70889(17)	1.58(3)
C1	0.9730(2)	0.8155(3)	0.5015(2)	2.19(4)
C2	0.9430(2)	0.6837(3)	0.5732(2)	1.98(4)
C3	0.8025(2)	0.6917(2)	0.5731(2)	1.52(4)
C4	0.7288(2)	0.8299(2)	0.4999(2)	1.57(4)
C5	0.5895(2)	0.8517(2)	0.47213(19)	1.50(4)
C6	0.4998(2)	0.9417(2)	0.3687(2)	1.71(4)
C7	0.3916(2)	0.8757(3)	0.3799(2)	1.70(4)
C8	0.2735(2)	0.9293(2)	0.29330(19)	1.45(4)
C9	0.2075(2)	1.0748(2)	0.2473(2)	1.71(4)
C10	0.0919(2)	1.1237(2)	0.1708(2)	1.89(4)
C11	0.0421(2)	1.0301(3)	0.1375(2)	1.98(4)
C12	0.1090(2)	0.8863(3)	0.1796(2)	1.90(4)
C13	0.2236(2)	0.8366(3)	0.2572(2)	1.76(4)
C14	0.4157(2)	0.7450(2)	0.4930(2)	1.55(4)
C15	0.3564(2)	0.6241(2)	0.5415(2)	1.56(4)
C16	0.4128(2)	0.5012(2)	0.6457(2)	1.51(4)
C17	0.3643(2)	0.3735(2)	0.7248(2)	1.53(4)
C18	0.2557(2)	0.3198(2)	0.7097(2)	1.79(4)
C19	0.2308(2)	0.1944(3)	0.8076(2)	2.12(4)
C20	0.3093(2)	0.1257(3)	0.9196(2)	2.17(4)
C21	0.4158(2)	0.1786(3)	0.9372(2)	2.03(4)
C22	0.4449(2)	0.3026(2)	0.8380(2)	1.76(4)
C23	0.5415(2)	0.3901(2)	0.8262(2)	1.70(4)
C24	0.6271(2)	0.3981(2)	0.9149(2)	1.57(4)
C25	0.6708(2)	0.2837(3)	1.0332(2)	1.96(4)
C26	0.7412(3)	0.3030(3)	1.1196(2)	2.10(4)
C27	0.7705(3)	0.4379(3)	1.0897(2)	2.24(4)
C28	0.7284(2)	0.5537(2)	0.9741(2)	1.85(4)
C29	0.6572(2)	0.5352(2)	0.8864(2)	1.65(4)

B1	0.6061(2)	0.6174(3)	0.6669(2)	1.37(4)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	1.06155	0.83159	0.49076	2.624
H2	1.00761	0.59790	0.61743	2.373
H6	0.51085	1.03108	0.30330	2.047
H9	0.24135	1.14036	0.26820	2.054
H10	0.04677	1.22221	0.14127	2.268
H11	-0.03719	1.06411	0.08620	2.376
H12	0.07664	0.82213	0.15566	2.279
H13	0.26862	0.73815	0.28602	2.118
H15	0.27679	0.62672	0.50234	1.874
H18	0.20078	0.36760	0.63496	2.144
H19	0.15934	0.15454	0.79833	2.544
H20	0.28909	0.04094	0.98511	2.600
H21	0.46742	0.13234	1.01395	2.438
H25	0.65140	0.19167	1.05376	2.353
H26	0.76961	0.22509	1.19891	2.518
H27	0.81973	0.45085	1.14879	2.690
H28	0.74825	0.64514	0.95527	2.219

Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	0.0222(3)	0.0277(3)	0.0223(3)	-0.0111(2)	0.0023(2)	-0.0064(3)
O1	0.0171(8)	0.0225(8)	0.0208(8)	-0.0041(6)	0.0014(6)	-0.0068(6)
O2	0.0215(8)	0.0189(8)	0.0171(8)	-0.0048(6)	-0.0002(6)	-0.0054(6)
N1	0.0158(9)	0.0194(9)	0.0191(9)	-0.0041(7)	0.0003(7)	-0.0072(7)
N2	0.0166(9)	0.0234(10)	0.0177(9)	-0.0030(7)	0.0005(7)	-0.0068(8)
C1	0.0190(11)	0.0371(14)	0.0299(12)	-0.0105(10)	0.0043(10)	-0.0151(11)
C2	0.0198(12)	0.0285(12)	0.0270(12)	-0.0051(9)	0.0023(9)	-0.0119(10)
C3	0.0212(11)	0.0193(10)	0.0175(10)	-0.0074(9)	0.0028(8)	-0.0067(9)
C4	0.0226(11)	0.0201(10)	0.0174(10)	-0.0107(9)	0.0014(8)	-0.0053(9)
C5	0.0211(11)	0.0200(10)	0.0171(10)	-0.0047(9)	0.0025(8)	-0.0089(9)
C6	0.0241(12)	0.0198(11)	0.0170(10)	-0.0022(9)	0.0007(9)	-0.0052(9)
C7	0.0171(11)	0.0282(12)	0.0159(10)	-0.0017(9)	-0.0010(8)	-0.0072(9)
C8	0.0190(11)	0.0199(10)	0.0169(10)	-0.0052(9)	0.0014(8)	-0.0079(9)
C9	0.0220(11)	0.0248(11)	0.0173(10)	-0.0043(9)	0.0004(9)	-0.0081(9)
C10	0.0227(12)	0.0219(11)	0.0214(11)	-0.0016(9)	-0.0020(9)	-0.0046(9)
C11	0.0176(11)	0.0341(13)	0.0202(11)	-0.0051(10)	-0.0016(9)	-0.0078(10)
C12	0.0219(12)	0.0328(13)	0.0199(11)	-0.0091(10)	0.0018(9)	-0.0119(10)
C13	0.0180(11)	0.0274(12)	0.0174(10)	-0.0027(9)	0.0018(8)	-0.0063(9)
C14	0.0165(10)	0.0233(11)	0.0184(10)	-0.0039(9)	0.0014(8)	-0.0084(9)
C15	0.0181(11)	0.0213(11)	0.0201(11)	-0.0054(9)	0.0012(9)	-0.0083(9)
C16	0.0181(11)	0.0199(11)	0.0229(11)	-0.0068(8)	0.0031(8)	-0.0113(9)
C17	0.0199(11)	0.0185(10)	0.0225(11)	-0.0054(9)	0.0042(9)	-0.0111(9)
C18	0.0239(12)	0.0193(11)	0.0299(12)	-0.0051(9)	0.0044(9)	-0.0154(10)
C19	0.0219(12)	0.0256(12)	0.0399(14)	-0.0102(10)	0.0090(10)	-0.0188(11)
C20	0.0265(12)	0.0228(12)	0.0308(13)	-0.0079(10)	0.0097(10)	-0.0090(10)
C21	0.0239(12)	0.0246(12)	0.0253(12)	-0.0039(10)	0.0051(9)	-0.0083(10)
C22	0.0181(11)	0.0255(12)	0.0223(11)	-0.0049(9)	0.0038(9)	-0.0094(10)
C23	0.0171(11)	0.0233(11)	0.0206(11)	-0.0033(9)	0.0039(9)	-0.0065(9)
C24	0.0187(11)	0.0172(10)	0.0221(11)	-0.0012(8)	0.0032(9)	-0.0081(9)
C25	0.0213(11)	0.0244(12)	0.0221(11)	-0.0022(9)	0.0018(9)	-0.0048(10)
C26	0.0287(13)	0.0222(11)	0.0222(11)	-0.0008(10)	0.0006(10)	-0.0051(9)
C27	0.0272(13)	0.0359(14)	0.0214(11)	-0.0029(10)	-0.0029(9)	-0.0126(10)
C28	0.0236(12)	0.0217(11)	0.0260(12)	-0.0024(9)	0.0022(9)	-0.0123(10)
C29	0.0176(10)	0.0234(11)	0.0175(10)	-0.0005(9)	0.0032(8)	-0.0065(9)
B1	0.0184(12)	0.0155(11)	0.0198(12)	-0.0040(9)	0.0006(9)	-0.0085(9)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
S1	C1	1.724(2)	S1	C4	1.727(3)
O1	C3	1.364(3)	O1	B1	1.488(3)
O2	C29	1.368(2)	O2	B1	1.466(4)
N1	C5	1.367(3)	N1	C14	1.385(3)
N1	B1	1.522(3)	N2	C16	1.400(3)
N2	C23	1.350(3)	N2	B1	1.536(3)
C1	C2	1.369(4)	C2	C3	1.425(3)
C3	C4	1.396(3)	C4	C5	1.433(3)
C5	C6	1.414(3)	C6	C7	1.401(4)
C7	C8	1.479(3)	C7	C14	1.431(3)
C8	C9	1.401(3)	C8	C13	1.400(4)
C9	C10	1.397(3)	C10	C11	1.388(4)
C11	C12	1.391(3)	C12	C13	1.395(3)
C14	C15	1.405(4)	C15	C16	1.384(3)
C16	C17	1.440(3)	C17	C18	1.402(4)
C17	C22	1.424(3)	C18	C19	1.392(3)
C19	C20	1.403(4)	C20	C21	1.388(4)
C21	C22	1.404(3)	C22	C23	1.452(4)
C23	C24	1.439(4)	C24	C25	1.413(3)
C24	C29	1.425(4)	C25	C26	1.381(4)
C26	C27	1.396(4)	C27	C28	1.394(3)
C28	C29	1.394(4)			

Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1	0.950	C2	H2	0.950
C6	H6	0.950	C9	H9	0.950
C10	H10	0.950	C11	H11	0.950
C12	H12	0.950	C13	H13	0.950
C15	H15	0.950	C18	H18	0.950
C19	H19	0.950	C20	H20	0.950
C21	H21	0.950	C25	H25	0.950
C26	H26	0.950	C27	H27	0.950
C28	H28	0.950			

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	S1	C4	91.69(12)	C3	O1	B1	111.17(17)
C29	O2	B1	114.77(19)	C5	N1	C14	109.61(17)
C5	N1	B1	121.8(2)	C14	N1	B1	127.61(19)
C16	N2	C23	111.4(2)	C16	N2	B1	125.71(16)
C23	N2	B1	121.5(2)	S1	C1	C2	113.03(19)
C1	C2	C3	111.33(19)	O1	C3	C2	123.40(17)
O1	C3	C4	123.2(2)	C2	C3	C4	113.3(2)
S1	C4	C3	110.62(18)	S1	C4	C5	128.12(14)
C3	C4	C5	120.3(2)	N1	C5	C4	113.65(16)
N1	C5	C6	108.1(2)	C4	C5	C6	136.34(19)
C5	C6	C7	107.75(18)	C6	C7	C8	127.34(18)
C6	C7	C14	106.9(2)	C8	C7	C14	125.7(2)
C7	C8	C9	120.2(3)	C7	C8	C13	121.3(2)
C9	C8	C13	118.5(2)	C8	C9	C10	120.2(3)
C9	C10	C11	120.8(2)	C10	C11	C12	119.6(2)
C11	C12	C13	119.8(3)	C8	C13	C12	121.1(2)
N1	C14	C7	107.2(2)	N1	C14	C15	119.38(17)
C7	C14	C15	132.7(2)	C14	C15	C16	120.6(2)
N2	C16	C15	120.6(2)	N2	C16	C17	106.23(17)
C15	C16	C17	132.0(2)	C16	C17	C18	131.77(19)
C16	C17	C22	107.5(2)	C18	C17	C22	120.64(19)
C17	C18	C19	118.0(2)	C18	C19	C20	121.2(3)
C19	C20	C21	121.6(2)	C20	C21	C22	118.0(2)
C17	C22	C21	120.5(2)	C17	C22	C23	106.62(18)
C21	C22	C23	132.7(2)	N2	C23	C22	107.6(2)
N2	C23	C24	117.6(2)	C22	C23	C24	133.83(19)
C23	C24	C25	124.1(2)	C23	C24	C29	117.19(17)
C25	C24	C29	118.3(2)	C24	C25	C26	121.2(2)
C25	C26	C27	119.6(2)	C26	C27	C28	120.9(3)
C27	C28	C29	119.9(2)	O2	C29	C24	121.4(2)
O2	C29	C28	118.6(2)	C24	C29	C28	120.02(18)
O1	B1	O2	107.2(2)	O1	B1	N1	107.69(17)
O1	B1	N2	114.4(2)	O2	B1	N1	115.7(2)

