Supplementary Information

A general approach to construct selenopheno[3,2-*b*]indole-cored molecules using Fischer indolization

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1. Experimental section

General information: Melting points were determined on combined heating stages and are uncorrected. NMR measurements were performed on NMR spectrometers in DMSO-d_6 with tetramethylsilane as an internal standard for ^{1}H, ^{13}C spectra, C_6F_6 for ^{19}F and H_2SeO_3 for ^{77}Se ones. Mass spectrometry was performed using a high-resolution Q-TOF LC-MS/MS spectrometer. Phenylhydrazine (**17a**), 4-(*tert*-butyl)phenylhydrazine (**17b**), 4-fluorophenylhydrazine (**17c**), naphthalen-1-ylhydrazine (**17d**), 4-hydrazinobenzoic acid (**17e**), 4-(trifluoromethoxy)-phenylhydrazine (**17f**), 4-methoxyphenylhydrazine (**17g**), 4-methylphenylhydrazine (**17h**), 4-cyanophenylhydrazine (**17i**) and 3,5-difluorophenylhydrazine (**17j**) (hydrochlorides) were used in this study. Unless otherwise stated, all reagents were purchased from commercial sources and used without further purification. Compounds **12a-d**,[1] **13**,[2] **14**,[3] and **15a,b**[4] were prepared in accordance with procedures described in the literature.

*General procedure for the synthesis of esters **12a-d** and **15a,b***

An appropriate 3-aryl-3-chloroacrylonitrile (20 mmol) or 4-chloro-3-cyanocoumarin (20 mmol) was added portion wise to a suspension of Na_2Se (2.50 g, 20 mmol) in dry DMF (40 ml) at room temperature. The thick suspension was vigorously stirred and heated under reflux at 80 °C for 1 hour under argon atmosphere. The reaction mixture was then cooled to 0 °C, methyl bromoacetate (2.03 ml, 22 mmol) was dropped to it and allowed to stir for 30 minutes, after that powered anhydrous K_2CO_3 (8.30 g, 60 mmol) was added and heated at 100°C for 5 hours. The reaction mixture was poured into ice water (100 ml) and neutralized with AcOH. The formed precipitate was filtered, washed with water (5×10 ml), MeOH (10 ml) and dried in air. The products were purified by crystallization from EtOH for products **12a-d** or DMF for products **15a,b** to give analytically pure forms.

*General procedure for the synthesis of esters **13** and **14***

Powered $NaBH_4$ (0.95 g, 25 mmol) was added portion wise to a stirred suspension of elemental Se (1.975 g, 25 mmol) in dry DMF (50 ml) at 0 °C during 10 min. An intensive hydrogen evolution was proceeded and thick suspension of NaHSe was formed during next 10 min. MeOH (10 ml) was dropped to this suspension causing rapid dissolution of NaHSe to form clear colorless solution. 2-Chloronicotinonitrile (20 mmol) or 3-chloropyrazine-2-carbonitrile (20 mmol) was added to a solution of NaHSe in DMF-MeOH at 0 °C, and a formed solution was stirred at room temperature for 1 h, and then treated with methyl bromoacetate (2.03 ml, 22 mmol). The reaction mixture was another stirred at room temperature for 30 min, treated with powered anhydrous K_2CO_3 (8.30 g, 60 mmol) and then stirred and heated at 80°C for 5 hours. Then, it was poured into

ice water (100 ml) and neutralized with AcOH. The formed precipitate was filtered, washed with water (5×20 ml) and dried in air. The products were purified by crystallization from EtOH to give analytically pure forms.

Methyl 3-amino-5-phenylselenophene-2-carboxylate (**12a**)

Yellow crystals, yield 1.681 g (30%), m.p. 145-146 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.57 (dd, J = 8.0, 1.3 Hz, 2H), 7.46 – 7.38 (m, 3H), 7.28 (s, 1H), 6.76 (s, 2H), 3.71 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.0, 157.3, 152.2, 134.6, 129.3, 125.9, 120.2, 95.7, 51.0. HRMS (ESI) calcd for $C_{12}H_{12}NO_2Se$ m/z 282.0028 $[M+H]^+$, found m/z 282.0033 $[M+H]^+$.

Methyl 3-amino-5-(4-fluorophenyl)selenophene-2-carboxylate (**12b**)

Light orange plates, yield 1.551 g (26%), m.p. 150-151 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.67 – 7.58 (m, 2H), 7.31 – 7.24 (m, 2H), 7.23 (s, 1H), 6.76 (s, 2H), 3.70 (s, 3H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 50.46 – 50.38 (m). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.0, 162.5 (d, J_{CF} = 247.3 Hz), 157.2, 150.9, 131.3 (d, J_{CF} = 3.3 Hz), 128.0 (d, J_{CF} = 8.5 Hz), 120.3, 116.2 (d, J_{CF} = 21.9 Hz), 95.6 (d, J_{CF} = 48.1 Hz), 51.0. HRMS (ESI) calcd for $C_{12}H_{11}FNO_2Se$ m/z 299.9934 $[M+H]^+$, found m/z 299.9938 $[M+H]^+$.

Methyl 3-amino-5-(4-chlorophenyl)selenophene-2-carboxylate (**12c**)

Yellowish cotton-like needles, yield 1.256 g (20%), m.p. 159-160 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.62 – 7.57 (m, 2H), 7.51 – 7.47 (m, 2H), 7.29 (s, 1H), 6.76 (s, 2H), 3.70 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.0, 157.1, 150.5, 133.7, 133.5, 129.2, 127.6, 120.8, 96.2, 51.1. HRMS (ESI) calcd for $C_{12}H_{11}ClNO_2Se$ m/z 315.9638 $[M+H]^+$, found m/z 315.9633 $[M+H]^+$.

Methyl 3-amino-5-(3-methoxyphenyl)selenophene-2-carboxylate (**12d**)

Deep orange plates, yield 1.985 g (32%), m.p. 70-71 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.34 (t, J = 8.0 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.15 – 7.12 (m, 1H), 7.09 – 7.07 (m, 1H), 7.00 – 6.96 (m, 1H), 6.75 (s, 2H), 3.80 (s, 3H), 3.70 (s, 3H).^{13}C NMR (126 MHz, DMSO-d_6) δ 165.1, 159.7, 157.2, 152.0, 136.0, 130.4, 120.5, 118.4, 114.9, 111.1, 95.8, 55.2, 51.0. HRMS (ESI) calcd for $C_{13}H_{14}NO_3Se$ m/z 312.0133 $[M+H]^+$, found m/z 312.0129 $[M+H]^+$.

Methyl 3-aminoselenopheno[2,3-b]pyridine-2-carboxylate (**13**)

Yellow crystals, yield 2.245 g (44%), m.p. 209-210 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.65 (dd, J = 4.6, 1.6 Hz, 1H), 8.50 (dd, J = 8.1, 1.6 Hz, 1H), 7.50 (dd, J = 8.1, 4.6 Hz, 1H), 7.40 (s, 2H), 3.77 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.9, 161.5, 150.6, 149.6, 132.6, 129.2,

120.0, 92.0, 51.5. HRMS (ESI) calcd for $C_9H_9N_2O_2Se$ m/z 256.9824 $[M+H]^+$, found m/z 256.9825 $[M+H]^+$.

Methyl 7-aminoselenopheno[2,3-b]pyrazine-6-carboxylate (**14**)

Orange crystals, yield 2.356 g (46%), m.p. 139-140 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.79 (d, J = 2.3 Hz, 1H), 8.77 (d, J = 2.3 Hz, 1H), 7.15 (s, 2H), 3.82 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.5, 157.2, 147.4, 145.2, 144.2, 141.8, 94.9, 51.9. HRMS (ESI) calcd for $C_8H_8N_3O_2Se$ m/z 257.9776 $[M+H]^+$, found m/z 257.9778 $[M+H]^+$.

Methyl 3-amino-4-oxo-4H-selenopheno[3,2-c]chromene-2-carboxylate (**15a**)

Yellowish solid, yield 322 mg (5%), m.p. 227-228 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (dd, J = 7.8, 1.3 Hz, 1H), 7.69 (ddd, J = 8.7, 7.4, 1.5 Hz, 1H), 7.50 (dd, J = 8.4, 0.7 Hz, 1H), 7.41 (td, J = 7.8, 1.1 Hz, 1H), 7.18 (s, 2H), 3.79 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.5, 157.8, 157.2, 153.9, 150.0, 132.8, 125.7, 125.3, 118.2, 117.0, 116.8, 96.0, 51.5. HRMS (ESI) calcd for $C_{13}H_{10}NO_4Se$ m/z 323.9770 $[M+H]^+$, found m/z 323.9766 $[M+H]^+$.

Methyl 3-amino-7-methoxy-4-oxo-4H-selenopheno[3,2-c]chromene-2-carboxylate (**15b**)

Yellowish crystals, yield 493 mg (7%), m.p. 202-203 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.86 (d, J = 8.7 Hz, 1H), 7.16 (s, 2H), 7.08 (d, J = 2.4 Hz, 1H), 7.00 (dd, J = 8.8, 2.5 Hz, 1H), 3.88 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.6, 163.1, 158.2, 157.4, 154.1, 152.0, 127.0, 114.4, 113.5, 111.7, 101.0, 56.1, 51.5. HRMS (ESI) calcd for $C_{14}H_{12}NO_5Se$ m/z 353.9875 $[M+H]^+$, found m/z 353.9878 $[M+H]^+$.

Methyl 3-aminobenzo[b]selenophene-2-carboxylate (**16**)

$NaBH_4$ (2.00 g, 53 mmol) was added portion wise to a solution of 2-(selenocyanato)benzonitrile (7.25 g, 35 mmol) in DMF-MeOH (100 ml, 4:1, v/v) and a mixture was stirred at room temperature for 24 h. The reaction mixture was cooled to 0 °C and treated with methyl bromoacetate (5.00 ml, 52.5 mmol) drop wise for 0.5 h, after that anhydrous K_2CO_3 (14.50 g, 105 mmol) was added in one portion and the obtained suspension was stirred at 100 °C for 5 h. Then, the reaction mixture was poured into ice water (100 ml) and neutralized with glacial AcOH (9 ml). The precipitate was filtered, washed with water (5×10 ml), MeOH (10 ml) and dried in air. Crude product was purified by crystallization from MeOH to give its analytically pure form.

Orange solid, yield 1.271 mg (25%), m.p. 109-110 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.14 – 8.11 (m, 1H), 7.96 – 7.93 (m, 1H), 7.49 – 7.40 (m, 2H), 7.27 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (126

MHz, DMSO-d_6) δ 166.2, 152.1, 138.8, 134.4, 128.7, 126.6, 124.7, 124.6, 92.5, 51.3. HRMS (APCI) calcd for $C_{10}H_9NO_2Se$ m/z 254.9793 $[M]^+$, found m/z 254.9796 $[M]^+$.

General procedure for the preparation of SeI derivatives **18**

NaOH (0.16 g, 4 mmol) in water (1 ml) was added to a stirred suspension of an appropriate ester **12** (1 mmol) in IPA (9 ml), and a reaction mixture was stirred and heated at reflux (100 °C) for 4 h. Then, the resulted solution was concentrated to dryness under reduced pressure. The solid residue was dissolved in glacial AcOH (7 ml). An appropriate arylhydrazine hydrochloride (1.2 mmol) was added, and the reaction mixture was stirred and heated at reflux (130 °C) for 2 h. The precipitate was filtered, washed with MeOH (3×4 ml) and dried at 120 °C to give product in an analytically pure form.

2-Phenyl-4H-selenopheno[3,2-b]indole (**18a**)

Light yellow powdery microcrystals, yield 275 mg (93%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.55 (s, 1H), 7.83 (s, 1H), 7.73 – 7.67 (m, 3H), 7.50 – 7.40 (m, 3H), 7.32 (t, J = 7.4 Hz, 1H), 7.22 – 7.16 (m, 1H), 7.11 – 7.05 (m, 1H). ^{77}Se NMR (114 MHz, DMSO-d_6) δ 430.12; ^{13}C NMR (126 MHz, DMSO-d_6) δ 148.6, 144.8, 140.0, 136.6, 129.2, 127.7, 125.4, 124.0, 122.3, 119.1, 118.8, 113.4, 112.1, 111.8. HRMS (ESI) calcd for $C_{16}H_{12}NSe$ m/z 298.0129 $[M+H]^+$, found m/z 298.0127 $[M+H]^+$.

7-(tert-Butyl)-2-phenyl-4H-selenopheno[3,2-b]indole (**18b**)

Beige plates, yield 282 mg (80%), m.p. 265-266 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.40 (s, 1H), 7.80 (s, 1H), 7.71 – 7.67 (m, 3H), 7.41 (dd, J = 16.0, 8.1 Hz, 3H), 7.33 – 7.26 (m, 2H), 1.36 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 148.1, 144.9, 141.6, 138.2, 136.6, 129.1, 127.6, 125.4, 123.9, 120.5, 114.7, 113.6, 111.8, 111.6, 34.4, 31.8. HRMS (ESI) calcd for $C_{20}H_{20}NSe$ m/z 354.0755 $[M+H]^+$, found m/z 354.0760 $[M+H]^+$.

7-Fluoro-2-phenyl-4H-selenopheno[3,2-b]indole (**18c**)

Beige powdery microcrystals, yield 251 mg (80%), m.p. >350 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.62 (s, 1H), 7.82 (s, 1H), 7.70 (dd, J = 8.2, 1.0 Hz, 2H), 7.58 (dd, J = 9.9, 2.6 Hz, 1H), 7.49 – 7.41 (m, 3H), 7.33 (t, J = 7.4 Hz, 1H), 7.02 (td, J = 9.2, 2.6 Hz, 1H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 38.29 (td, J = 9.7, 4.6 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.7 (d, J_{CF}= 245.2 Hz), 147.3, 144.8, 140.0, 133.2 (d, J_{CF} = 3.1 Hz), 127.4 (d, J_{CF} = 8.2 Hz), 124.0, 122.3, 119.1, 118.8, 116.0 (d, J_{CF} = 21.8 Hz), 113.5, 112.1, 112.0. HRMS (ESI) calcd for $C_{16}H_{11}FNSe$ m/z 316.0035 $[M+H]^+$, found m/z 316.0038 $[M+H]^+$.

8-Phenyl-10H-benzo[g]selenopheno[3,2-b]indole (**18d**)

Beige crystals, yield 260 mg (75%), m.p. 325-326 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.53 (s, 1H), 8.42 (d, J = 8.2 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.91 (s, 1H), 7.85 (d, J = 8.6 Hz, 1H), 7.71 (dd, J = 8.2, 1.0 Hz, 2H), 7.61 – 7.53 (m, 2H), 7.48 – 7.40 (m, 3H), 7.32 (t, J = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 147.5, 143.4, 136.6, 134.6, 130.1, 129.1, 128.5, 127.6, 125.5, 125.4, 124.1, 122.2, 120.9, 119.9, 119.8, 119.2, 115.2, 111.6. HRMS (ESI) calcd for $C_{20}H_{14}NSe$ m/z 348.0286 $[M+H]^+$, found m/z 348.0282 $[M+H]^+$.

2-Phenyl-4H-selenopheno[3,2-b]indole-7-carboxylic acid (**18e**)

Light beige powder, yield 309 mg (91%), m.p. 336-337 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.36 (s, 1H), 11.95 (s, 1H), 8.43 (d, J = 0.7 Hz, 1H), 7.87 (s, 1H), 7.81 (dd, J = 8.6, 1.6 Hz, 1H), 7.72 (d, J = 7.3 Hz, 2H), 7.54 (d, J = 8.6 Hz, 1H), 7.44 (t, J = 7.7 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.2, 150.1, 146.0, 142.6, 136.4, 129.2, 127.9, 125.5, 123.7, 123.5, 121.5, 121.4, 114.4, 111.8, 111.7. HRMS (ESI) calcd for $C_{17}H_{12}NO_2Se$ m/z 342.0028 $[M+H]^+$, found m/z 342.0026 $[M+H]^+$.

2-Phenyl-7-(trifluoromethoxy)-4H-selenopheno[3,2-b]indole (**18f**)

White powder, yield 308 mg (81%), m.p. 285-286 °C. ^{1}H NMR (500 MHz, DMSO-d_6) ^{1}H NMR (500 MHz, DMSO) δ 11.80 (s, 1H), 7.85 (s, 2H), 7.72 – 7.69 (m, 2H), 7.55 (d, J = 8.8 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.37 – 7.32 (m, 1H), 7.14 (dd, J = 8.8, 1.6 Hz, 1H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 105.68 (s). ^{13}C NMR (126 MHz, DMSO-d_6) δ 150.4, 146.7, 141.5, 138.5, 136.3, 129.2, 128.0, 125.6, 124.2, 120.4 (q, J_{CF} = 254.3 Hz), 115.6, 113.2, 112.9, 111.6, 111.5. HRMS (ESI) calcd for $C_{17}H_{11}F_3NOSe$ m/z 381.9952 $[M+H]^+$, found m/z 381.9955 $[M+H]^+$.

*7-Methoxy-2-phenyl-4H-selenopheno[3,2-b]indole (**18g**)*

Grayish microcrystals, yield 235 mg (72%), m.p. 261-262 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.35 (s, 1H), 7.79 (s, 1H), 7.68 (dd, J = 8.2, 1.0 Hz, 2H), 7.42 (t, J = 7.7 Hz, 2H), 7.37 (d, J = 8.8 Hz, 1H), 7.30 (d, J = 7.3 Hz, 1H), 7.27 (d, J = 2.4 Hz, 1H), 6.82 (dd, J = 8.8, 2.5 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 153.4, 148.3, 145.4, 136.6, 135.0, 129.1, 127.6, 125.4, 124.4, 113.0, 112.8, 112.3, 111.9, 100.9, 55.4. HRMS (ESI) calcd for $C_{17}H_{14}NOSe$ m/z 328.0235 $[M+H]^+$, found m/z 328.0234 $[M+H]^+$.

7-Methyl-2-phenyl-4H-selenopheno[3,2-b]indole (**18h**)

White powder, yield 291 mg (94%), m.p. 313-314 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.41 (s, 1H), 7.80 (s, 1H), 7.70 – 7.66 (m, 2H), 7.49 (s, 1H), 7.42 (t, J = 7.7 Hz, 2H), 7.37 (d, J = 8.3 Hz,

1H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.02 (dd, *J* = 8.3, 1.2 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 148.3, 145.0, 138.4, 136.6, 129.1, 127.7, 127.6, 125.3, 124.2, 123.9, 118.5, 113.0, 111.9, 111.8, 21.1. HRMS (ESI) calcd for $C_{17}H_{14}NSe$ m/z 312.0286 $[M+H]^+$, found m/z 312.0287 $[M+H]^+$.

2-Phenyl-4H-selenopheno[3,2-b]indole-7-carbonitrile (**18i**)

Brownish powder, yield 225 mg (70%), m.p. 283-284 °C. ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 12.17 (s, 1H), 8.39 (d, *J* = 0.6 Hz, 1H), 7.89 (s, 1H), 7.73 (d, *J* = 7.3 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.53 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 151.4, 146.6, 141.9, 136.2, 129.2, 128.2, 125.7, 124.9, 124.3, 124.0, 120.6, 113.7, 113.1, 111.6, 100.8. HRMS (ESI) calcd for $C_{17}H_{11}N_2Se$ m/z 323.0082 $[M+H]^+$, found m/z 323.0081 $[M+H]^+$.

6,8-Difluoro-2-phenyl-4H-selenopheno[3,2-b]indole (**18j**)

Brownish powder, yield 226 mg (68%), m.p. 259-260 °C. ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 12.00 (s, 1H), 7.87 (s, 1H), 7.71 (dd, *J* = 8.2, 0.9 Hz, 2H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.19 (dd, *J* = 9.7, 2.0 Hz, 1H), 6.96 (td, *J* = 10.3, 2.0 Hz, 1H). ^{19}F NMR (471 MHz, DMSO-*d*$_6$) δ 45.37 (td, *J* = 9.9, 3.9 Hz), 42.49 (ddd, *J* = 10.3, 3.5, 2.7 Hz). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 158.6 (dd, J_{CF} = 237.6, 12.2 Hz), 153.7 (dd, J_{CF} = 245.8, 15.7 Hz), 149.9, 145.2 (d, J_{CF} = 2.6 Hz), 141.5 (dd, J_{CF} = 14.8, 12.9 Hz), 136.1, 129.2, 128.0, 125.5, 111.6, 110.0 (dd, J_{CF} = 22.0, 1.2 Hz), 108.9, 95.2 (dd, J_{CF} = 26.4, 4.1 Hz), 94.5 (dd, J_{CF} = 29.3, 22.9 Hz).

HRMS (ESI) calcd for $C_{16}H_{10}F_2NSe$ m/z 333.9941 $[M+H]^+$, found m/z 333.9941 $[M+H]^+$.

2-(4-Fluorophenyl)-4H-selenopheno[3,2-b]indole (**18k**)

White powder, yield 279 mg (89%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.56 (s, 1H), 7.79 (s, 1H), 7.76 – 7.69 (m, 3H), 7.48 (d, *J* = 8.1 Hz, 1H), 7.30 – 7.23 (m, 2H), 7.22 – 7.15 (m, 2H), 7.11 – 7.05 (m, 1H). ^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ 48.11 – 48.02 (m). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 161.7 (d, J_{CF} = 245.4 Hz), 147.3, 144.8, 140.0, 133.2 (d, J_{CF} = 3.3 Hz), 127.4 (d, J_{CF} = 8.0 Hz), 124.0, 122.3, 119.1, 118.8, 116.1, 115.9, 113.5, 112.1, 112.0. HRMS (ESI) calcd for $C_{16}H_{11}FNSe$ m/z 316.0035 $[M+H]^+$, found m/z 316.0034 $[M+H]^+$

2-(4-Chlorophenyl)-4H-selenopheno[3,2-b]indole (**18l**)

Yellowish powder, yield 314 mg (95%), m.p. >350 °C. ^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 11.59 (s, 1H), 7.87 (s, 1H), 7.75 – 7.69 (m, 3H), 7.51 – 7.45 (m, 3H), 7.23 – 7.17 (m, 1H), 7.11 – 7.06 (m, 1H). ^{13}C NMR (126 MHz, DMSO-*d*$_6$) δ 146.9, 144.8, 140.1, 135.5, 132.0, 129.1, 127.0, 124.0,

122.5, 119.1, 119.0, 114.0, 112.5, 112.2. HRMS (ESI) calcd for $C_{16}H_{11}ClNSe$ m/z 331.9740 $[M+H]^+$, found m/z 331.9732 $[M+H]^+$.

2-(3-Methoxyphenyl)-4H-selenopheno[3,2-b]indole (**18m**)

Beige plates, yield 271 mg (83%), m.p. 224-225 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.55 (s, 1H), 7.85 (s, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.1 Hz, 1H), 7.38 – 7.31 (m, 1H), 7.27 – 7.16 (m, 3H), 7.11 – 7.05 (m, 1H), 6.93 – 6.87 (m, 1H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.8, 148.4, 144.7, 140.1, 137.9, 130.3, 124.1, 122.4, 119.1, 118.9, 118.1, 113.5, 113.3, 112.2, 110.7, 55.2. HRMS (ESI) calcd for $C_{17}H_{14}NOSe$ m/z 328.0235 $[M+H]^+$, found m/z 328.0234 $[M+H]^+$.

General procedure for the preparation of PySeI compounds **19**

Ester **13** (255 mg, 1 mmol) was immersed in IPA (9 ml) and suspended. Then, a solution of NaOH (160 mg, 4 mmol) in water (1 ml) was added in one portion to this suspension, and the resulting mixture was stirred and heated at reflux (100 °C) for 2 h. The resulting solution was evaporated to dryness under reduced pressure, and the obtained residue was dissolved in glacial AcOH (7 ml). An appropriate arylhydrazine hydrochloride (1.2 mmol) was added, and the reaction mixture was stirred and heated at reflux (130 °C) for 2 h. After that a mixture was cooled to ambient temperature and diluted with MeOH (14 ml). The formed precipitate was filtered, washed with a 50% aqueous MeOH (3 × 4 ml) and dried at 120 °C to afford product in an analytically pure form.

5H-Pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19a**)

Greenish microcrystals, yield 260 mg (96%), m.p. 317-318 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.31 (s, 1H), 8.48 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.37 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.62 (d, *J* = 8.2 Hz, 1H), 7.54 (dd, *J* = 7.9, 4.7 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.18 – 7.13 (m, 1H). ^{77}Se NMR (114 MHz, DMSO-d_6) δ 404.45; ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.7, 145.5, 139.4, 135.0, 128.5, 124.6, 124.3, 123.3, 120.2, 119.8, 119.7, 1125, 110.1. HRMS (ESI) calcd for $C_{13}H_9N_2Se$ m/z 272.9925 $[M+H]^+$, found m/z 272.9930 $[M+H]^+$.

8-(tert-Butyl)-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19b**)

Yellowish microcrystals, yield 307 mg (94%), m.p. 299-300 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.13 (s, 1H), 8.46 (dd, *J* = 4.7, 1.7 Hz, 1H), 8.34 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.80 (d, *J* = 1.6 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.38 (dd, *J* = 8.7, 1.9 Hz, 1H), 1.38 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.7, 145.2, 142.2, 137.5, 135.1, 128.2, 124.8, 124.2, 121.6, 120.2, 115.6, 112.0, 110.3,

34.5, 31.7. HRMS (ESI) calcd for $C_{17}H_{17}N_2Se$ m/z 329.0551 $[M+H]^+$, found m/z 329.0552 $[M+H]^+$.

8-Fluoro-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19c**)

Light yellow solid, yield 231 mg (80%), m.p. 314-315 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.39 (s, 1H), 8.49 (dd, J = 4.7, 1.7 Hz, 1H), 8.38 (dd, J = 7.9, 1.7 Hz, 1H), 7.71 (dd, J = 9.8, 2.5 Hz, 1H), 7.61 (dd, J = 8.9, 4.5 Hz, 1H), 7.54 (dd, J = 7.9, 4.7 Hz, 1H), 7.13 (td, J = 9.2, 2.6 Hz, 1H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 39.07 (td, J = 9.6, 4.6 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.0, 156.9 (d, J_{CF} = 232.8 Hz), 145.9, 136.9, 136.0, 128.7, 124.5 (d, J_{CF} = 11.2 Hz), 124.4, 120.3, 113.4 (d, J_{CF} = 9.8 Hz), 111.4 (d, J_{CF} = 26.2 Hz), 109.7 (d, J_{CF} = 4.7 Hz), 104.8 (d, J_{CF} = 24.7 Hz). HRMS (ESI) calcd for $C_{13}H_8FN_2Se$ m/z 290.9831 $[M+H]^+$, found m/z 290.9836 $[M+H]^+$.

12H-Benzo[g]pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19d**)

Pink microcrystals, yield 289 mg (90%), m.p. >350 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.09 (s, 1H), 8.50 – 8.42 (m, 3H), 8.02 (d, J = 8.1 Hz, 1H), 7.94 (d, J = 8.6 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.57 (dd, J = 7.9, 4.7 Hz, 1H), 7.52 (dd, J = 11.1, 3.9 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.4, 145.1, 134.4, 133.5, 130.5, 128.7, 128.0, 125.9, 124.8, 124.7, 122.3, 120.9, 120.6, 120.3, 120.2, 119.7, 111.9. HRMS (ESI) calcd for $C_{17}H_{11}N_2Se$ m/z 323.0082 $[M+H]^+$, found m/z 323.0083 $[M+H]^+$.

5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole-8-carboxylic acid (**19e**)

Grayish powder, yield 274 mg (87%), m.p. >350 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.68 (s, 1H), 12.60 (s, 1H), 8.57 (s, 1H), 8.51 (dd, J = 4.6, 1.6 Hz, 1H), 8.40 (dd, J = 7.9, 1.5 Hz, 1H), 7.90 (dd, J = 8.6, 1.5 Hz, 1H), 7.68 (d, J = 8.6 Hz, 1H), 7.56 (dd, J = 7.9, 4.7 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.0, 165.1, 145.9, 141.8, 136.4, 128.8, 124.3, 124.0, 122.6, 122.2, 120.3, 112.2, 111.3. HRMS (ESI) calcd for $C_{14}H_9N_2O_2Se$ m/z 316.9824 $[M+H]^+$, found m/z 316.9824 $[M+H]^+$.

8-(Trifluoromethoxy)-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19f**)

Yellowish powder, yield 316 mg (89%), m.p. 266-267 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.57 (s, 1H), 8.52 (dd, J = 4.7, 1.6 Hz, 1H), 8.40 (dd, J = 7.9, 1.6 Hz, 1H), 7.99 (s, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.55 (dd, J = 7.9, 4.7 Hz, 1H), 7.25 (dd, J = 8.8, 1.5 Hz, 1H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 105.71 (s). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.2, 146.1, 141.8, 137.8, 137.1, 128.9, 124.5, 124.3, 120.4 (q, J = 254.7 Hz), 120.3, 116.8, 113.5, 112.5, 110.1. HRMS (ESI) calcd for $C_{14}H_8F_3N_2OSe$ m/z 356.9748 $[M+H]^+$, found m/z 356.9754 $[M+H]^+$.

8-Methoxy-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19g**)

Brownish microcrystals, yield 232 mg (77%), m.p. 242-243 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.46 (dd, J = 4.7, 1.7 Hz, 1H), 8.33 (dd, J = 7.9, 1.7 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.38 (d, J = 2.4 Hz, 1H), 6.93 (dd, J = 8.8, 2.5 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.7, 153.7, 145.4, 135.6, 134.3, 128.3, 124.8, 124.7, 120.2, 113.7, 113.2, 109.6, 101.4, 55.4. HRMS (ESI) calcd for $C_{14}H_{11}N_2OSe$ m/z 303.0031 $[M+H]^+$, found m/z 303.0034 $[M+H]^+$.

8-Methyl-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19h**)

Beige cotton-like needles, yield 257 mg (90%), m.p. 300-301 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.16 (s, 1H), 8.46 (dd, J = 4.7, 1.6 Hz, 1H), 8.34 (dd, J = 7.9, 1.6 Hz, 1H), 7.60 (s, 1H), 7.54 – 7.48 (m, 2H), 7.12 (dd, J = 8.4, 1.2 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.6, 145.3, 137.7, 135.1, 128.4, 128.3, 124.9, 124.7, 124.5, 120.2, 119.3, 112.2, 109.6, 21.1. HRMS (ESI) calcd for $C_{14}H_{11}N_2Se$ m/z 287.0082 $[M+H]^+$, found m/z 287.0086 $[M+H]^+$.

5H-Pyrido[3',2':4,5]selenopheno[3,2-b]indole-8-carbonitrile (**19i**)

Brown solid, yield 201 mg (68%), m.p. >350 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.91 (s, 1H), 8.57 – 8.51 (m, 2H), 8.43 (dd, J = 7.9, 1.7 Hz, 1H), 7.78 (d, J = 8.5 Hz, 1H), 7.63 (dd, J = 8.5, 1.6 Hz, 1H), 7.57 (dd, J = 7.9, 4.7 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.3, 146.4, 141.1, 137.1, 129.1, 125.7, 125.6, 124.3, 124.0, 120.4, 120.4, 113.6, 110.7, 101.6. HRMS (ESI) calcd for $C_{14}H_8N_3Se$ m/z 297.9878 $[M+H]^+$, found m/z 297.9879 $[M+H]^+$.

7,9-Difluoro-5H-pyrido[3',2':4,5]selenopheno[3,2-b]indole (**19j**)

Pinkish microneedles, yield 276 mg (90%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.77 (s, 1H), 8.52 (dd, J = 4.7, 1.7 Hz, 1H), 8.42 (dd, J = 7.9, 1.7 Hz, 1H), 7.57 (dd, J = 7.9, 4.7 Hz, 1H), 7.37 (dd, J = 9.6, 2.0 Hz, 1H), 7.05 (td, J = 10.4, 2.0 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 46.73 (td, J = 9.9, 4.4 Hz), 42.74 (ddd, J = 10.5, 4.3, 2.4 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.6, 159.2 (dd, J_{CF} = 238.7, 12.4 Hz), 154.3 (dd, J_{CF} = 247.1, 15.7 Hz), 145.8, 140.8 (dd, J_{CF} = 14.9, 12.6 Hz), 135.5 (d, J_{CF} = 2.9 Hz), 129.0, 123.8, 120.5, 110.4 (d, J_{CF} = 21.8 Hz), 105.7, 95.6 (dd, J_{CF} = 26.4, 4.3 Hz), 95.2 (dd, J_{CF} = 29.6, 22.8 Hz). HRMS (ESI) calcd for $C_{13}H_7F_2N_2Se$ m/z 308.9737 $[M+H]^+$, found m/z 308.9743 $[M+H]^+$

General procedure for the preparation of PzSeI compounds **20**

Ester **14** (256 mg, 1 mmol) was suspended in IPA (9 ml) and a solution of NaOH (160 mg, 4 mmol) in water (1 ml) was added in one portion to this suspension. The resulting mixture was stirred and heated at reflux (100 °C) for 2 h. The formed solution was concentrated under vacuum,

and the residue was dissolved in glacial AcOH (7 ml). An appropriate arylhydrazine hydrochloride (1.2 mmol) was added, and the reaction mixture was stirred and heated at reflux (130 °C) for 2 h. After that a mixture was cooled to ambient temperature and diluted with MeOH (14 ml). The formed precipitate was filtered off, washed with a 50% aqueous MeOH (3 × 4 ml) and dried at 120 °C to afford product in an analytically pure form.

10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20a**)

Light yellow solid, yield 264 mg (97%), m.p. 266-267 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 8.73 (d, J = 2.5 Hz, 1H), 8.50 (d, J = 2.5 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.3 Hz, 1H), 7.39 – 7.33 (m, 1H), 7.22 – 7.17 (m, 1H). ^{77}Se NMR (114 MHz, DMSO-d_6) δ 384.55; ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.0, 141.7, 141.1, 140.3, 139.2, 133.5, 124.7, 124.0, 120.4, 120.0, 114.2, 113.0. HRMS (ESI) calcd for $C_{12}H_8N_3Se$ m/z 273.9878 $[M+H]^+$, found m/z 273.9880 $[M+H]^+$.

7-(tert-Butyl)-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20b**)

Light yellow powder, yield 321 mg (98%), m.p. 251-252 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.45 (s, 1H), 8.71 (d, J = 2.5 Hz, 1H), 8.48 (d, J = 2.5 Hz, 1H), 7.94 (s, 1H), 7.53 (d, J = 8.7 Hz, 1H), 7.46 (dd, J = 8.7, 1.8 Hz, 1H), 1.38 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.0, 142.6, 141.8, 141.0, 138.9, 138.5, 133.5, 123.9, 123.1, 116.1, 114.4, 112.5, 34.5, 31.7. HRMS (ESI) calcd for $C_{16}H_{16}N_3Se$ m/z 330.0504 $[M+H]^+$, found m/z 330.0510 $[M+H]^+$.

7-Fluoro-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20c**)

Yellowish powder microneedles, yield 264mg (91%), m.p. 280-281 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.70 (s, 1H), 8.74 (d, J = 2.5 Hz, 1H), 8.53 (d, J = 2.5 Hz, 1H), 7.86 (dd, J = 9.8, 2.6 Hz, 1H), 7.59 (dd, J = 9.0, 4.5 Hz, 1H), 7.22 (td, J = 9.2, 2.6 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 39.63 (td, J = 9.6, 4.6 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.3, 156.9 (d, J_{CF} = 233.4 Hz), 141.5, 141.1, 139.6, 136.9, 135.1, 124.1 (d, J_{CF} = 11.2 Hz), 114.0 (d, J_{CF} = 9.7 Hz), 113.6 (d, J_{CF} = 5.1 Hz), 113.0 (d, J_{CF} = 26.4 Hz), 105.3 (d, J_{CF} = 24.7 Hz). HRMS (ESI) calcd for $C_{12}H_7FN_3OSe$ m/z 291.9784 $[M+H]^+$, found m/z 291.9783 $[M+H]^+$.