O2	B1	N2	106.25(17)	N1	B1	N2	105.9(2)

Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
S1	C1	H1	123.5	C2	C1	H1	123.5
C1	C2	H2	124.3	C3	C2	H2	124.3
C5	C6	H6	126.1	C7	C6	H6	126.1
C8	C9	H9	119.9	C10	C9	H9	119.9
C9	C10	H10	119.6	C11	C10	H10	119.6
C10	C11	H11	120.2	C12	C11	H11	120.2
C11	C12	H12	120.1	C13	C12	H12	120.1
C8	C13	H13	119.5	C12	C13	H13	119.4
C14	C15	H15	119.7	C16	C15	H15	119.7
C17	C18	H18	121.0	C19	C18	H18	121.0
C18	C19	H19	119.4	C20	C19	H19	119.4
C19	C20	H20	119.2	C21	C20	H20	119.2
C20	C21	H21	121.0	C22	C21	H21	121.0
C24	C25	H25	119.4	C26	C25	H25	119.4
C25	C26	H26	120.2	C27	C26	H26	120.2
C26	C27	H27	119.6	C28	C27	H27	119.6
C27	C28	H28	120.0	C29	C28	H28	120.0

Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	S1	C4	C3	0.19(19)	C1	S1	C4	C5	-168.6(2)
C4	S1	C1	C2	0.1(2)	C3	O1	B1	O2	-74.33(19)
C3	O1	B1	N1	50.8(3)	C3	O1	B1	N2	168.12(17)
B1	O1	C3	C2	154.4(2)	B1	O1	C3	C4	-29.8(3)
C29	O2	B1	O1	-71.5(2)	C29	O2	B1	N1	168.33(17)
C29	O2	B1	N2	51.2(2)	B1	O2	C29	C24	-33.3(3)
B1	O2	C29	C28	148.96(18)	C5	N1	C14	C7	-6.1(3)
C5	N1	C14	C15	165.8(2)	C14	N1	C5	C4	-160.02(19)
C14	N1	C5	C6	6.8(3)	C5	N1	B1	O1	-43.8(3)
C5	N1	B1	O2	76.1(3)	C5	N1	B1	N2	-166.5(2)
B1	N1	C5	C4	9.7(3)	B1	N1	C5	C6	176.5(2)
C14	N1	B1	O1	124.0(2)	C14	N1	B1	O2	-116.1(3)
C14	N1	B1	N2	1.2(3)	B1	N1	C14	C7	-175.1(2)
B1	N1	C14	C15	-3.2(4)	C16	N2	C23	C22	8.1(3)
C16	N2	C23	C24	-162.06(19)	C23	N2	C16	C15	161.3(2)
C23	N2	C16	C17	-7.8(3)	C16	N2	B1	O1	-115.2(2)
C16	N2	B1	O2	126.7(2)	C16	N2	B1	N1	3.2(3)
B1	N2	C16	C15	-5.7(3)	B1	N2	C16	C17	-174.85(19)
C23	N2	B1	O1	79.0(3)	C23	N2	B1	O2	-39.1(3)
C23	N2	B1	N1	-162.64(19)	B1	N2	C23	C22	175.82(17)
B1	N2	C23	C24	5.6(3)	S1	C1	C2	C3	-0.4(3)
C1	C2	C3	O1	176.8(2)	C1	C2	C3	C4	0.6(3)
O1	C3	C4	S1	-176.7(2)	O1	C3	C4	C5	-6.8(4)
C2	C3	C4	S1	-0.5(3)	C2	C3	C4	C5	169.4(2)
S1	C4	C5	N1	-174.79(18)	S1	C4	C5	C6	23.6(5)
C3	C4	C5	N1	17.3(3)	C3	C4	C5	C6	-144.3(3)
N1	C5	C6	C7	-4.7(3)	C4	C5	C6	C7	157.6(3)
C5	C6	C7	C8	-179.6(2)	C5	C6	C7	C14	0.9(3)
C6	C7	C8	C9	-44.6(4)	C6	C7	C8	C13	136.6(3)
C6	C7	C14	N1	3.1(3)	C6	C7	C14	C15	-167.3(2)
C8	C7	C14	N1	-176.4(2)	C8	C7	C14	C15	13.2(4)
C14	C7	C8	C9	134.7(2)	C14	C7	C8	C13	-44.1(3)
C7	C8	C9	C10	-176.67(17)	C7	C8	C13	C12	177.36(17)
C9	C8	C13	C12	-1.5(3)	C13	C8	C9	C10	2.2(3)
C8	C9	C10	C11	-1.1(3)	C9	C10	C11	C12	-0.7(3)