12H-benzo[g]pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20d**)

Yellowish solid, yield 306 mg (95%), m.p. 269-270 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.58 (s, 1H), 8.73 (t, J = 6.4 Hz, 2H), 8.49 (d, J = 2.5 Hz, 1H), 8.02 (dd, J = 8.3, 4.9 Hz, 2H), 7.64 (t, J = 7.7 Hz, 2H), 7.55 (t, J = 7.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.7, 141.8, 140.9,

138.7, 135.8, 132.0, 131.2, 128.6, 126.0, 125.4, 122.5, 121.9, 121.1, 120.1, 119.7, 115.8. HRMS (ESI) calcd for $C_{16}H_{10}N_3Se$ m/z 324.0034 $[M+H]^+$, found m/z 324.0038 $[M+H]^+$.

10H-Pyrazino[2',3':4,5]selenopheno[3,2-b]indole-7-carboxylic acid (**20e**)

Orange powder, yield 303 mg (96%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.98 (s, 1H), 12.64 (s, 1H), 8.75 (d, J = 2.5 Hz, 1H), 8.71 (s, 1H), 8.54 (d, J = 2.5 Hz, 1H), 7.95 (d, J = 8.7 Hz, 1H), 7.65 (d, J = 8.7 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.9, 160.4, 142.6, 141.3, 141.2, 139.6, 134.8, 125.5, 123.7, 123.4, 122.5, 115.4, 112.7. HRMS (ESI) calcd for $C_{13}H_6N_3O_2Se$ m/z 315.9631 $[M-H]^+$, found m/z 315.9627 $[M-H]^+$.

7-(Trifluoromethoxy)-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20f**)

Light yellow powder, yield 253 mg (71%), m.p. 254-255 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.89 (s, 1H), 8.75 (d, J = 2.5 Hz, 1H), 8.55 (d, J = 2.5 Hz, 1H), 8.16 (s, 1H), 7.67 (d, J = 9.0 Hz, 1H), 7.33 (dd, J = 8.9, 1.6 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 105.66 (s). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.5, 142.0, 141.3, 141.2, 139.8, 138.7, 135.4, 124.1, 120.4 (q, J_{CF} = 254.8 Hz), 118.2, 114.0, 114.0, 113.1. HRMS (ESI) calcd for $C_{13}H_7F_3N_3OSe$ m/z 357.9701 $[M+H]^+$, found m/z 357.9706 $[M+H]^+$

7-Methoxy-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20g**)

Light orange powder, yield 236 mg (78%), m.p. 285-286 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.44 (s, 1H), 8.70 (d, J = 2.5 Hz, 1H), 8.48 (d, J = 2.5 Hz, 1H), 7.50 (dd, J = 7.5, 5.8 Hz, 2H), 7.00 (dd, J = 8.9, 2.5 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.0, 153.8, 141.8, 141.0, 139.0, 135.3, 133.9, 124.4, 115.5, 113.6, 113.5, 101.5, 55.5. HRMS (ESI) calcd for $C_{13}H_{10}N_3OSe$ m/z 303.9984 $[M+H]^+$, found m/z 303.9983 $[M+H]^+$.

7-Methyl-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20h**)

Yellow powder, yield 180 mg (63%), m.p. 229-230 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.48 (s, 1H), 8.71 (d, J = 2.5 Hz, 1H), 8.48 (d, J = 2.5 Hz, 1H), 7.72 (s, 1H), 7.49 (d, J = 8.4 Hz, 1H), 7.19 (dd, J = 8.4, 1.1 Hz, 1H), 2.44 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.9, 141.7, 141.0, 139.0, 138.6, 133.5, 128.8, 126.4, 124.2, 119.7, 113.6, 112.7, 21.1. HRMS (ESI) calcd for $C_{13}H_{10}N_3Se$ m/z 288.0034 $[M+H]^+$, found m/z 288.0039 $[M+H]^+$

10H-Pyrazino[2',3':4,5]selenopheno[3,2-b]indole-7-carbonitrile (**20i**)

Grayish powder, yield 235 mg (79%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.23 (s, 1H), 8.79 (d, J = 2.5 Hz, 1H), 8.68 (s, 1H), 8.58 (d, J = 2.5 Hz, 1H), 7.76 – 7.67 (m, 2H). ^{13}C NMR

(126 MHz, DMSO-d_6) δ 160.6, 141.9, 141.4, 141.1, 140.2, 135.6, 126.8, 126.6, 124.0, 120.2, 114.7, 114.1, 101.9. HRMS (ESI) calcd for $C_{13}H_7N_4Se$ m/z 298.9830 $[M+H]^+$, found m/z 298.9830 $[M+H]^+$.

6,8-Difluoro-10H-pyrazino[2',3':4,5]selenopheno[3,2-b]indole (**20j**)

Brown microcrystals, yield 274 mg (89%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.10 (s, 1H), 8.77 (d, J = 2.5 Hz, 1H), 8.55 (d, J = 2.5 Hz, 1H), 7.24 (dd, J = 9.5, 2.0 Hz, 1H), 7.10 (td, J = 10.3, 2.0 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 48.85 (td, J = 9.8, 5.1 Hz), 44.02 (ddd, J = 10.5, 5.1, 2.3 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.9 (dd, J_{CF} = 240.8, 12.2 Hz), 159.7, 154.8 (dd, J_{CF} = 248.5, 15.8 Hz), 141.6 (dd, J_{CF} = 14.9, 12.1 Hz), 141.4, 140.7, 139.5, 133.9, 110.3 (d, J_{CF} = 22.0 Hz), 109.9, 95.9 – 95.7 (m), 95.6 – 95.4 (m). HRMS (ESI) calcd for $C_{12}H_6F_2N_3Se$ m/z 309.9690 $[M+H]^+$, found m/z 309.9691 $[M+H]^+$.

General procedure for the synthesis of CSeI compounds **21**

NaOH (0.08 g, 2 mmol) in water (1 ml) was added to a stirred suspension of ester **15a** (161 mg, 0.5 mmol) or ester **15b** (141 mg, 0.4 mmol) in IPA (9 ml), and the reaction mixture was stirred and heated at reflux (100 °C) for 2 h. Then, the solution was concentrated to dryness under reduced pressure. The residue was dissolved in glacial AcOH (7 ml) and phenylhydrazine hydrochloride **17a** (0.6 mmol or 0.5 mmol) was added to the formed solution. The reaction mixture was stirred and heated at reflux (130 °C) for 2 h, after that it cooled to ambient temperature. The precipitate was filtered, washed with 50% aqueous MeOH (3×10 ml) and dried at 120 °C to give compound in an analytically pure form.

6H,7H-Chromeno[3',4':4,5]selenopheno[3,2-b]indol-6-one (**21a**)

Yellow crystals, yield 159 mg (94%), m.p. 330-331 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.05 (s, 1H), 8.01 – 7.94 (m, 2H), 7.66 – 7.57 (m, 2H), 7.53 (dd, J = 8.3, 1.0 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.31 – 7.25 (m, 1H), 7.19 – 7.13 (m, 1H). ^{77}Se NMR (114 MHz, DMSO-d_6) δ 445.95; ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.2, 153.8, 149.6, 140.5, 139.7, 130.5, 125.2, 124.4, 123.3, 119.9, 119.7, 119.4, 116.9, 114.1, 113.8, 113.1. HRMS (ESI) calcd for $C_{17}H_{10}NO_2Se$ m/z 339.9871 $[M+H]^+$, found m/z 339.9873 $[M+H]^+$.

3-Methoxy-6H,7H-chromeno[3',4':4,5]selenopheno[3,2-b]indol-6-one (**21b**)

Yellow powder, yield 90 mg (61%), m.p. 336-337 °C. ^{1}H NMR (500 MHz, DMSO) δ 11.97 (s, 1H), 7.90 (dd, J = 12.6, 8.3 Hz, 2H), 7.63 (d, J = 8.2 Hz, 1H), 7.28 – 7.23 (m, 1H), 7.14 (dd, J = 14.5, 5.1 Hz, 2H), 7.02 (dd, J = 8.7, 2.5 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (126 MHz, DMSO) δ

161.4, 156.4, 154.8, 151.3, 140.3, 139.7, 125.6, 123.4, 122.9, 119.6, 119.1, 113.3, 113.0, 112.4, 111.6, 101.3, 56.0. HRMS (ESI) calcd for $C_{18}H_{12}NO_3Se$ m/z 369.9977 $[M+H]^+$, found m/z 369.9972 $[M+H]^+$.

General procedure for the preparation of BSeI compounds **22**

Ester **16** (254 mg, 1 mmol) was placed in IPA (9 ml) and suspended. A solution of NaOH (160 mg, 4 mmol) in water (1 ml) was added in one portion, and the resulting mixture was stirred and heated at reflux (100 °C) for 2 h. The obtained solution was evaporated to dryness under reduced pressure, and the residue was dissolved in glacial AcOH (7 ml). An appropriate arylhydrazine hydrochloride (1.2 mmol) was added, and the reaction mixture was stirred and heated at reflux (130 °C) for 2 h. After that the obtained mixture was cooled to ambient temperature and diluted with MeOH (14 ml). The formed precipitate was filtered off, washed with a 50% aqueous MeOH (3 × 4 ml) and dried at 120 °C to afford product in an analytically pure form.

10H-benzo[4,5]selenopheno[3,2-b]indole (**22a**)

Light beige plates, yield 143 mg (53%), m.p. 246-247 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (s, 1H), 8.13 – 8.04 (m, 1H), 7.76 (d, J = 7.8 Hz, 1H), 7.57 (d, J = 8.2 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.34 – 7.21 (m, 1H), 7.16 – 7.09 (m, 1H). ^{77}Se NMR (114 MHz, DMSO-d_6) δ 378.88. ^{13}C NMR (126 MHz, DMSO-d_6) δ 141.7, 139.9, 139.1, 129.3, 127.7, 125.0, 124.4, 124.3, 122.7, 121.4, 119.4, 119.3, 112.4, 111.0. HRMS (ESI) calcd for $C_{14}H_9NSe$ m/z 270.9895 $[M]^+$, found m/z 270.9896 $[M]^+$.

3-(tert-Butyl)-10H-benzo[4,5]selenopheno[3,2-b]indole (**22b**)

White plates, yield 231 mg (71%), m.p. 223-224 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.99 (s, 1H), 8.06 (dd, J = 15.6, 7.6 Hz, 2H), 7.73 (d, J = 1.7 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.36 – 7.25 (m, 2H), 1.38 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 141.8, 141.6, 139.1, 138.0, 129.4, 127.6, 124.9, 124.2, 124.2, 121.3, 120.9, 115.2, 111.8, 111.1, 34.4, 31.8. HRMS (ESI) calcd for $C_{18}H_{17}NSe$ m/z 327.0521 $[M]^+$, found m/z 327.0525 $[M]^+$.

3-Fluoro-10H-benzo[4,5]selenopheno[3,2-b]indole (**22c**)

Light beige microcystals, yield 181 mg (63%), m.p. 248-249 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.23 (s, 1H), 8.08 (dd, J = 12.0, 7.9 Hz, 2H), 7.64 (dd, J = 9.9, 2.6 Hz, 1H), 7.56 (dd, J = 8.9, 4.5 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.35 – 7.29 (m, 1H), 7.08 (td, J = 9.3, 2.6 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 38.64 (td, J = 9.7, 4.6 Hz). ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.8 (d, J_{CF} = 232.2 Hz), 142.1, 140.9, 136.5, 129.0, 127.7, 125.0, 124.8, 124.5 (d, J_{CF} = 11.0 Hz), 113.2

(d, J_{CF} = 9.7 Hz), 110.7, 110.6 (d, J_{CF} = 4.7 Hz), 110.5, 104.5 (d, J_{CF} = 24.5 Hz). HRMS (APCI) calcd for $C_{14}H_8FNSe$ m/z 288.9801 $[M]^+$, found m/z 288.9802 $[M]^+$.

12H-benzo[g]benzo[4,5]selenopheno[3,2-b]indole (**22d**)

Pink powder, yield 179 mg (56%), m.p. 240-241 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.91 (s, 1H), 8.49 (d, J = 8.2 Hz, 1H), 8.19 (d, J = 7.3 Hz, 1H), 8.11 (d, J = 7.9 Hz, 1H), 8.00 (d, J = 8.1 Hz, 1H), 7.90 (d, J = 8.6 Hz, 1H), 7.68 – 7.57 (m, 2H), 7.55 – 7.46 (m, 2H), 7.34 – 7.27 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 141.4, 137.6, 134.6, 130.3, 129.5, 128.7, 127.7, 125.7, 125.1, 124.3, 124.1, 122.4, 121.1, 120.9, 120.2, 120.1, 119.6, 112.9. HRMS (APCI) calcd for $C_{18}H_{12}NSe$ m/z 322.0129 $[M+H]^+$, found m/z 322.0133 $[M+H]^+$.

Benzo[4,5]selenopheno[3,2-b]indole-3-carboxylic acid (**22e**)

Light orange microcrystals, yield 182 mg (58%), m.p. >350 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.57 (s, 1H), 12.54 (s, 1H), 8.49 (d, J = 1.4 Hz, 1H), 8.12 (dd, J = 12.8, 7.9 Hz, 2H), 7.87 (dd, J = 8.6, 1.6 Hz, 1H), 7.63 (d, J = 8.6 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.36 – 7.30 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.1, 142.4, 142.3, 140.4, 129.0, 127.7, 125.1, 124.9, 124.0, 123.8, 122.1, 121.9, 121.6, 112.3, 112.1. HRMS (ESI) calcd for $C_{15}H_8NO_2Se$ m/z 313.9726 $[M-H]^+$, found m/z 313.9724 $[M-H]^+$.

3-(Trifluoromethoxy)-10H-benzo[4,5]selenopheno[3,2-b]indole (**22f**)

Light yellow solid, yield 273 mg (77%), m.p. 220-221 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.43 (s, 1H), 8.15 – 8.07 (m, 2H), 7.91 (s, 1H), 7.64 (d, J = 8.8 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.37 – 7.31 (m, 1H), 7.21 (dd, J = 8.8, 1.5 Hz, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ 105.72 (s). ^{13}C NMR (126 MHz, DMSO-d_6) δ 142.4, 141.7 (d, J_{CF} = 1.6 Hz), 141.1, 138.3, 128.9, 127.7, 125.0, 125.0, 124.4, 121.7, 120.5 (q, J = 254.5 Hz), 116.0, 113.2, 112.1, 111.0. HRMS (APCI) calcd for $C_{15}H_8F_3NOSe$ m/z 354.9718 $[M]^+$, found m/z 354.9720 $[M]^+$.

2. References

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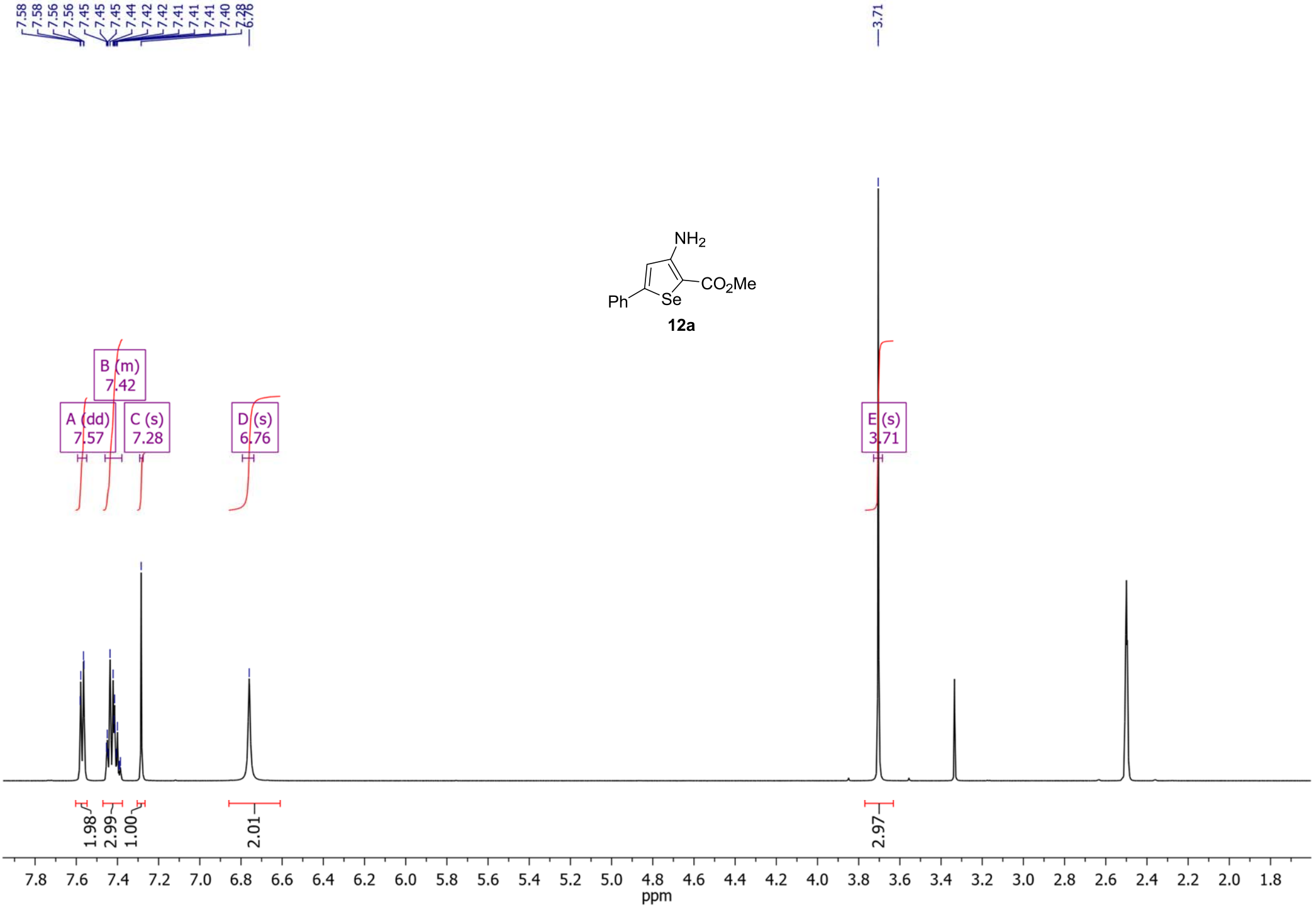
2 V. P. Litvinov, V. Y. Mortikov, Y. A. Sharanin and A. M. Shestopalov, *Synthesis (Stuttg).*, 1985, **1985**, 98–99.

3 M. A. Abd ul-Malik, A. M. Kamal El-Dean, S. M. Radwan and R. M. Zaki, *J. Heterocycl. Chem.*, 2021, **58**, 2067–2077.

4 S. H. Abdel-Hafez, A. Elkhateeb, A. A. Gobouri, I. H. El Azab and G. Kirsch, *Heterocycles*, 2016, **92**, 1054–1062.

3. Copies of NMR spectra

^{1}H NMR (solvent: DMSO-d_6)



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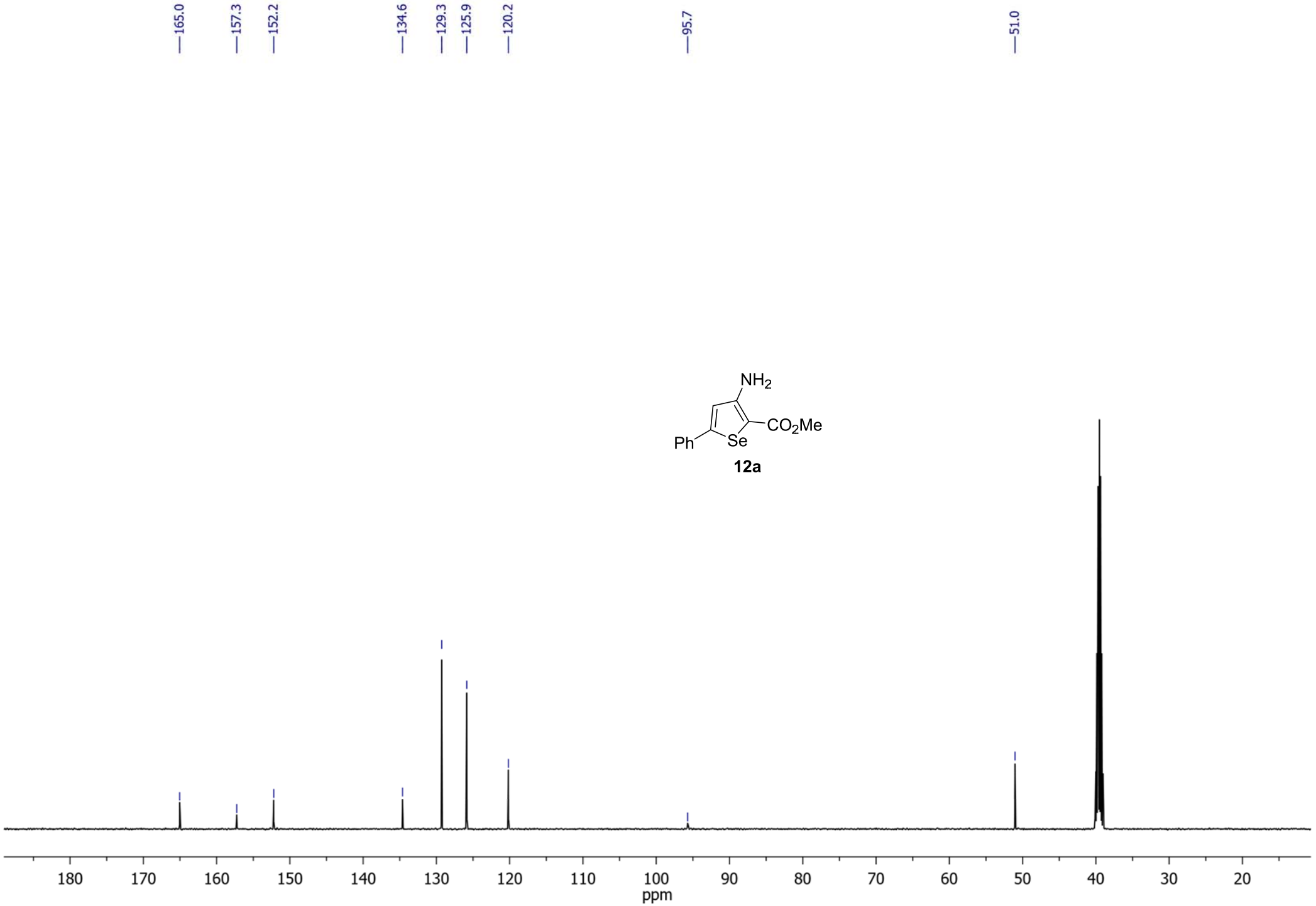

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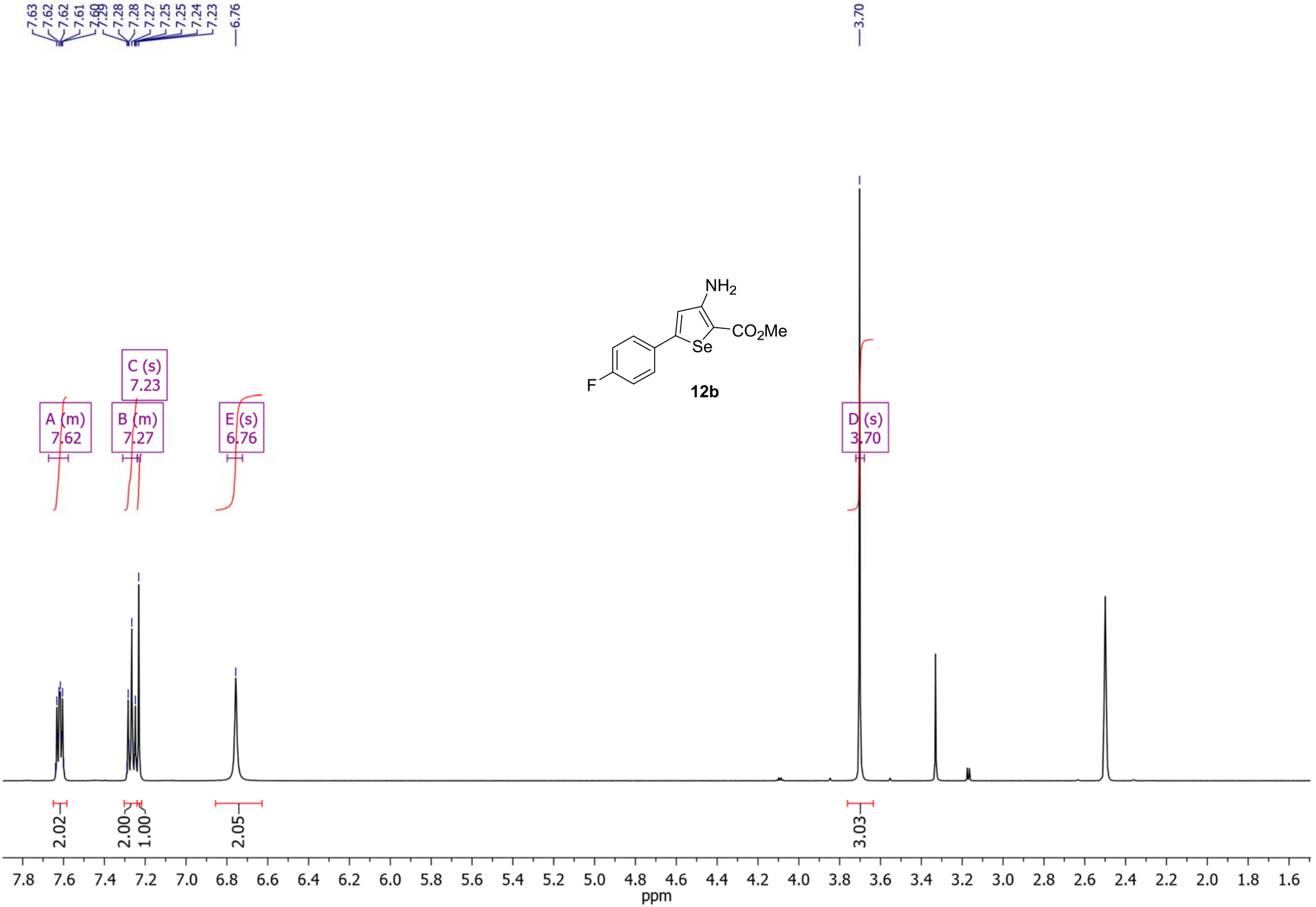

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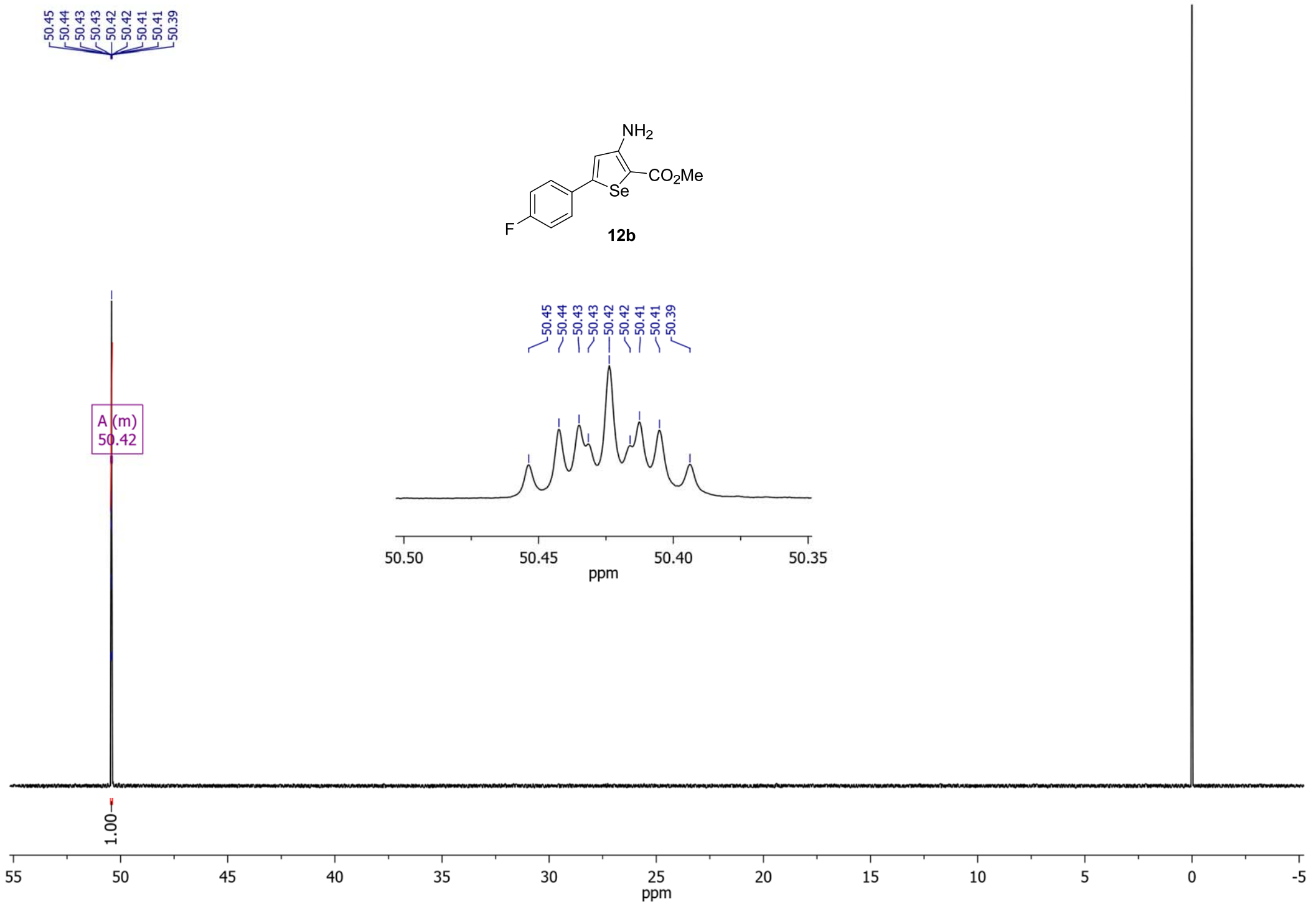

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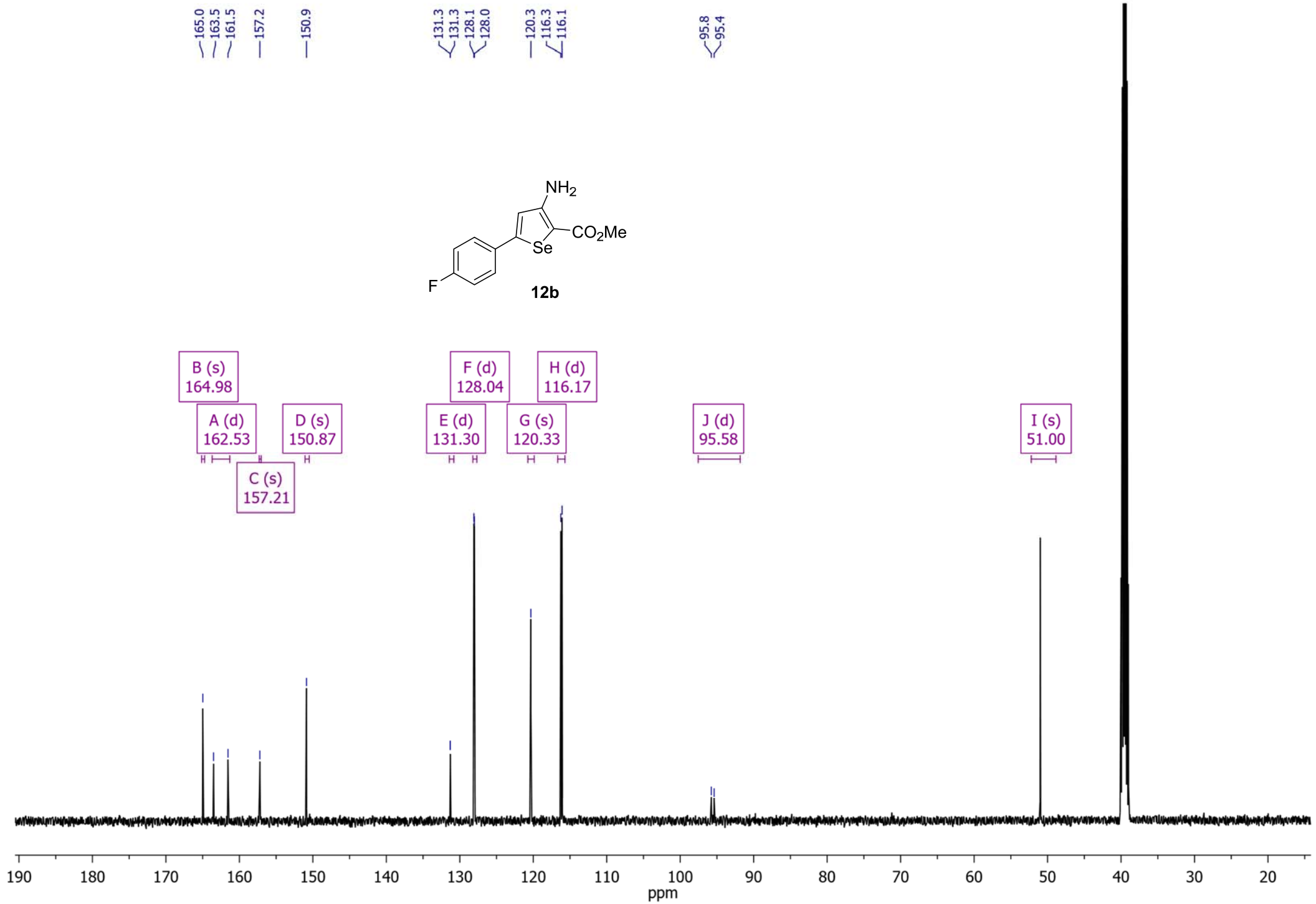