C10	C11	C12	C13	1.4(3)	C11	C12	C13	C8	-0.3(3)
N1	C14	C15	C16	0.7(4)	C7	C14	C15	C16	170.2(2)
C14	C15	C16	N2	3.5(4)	C14	C15	C16	C17	169.4(2)
N2	C16	C17	C18	-179.5(2)	N2	C16	C17	C22	4.2(2)
C15	C16	C17	C18	13.2(5)	C15	C16	C17	C22	-163.2(3)
C16	C17	C18	C19	-177.0(2)	C16	C17	C22	C21	176.0(2)
C16	C17	C22	C23	0.5(3)	C18	C17	C22	C21	-0.8(4)
C18	C17	C22	C23	-176.4(2)	C22	C17	C18	C19	-1.1(4)
C17	C18	C19	C20	1.8(4)	C18	C19	C20	C21	-0.8(4)
C19	C20	C21	C22	-1.1(4)	C20	C21	C22	C17	1.8(4)
C20	C21	C22	C23	176.1(2)	C17	C22	C23	N2	-5.2(3)
C17	C22	C23	C24	162.7(2)	C21	C22	C23	N2	-180.0(3)
C21	C22	C23	C24	-12.1(5)	N2	C23	C24	C25	-169.15(19)
N2	C23	C24	C29	17.8(3)	C22	C23	C24	C25	23.9(4)
C22	C23	C24	C29	-149.2(2)	C23	C24	C25	C26	-173.1(2)
C23	C24	C29	O2	-4.0(3)	C23	C24	C29	C28	173.62(18)
C25	C24	C29	O2	-177.51(19)	C25	C24	C29	C28	0.2(3)
C29	C24	C25	C26	-0.1(3)	C24	C25	C26	C27	-0.3(3)
C25	C26	C27	C28	0.6(4)	C26	C27	C28	C29	-0.6(4)
C27	C28	C29	O2	177.9(2)	C27	C28	C29	C24	0.2(3)

Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
S1	C6	3.574(3)	O1	C5	2.871(3)
O1	C14	3.592(3)	O1	C23	3.275(3)
O1	C24	3.337(3)	O1	C29	2.932(3)
O2	C3	2.907(3)	O2	C4	3.265(3)
O2	C5	3.262(3)	O2	C16	3.581(4)
O2	C23	2.798(4)	N1	C3	2.712(3)
N1	C16	2.789(3)	N2	C14	2.813(3)
N2	C29	2.742(4)	C4	C14	3.527(4)
C4	B1	2.754(3)	C5	C15	3.555(4)
C6	C9	3.161(4)	C8	C11	2.811(4)
C8	C15	3.263(3)	C9	C12	2.790(4)
C10	C13	2.771(4)	C13	C14	3.167(4)
C13	C15	3.296(3)	C15	C18	3.308(4)
C15	C23	3.547(3)	C15	B1	3.004(4)
C16	C24	3.588(4)	C17	C20	2.778(3)
C18	C21	2.852(4)	C19	C22	2.782(4)
C21	C24	3.407(4)	C21	C25	3.458(4)
C22	C25	3.271(4)	C24	C27	2.803(4)
C24	B1	2.823(3)	C25	C28	2.794(4)
C26	C29	2.806(3)			

Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
S1	H2	3.504	S1	H6	3.504
O1	H2	2.736	O2	H28	2.553
N1	H6	3.165	N1	H15	3.265
N2	H15	3.272	C3	H1	3.211
C4	H1	3.410	C4	H2	3.255
C4	H6	3.038	C6	H9	2.940
C7	H9	2.659	C7	H13	2.671
C7	H15	2.861	C8	H6	2.887
C8	H10	3.279	C8	H12	3.289
C8	H15	3.070	C9	H6	3.115
C9	H11	3.278	C9	H13	3.266
C10	H12	3.261	C11	H9	3.275
C11	H13	3.265	C12	H10	3.259
C13	H9	3.268	C13	H11	3.271
C13	H15	2.775	C14	H6	3.197
C14	H13	2.962	C15	H13	2.831
C15	H18	3.177	C16	H18	2.862
C17	H15	2.834	C17	H19	3.256
C17	H21	3.319	C18	H15	3.145
C18	H20	3.283	C19	H21	3.296
C20	H18	3.295	C21	H19	3.283
C21	H25	2.903	C22	H18	3.318
C22	H20	3.253	C22	H25	3.055
C23	H21	2.890	C23	H25	2.713
C24	H21	3.281	C24	H26	3.291
C24	H28	3.301	C25	H21	2.948
C25	H27	3.255	C26	H28	3.282
C27	H25	3.256	C28	H26	3.283
C29	H25	3.296	C29	H27	3.269
H1	H2	2.428	H6	H9	2.734
H9	H10	2.340	H10	H11	2.336
H11	H12	2.346	H12	H13	2.338
H13	H15	2.293	H15	H18	2.751
H18	H19	2.348	H19	H20	2.333
H20	H21	2.341	H21	H25	2.241

H25	H26	2.325	H26	H27	2.343
H27	H28	2.339			

Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C3	C18[1]	3.447(4)	C4	C18[1]	3.390(4)
C5	C5[2]	3.522(4)	C5	C6[2]	3.348(4)
C5	C18[1]	3.425(4)	C6	C5[2]	3.348(4)
C10	C20[3]	3.564(4)	C13	C23[1]	3.387(4)
C15	C16[1]	3.529(4)	C16	C15[1]	3.529(4)
C17	C27[4]	3.531(4)	C18	C3[1]	3.447(4)
C18	C4[1]	3.390(4)	C18	C5[1]	3.425(4)
C20	C10[5]	3.564(4)	C21	C21[6]	3.455(4)
C21	C28[4]	3.386(4)	C22	C27[4]	3.460(4)
C22	C28[4]	3.361(4)	C23	C13[1]	3.387(4)
C27	C17[4]	3.531(4)	C27	C22[4]	3.460(4)
C28	C21[4]	3.386(4)	C28	C22[4]	3.361(4)