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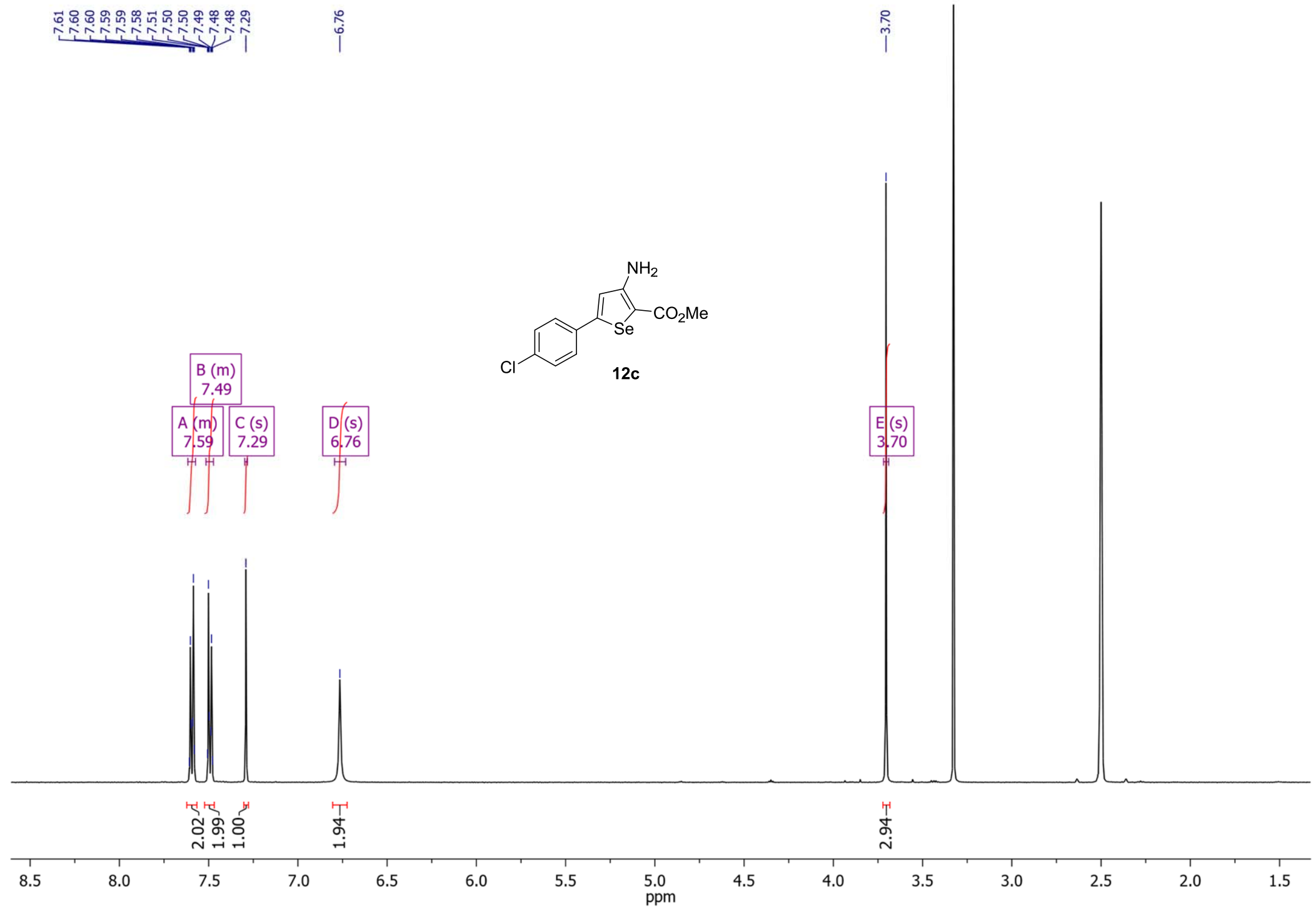

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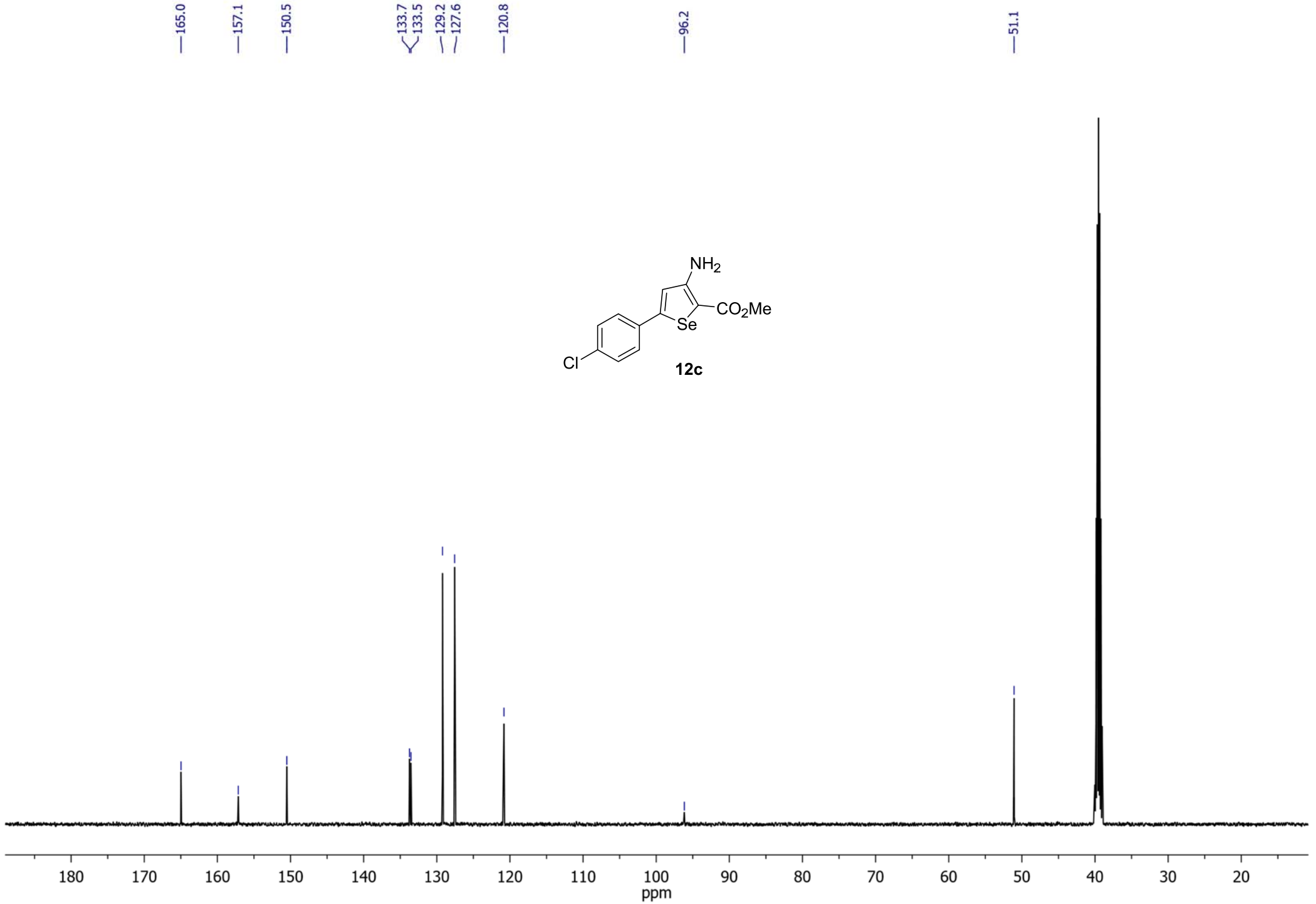

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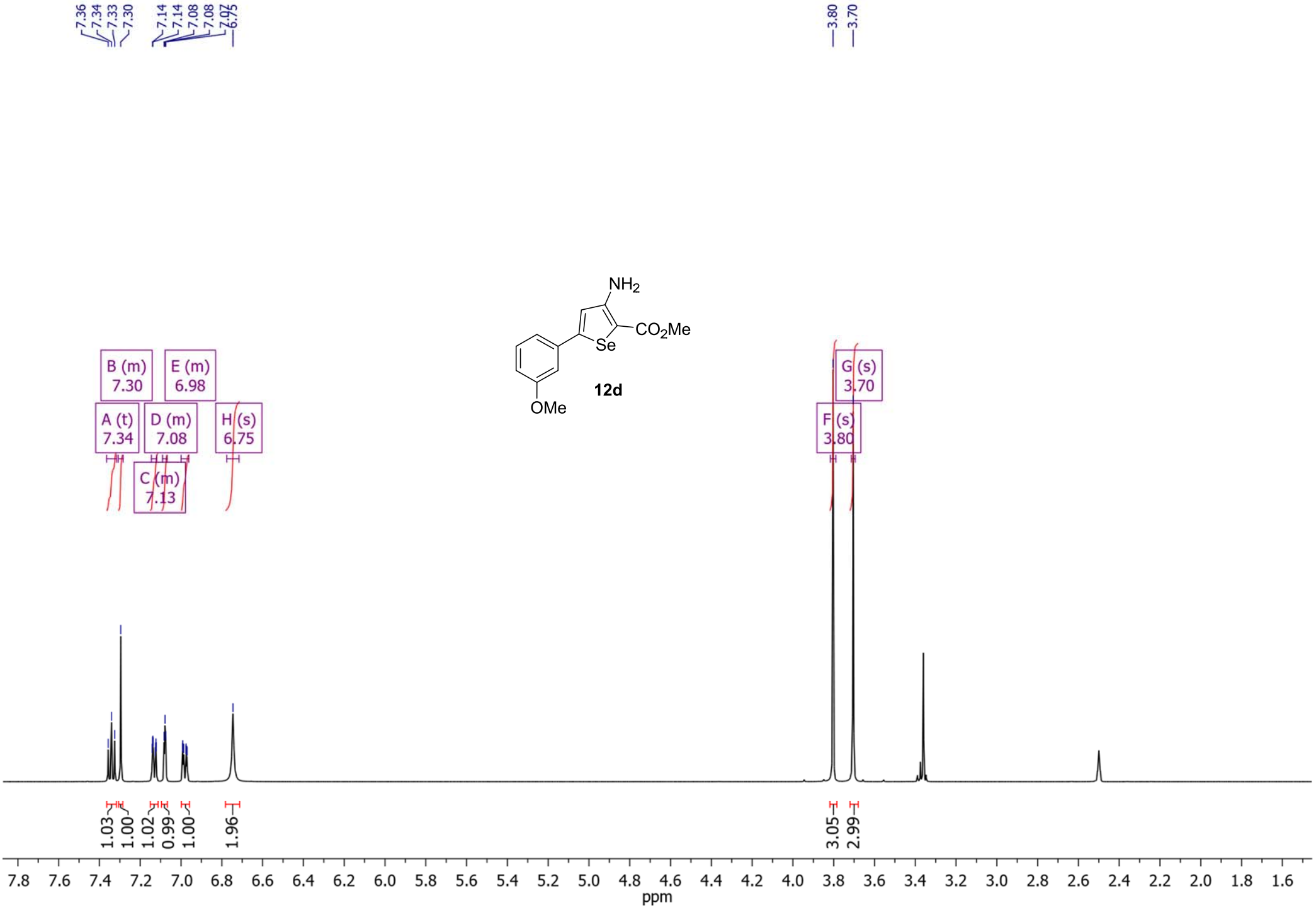

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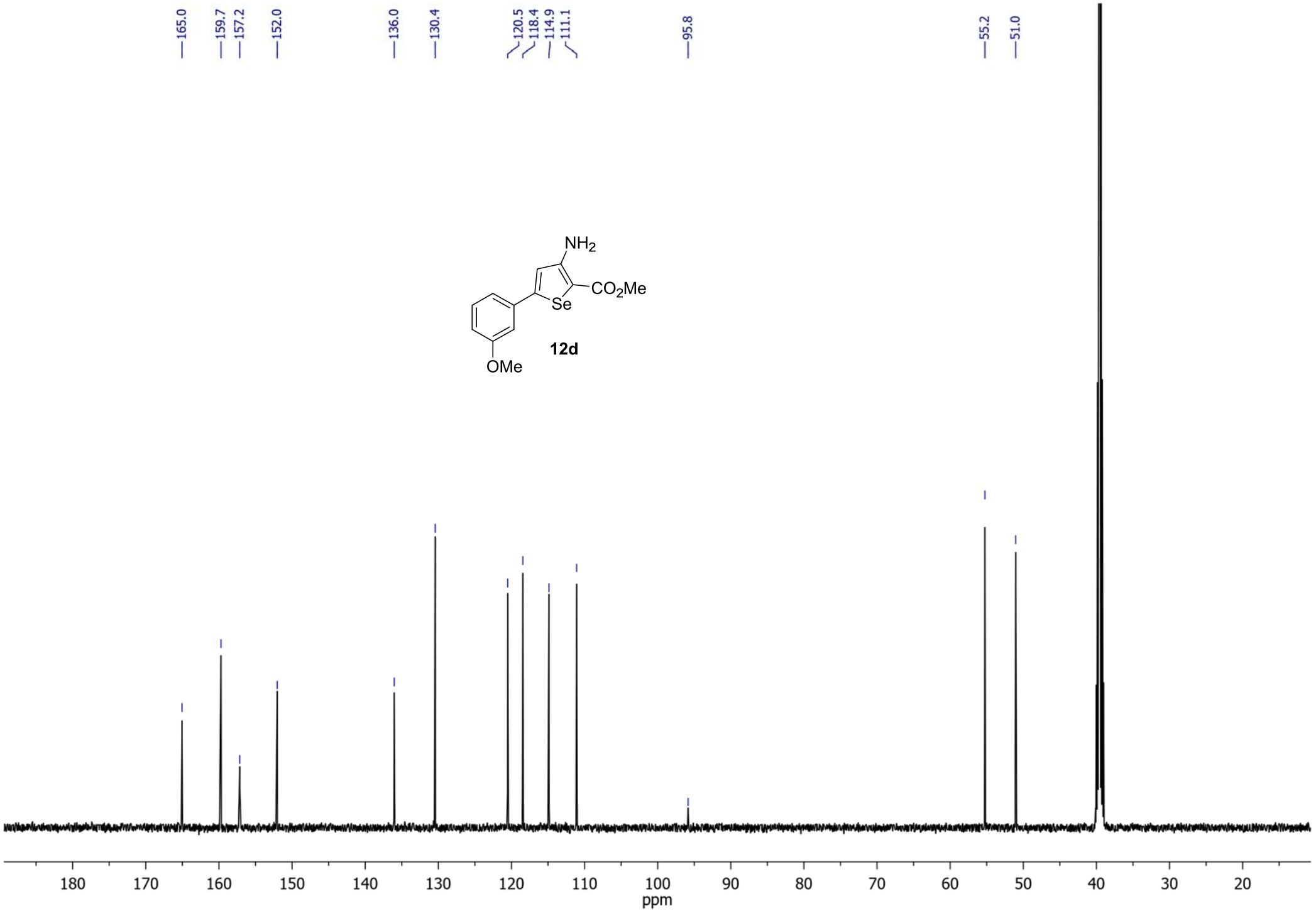

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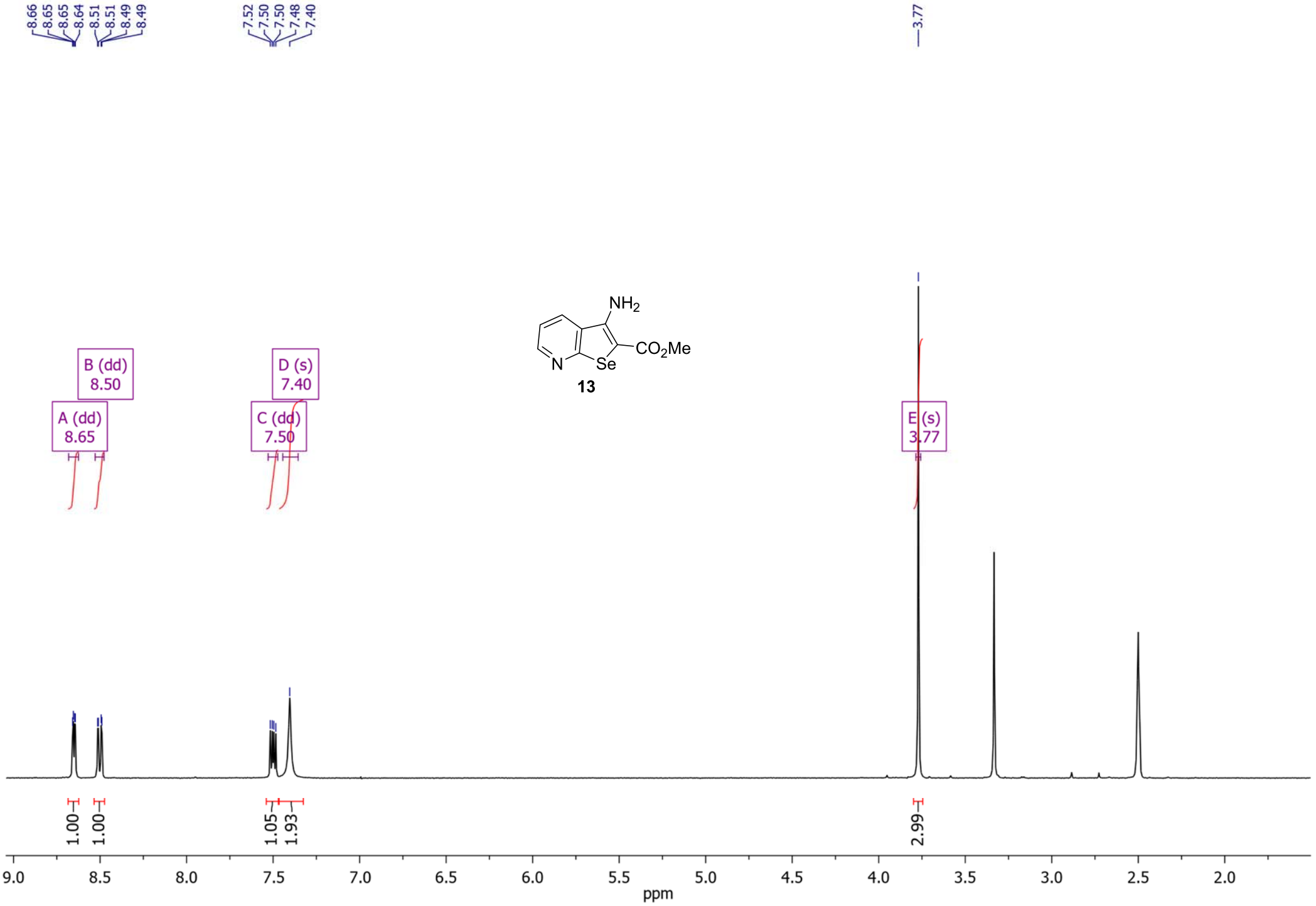

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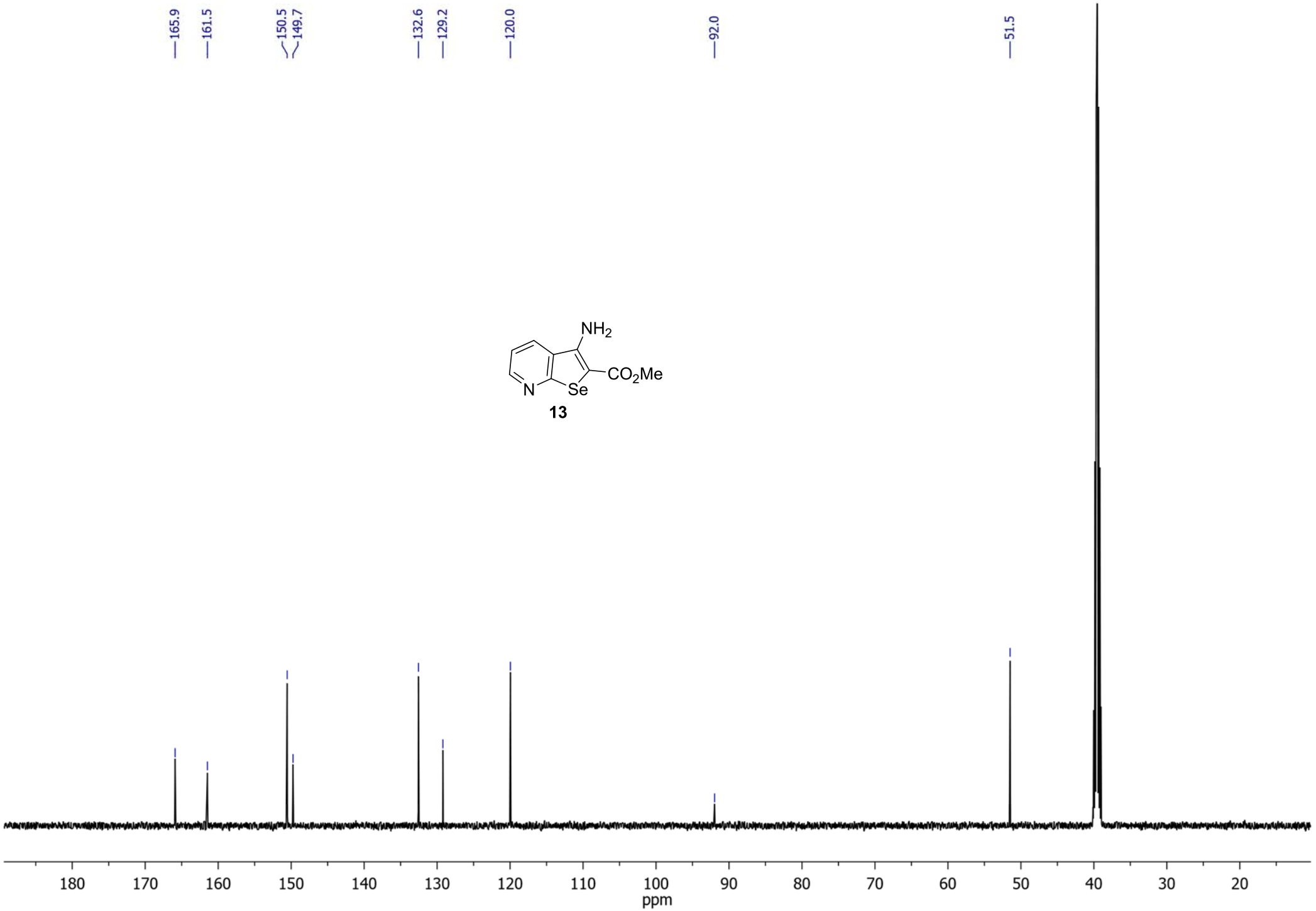

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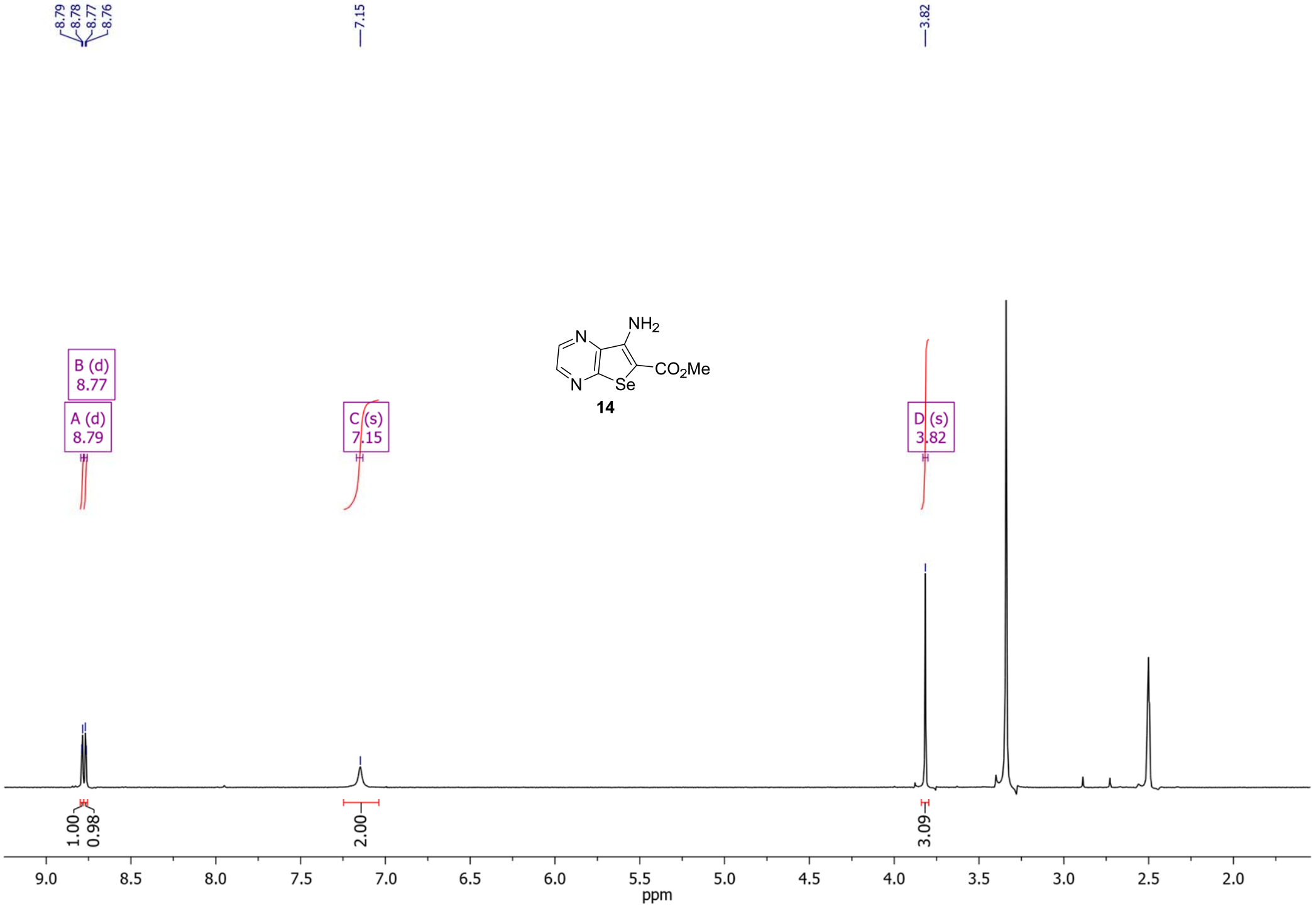

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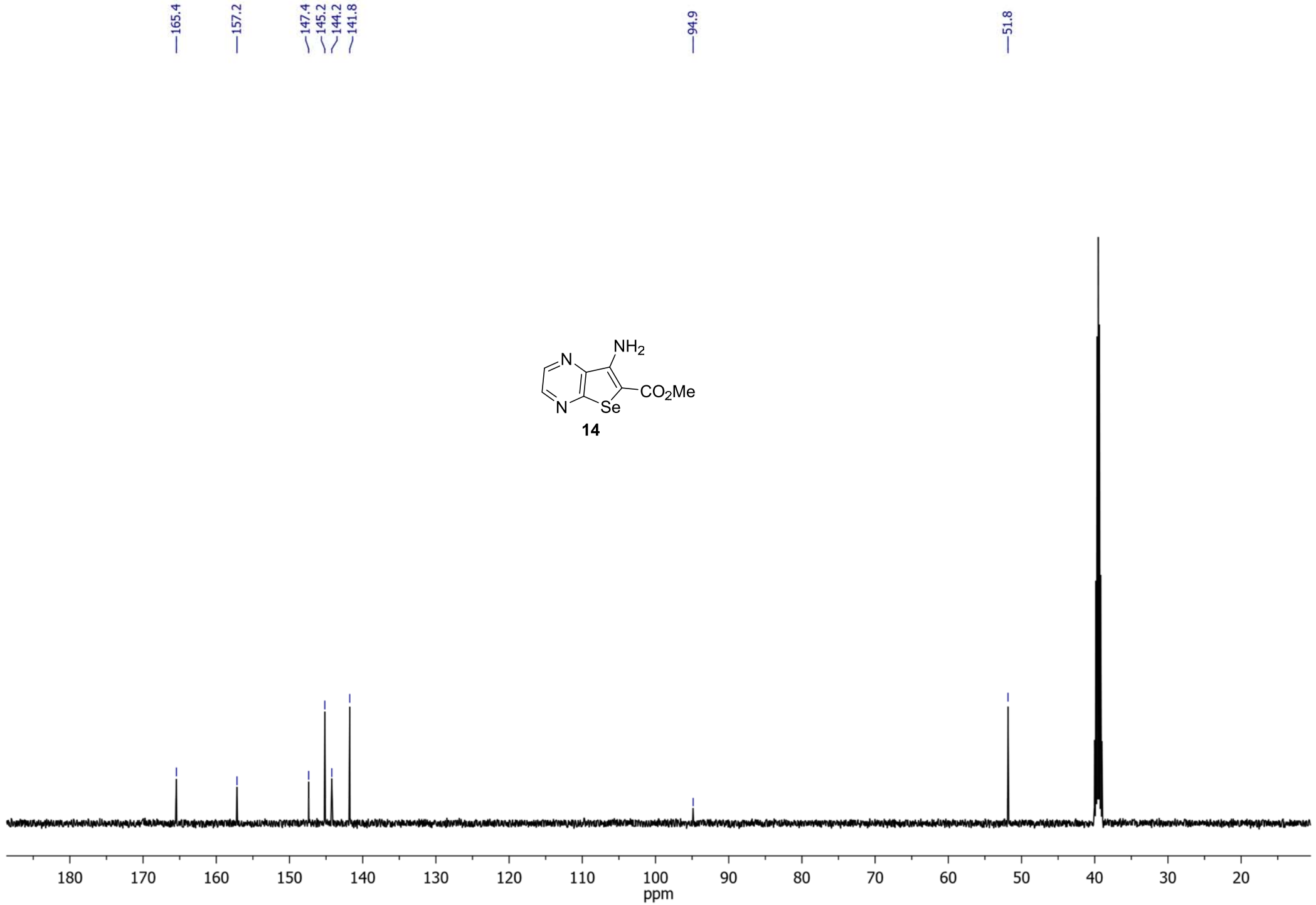

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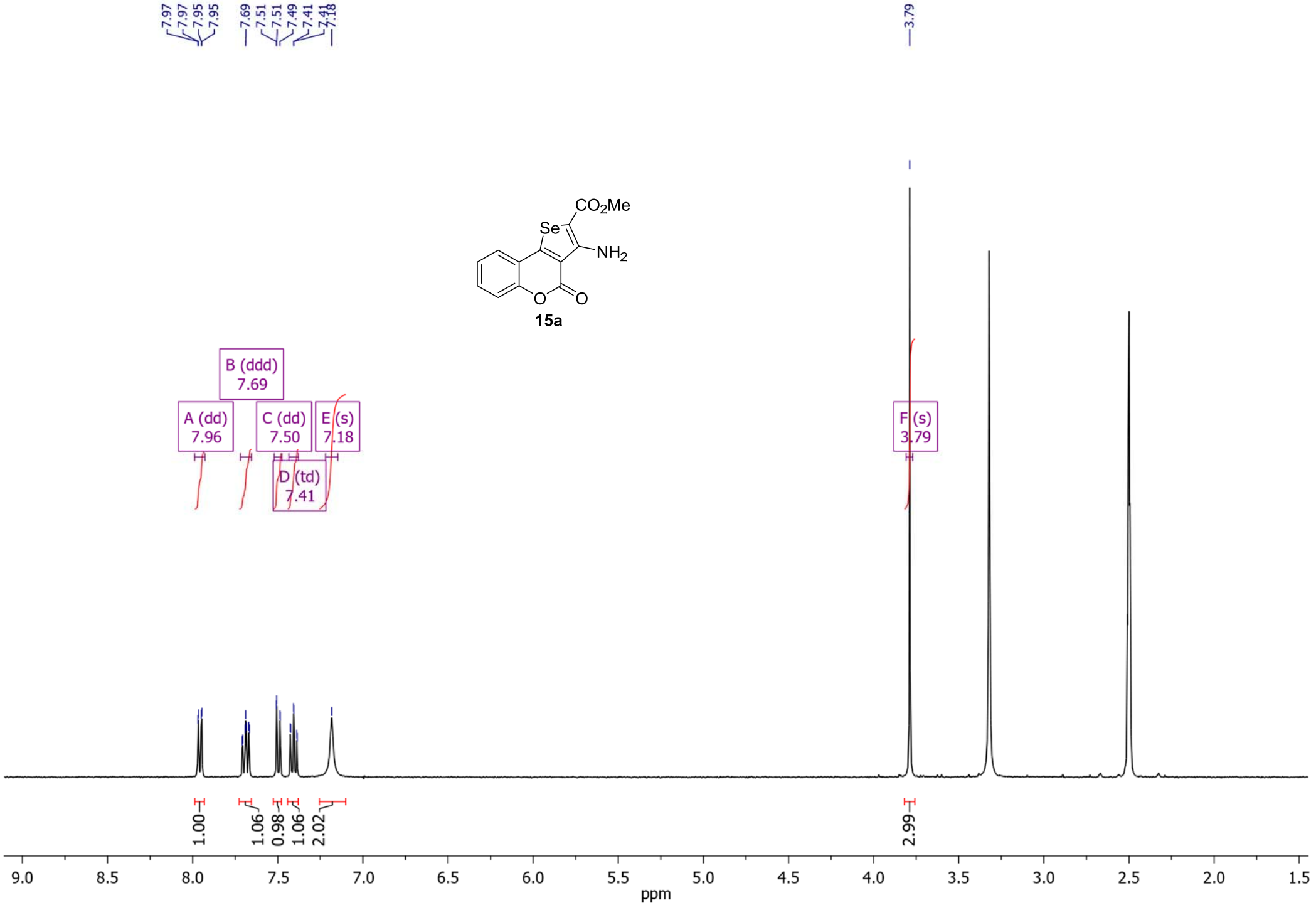

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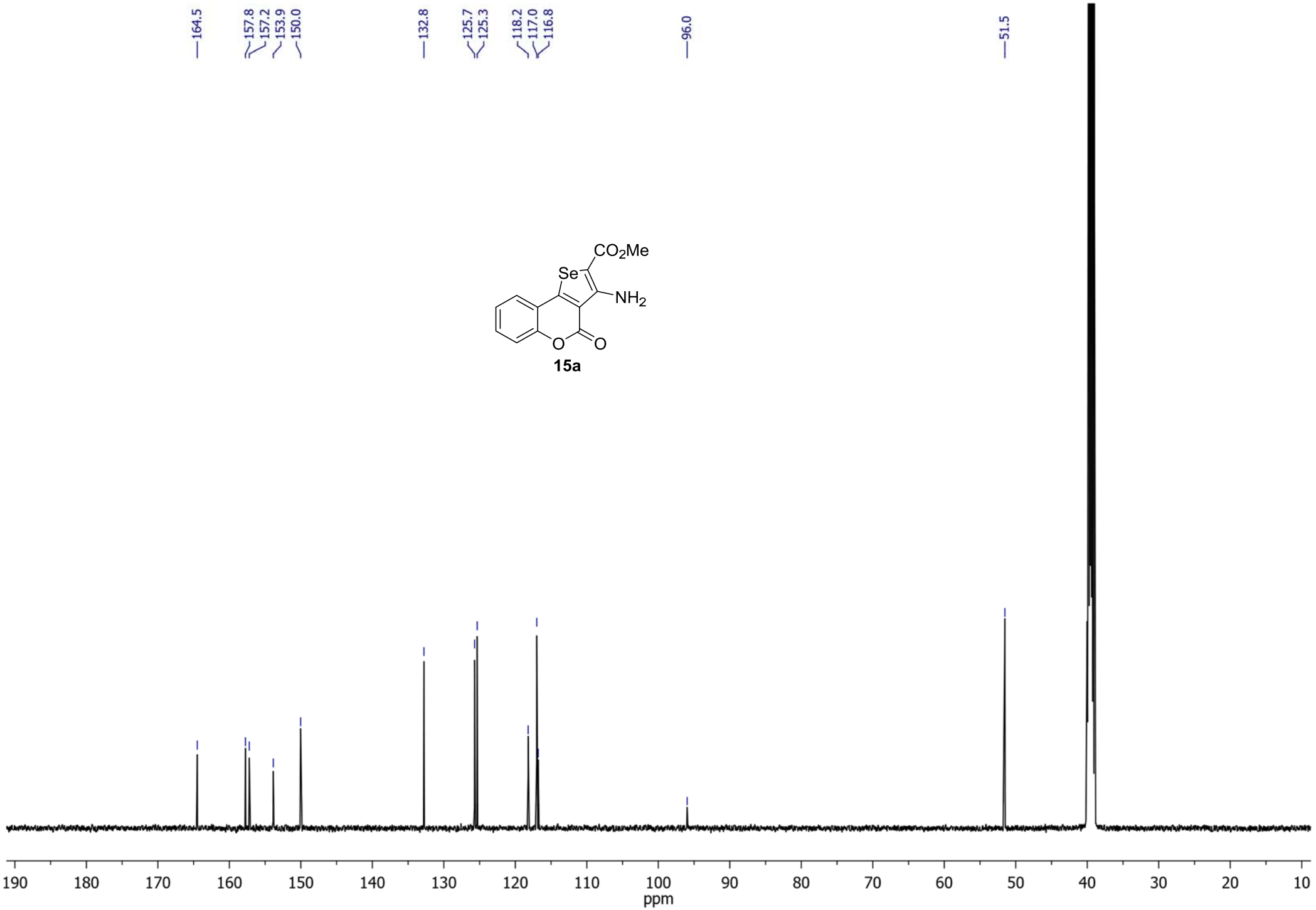

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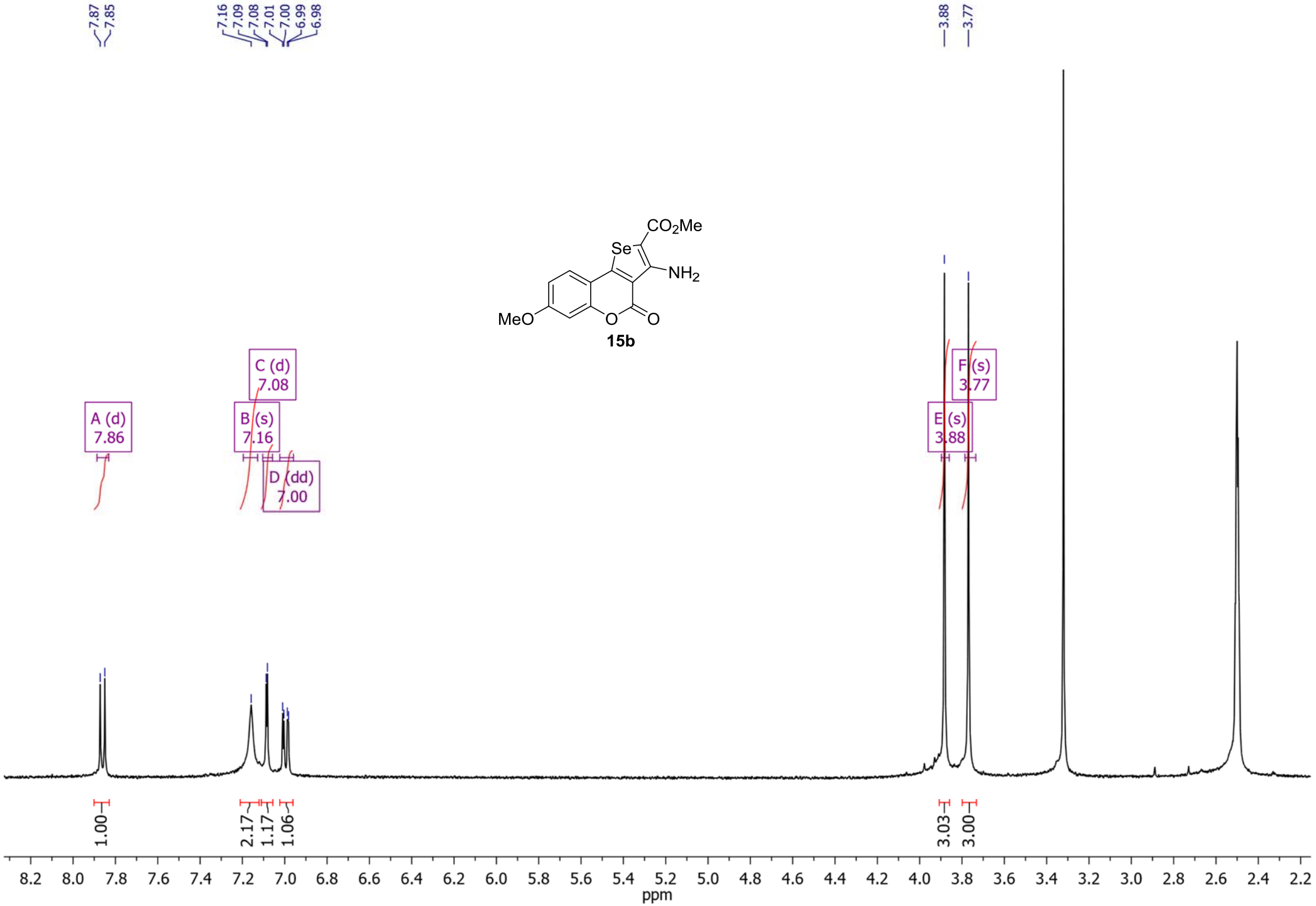

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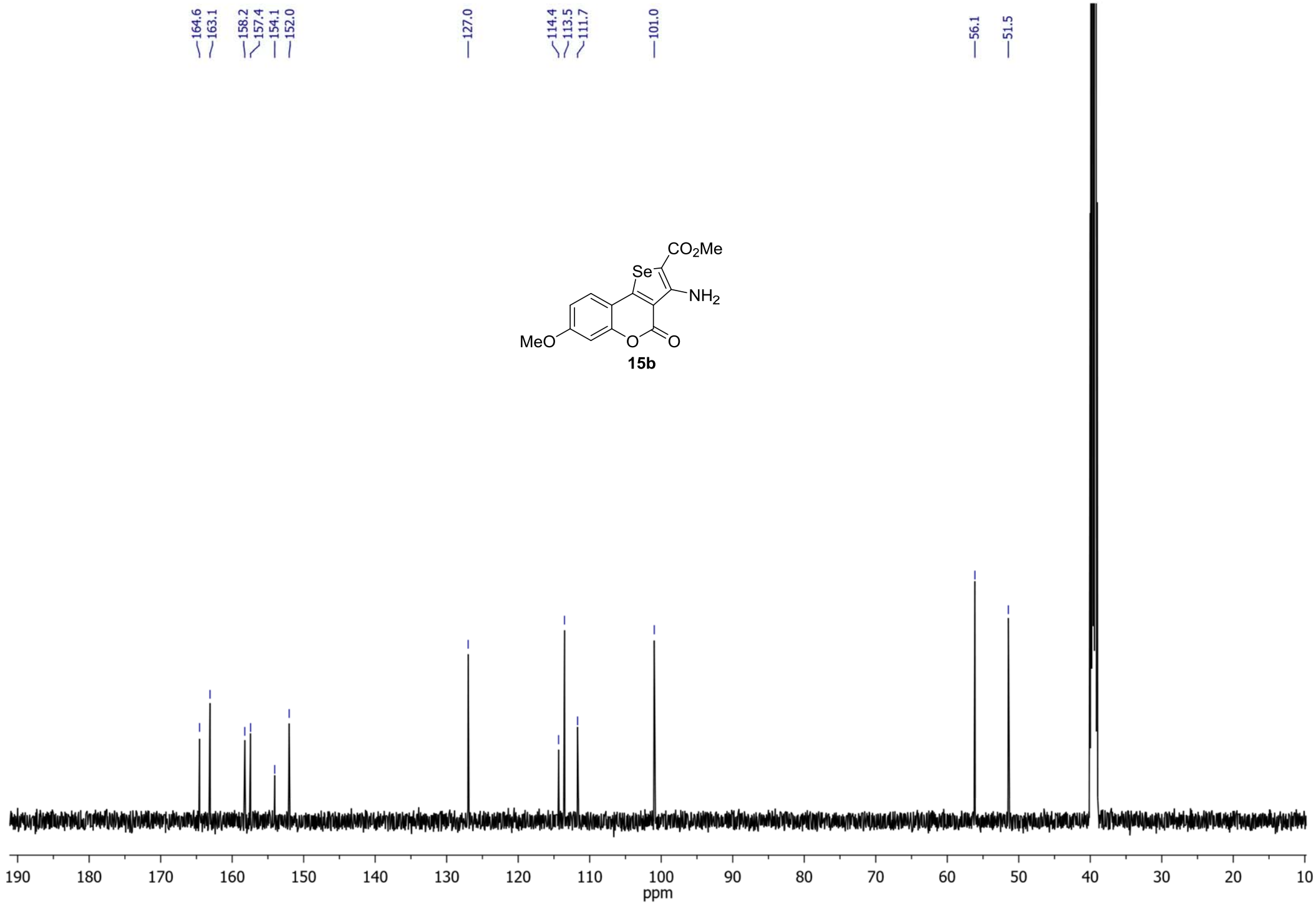

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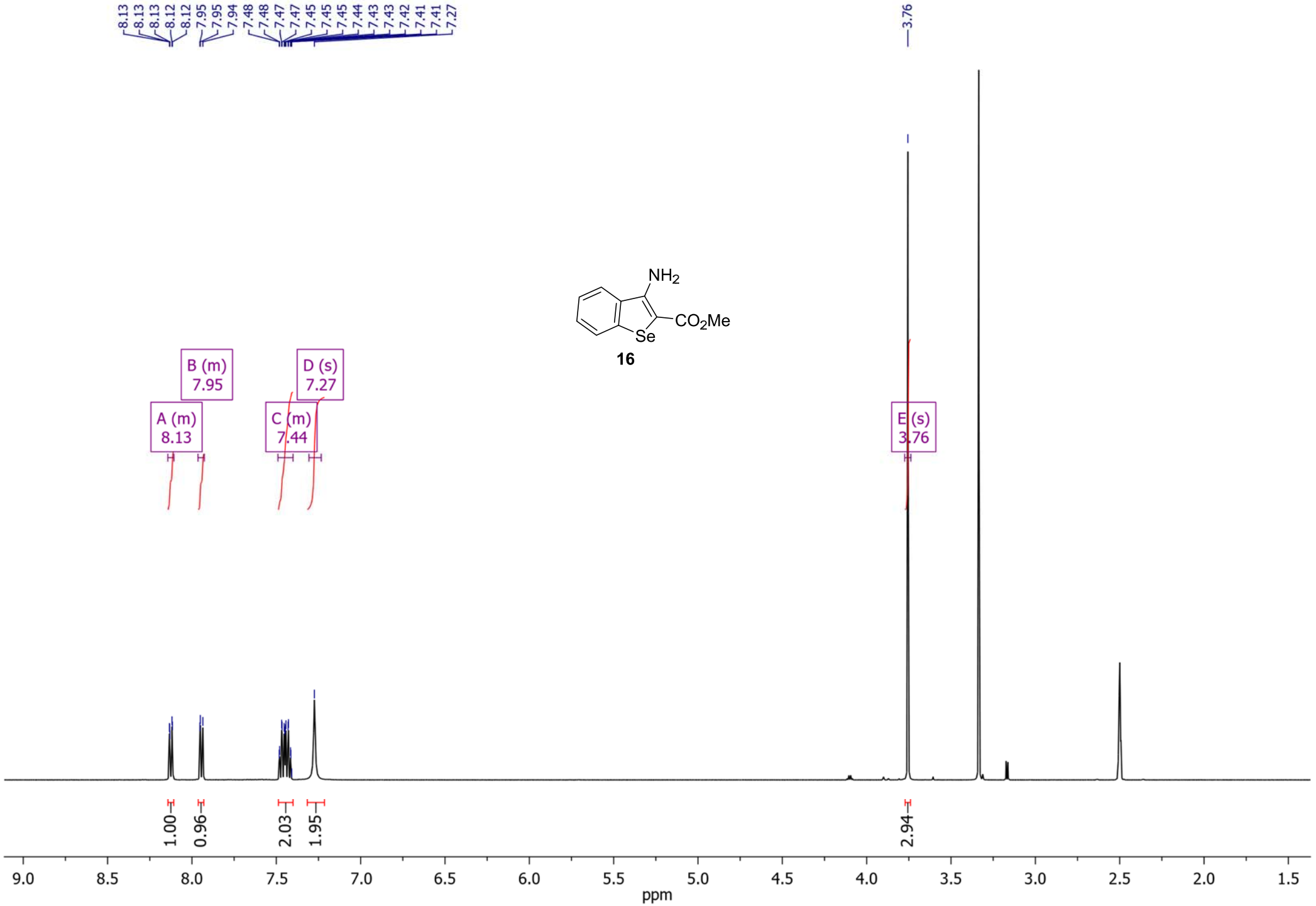

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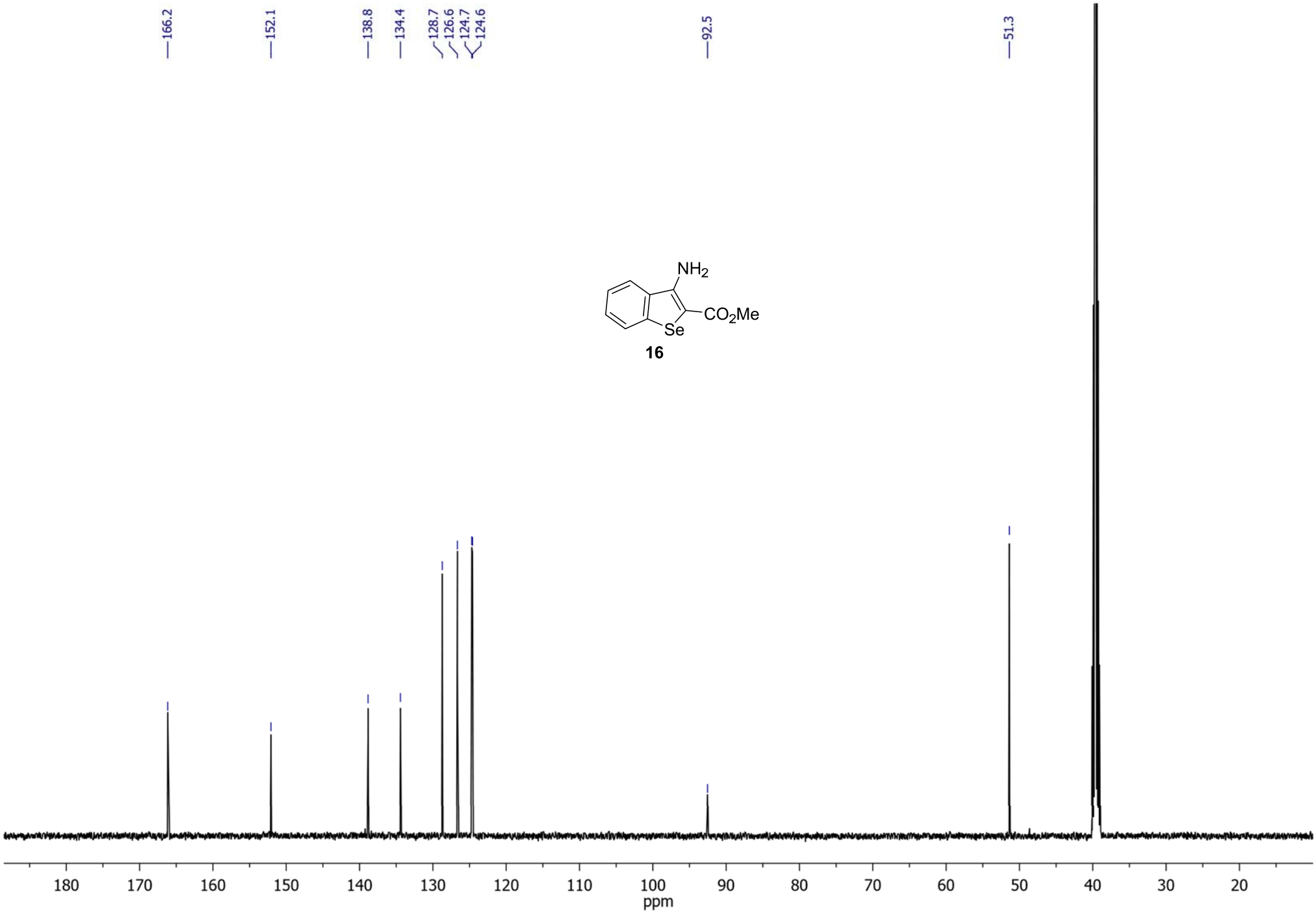

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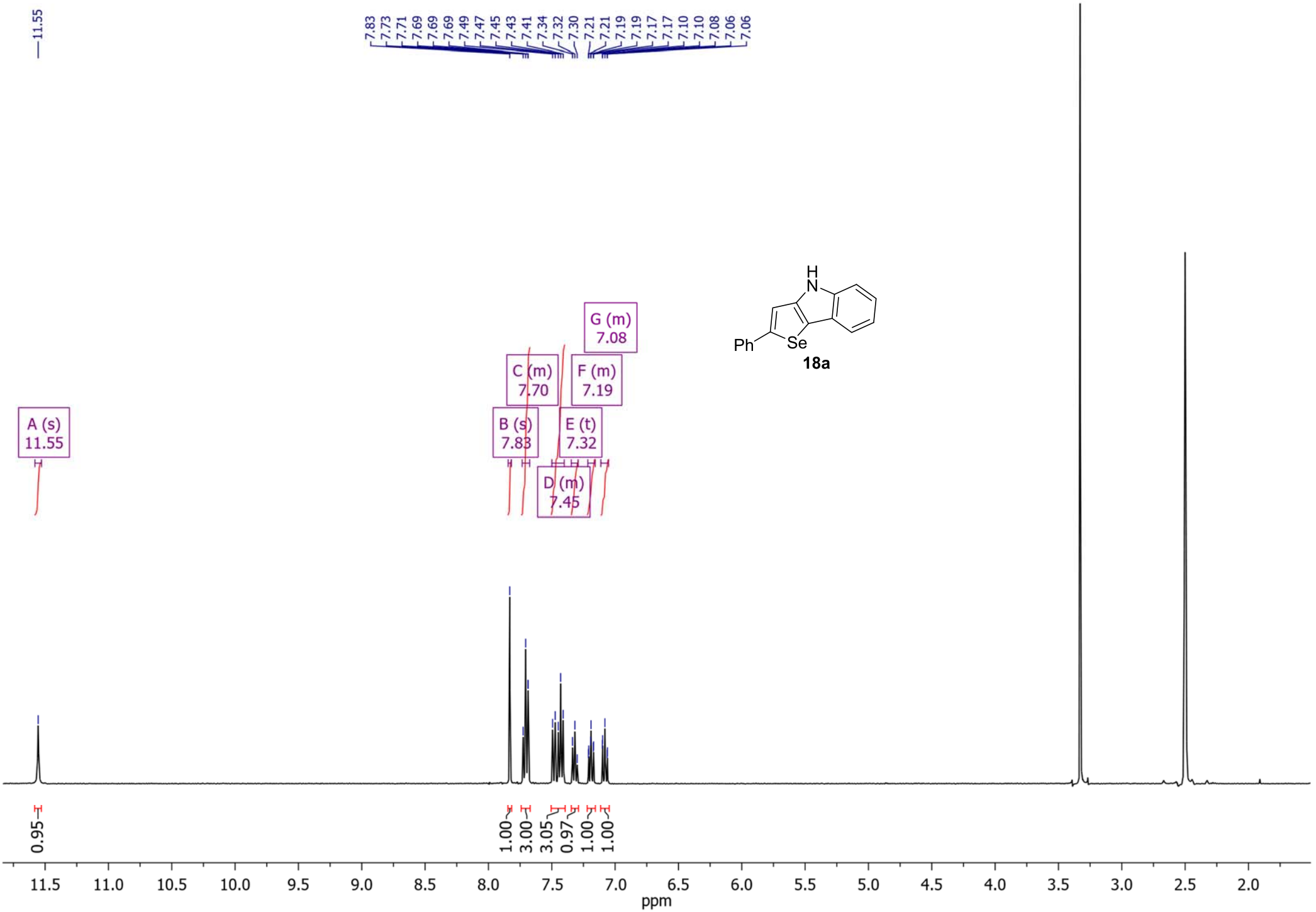

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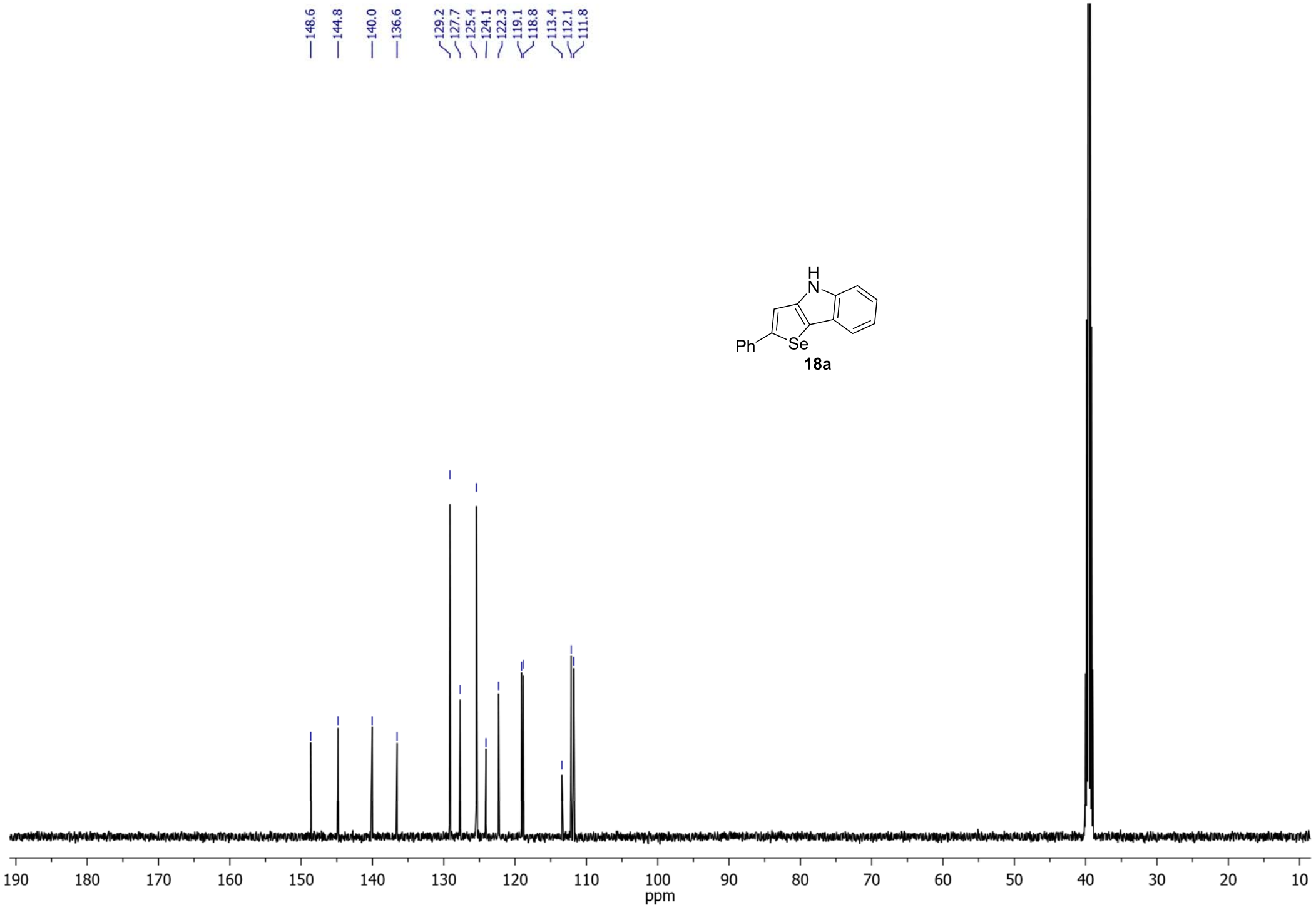

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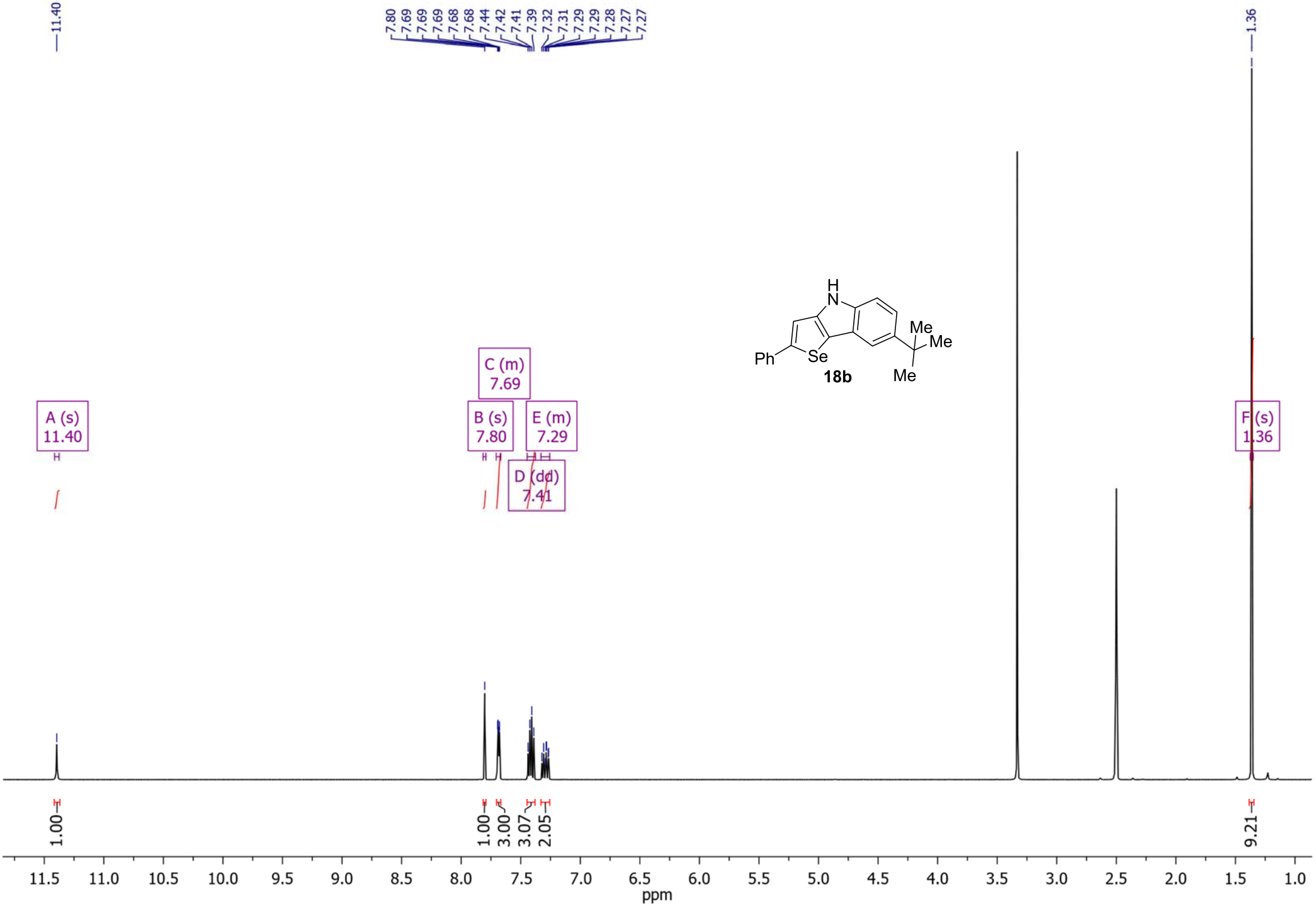

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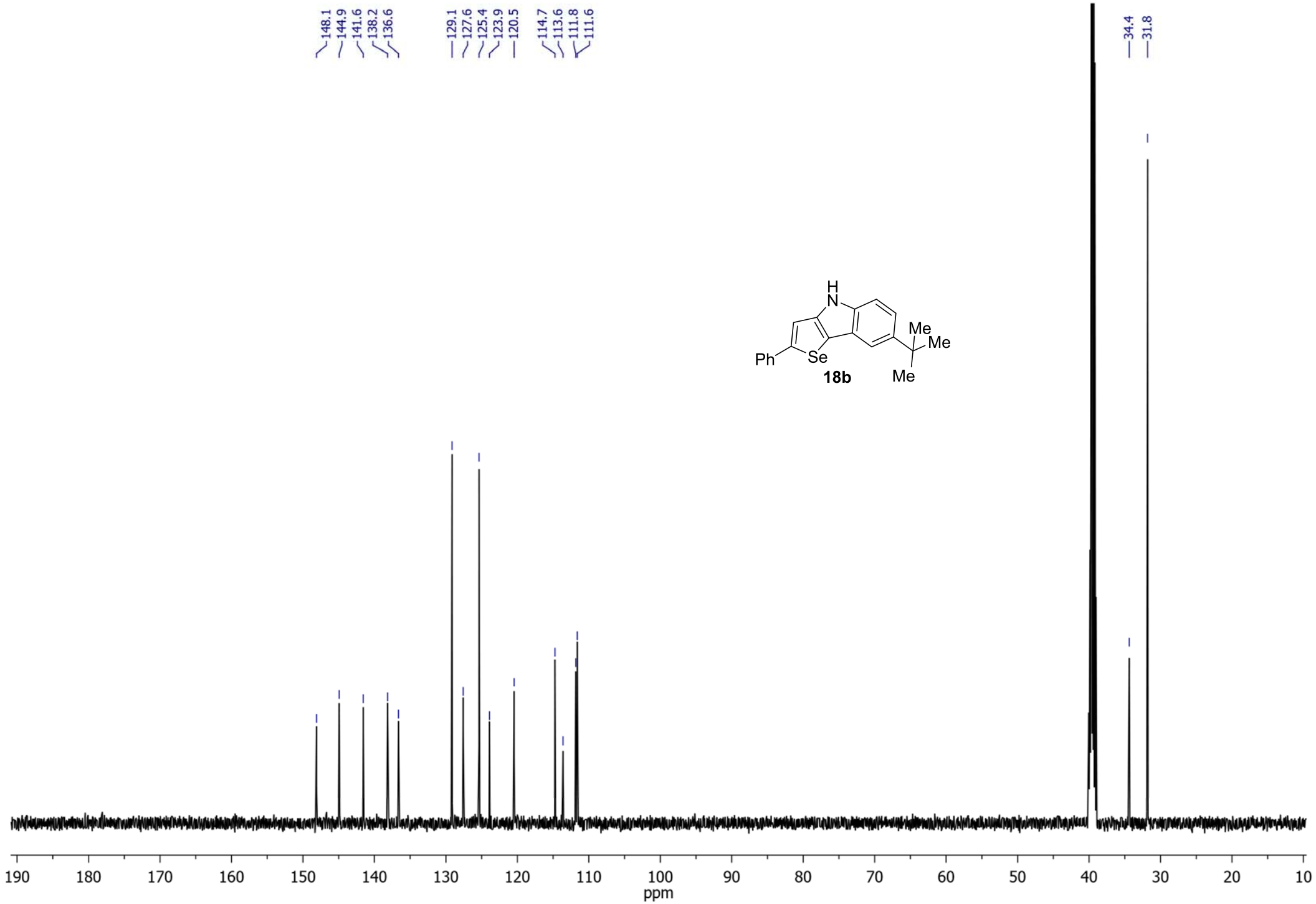

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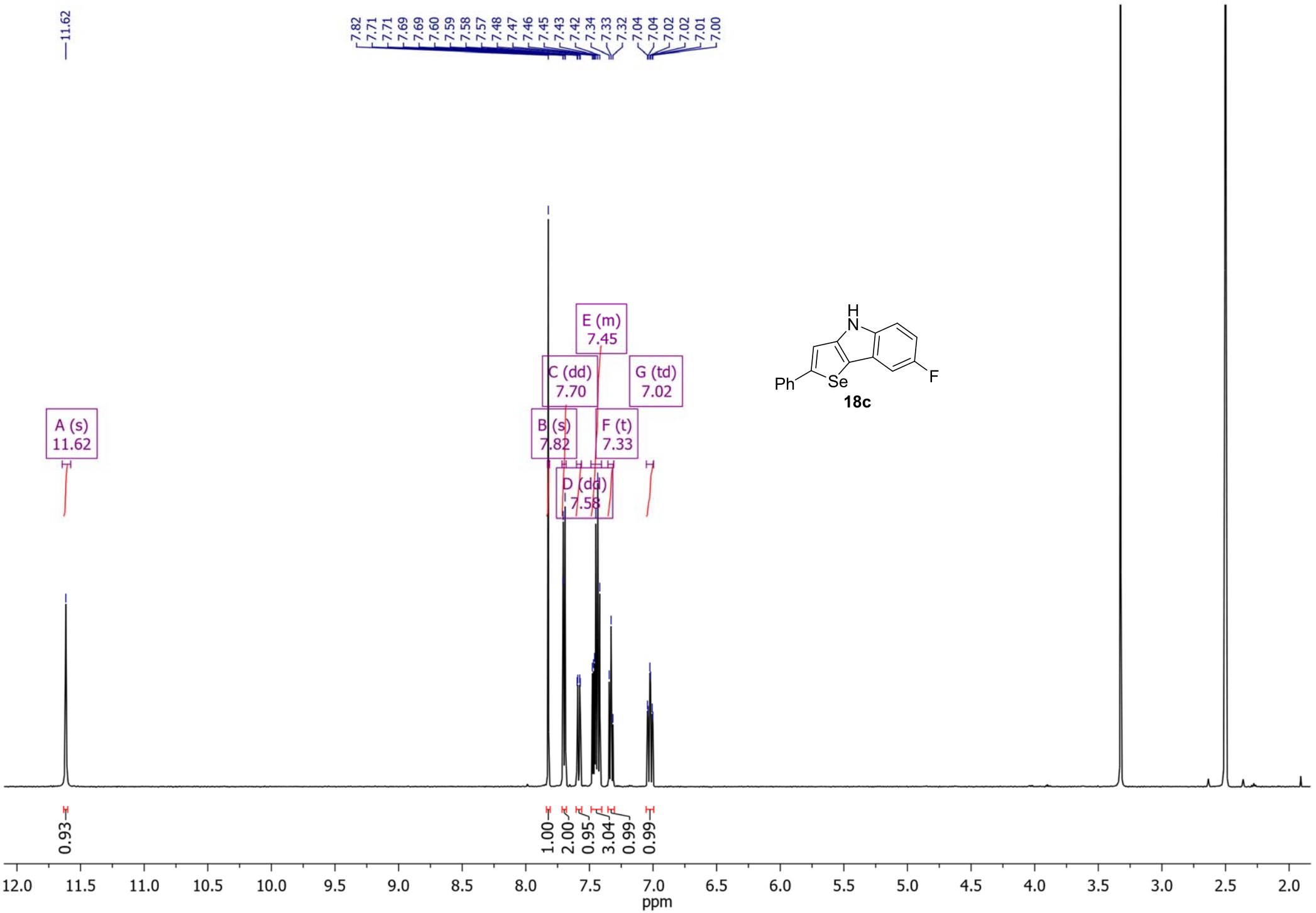
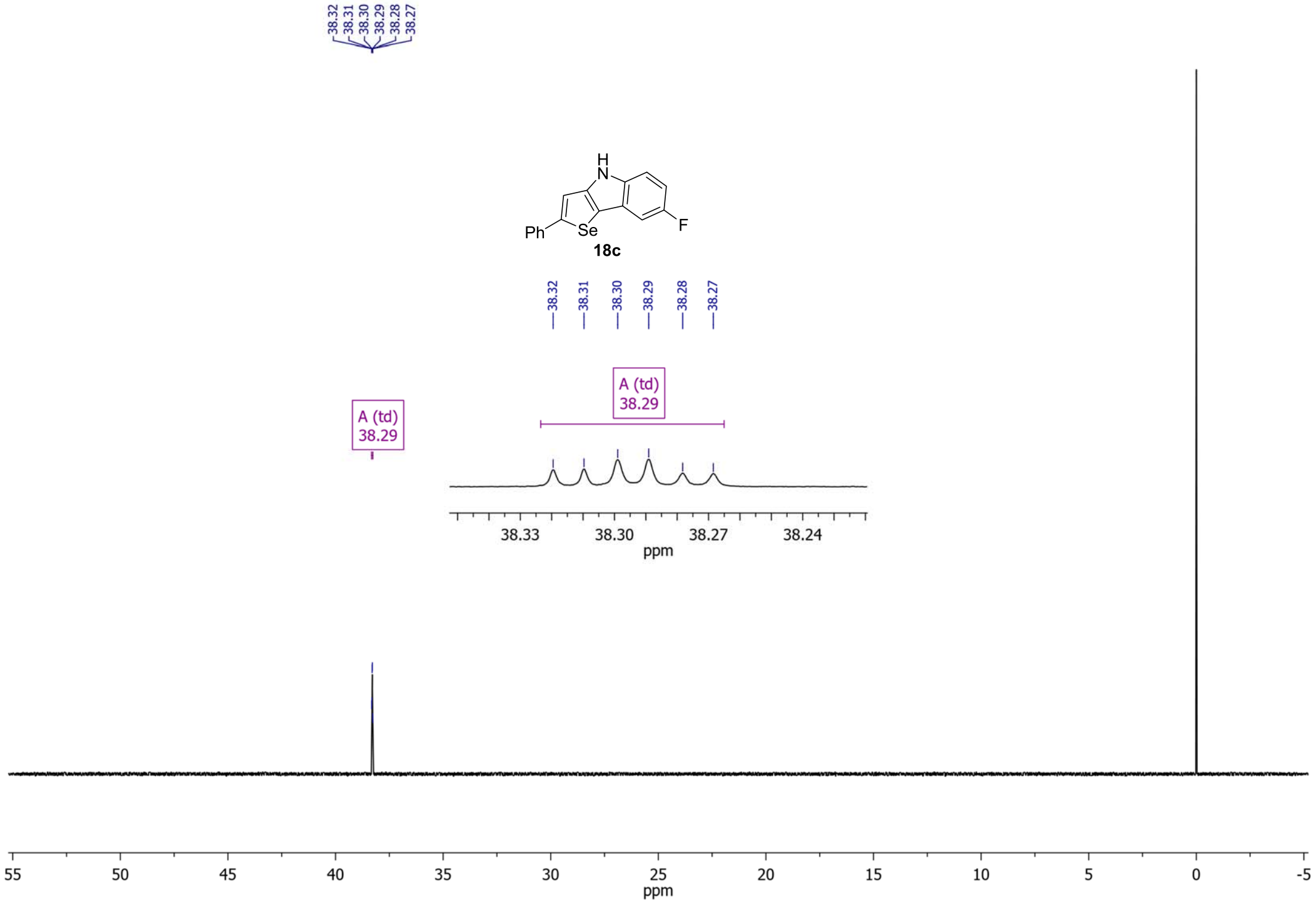