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1 (2) -X+1,-Y+2,-Z+1
(3) X,Y+1,Z-1 (4) -X+1,-Y+1,-Z+2
(5) X,Y-1,Z+1 (6) -X+1,-Y,-Z+2

Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
S1	H1[1]	3.176	S1	H9[2]	3.300
S1	H19[3]	3.293	S1	H26[4]	2.994
O1	H13[3]	3.024	O1	H15[3]	3.153
O1	H18[3]	2.955	O2	H6[2]	3.025
O2	H9[2]	2.748	N1	H6[2]	3.425
N2	H13[3]	2.849	N2	H15[3]	3.571
C1	H9[2]	3.479	C1	H15[5]	3.298
C2	H9[2]	3.353	C2	H15[5]	3.451
C2	H18[5]	3.578	C2	H18[3]	3.203
C3	H9[2]	2.995	C3	H18[3]	2.750
C4	H9[2]	2.893	C4	H18[3]	3.027
C4	H19[3]	3.543	C5	H6[2]	3.349
C5	H18[3]	3.363	C8	H1[6]	3.072
C8	H20[4]	3.289	C9	H1[6]	3.439
C9	H20[4]	3.262	C9	H28[2]	2.997
C10	H20[4]	3.127	C10	H26[7]	3.281
C10	H28[2]	3.019	C11	H11[8]	3.159
C11	H12[8]	3.295	C11	H19[9]	2.979
C11	H20[4]	2.995	C11	H26[7]	3.306
C12	H1[6]	3.451	C12	H11[8]	3.036
C12	H19[9]	2.855	C12	H20[4]	2.978
C13	H1[6]	3.088	C13	H20[4]	3.124
C14	H1[6]	3.544	C15	H1[6]	3.234
C16	H13[3]	3.553	C16	H27[10]	3.383
C17	H27[10]	3.080	C18	H2[6]	3.246
C18	H27[10]	3.374	C19	H11[9]	3.461
C19	H12[9]	3.187	C19	H25[11]	3.597
C20	H21[11]	2.977	C20	H25[11]	3.128
C20	H28[10]	3.223	C21	H20[11]	3.285
C21	H21[11]	3.018	C21	H28[10]	2.845
C22	H13[3]	3.214	C22	H27[10]	3.349
C22	H28[10]	3.172	C23	H13[3]	2.701
C24	H13[3]	3.236	C25	H11[12]	3.261
C25	H12[3]	3.583	C25	H20[11]	3.415
C26	H10[12]	3.058	C26	H11[12]	3.121

C27	H10[12]	3.120	C28	H9[2]	3.322
C28	H10[2]	3.452	C28	H21[10]	3.498
C29	H9[2]	3.460	B1	H9[2]	3.590
B1	H13[3]	3.463	H1	S1[1]	3.176
H1	C8[5]	3.072	H1	C9[5]	3.439
H1	C12[5]	3.451	H1	C13[5]	3.088
H1	C14[5]	3.544	H1	C15[5]	3.234
H1	H1[1]	3.554	H1	H13[5]	3.401
H1	H15[5]	2.680	H2	C18[5]	3.246
H2	H15[5]	3.011	H2	H18[5]	2.699
H2	H18[3]	3.599	H2	H27[13]	3.147
H6	O2[2]	3.025	H6	N1[2]	3.425
H6	C5[2]	3.349	H6	H21[4]	3.117
H6	H25[4]	3.130	H6	H26[4]	3.535
H9	S1[2]	3.300	H9	O2[2]	2.748
H9	C1[2]	3.479	H9	C2[2]	3.353
H9	C3[2]	2.995	H9	C4[2]	2.893
H9	C28[2]	3.322	H9	C29[2]	3.460
H9	B1[2]	3.590	H9	H28[2]	2.645
H10	C26[7]	3.058	H10	C27[7]	3.120
H10	C28[2]	3.452	H10	H26[7]	2.875
H10	H27[7]	2.971	H10	H28[2]	2.696
H11	C11[8]	3.159	H11	C12[8]	3.036
H11	C19[9]	3.461	H11	C25[7]	3.261
H11	C26[7]	3.121	H11	H11[8]	2.834
H11	H12[8]	2.583	H11	H19[9]	2.654
H11	H20[4]	3.467	H11	H20[9]	3.293
H11	H25[7]	3.159	H11	H26[7]	2.921
H12	C11[8]	3.295	H12	C19[9]	3.187
H12	C25[3]	3.583	H12	H11[8]	2.583
H12	H19[9]	2.426	H12	H20[4]	3.425
H13	O1[3]	3.024	H13	N2[3]	2.849
H13	C16[3]	3.553	H13	C22[3]	3.214
H13	C23[3]	2.701	H13	C24[3]	3.236
H13	B1[3]	3.463	H13	H1[6]	3.401
H15	O1[3]	3.153	H15	N2[3]	3.571
H15	C1[6]	3.298	H15	C2[6]	3.451