^{19}F NMR (solvent: DMSO-d_6)



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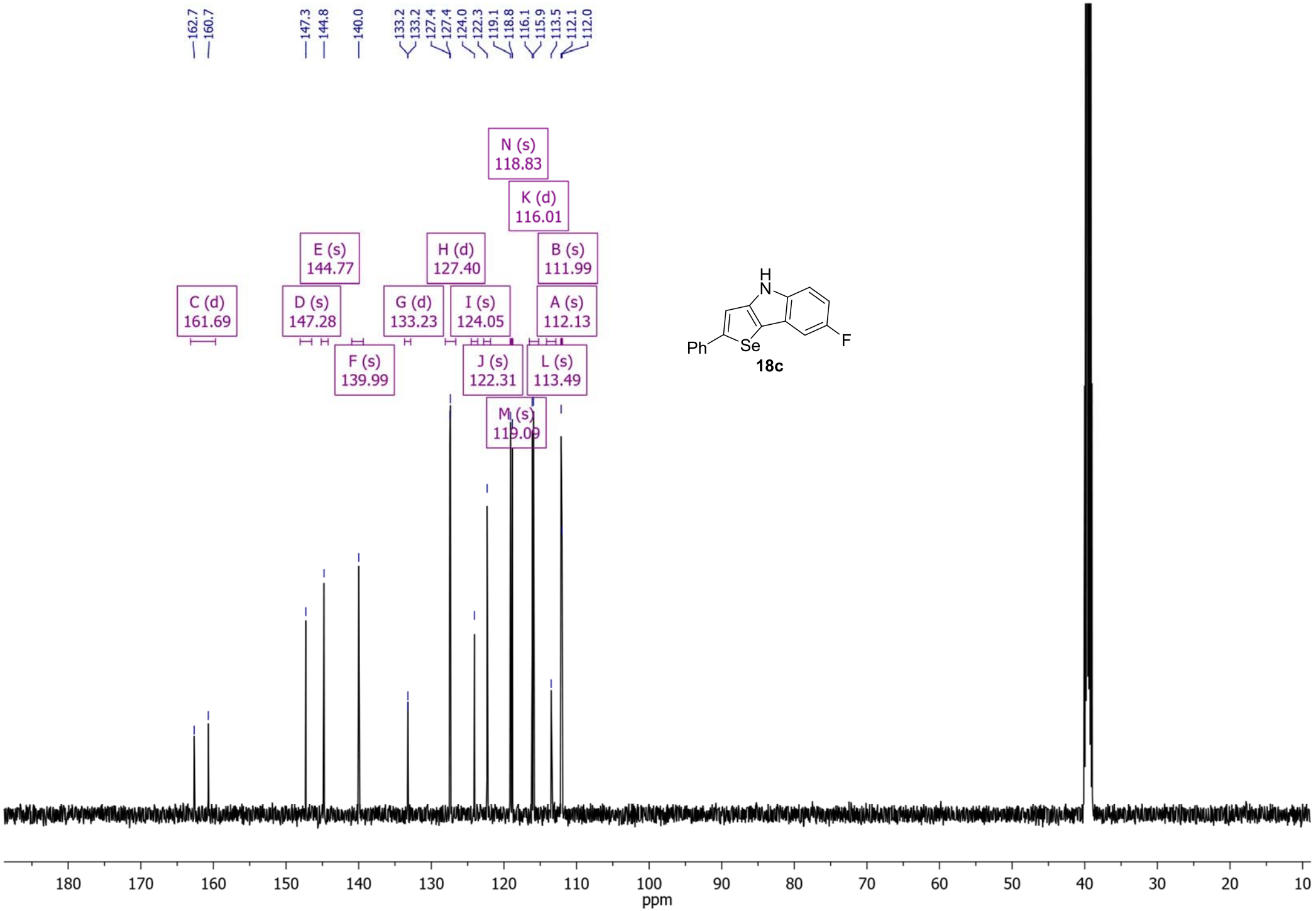

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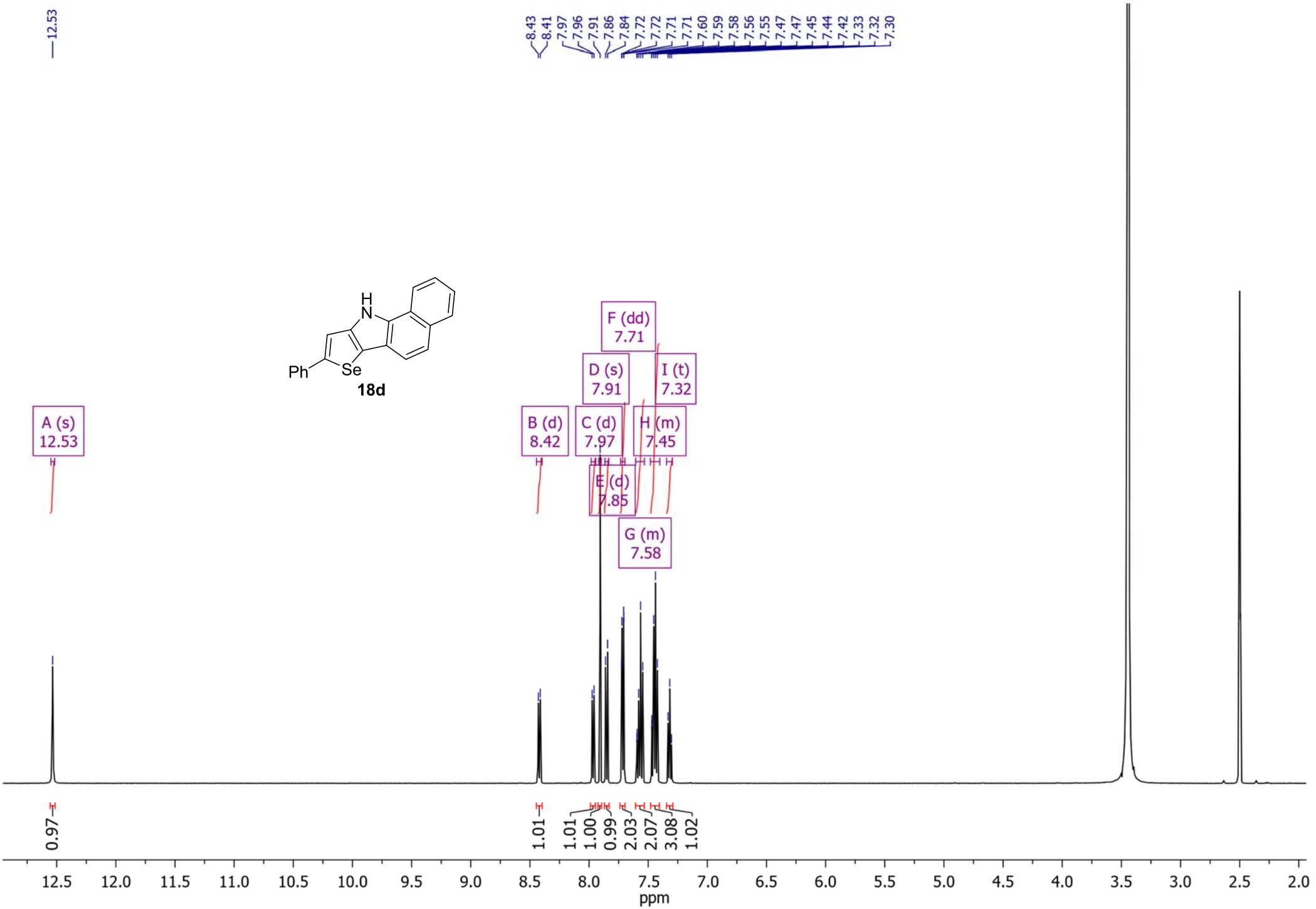

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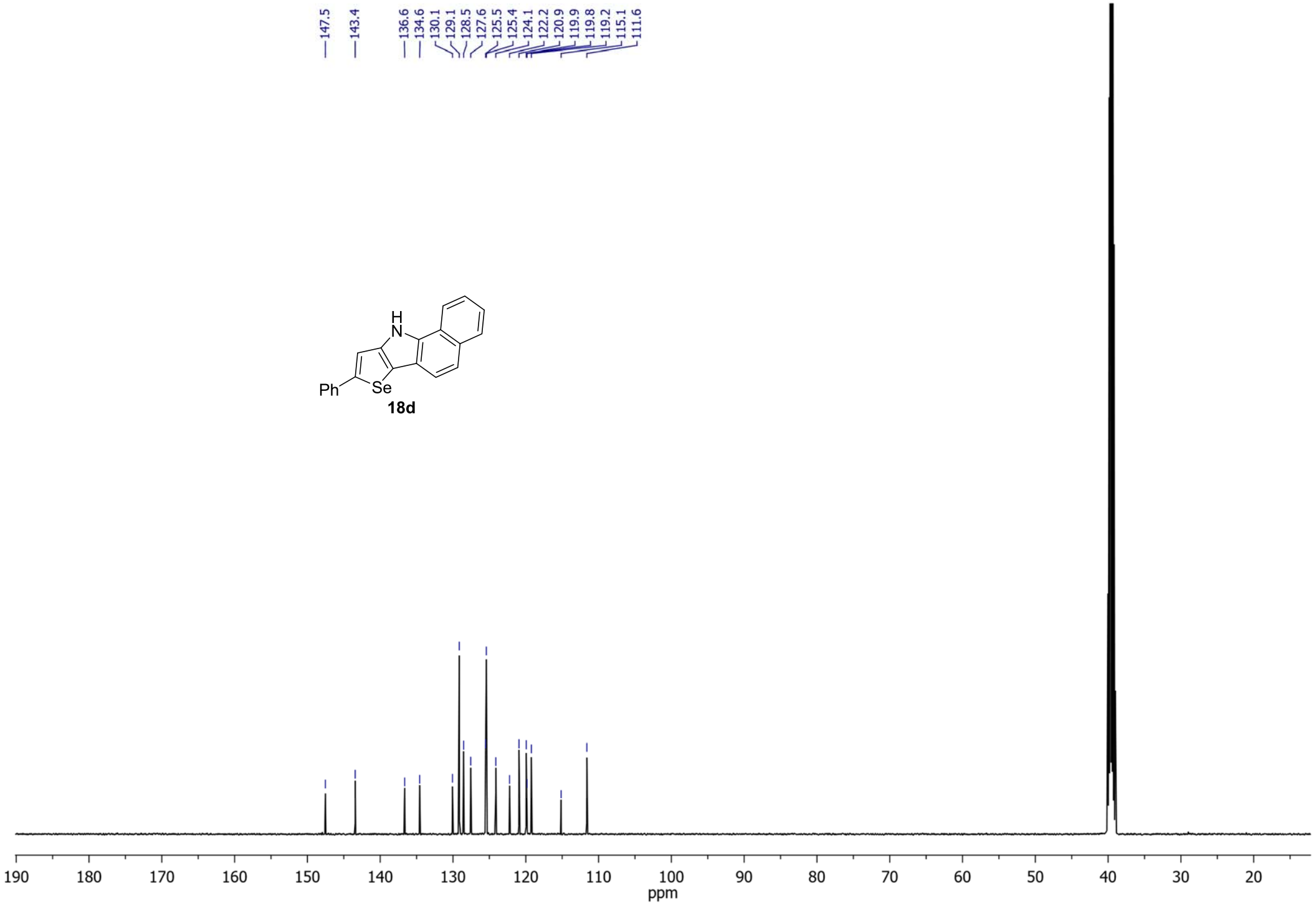

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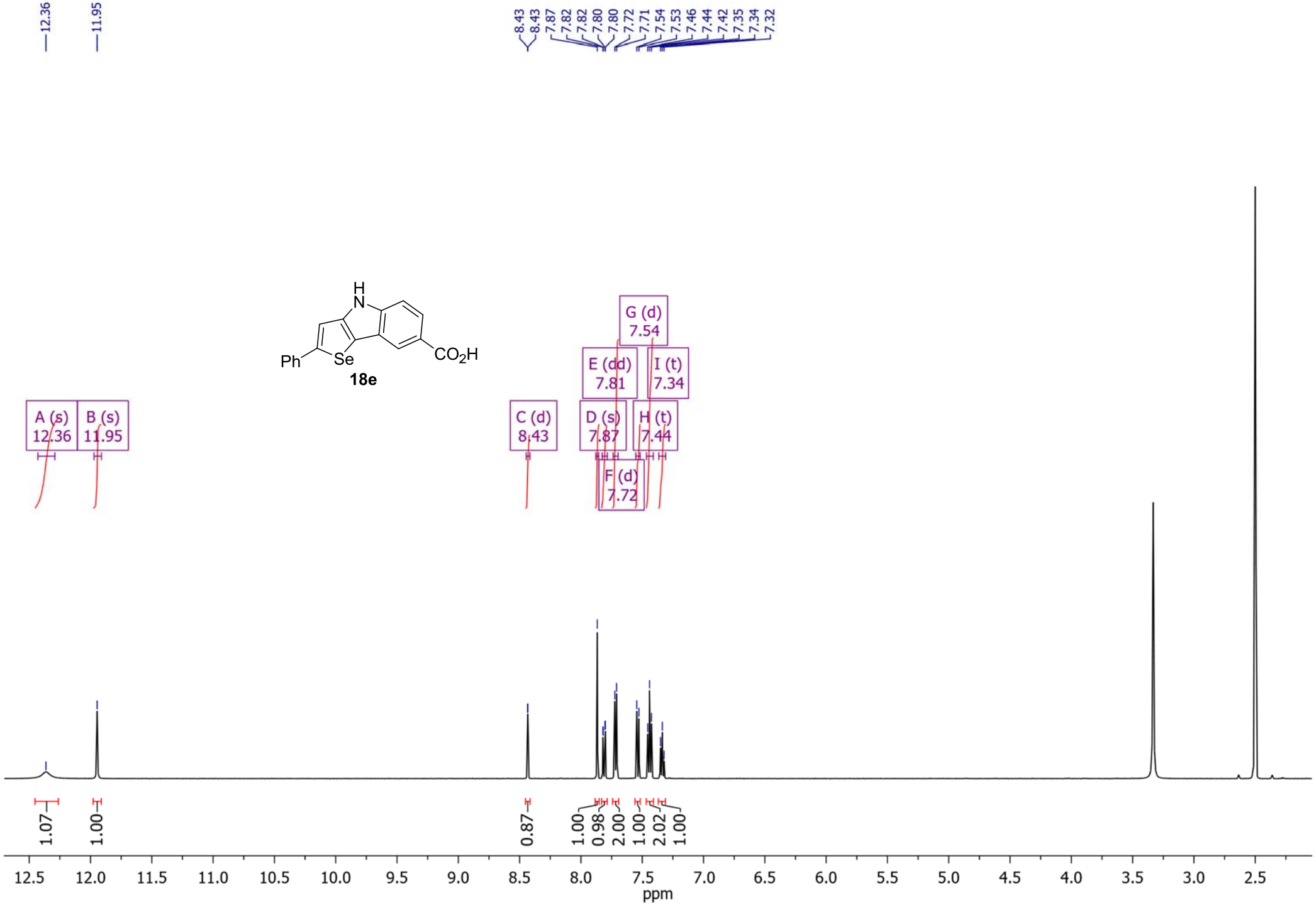

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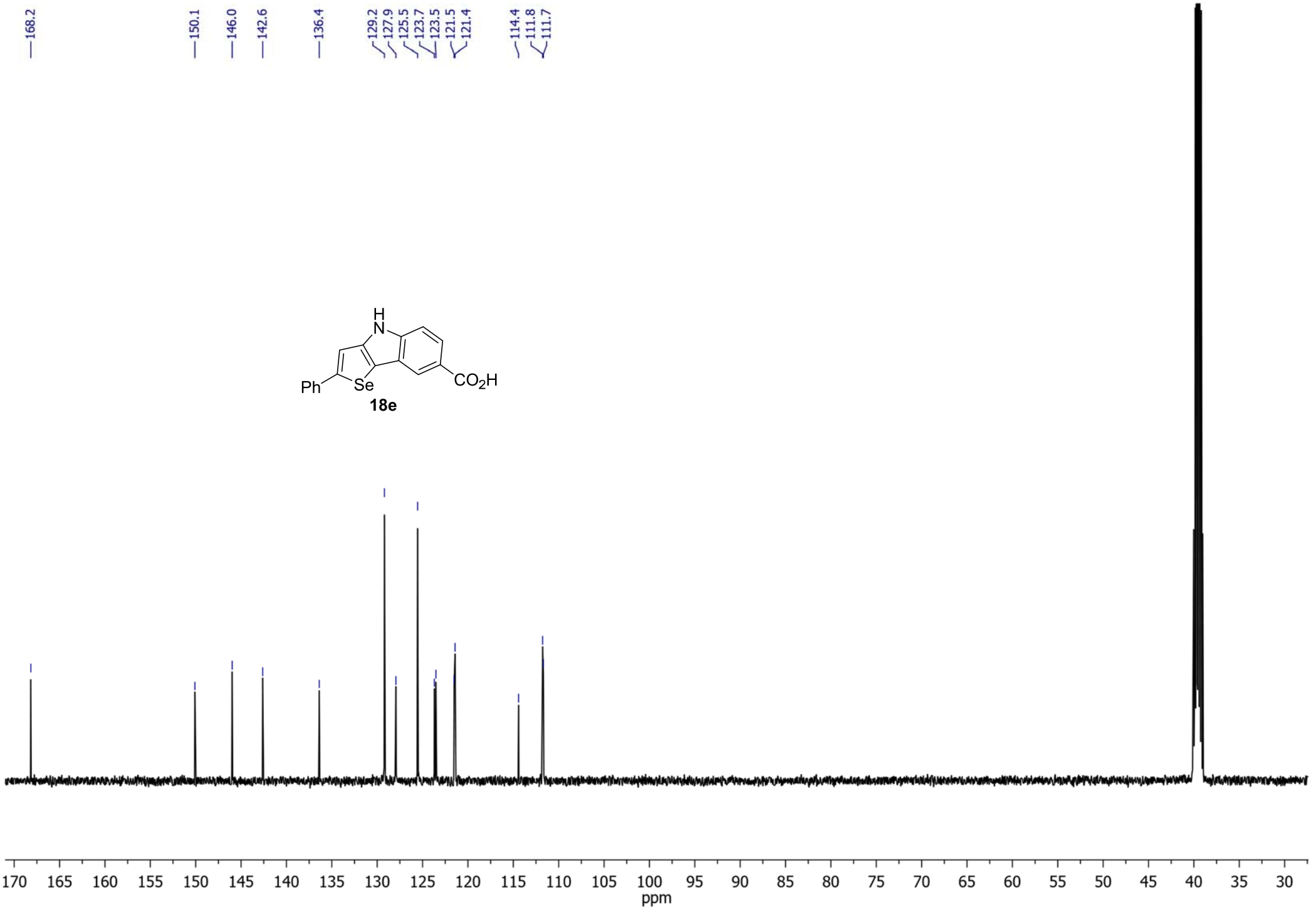

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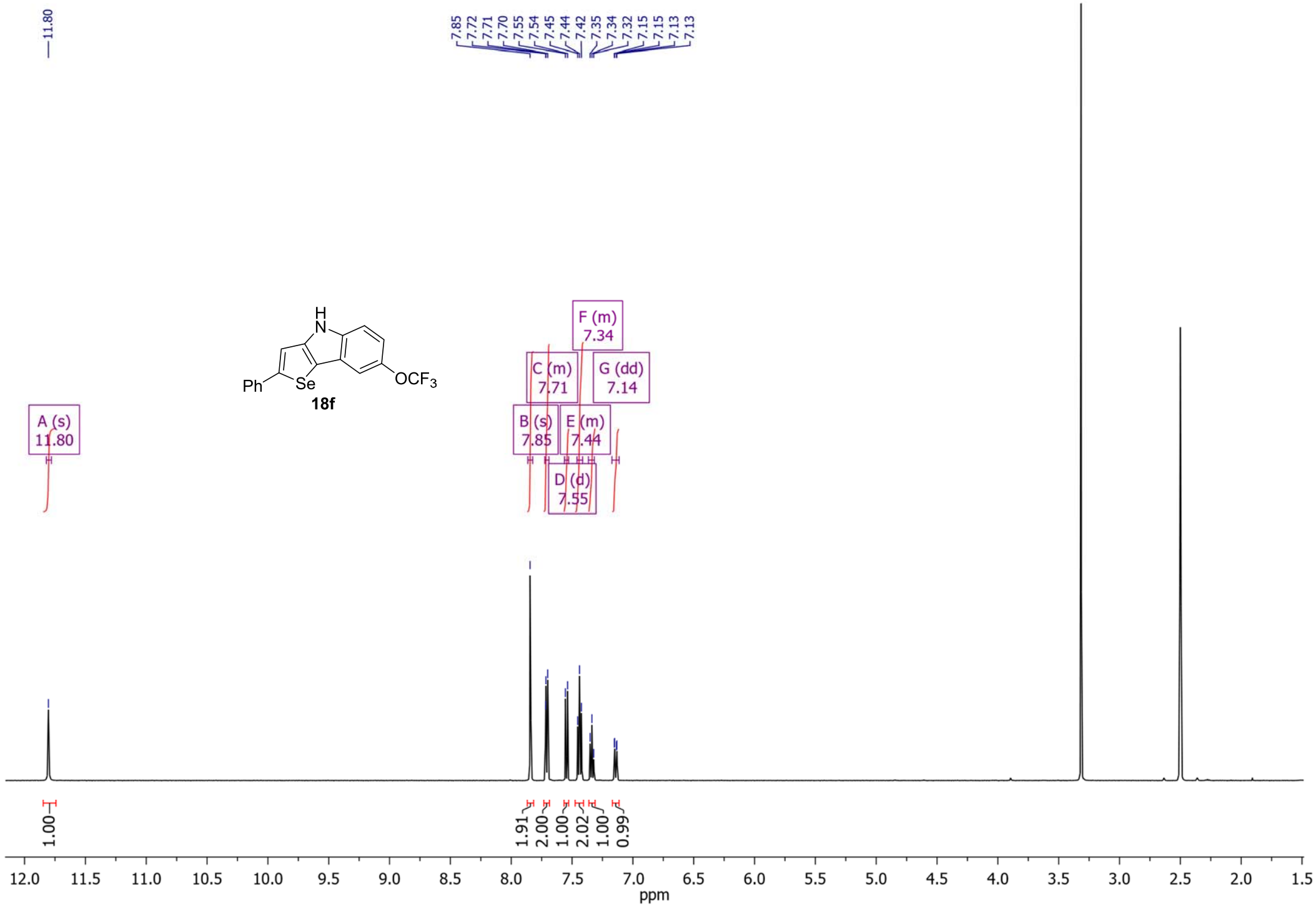

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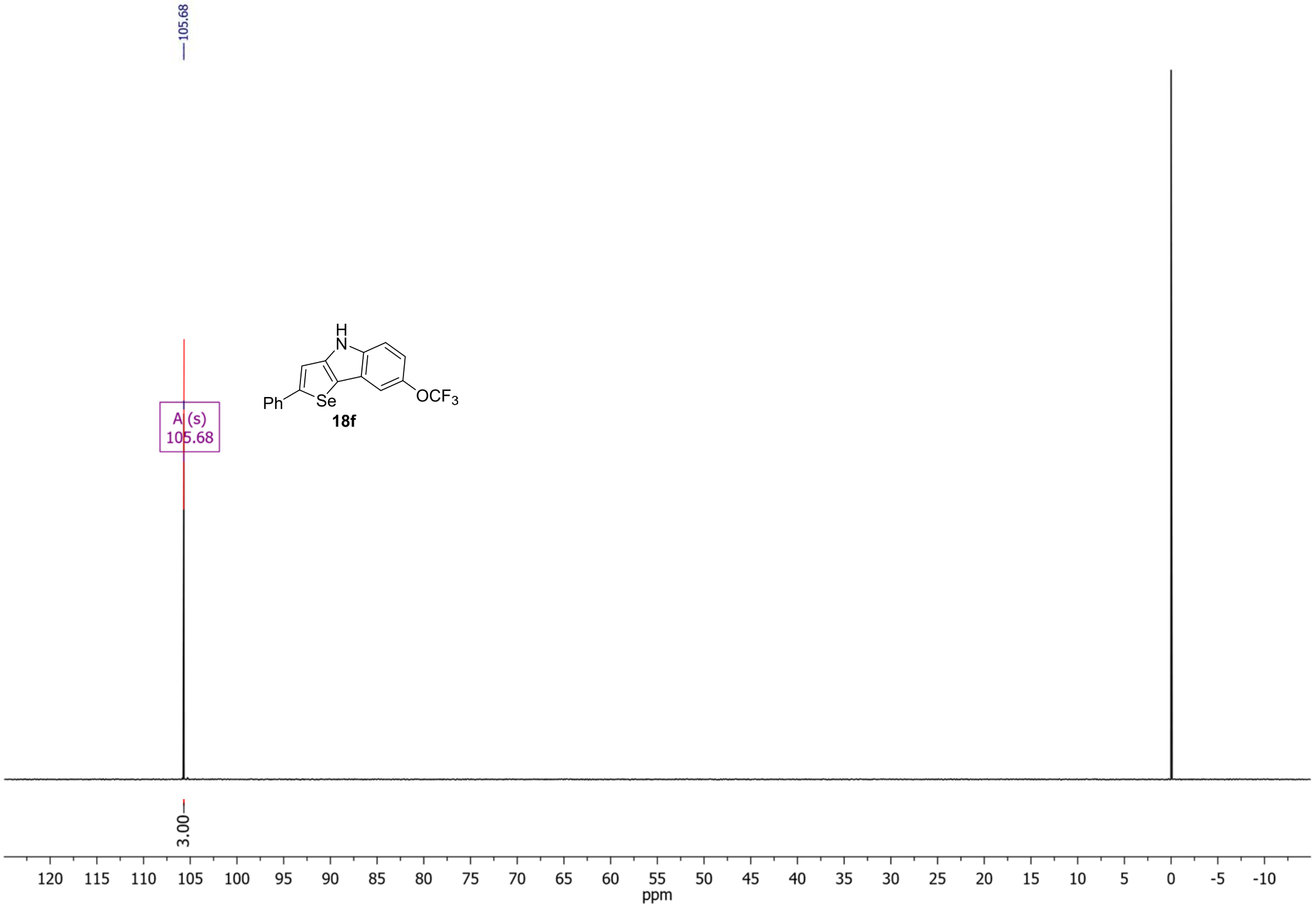

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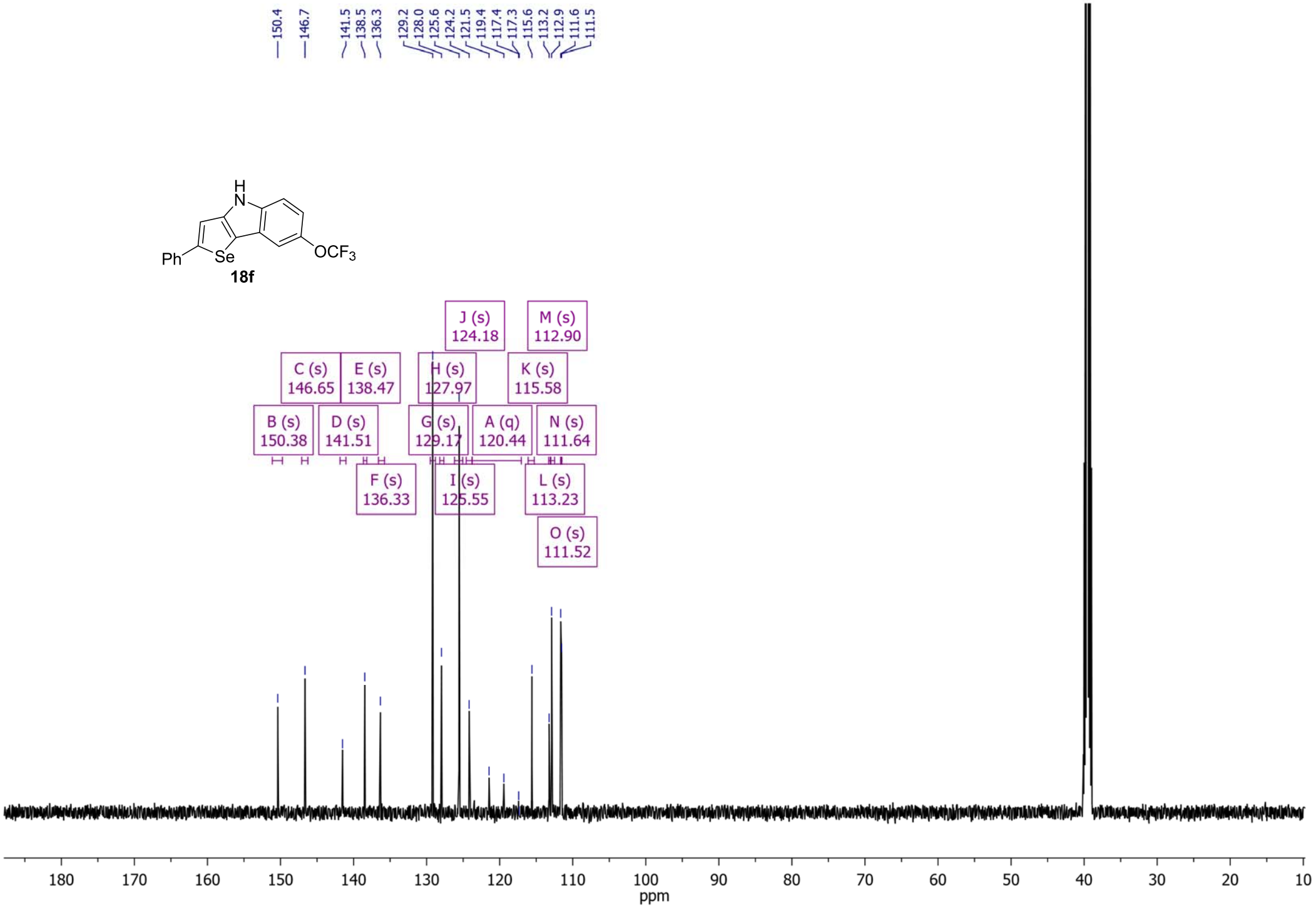

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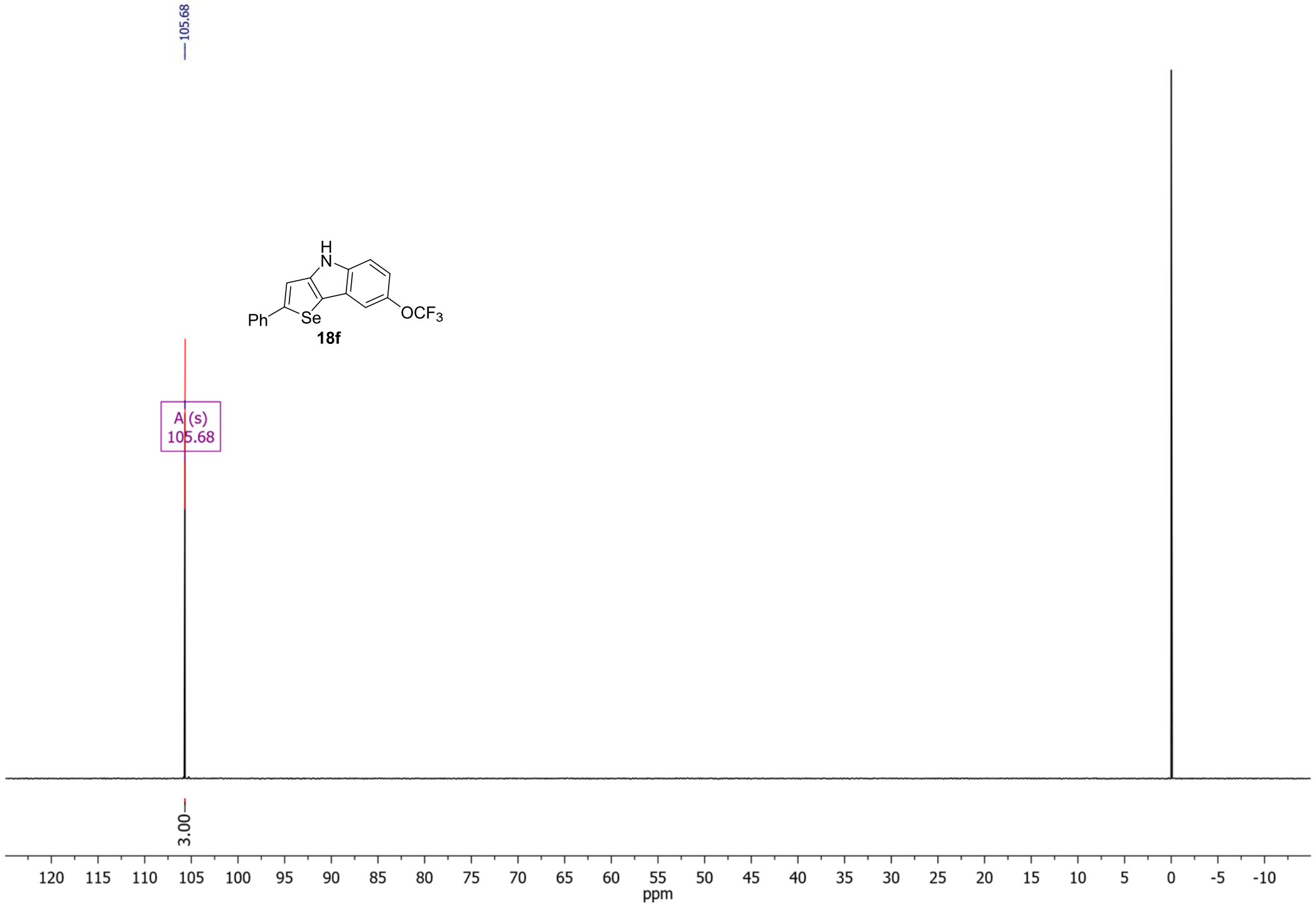

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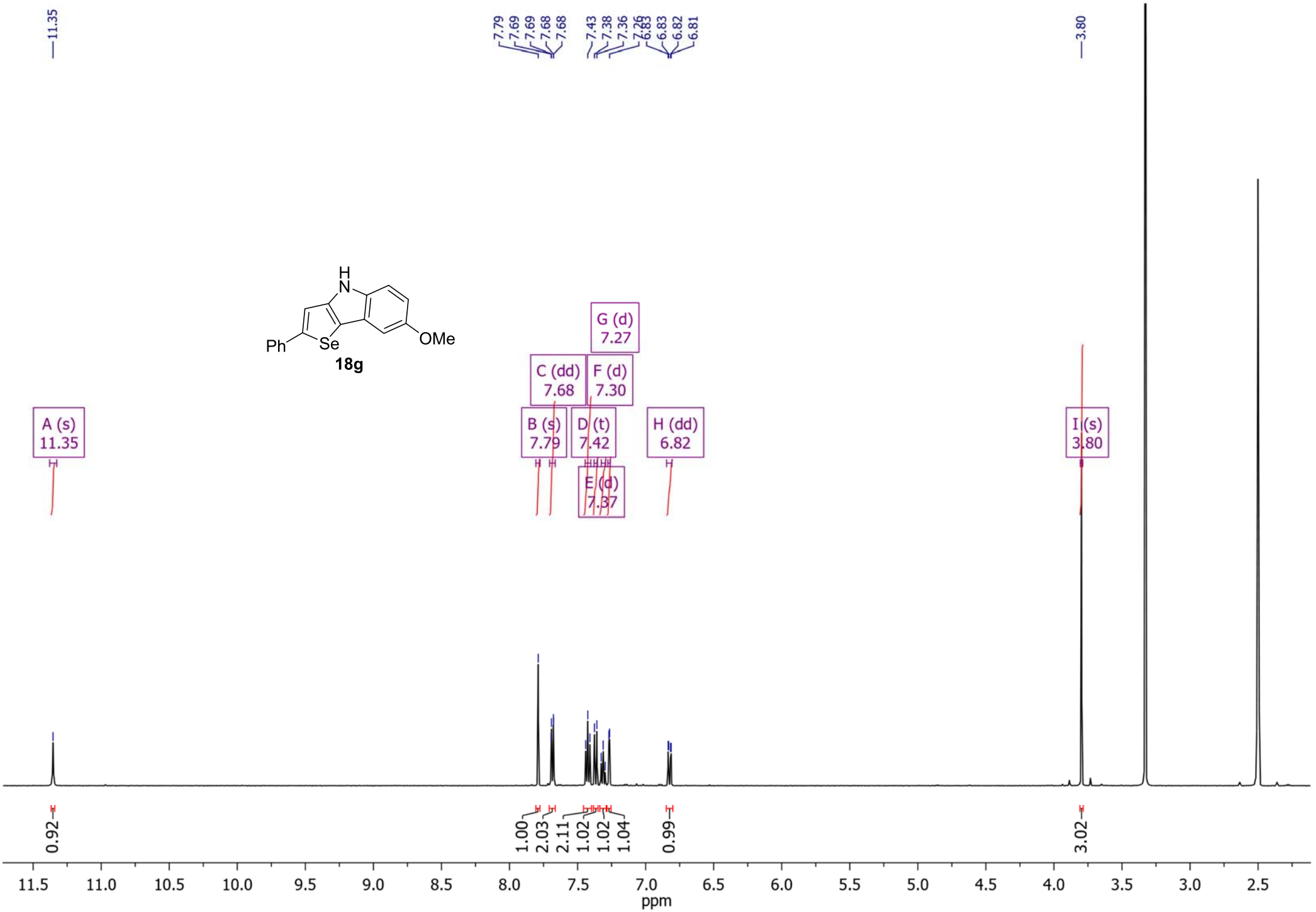

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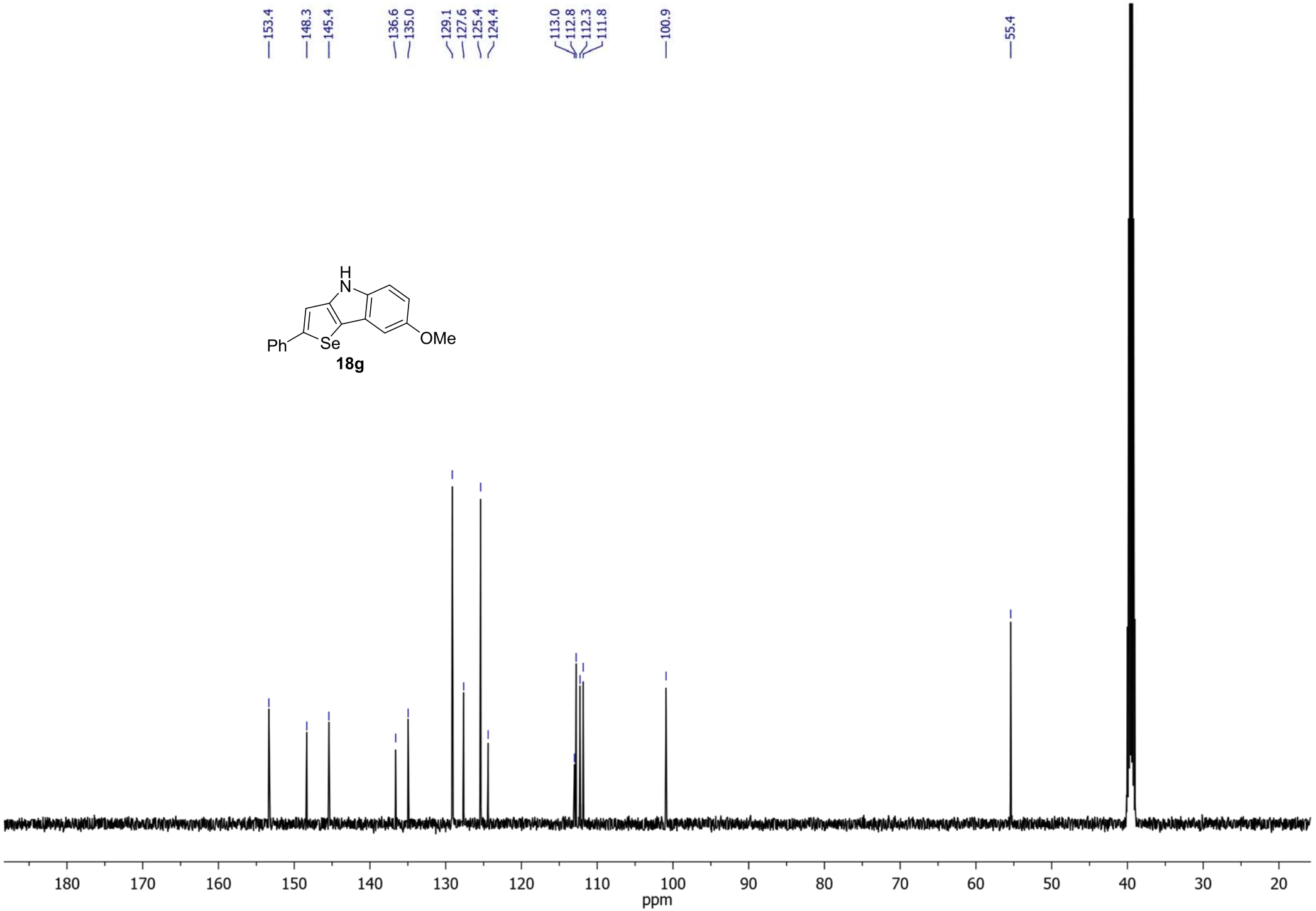

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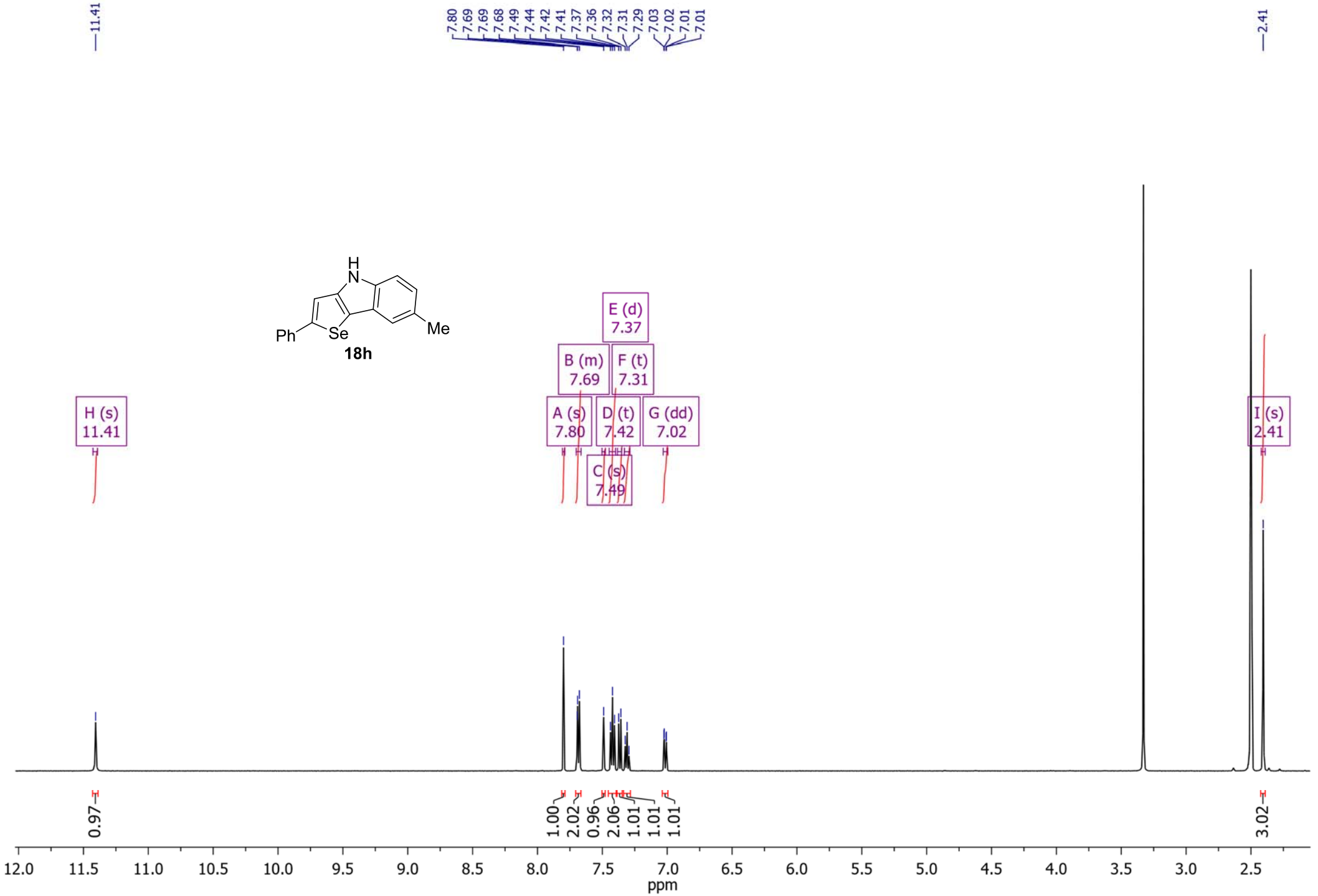

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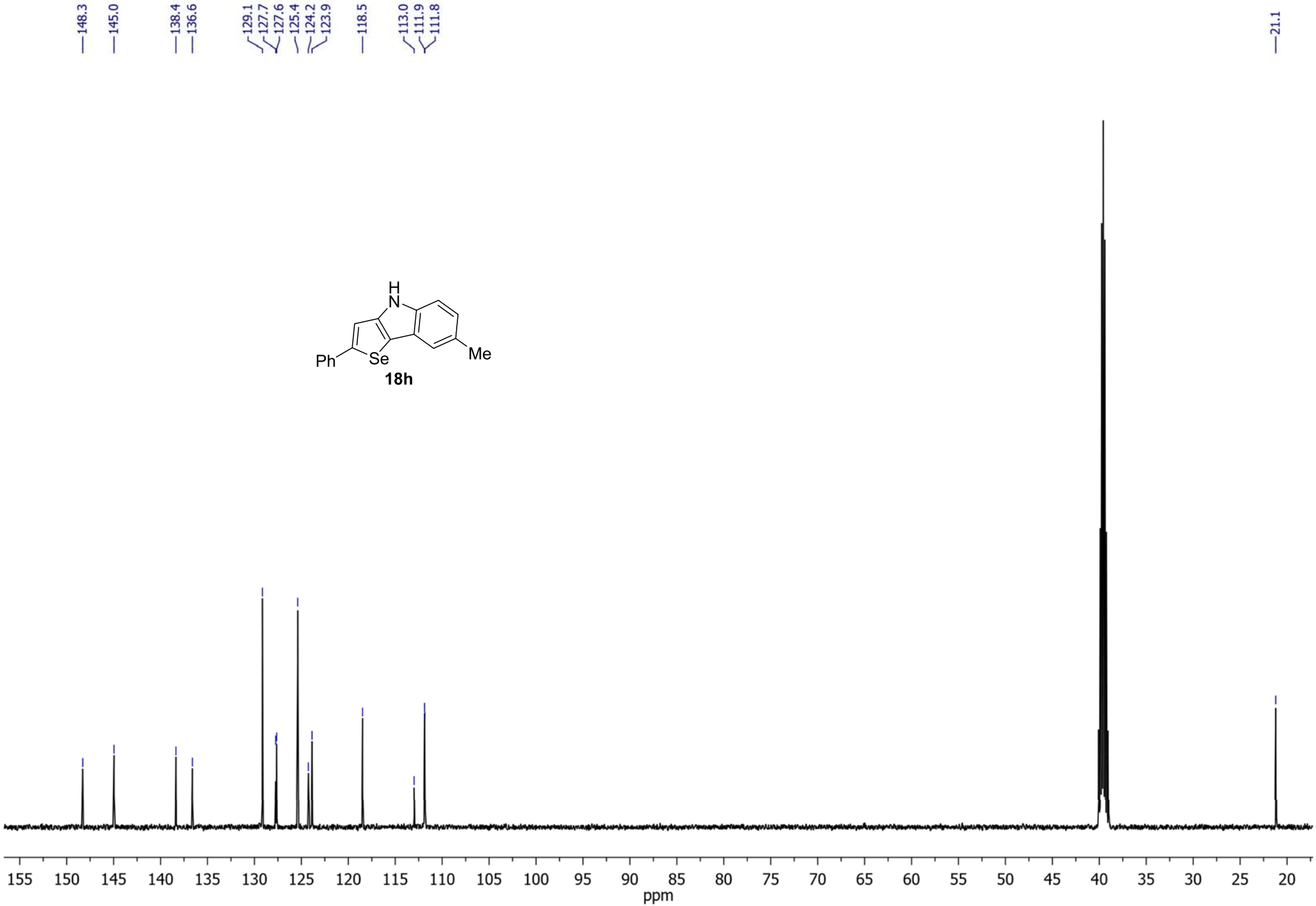
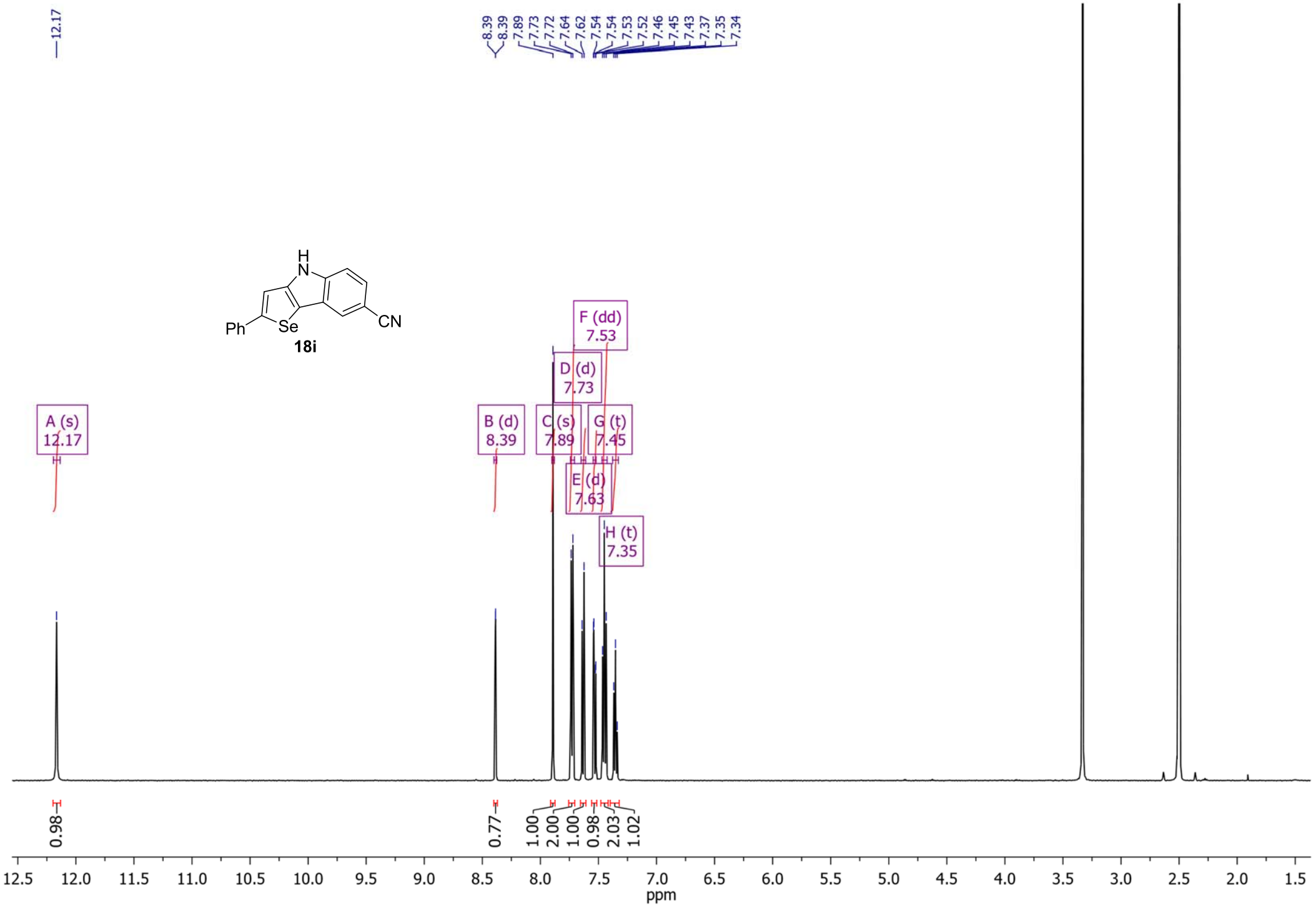
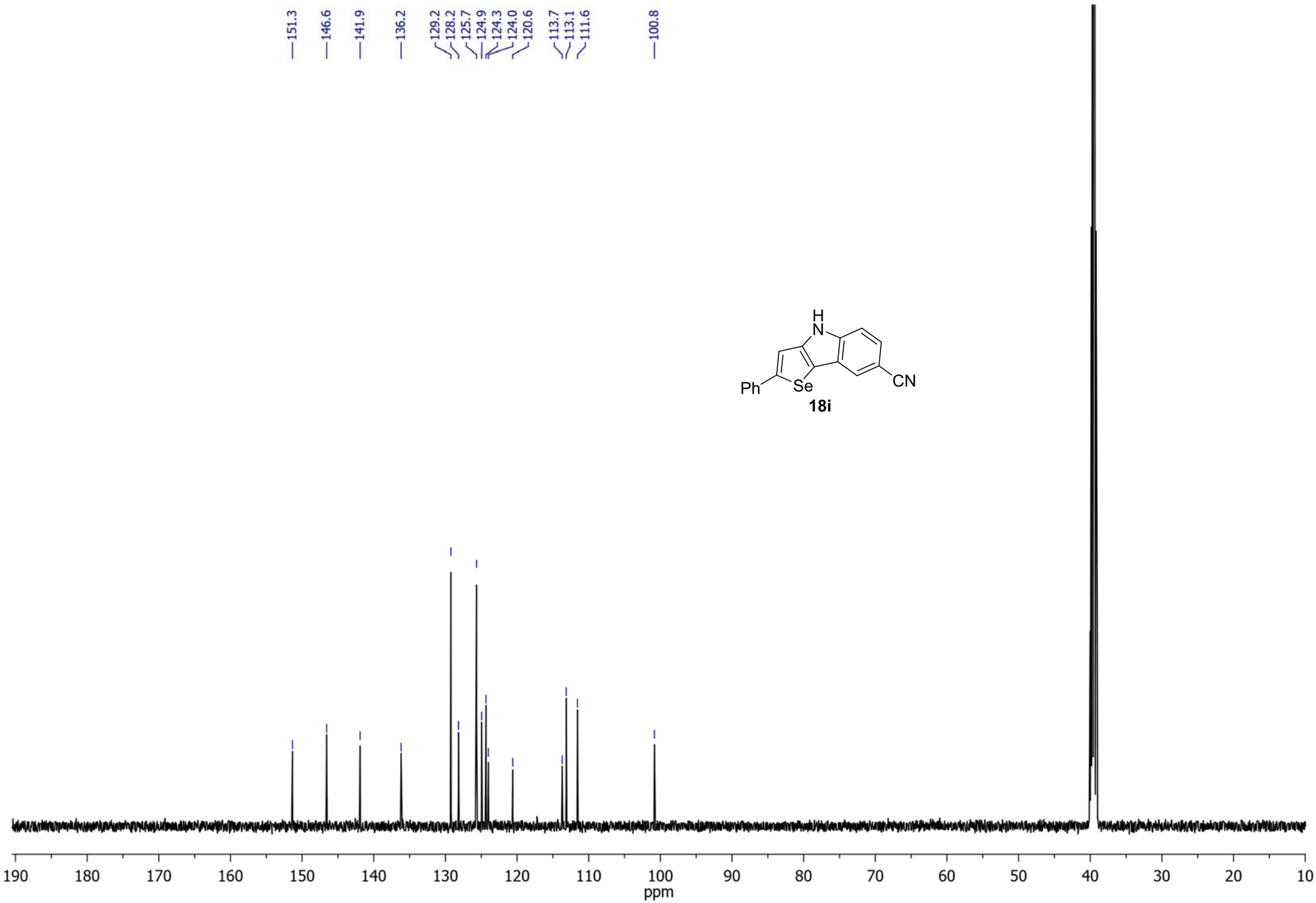


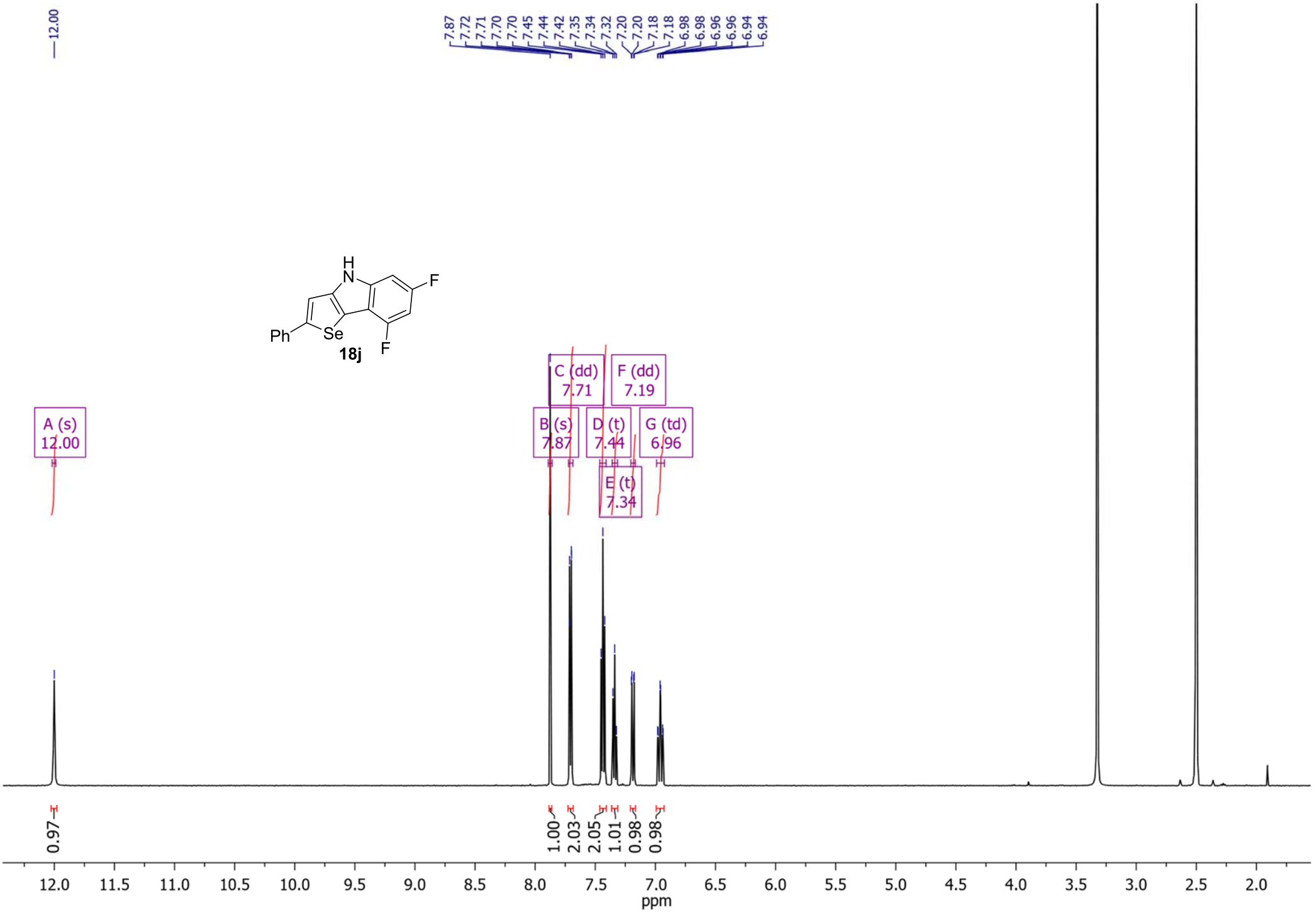
^{1}H NMR (solvent: DMSO-d_6)



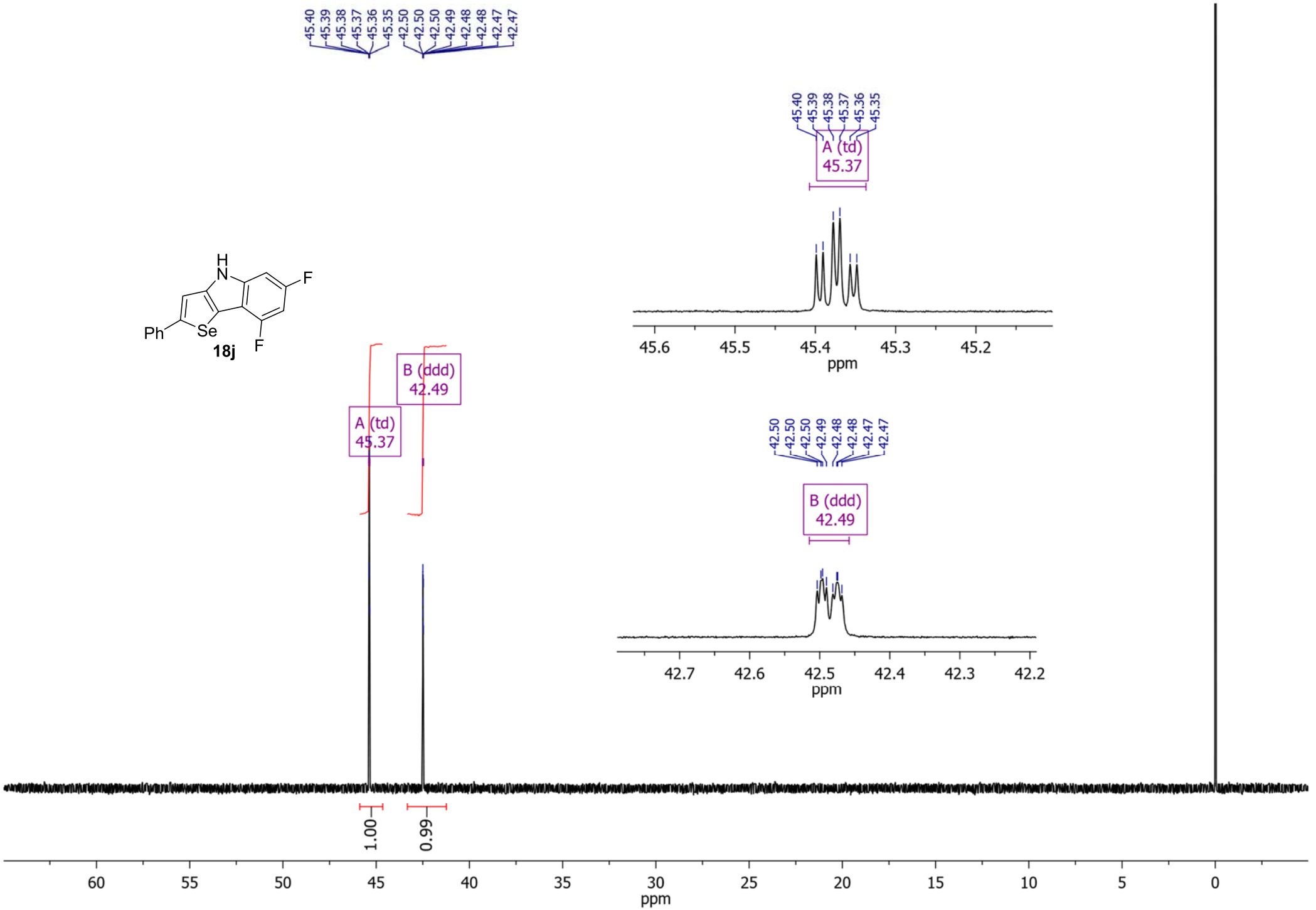
^{13}C NMR (solvent: DMSO-d_6)



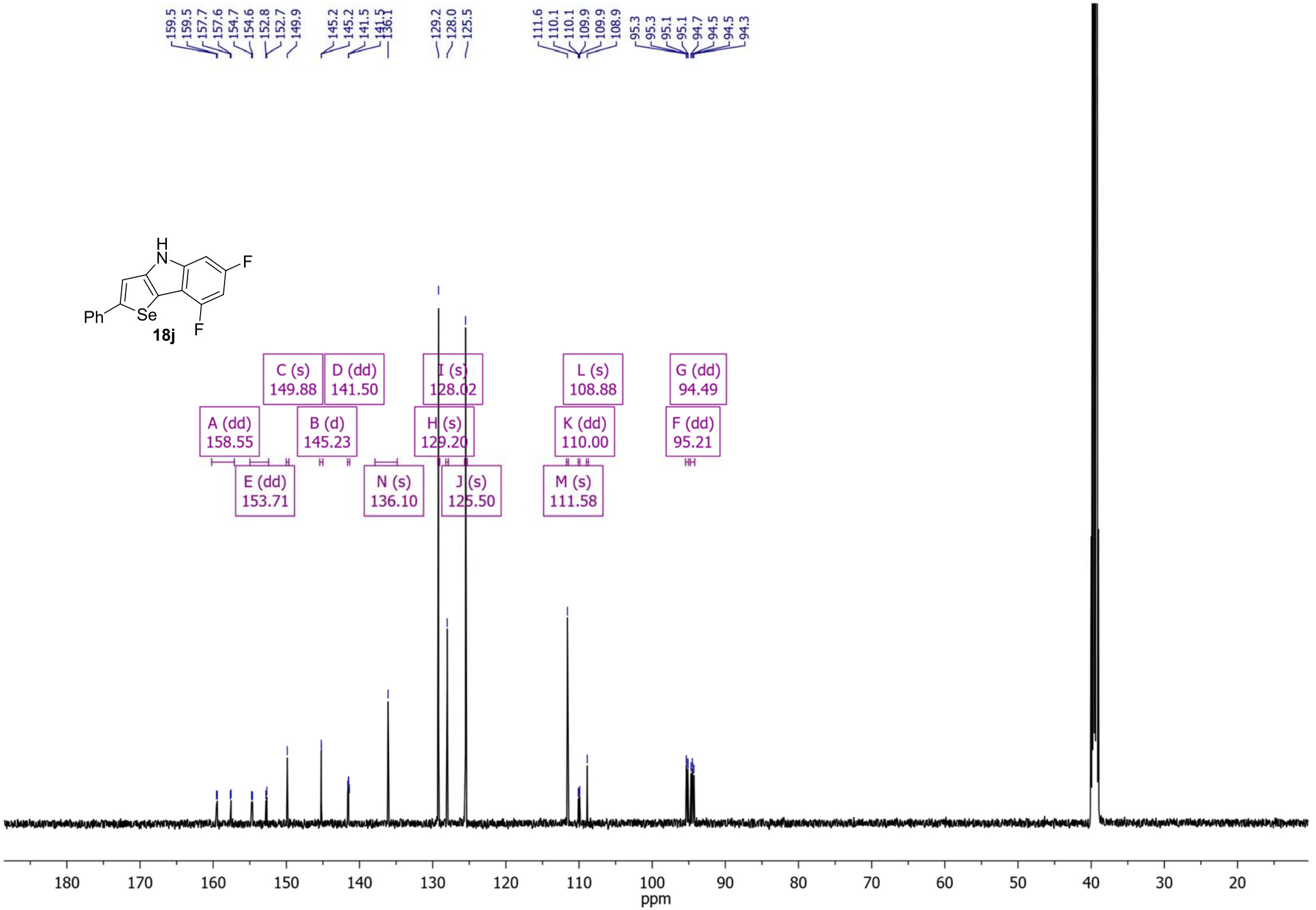
^{1}H NMR (solvent: DMSO-d_6)