H15	H1[6]	2.680	H15	H2[6]	3.011
H18	O1[3]	2.955	H18	C2[6]	3.578

Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H18	C2[3]	3.203	H18	C3[3]	2.750
H18	C4[3]	3.027	H18	C5[3]	3.363
H18	H2[6]	2.699	H18	H2[3]	3.599
H19	S1[3]	3.293	H19	C4[3]	3.543
H19	C11[9]	2.979	H19	C12[9]	2.855
H19	H11[9]	2.654	H19	H12[9]	2.426
H19	H25[11]	3.451	H20	C8[14]	3.289
H20	C9[14]	3.262	H20	C10[14]	3.127
H20	C11[14]	2.995	H20	C12[14]	2.978
H20	C13[14]	3.124	H20	C21[11]	3.285
H20	C25[11]	3.415	H20	H11[14]	3.467
H20	H11[9]	3.293	H20	H12[14]	3.425
H20	H21[11]	2.740	H20	H25[11]	2.589
H20	H28[10]	3.560	H21	C20[11]	2.977
H21	C21[11]	3.018	H21	C28[10]	3.498
H21	H6[14]	3.117	H21	H20[11]	2.740
H21	H21[11]	2.844	H21	H28[10]	2.958
H25	C19[11]	3.597	H25	C20[11]	3.128
H25	H6[14]	3.130	H25	H11[12]	3.159
H25	H19[11]	3.451	H25	H20[11]	2.589
H26	S1[14]	2.994	H26	C10[12]	3.281
H26	C11[12]	3.306	H26	H6[14]	3.535
H26	H10[12]	2.875	H26	H11[12]	2.921
H27	C16[10]	3.383	H27	C17[10]	3.080
H27	C18[10]	3.374	H27	C22[10]	3.349
H27	H2[13]	3.147	H27	H10[12]	2.971
H28	C9[2]	2.997	H28	C10[2]	3.019
H28	C20[10]	3.223	H28	C21[10]	2.845
H28	C22[10]	3.172	H28	H9[2]	2.645
H28	H10[2]	2.696	H28	H20[10]	3.560

H28	H21[10]	2.958

Symmetry Operators:

(1) -X+2,-Y+2,-Z+1	(2) -X+1,-Y+2,-Z+1
(3) -X+1,-Y+1,-Z+1	(4) X,Y+1,Z-1
(5) X+1,Y,Z	(6) X-1,Y,Z
(7) X-1,Y+1,Z-1	(8) -X,-Y+2,-Z
(9) -X,-Y+1,-Z+1	(10) -X+1,-Y+1,-Z+2
(11) -X+1,-Y,-Z+2	(12) X+1,Y-1,Z+1
(13) -X+2,-Y+1,-Z+2	(14) X,Y-1,Z+1

Calculation results

Table S6. Atom coordinates and absolute energy levels for **1** optimized in the S_0 state.
E(RCAM-B3LYP) = −1476.95930873

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.818228	5.002385	-0.555804
2	6	0	-3.215522	3.688237	-0.410199
3	6	0	-2.233808	2.690565	-0.392110
4	6	0	-0.862611	3.032169	-0.489648
5	6	0	-0.474651	4.367924	-0.626708
6	6	0	-1.457307	5.337464	-0.666904
7	6	0	-2.288055	1.256432	-0.217024
8	7	0	-1.049938	0.780305	-0.305185
9	6	0	-0.109112	1.811773	-0.368197
10	5	0	-0.740773	-0.697362	-0.018553
11	7	0	0.755606	-0.777705	0.184555
12	6	0	1.665521	0.259114	0.185463
13	6	0	1.211056	1.561912	-0.082439
14	6	0	1.409267	-1.955646	0.141694
15	6	0	2.784913	-1.703012	0.262409
16	6	0	2.958385	-0.315507	0.273643
17	6	0	-3.311770	0.365743	0.280553
18	6	0	0.639304	-3.117119	-0.268122
19	6	0	4.245063	0.396960	0.315959
20	6	0	-4.688593	0.613303	0.185796
21	6	0	-5.598181	-0.182658	0.852108
22	6	0	-5.137075	-1.234918	1.649634
23	6	0	-3.786206	-1.507800	1.753808
24	6	0	-2.855022	-0.736006	1.053346
25	6	0	-0.577634	-2.869307	-0.950515
26	6	0	-1.269128	-3.935902	-1.523786
27	6	0	-0.784632	-5.228128	-1.404304
28	6	0	0.401297	-5.483433	-0.714730
29	6	0	1.106811	-4.429892	-0.161081
30	6	0	5.231104	-0.000632	1.225078
31	6	0	6.455007	0.651801	1.276501

32	6	0	6.718063	1.715180	0.419744
33	6	0	5.750566	2.114226	-0.494694
34	6	0	4.527005	1.458926	-0.550085
35	8	0	-1.553987	-1.035684	1.157268
36	8	0	-1.079658	-1.621700	-1.089312
37	1	0	-3.563556	5.789919	-0.579057
38	1	0	-4.265480	3.444531	-0.303635
39	1	0	0.573251	4.639060	-0.702280
40	1	0	-1.176464	6.379472	-0.780019
41	1	0	1.916052	2.384456	-0.063540
42	1	0	3.572863	-2.441147	0.231759
43	1	0	-5.038092	1.427673	-0.438603
44	1	0	-6.661212	0.009392	0.760844
45	1	0	-5.848361	-1.856776	2.183862
46	1	0	-3.415349	-2.331288	2.352806
47	1	0	-2.192259	-3.721526	-2.050057
48	1	0	-1.340320	-6.048834	-1.846739
49	1	0	0.771288	-6.498182	-0.618351
50	1	0	2.038026	-4.612502	0.366419
51	1	0	5.020308	-0.818766	1.906030
52	1	0	7.205093	0.331947	1.992674
53	1	0	7.674500	2.225920	0.460685
54	1	0	5.953363	2.931777	-1.179131
55	1	0	3.794739	1.747632	-1.296434

Table S7. Atom coordinates and absolute energy levels for **2** optimized in the S_0 state.
E(RCAM-B3LYP) = −1797.74818873