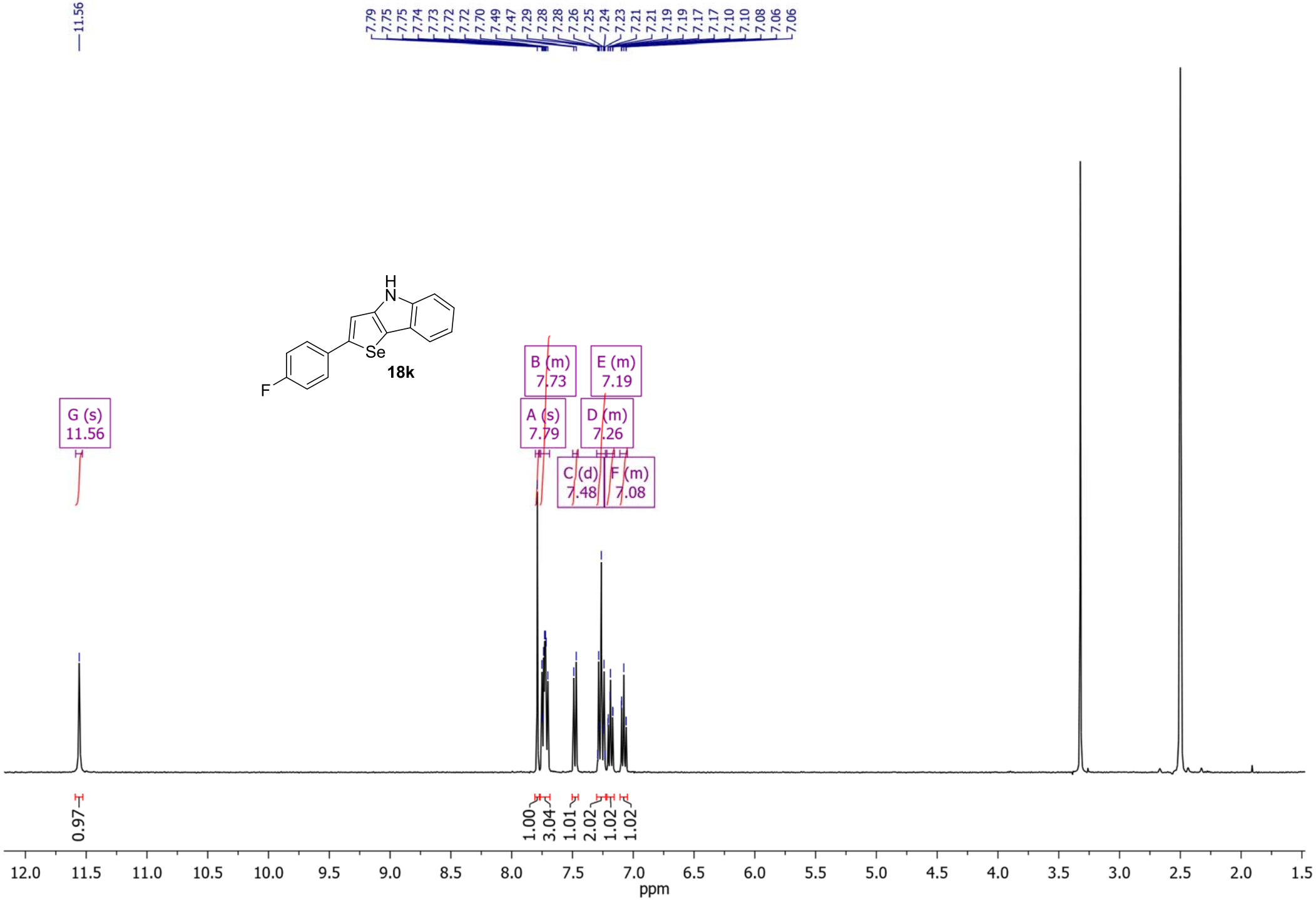
^{19}F NMR (solvent: DMSO-d_6)



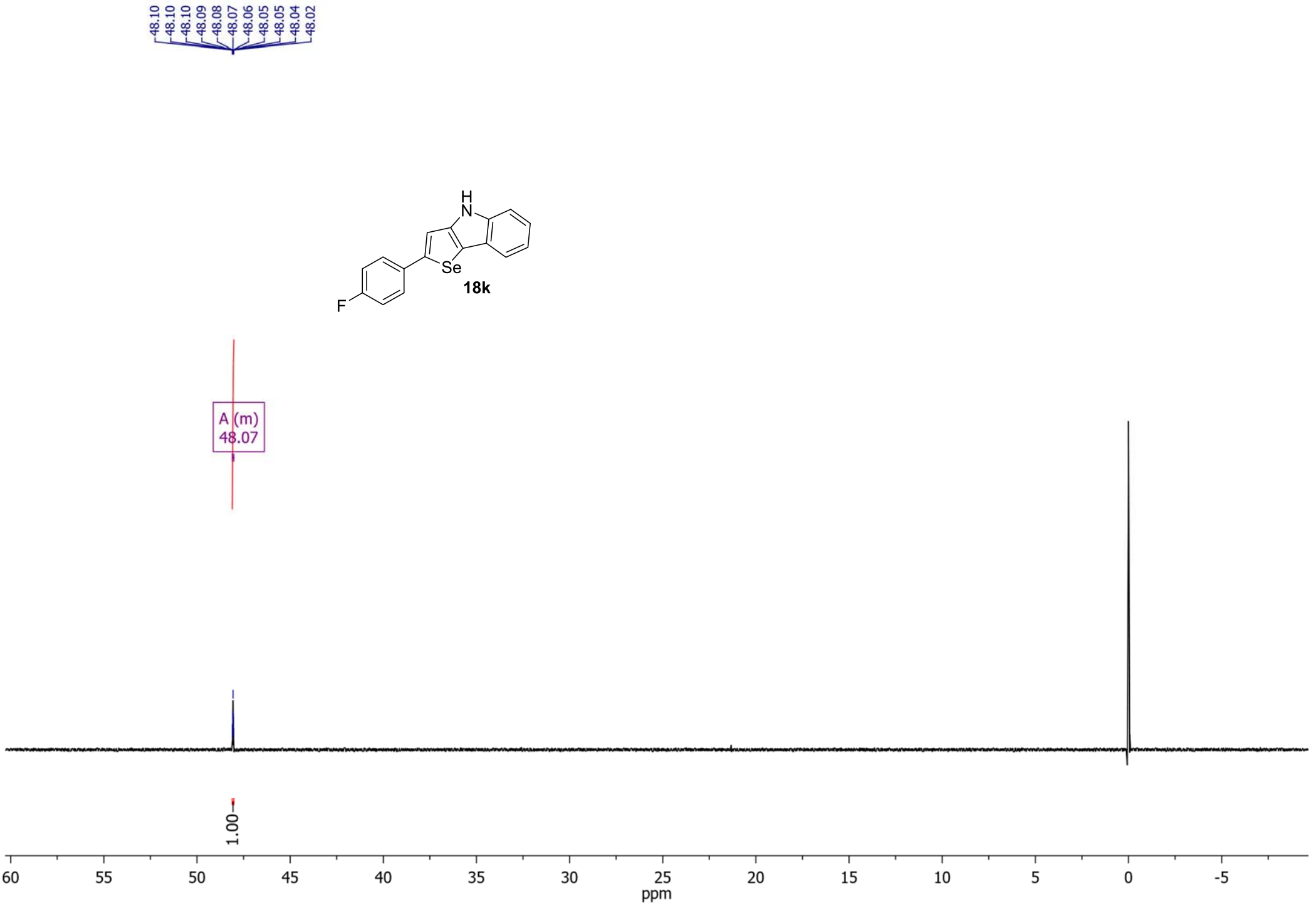
^{13}C NMR (solvent: DMSO-d_6)



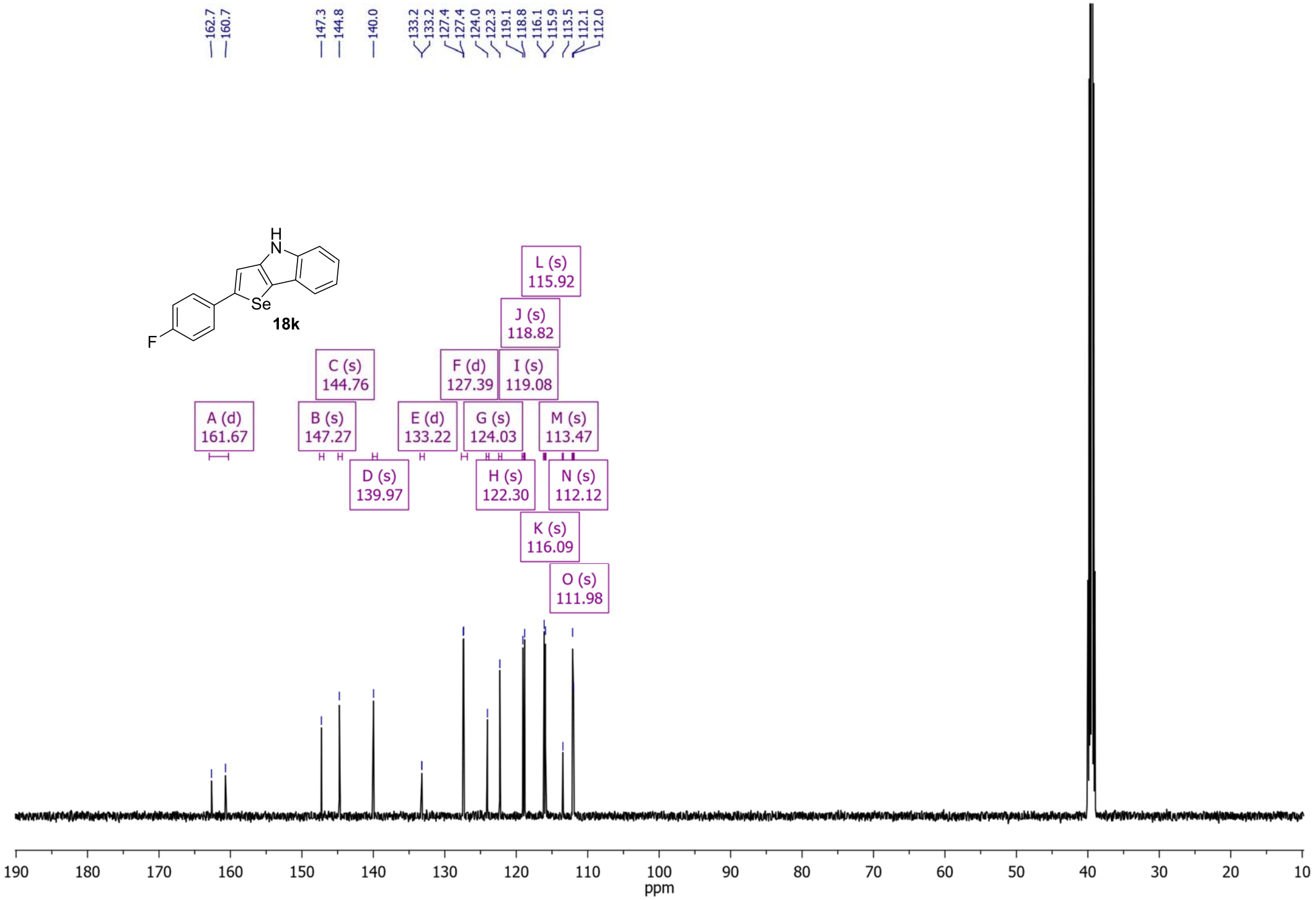
^{1}H NMR (solvent: DMSO-d_6)



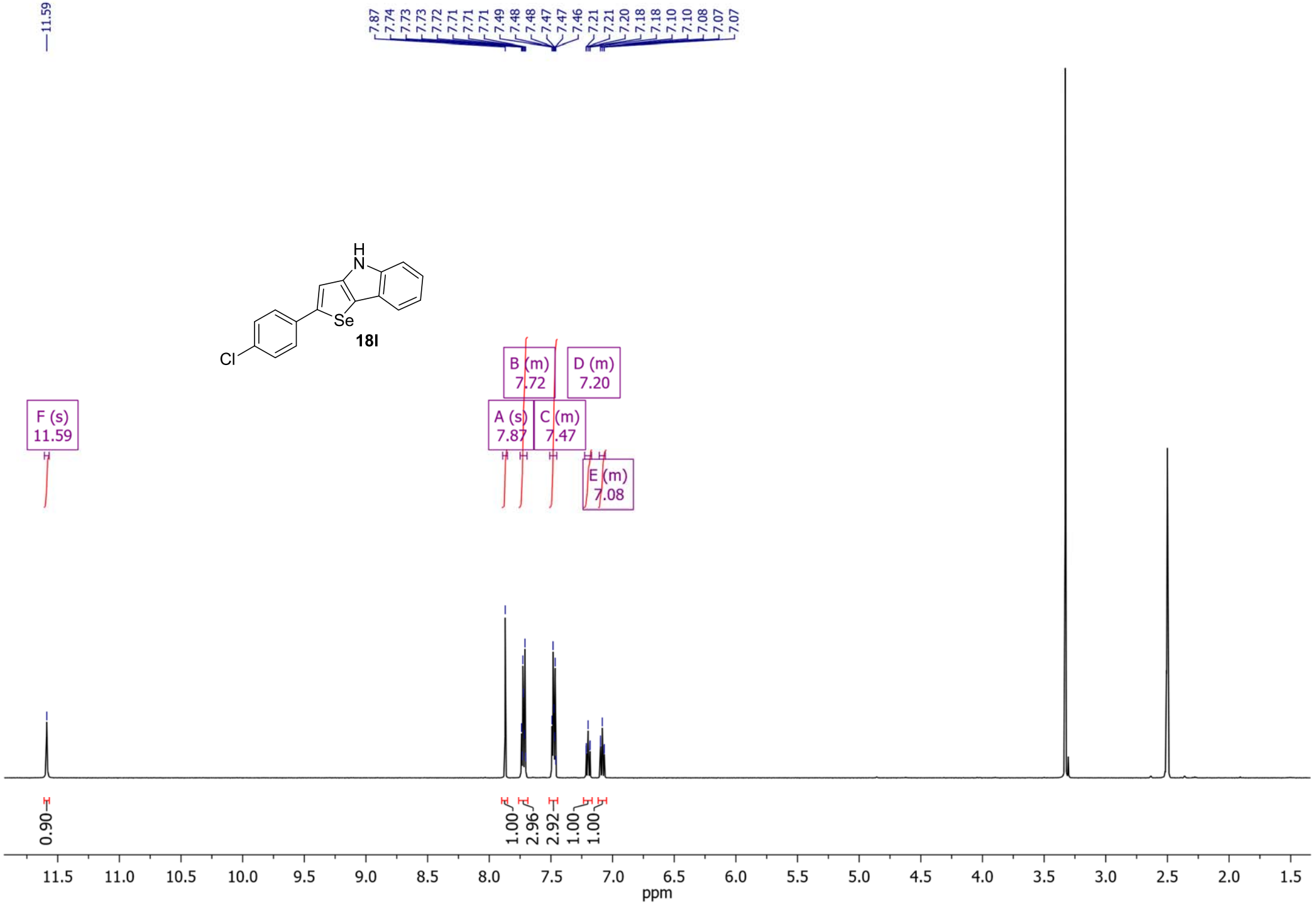
^{19}F NMR (solvent: DMSO-d_6)



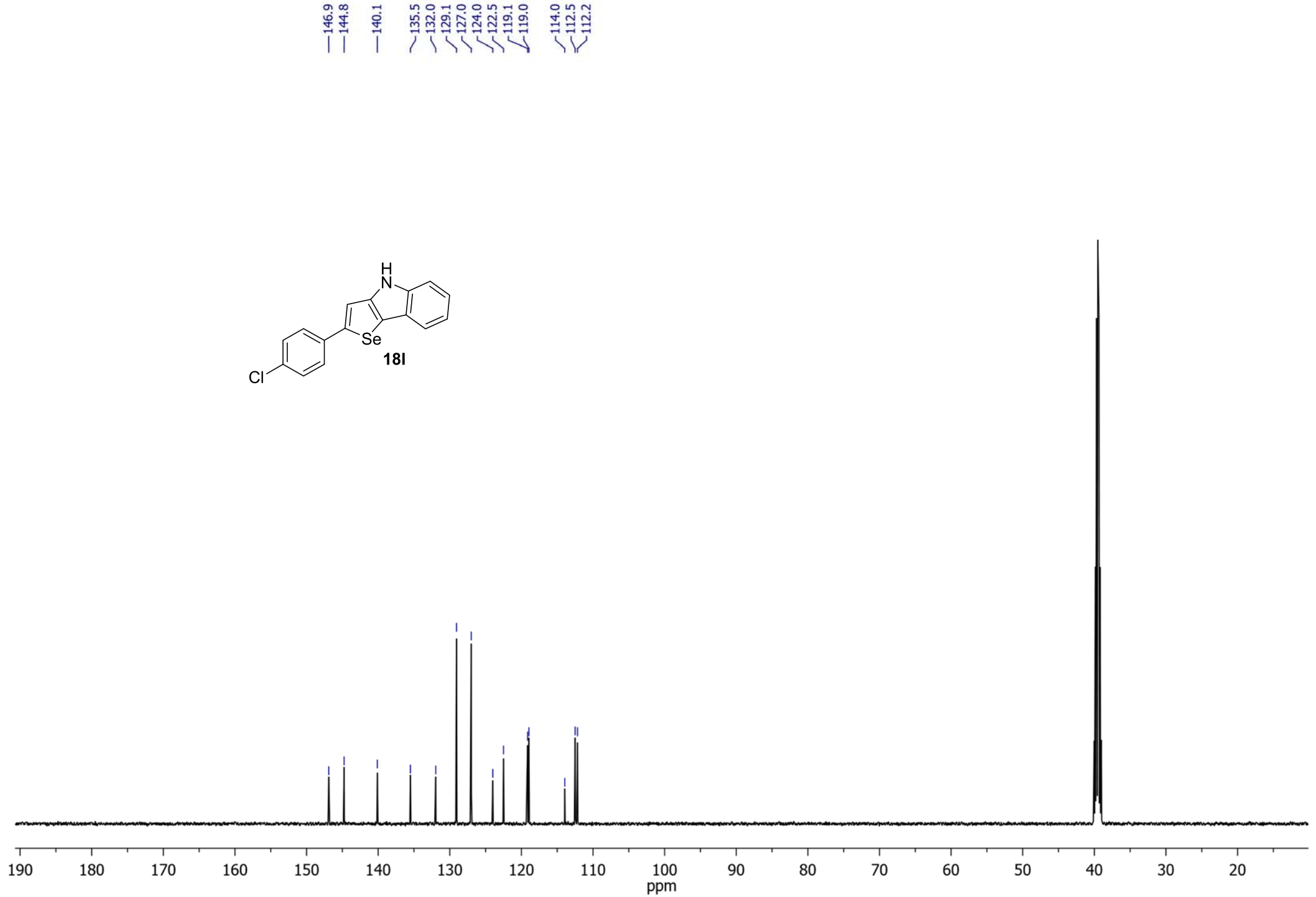
^{13}C NMR (solvent: DMSO-d_6)



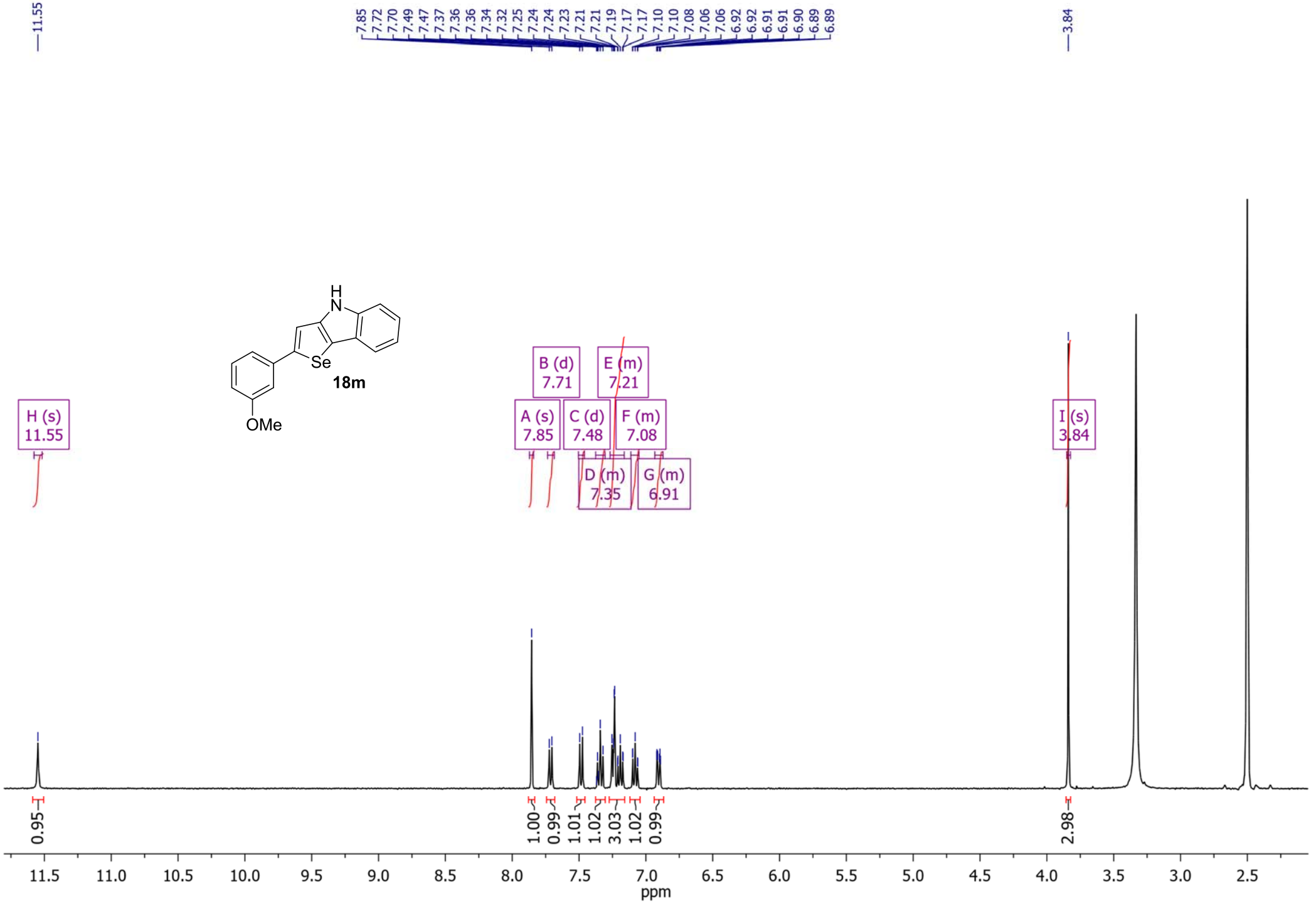
^{1}H NMR (solvent: DMSO-d_6)



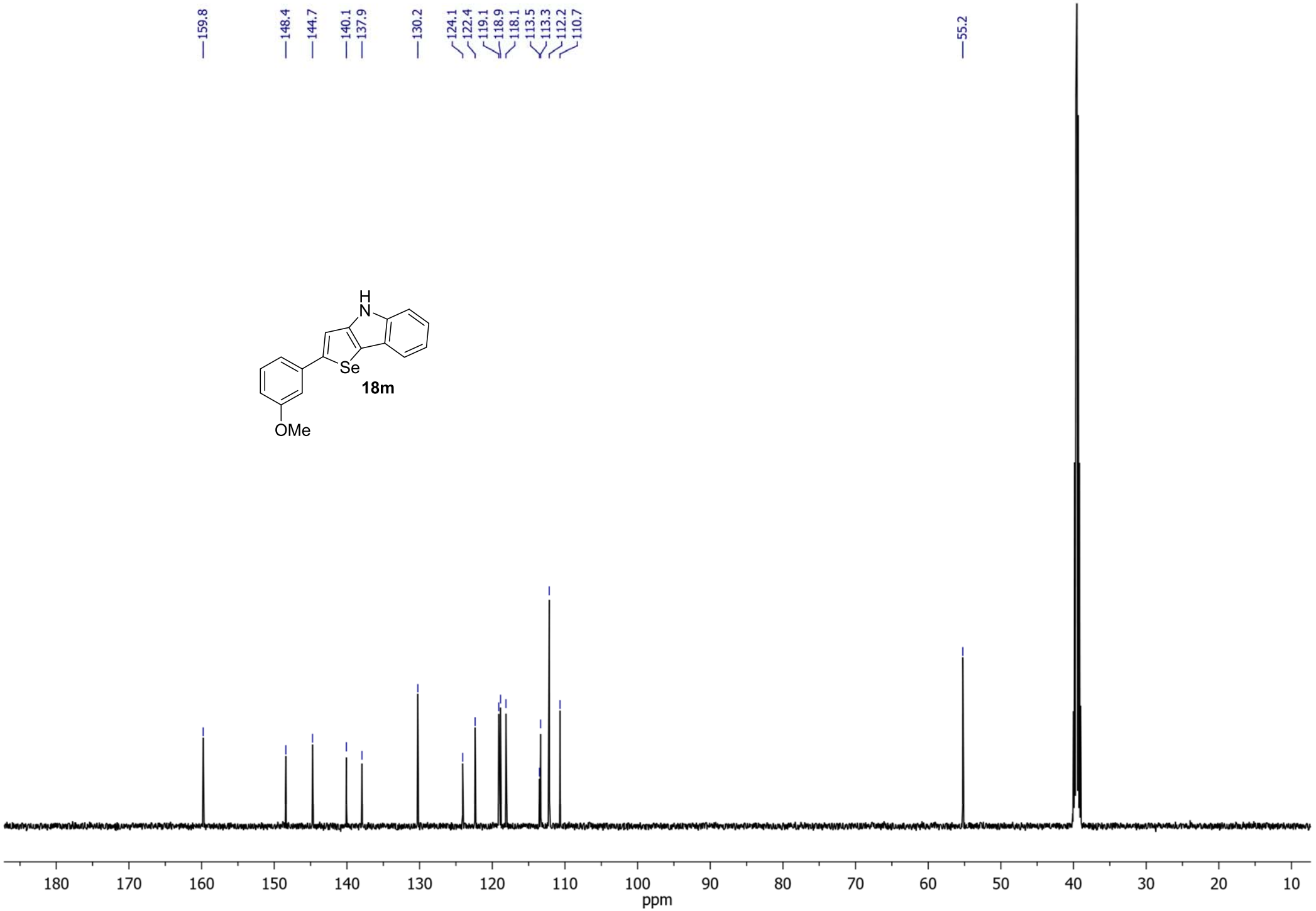
^{13}C NMR (solvent: DMSO-d_6)



^{1}H NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)



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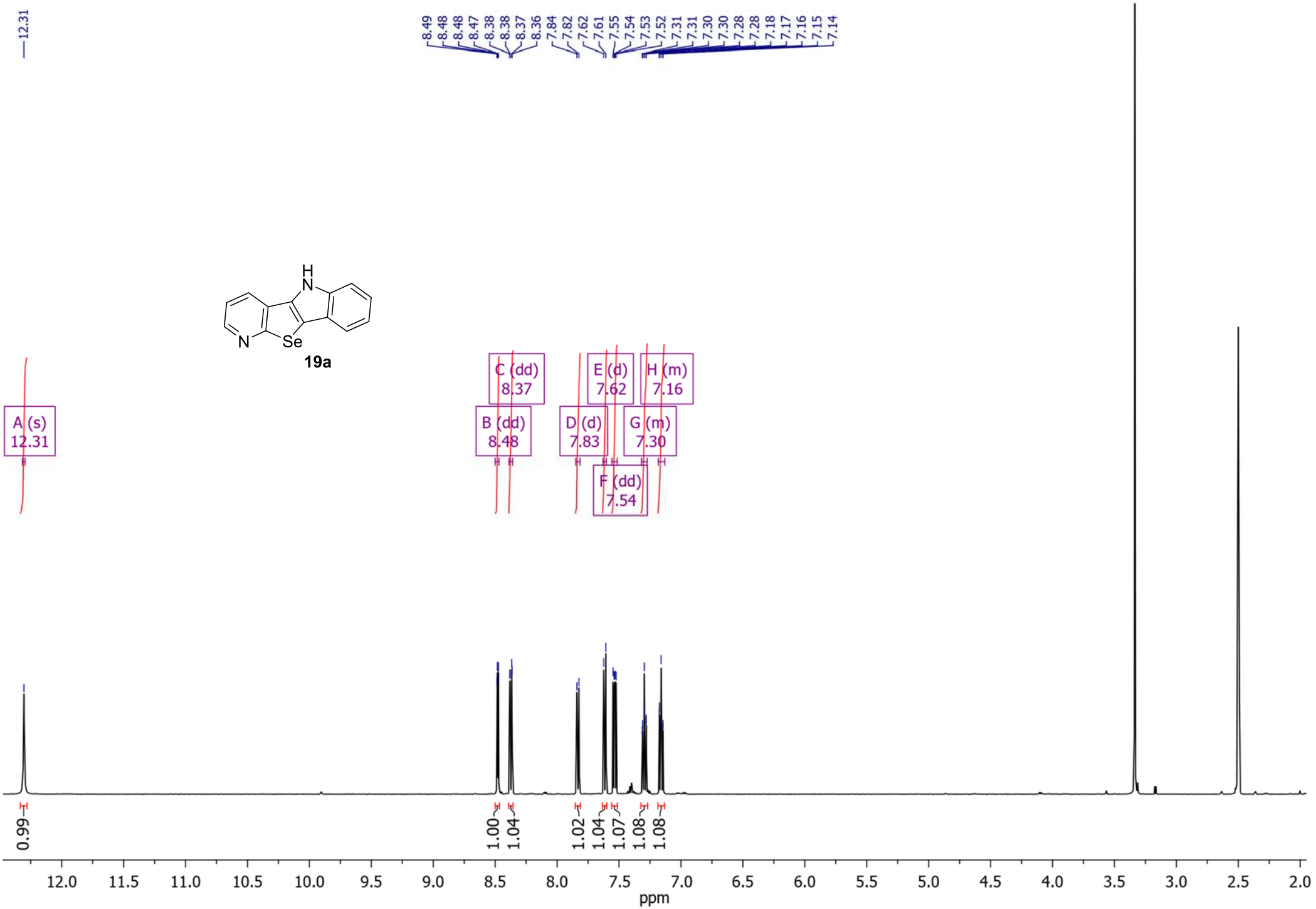
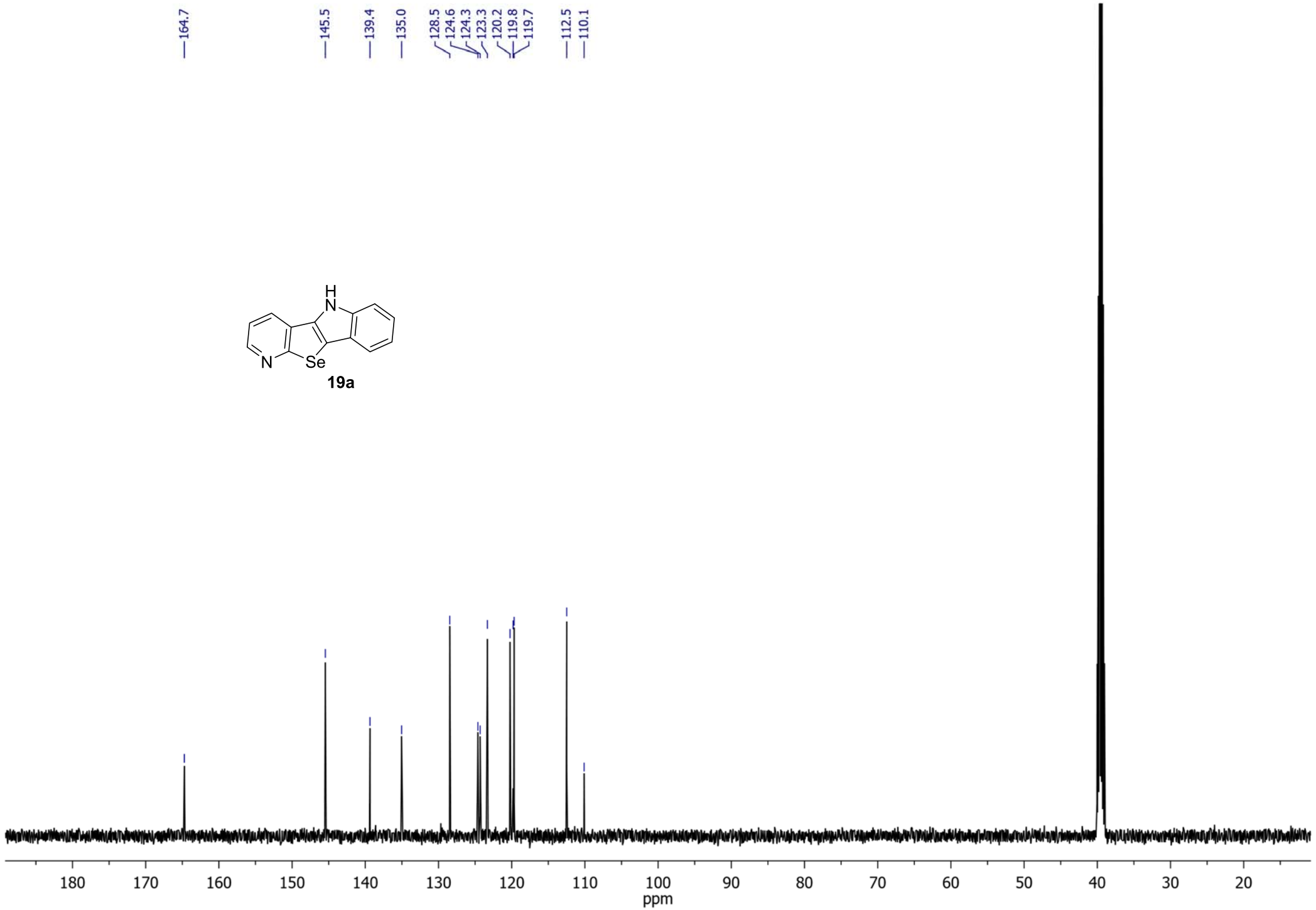
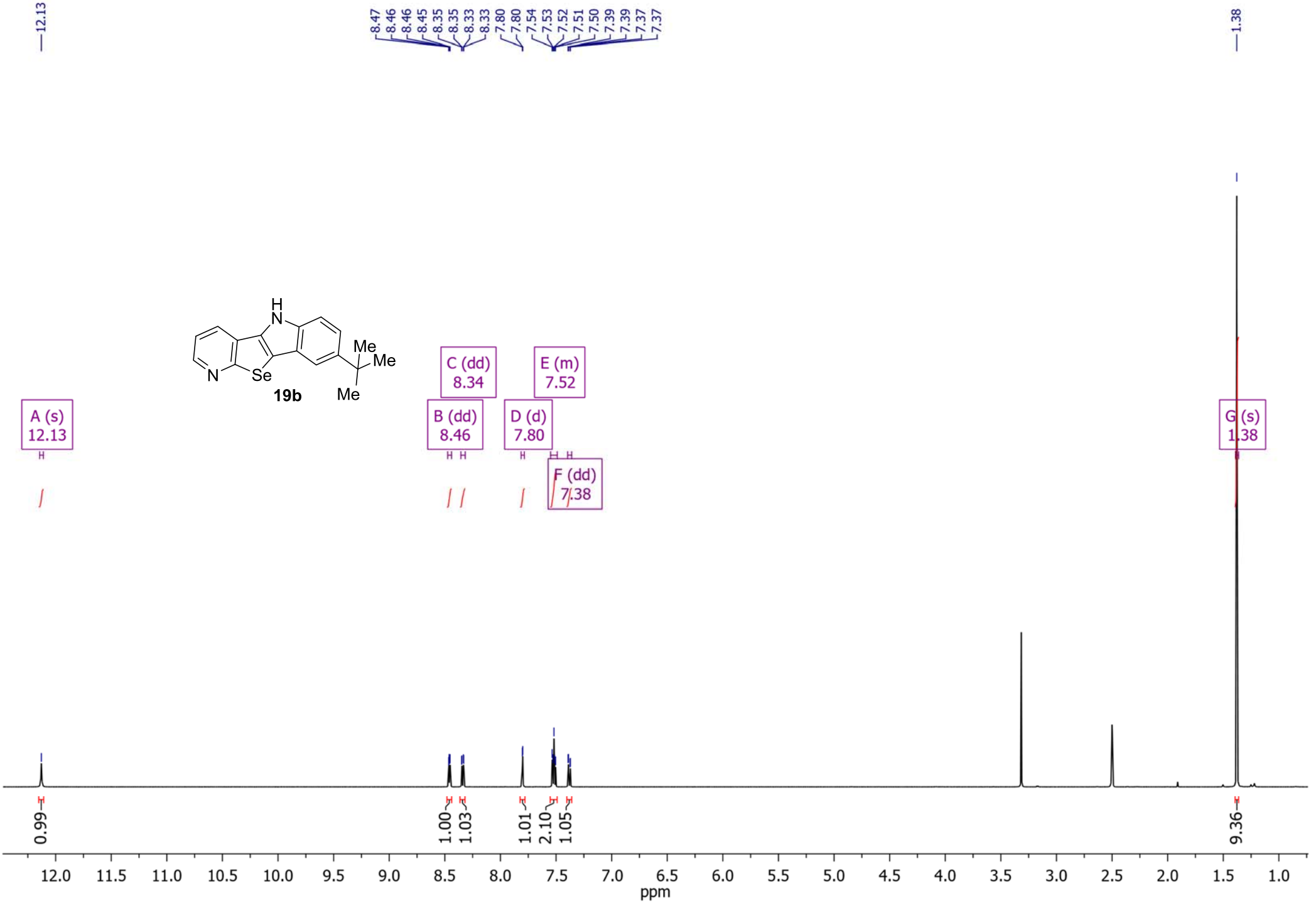