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.137740	4.849419	-0.564491
2	6	0	-3.462200	3.516641	-0.417276
3	6	0	-2.427129	2.572528	-0.398944
4	6	0	-1.075812	2.989591	-0.498698
5	6	0	-0.762583	4.345873	-0.638179
6	6	0	-1.796323	5.259174	-0.677997
7	6	0	-2.402499	1.140903	-0.221207
8	7	0	-1.137247	0.734406	-0.307604
9	6	0	-0.257179	1.815186	-0.376822
10	5	0	-0.748253	-0.720924	-0.022287
11	7	0	0.754180	-0.721833	0.179079
12	6	0	1.602988	0.369969	0.181221
13	6	0	1.078974	1.639759	-0.091597
14	6	0	1.487753	-1.857592	0.139549
15	6	0	2.845190	-1.519694	0.282289
16	6	0	2.928889	-0.126532	0.288183
17	6	0	-3.374957	0.193882	0.278559
18	6	0	0.768886	-3.016324	-0.297771
19	6	0	4.168340	0.664528	0.344350
20	6	0	-4.763023	0.364011	0.185529
21	6	0	-5.626914	-0.484079	0.849866
22	6	0	-5.108298	-1.512495	1.641836
23	6	0	-3.743487	-1.710504	1.742401
24	6	0	-2.858467	-0.883798	1.046387
25	6	0	4.396829	1.736075	-0.525419
26	6	0	5.577179	2.465205	-0.457361
27	6	0	6.553419	2.132131	0.474064
28	6	0	6.343386	1.060415	1.335044
29	6	0	5.162820	0.333549	1.270642
30	6	0	-0.427239	-2.845950	-0.980753
31	6	0	-0.895109	-4.052455	-1.579700
32	6	0	-0.059862	-5.097196	-1.341004
33	16	0	1.316509	-4.658782	-0.390191

34	8	0	-1.540942	-1.112619	1.146859
35	8	0	-1.051610	-1.666802	-1.102712
36	1	0	-3.925022	5.595078	-0.587557
37	1	0	-4.497287	3.216233	-0.309587
38	1	0	0.268757	4.674151	-0.715773
39	1	0	-1.573701	6.315007	-0.792668
40	1	0	1.736349	2.500713	-0.074853
41	1	0	3.675824	-2.209958	0.266890
42	1	0	-5.158071	1.160531	-0.434694
43	1	0	-6.698991	-0.349744	0.760611
44	1	0	-5.783230	-2.174812	2.174584
45	1	0	-3.326431	-2.514326	2.337837
46	1	0	3.658854	1.974738	-1.283647
47	1	0	5.739734	3.289217	-1.144737
48	1	0	7.476041	2.700867	0.525054
49	1	0	7.100866	0.791982	2.064380
50	1	0	4.992469	-0.491762	1.954218
51	1	0	-1.814851	-4.113774	-2.146021
52	1	0	-0.187305	-6.124970	-1.649234

Table S8. Atom coordinates and absolute energy levels for **3** optimized in the S_0 state.
E(RCAM-B3LYP) = −1797.75150905

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.170804	-4.712021	-0.689331
2	6	0	3.462388	-3.372872	-0.509776
3	6	0	2.400029	-2.469315	-0.439785
4	6	0	1.059474	-2.908984	-0.532426
5	6	0	0.779971	-4.266615	-0.701646
6	6	0	1.839815	-5.151295	-0.784066
7	6	0	2.347777	-1.042209	-0.214384
8	7	0	1.075158	-0.645084	-0.310007
9	6	0	0.213066	-1.749373	-0.378558
10	5	0	0.648164	0.802332	-0.030380
11	7	0	-0.844048	0.766154	0.178709
12	6	0	-1.671424	-0.336991	0.183090
13	6	0	-1.116152	-1.606743	-0.088037
14	6	0	-1.588487	1.893557	0.142005
15	6	0	-2.935416	1.534925	0.267683
16	6	0	-3.000533	0.134068	0.277404
17	6	0	3.255467	-0.100349	0.329484
18	6	0	-0.909832	3.112000	-0.268817
19	6	0	-4.229364	-0.674113	0.323916
20	6	0	2.730794	0.947300	1.092568
21	6	0	0.323428	2.962318	-0.948905
22	6	0	0.934020	4.079598	-1.515556
23	6	0	0.351457	5.331315	-1.395283
24	6	0	-0.851750	5.491602	-0.708504
25	6	0	-1.475440	4.384766	-0.158762
26	6	0	-4.433234	-1.755121	-0.540614
27	6	0	-5.603227	-2.501599	-0.481207
28	6	0	-6.596033	-2.176396	0.435379
29	6	0	-6.411837	-1.095146	1.290325
30	6	0	-5.240766	-0.352198	1.235259
31	8	0	1.441866	1.230018	1.157493
32	8	0	0.923003	1.755880	-1.088271
33	16	0	4.976629	-0.233055	0.539255

34	6	0	4.969686	1.102798	1.636558
35	6	0	3.734728	1.625537	1.847141
36	1	0	3.976373	-5.434989	-0.755932
37	1	0	4.490394	-3.036660	-0.428595
38	1	0	-0.242787	-4.621522	-0.773036
39	1	0	1.641551	-6.208923	-0.924145
40	1	0	-1.755813	-2.480796	-0.070860
41	1	0	-3.779622	2.208241	0.239743
42	1	0	1.871885	3.937601	-2.040477
43	1	0	0.843255	6.193304	-1.834806
44	1	0	-1.299835	6.474277	-0.610406
45	1	0	-2.418926	4.494087	0.367197
46	1	0	-3.683331	-1.987989	-1.288978
47	1	0	-5.745148	-3.332850	-1.164568
48	1	0	-7.510921	-2.758128	0.479269
49	1	0	-7.182215	-0.832026	2.008133
50	1	0	-5.090997	0.480326	1.914984
51	1	0	5.906068	1.450411	2.049545
52	1	0	3.520000	2.467508	2.491121

Table S9. Atom coordinates and absolute energy levels for **4** optimized in the S_0 state.
E(RCAM-B3LYP) = −2118.53992626

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.455395	-4.551695	-0.693384
2	6	0	3.678158	-3.200622	-0.511947
3	6	0	2.570855	-2.350630	-0.444570
4	6	0	1.253733	-2.858243	-0.541961
5	6	0	1.044723	-4.229389	-0.713724
6	6	0	2.147692	-5.058315	-0.793232
7	6	0	2.446085	-0.931033	-0.217620
8	7	0	1.153198	-0.599700	-0.312784
9	6	0	0.350464	-1.745528	-0.388998
10	5	0	0.654143	0.822903	-0.035705
11	7	0	-0.839385	0.712325	0.170926
12	6	0	-1.605691	-0.438263	0.177681
13	6	0	-0.987640	-1.672084	-0.098487
14	6	0	-1.656916	1.793715	0.137120
15	6	0	-2.980152	1.356817	0.284018
16	6	0	-2.959838	-0.043178	0.289810
17	6	0	3.303541	0.057292	0.329698
18	6	0	-1.023226	3.003138	-0.303230
19	6	0	-4.138482	-0.922189	0.351131
20	6	0	0.183276	2.925127	-0.980386
21	6	0	2.726496	1.080769	1.084494
22	6	0	-4.292516	-2.008806	-0.516478
23	6	0	-5.416319	-2.821991	-0.443151
24	6	0	-6.411319	-2.559409	0.490973
25	6	0	-6.276609	-1.473606	1.349361
26	6	0	-5.151845	-0.663379	1.280078
27	8	0	1.422427	1.298506	1.144958
28	8	0	0.895152	1.792645	-1.103728
29	6	0	0.569419	4.166579	-1.565516
30	6	0	-0.338787	5.148157	-1.324143
31	16	0	-1.684394	4.603683	-0.384230
32	16	0	5.029054	0.017006	0.538094
33	6	0	4.954089	1.358885	1.625230

34	6	0	3.693069	1.817955	1.831706
35	1	0	4.296596	-5.233122	-0.757839
36	1	0	4.687625	-2.812893	-0.427238
37	1	0	0.041566	-4.635813	-0.789122
38	1	0	2.004229	-6.124564	-0.934938
39	1	0	-1.580679	-2.578348	-0.083201
40	1	0	-3.860927	1.981979	0.270455
41	1	0	-3.542052	-2.194197	-1.277376
42	1	0	-5.520803	-3.656723	-1.128969
43	1	0	-7.290089	-3.193519	0.545881
44	1	0	-7.049340	-1.259253	2.080681
45	1	0	-5.039849	0.173429	1.961777
46	1	0	1.484725	4.296705	-2.127532
47	1	0	-0.285095	6.184160	-1.625826
48	1	0	5.871094	1.756741	2.036176
49	1	0	3.434451	2.651859	2.470104

Table S10. Atom coordinates and absolute energy levels for **5** optimized in the S_0 state.
E(RCAM-B3LYP) = −1527.42997880

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.587185	-4.535103	-0.061715
2	6	0	3.791529	-3.171729	-0.082834
3	6	0	2.668979	-2.332184	-0.047625
4	6	0	1.366640	-2.869716	-0.020826
5	6	0	1.171168	-4.255274	0.000973
6	6	0	2.284709	-5.070350	-0.014777
7	6	0	2.534229	-0.899150	-0.075511
8	7	0	1.239962	-0.584486	-0.087144
9	6	0	0.470323	-1.753025	-0.034550
10	5	0	0.611056	0.873194	0.023422
11	7	0	-0.939143	0.723017	0.080699
12	6	0	-1.602354	-0.493642	0.054060
13	6	0	-0.894253	-1.697719	0.038297
14	6	0	-1.877661	1.705663	0.077120
15	6	0	-3.150949	1.118495	0.073555
16	6	0	-2.994925	-0.263398	0.051742
17	6	0	3.661790	0.046139	-0.064065
18	6	0	-1.632485	3.157602	0.042107
19	6	0	-4.063704	-1.272991	0.035137
20	6	0	4.688964	-0.158329	0.865284
21	6	0	5.797126	0.676100	0.886184
22	6	0	5.901923	1.715015	-0.031480
23	6	0	4.889372	1.919242	-0.961516
24	6	0	3.772614	1.095380	-0.980932
25	6	0	-0.620093	3.785782	0.773918
26	6	0	-0.484500	5.167076	0.736317
27	6	0	-1.350001	5.944266	-0.023866
28	6	0	-2.360289	5.329289	-0.754469
29	6	0	-2.500771	3.949935	-0.719671
30	6	0	-5.171277	-1.131808	0.878361
31	6	0	-6.194943	-2.068611	0.868957
32	6	0	-6.132559	-3.165783	0.016237
33	6	0	-5.042567	-3.313328	-0.832968

34	6	0	-4.019249	-2.373625	-0.827761
35	9	0	0.944244	1.617275	-1.089005
36	9	0	1.114045	1.416940	1.191371
37	1	0	4.436895	-5.208668	-0.087186
38	1	0	4.792190	-2.757642	-0.132336
39	1	0	0.173653	-4.681612	0.025841
40	1	0	2.157822	-6.147982	0.001358
41	1	0	-1.454484	-2.624279	0.086682
42	1	0	-4.084582	1.661293	0.079838
43	1	0	4.601767	-0.960159	1.590385
44	1	0	6.577883	0.515721	1.622272
45	1	0	6.770233	2.365775	-0.019839
46	1	0	4.965894	2.729058	-1.679367
47	1	0	2.978458	1.267715	-1.693274
48	1	0	0.058661	3.190890	1.368697
49	1	0	0.305391	5.638887	1.311809
50	1	0	-1.237256	7.023388	-0.048884
51	1	0	-3.037975	5.923993	-1.358463
52	1	0	-3.278480	3.472735	-1.306234
53	1	0	-5.213081	-0.285884	1.556639
54	1	0	-7.043237	-1.944704	1.534413
55	1	0	-6.932824	-3.898477	0.009847
56	1	0	-4.993522	-4.157081	-1.513852
57	1	0	-3.192840	-2.471892	-1.523719