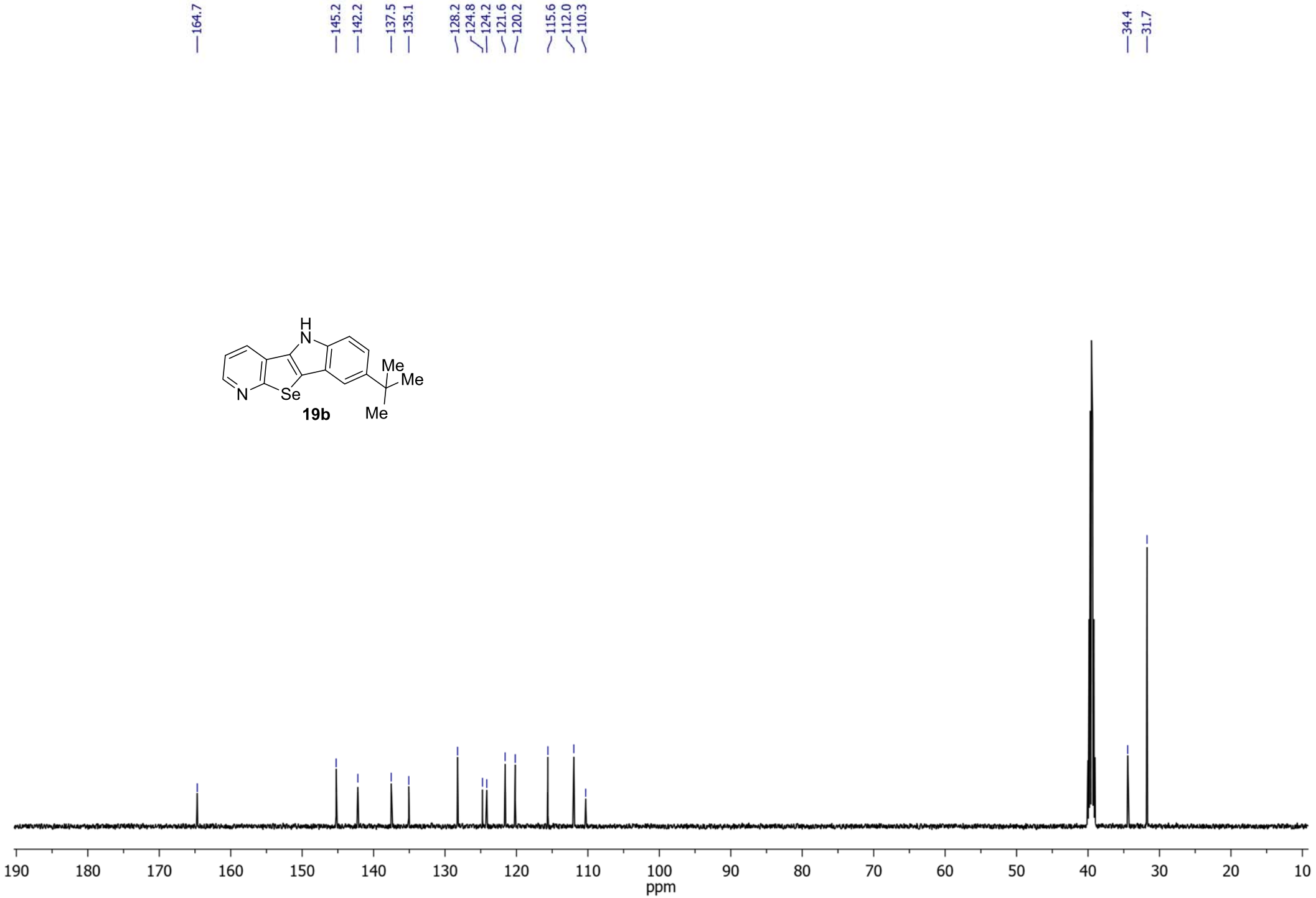
^{13}C NMR (solvent: DMSO-d_6)



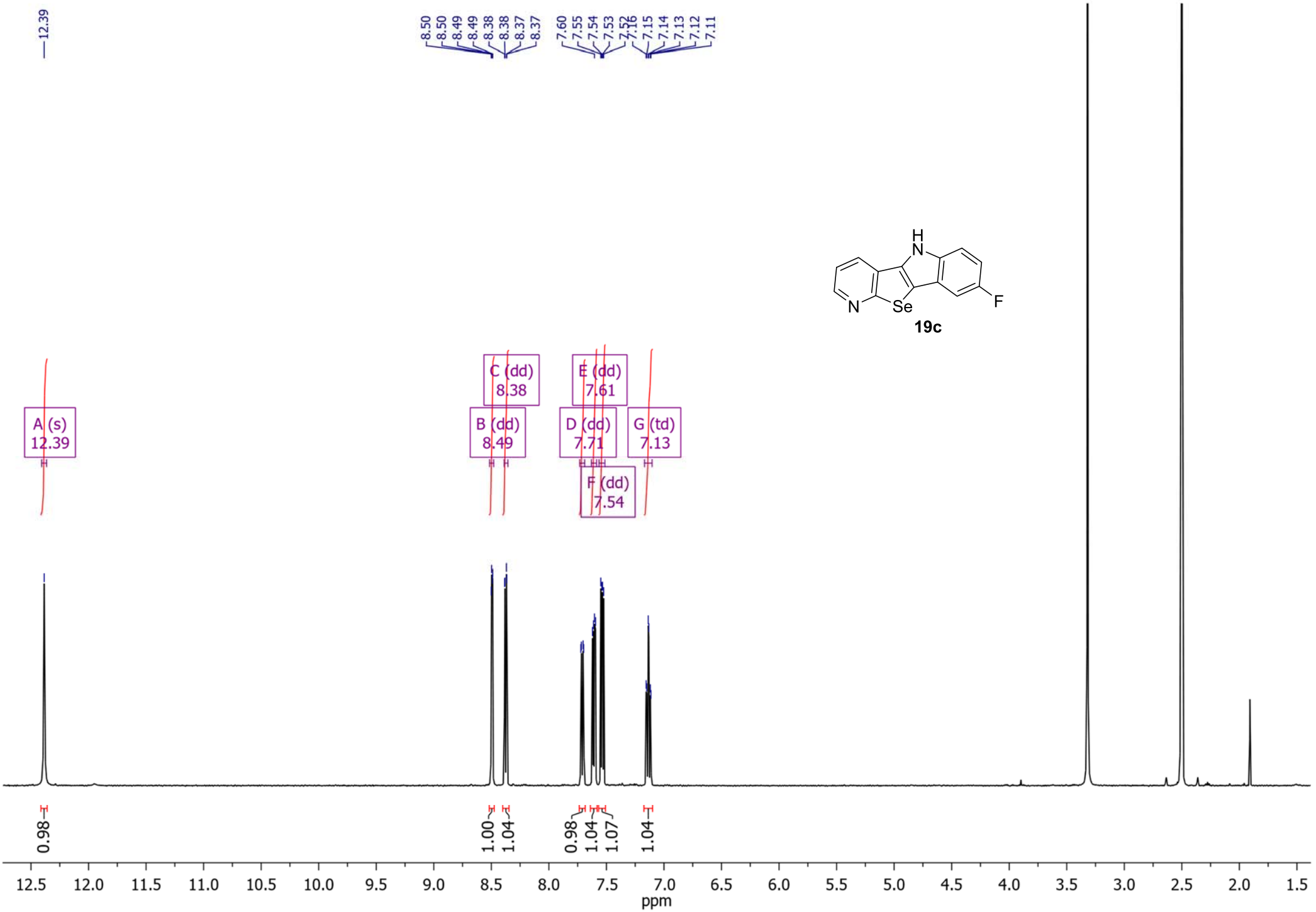
^{1}H NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)

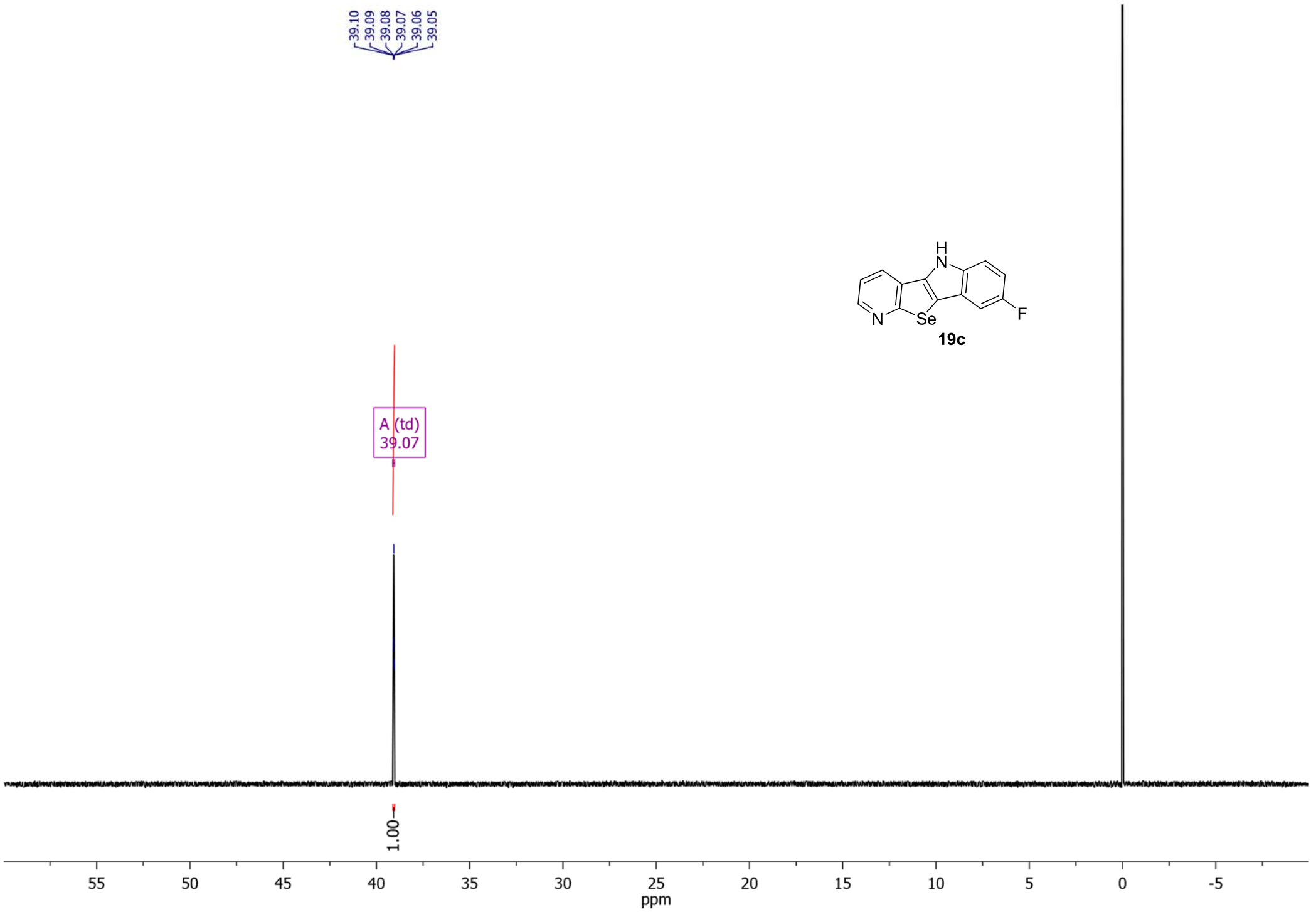


^{1}H NMR (solvent: DMSO-d_6)

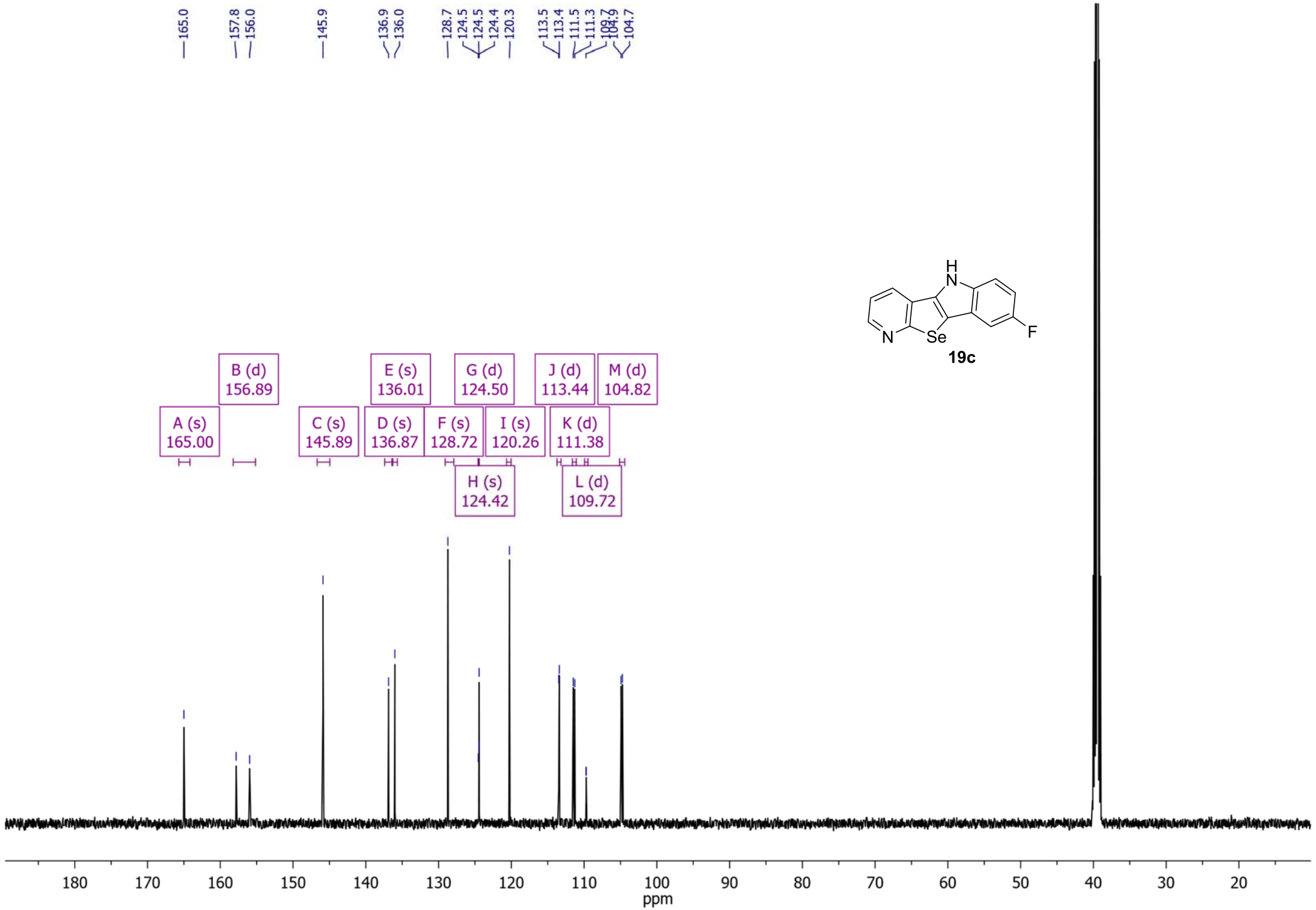


19c

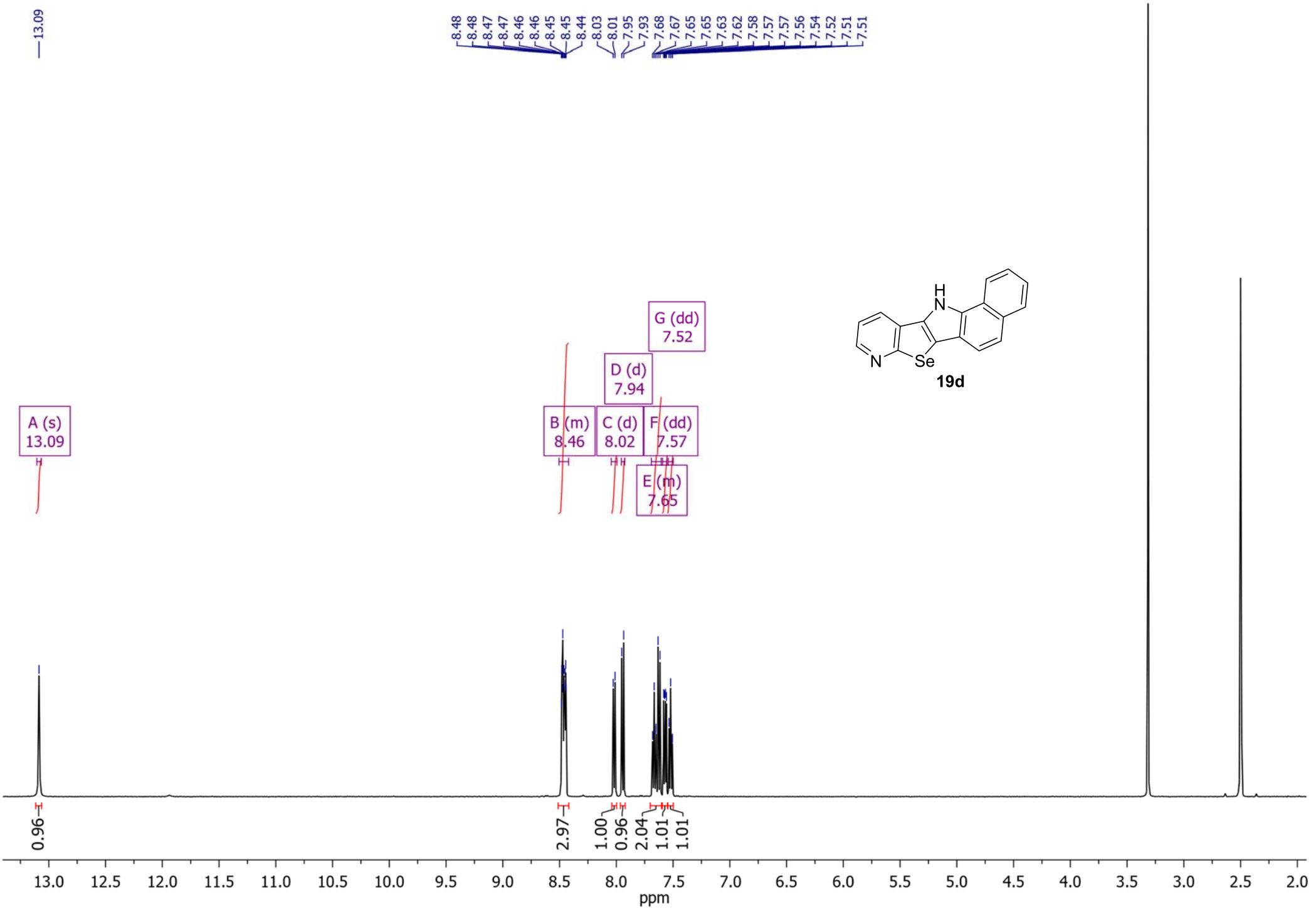
^{19}F NMR (solvent: DMSO-d_6)



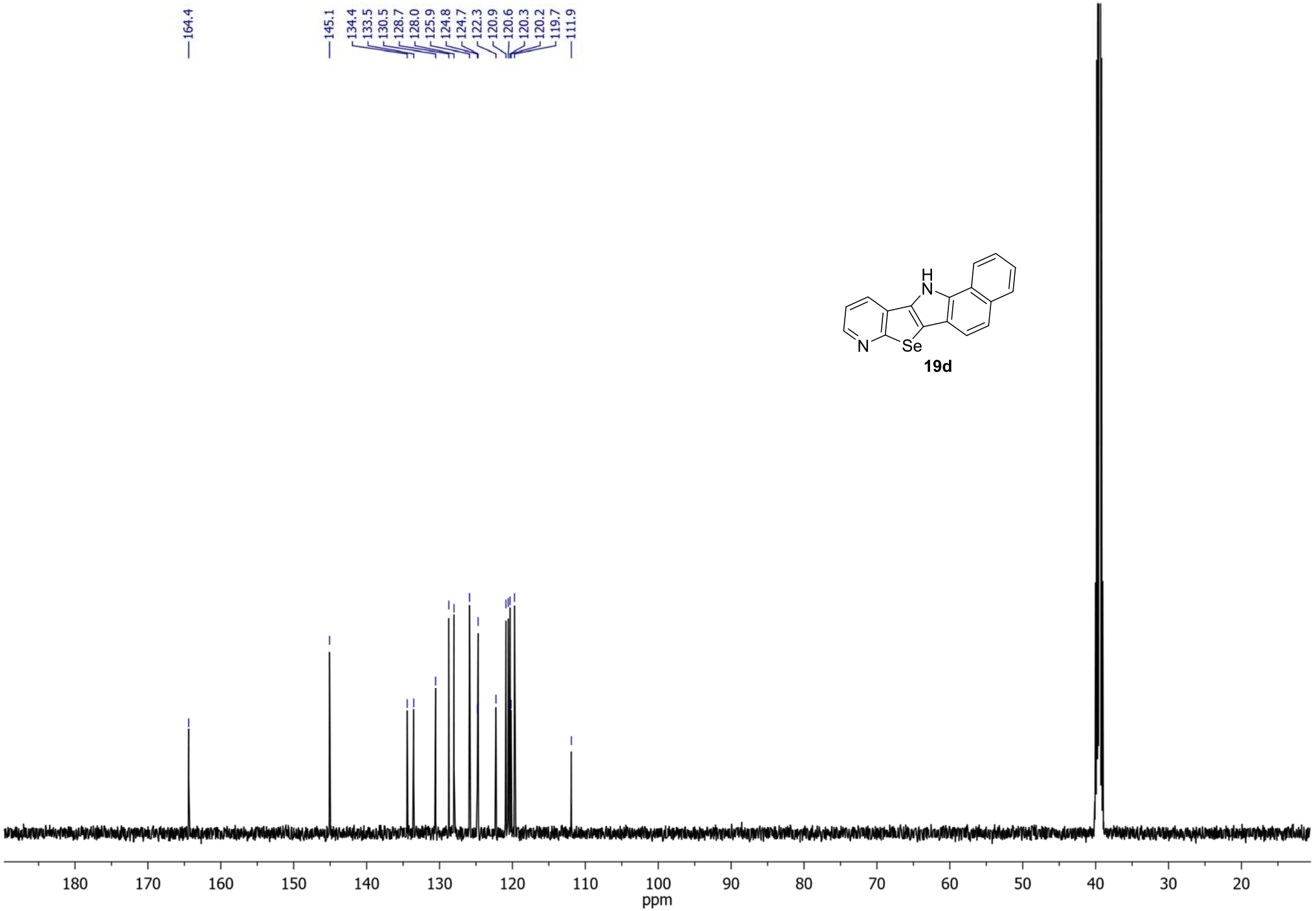
^{13}C NMR (solvent: DMSO-d_6)



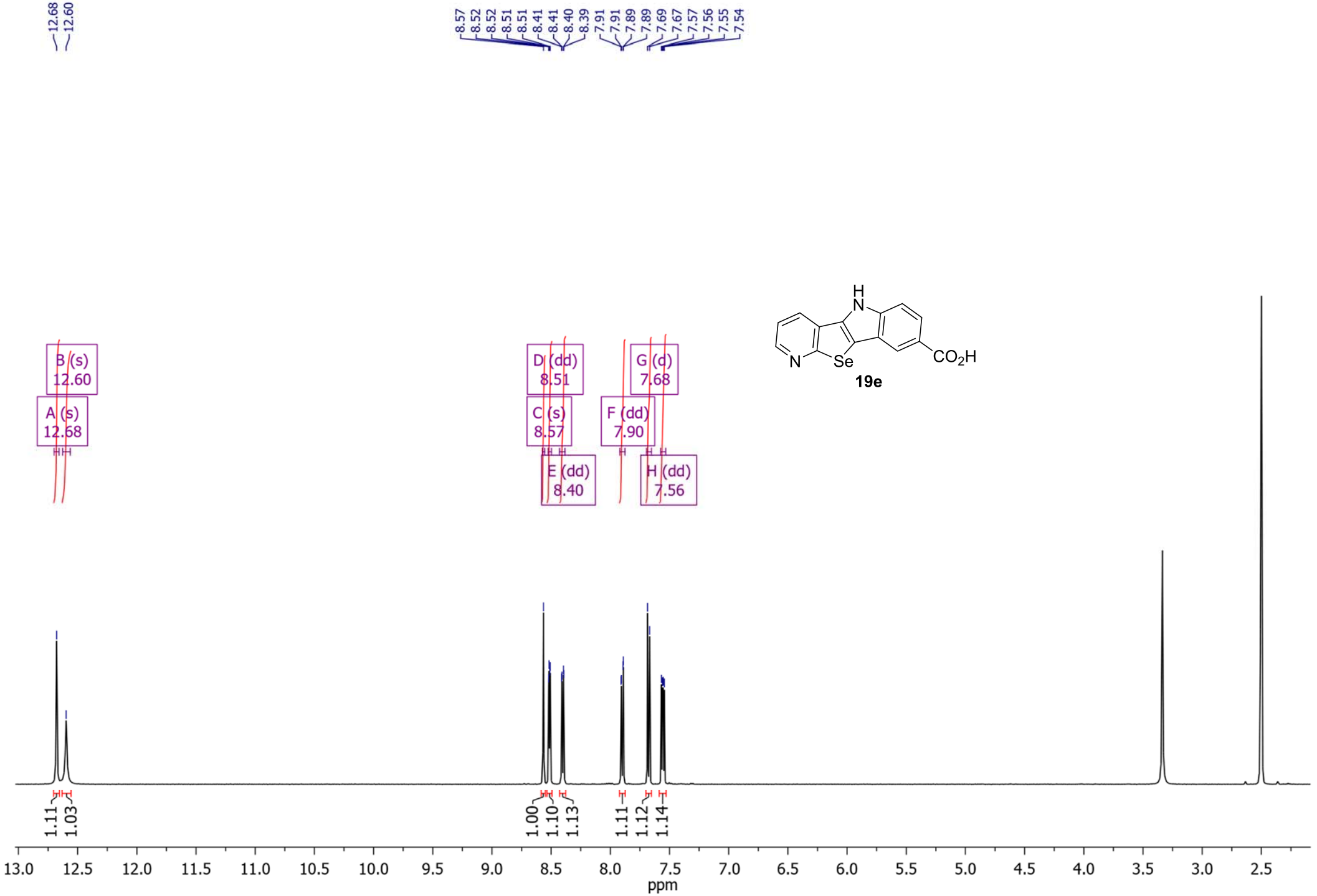
^{1}H NMR (solvent: DMSO-d_6)



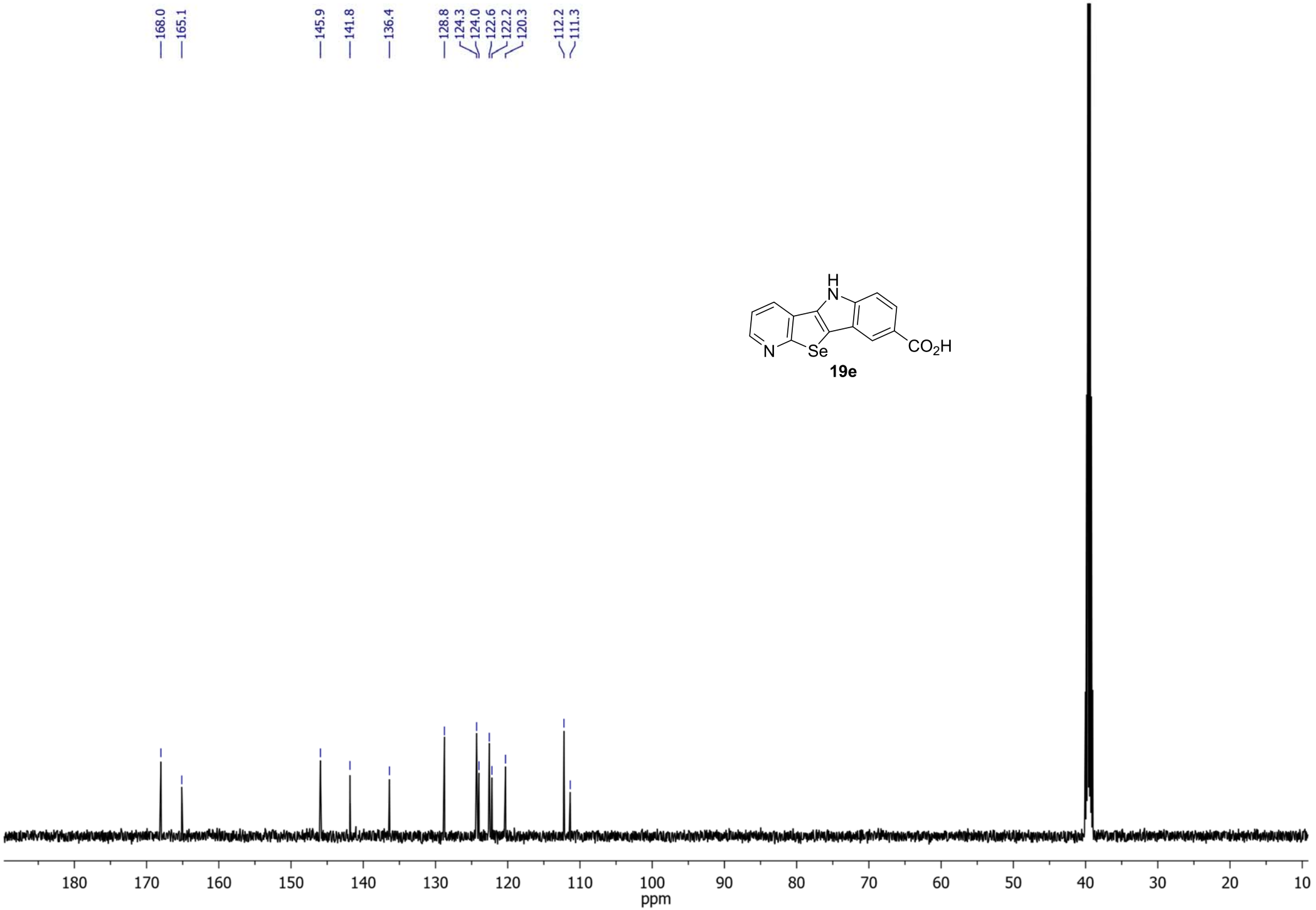
^{13}C NMR (solvent: DMSO-d_6)



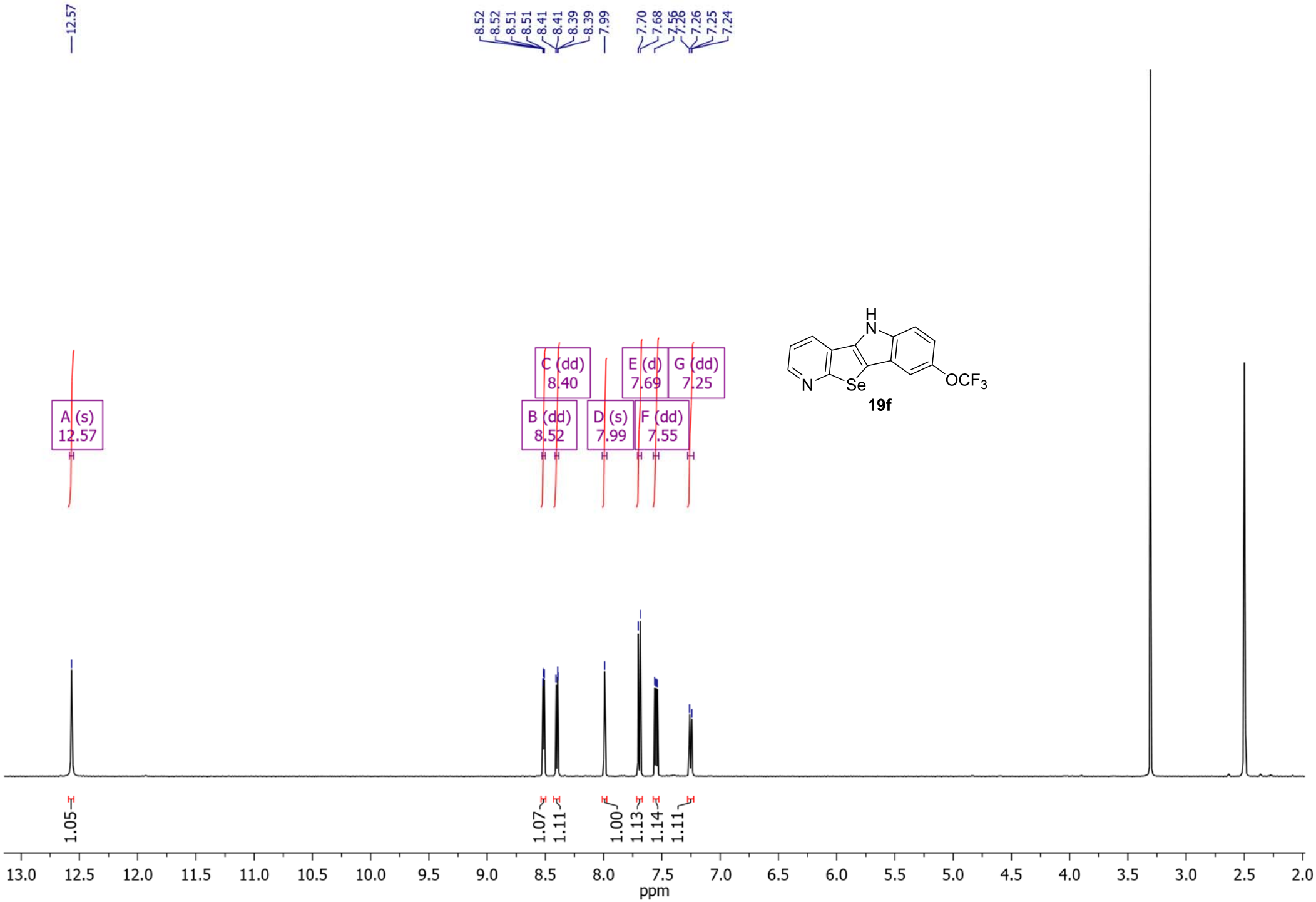
^{1}H NMR (solvent: DMSO-d_6)



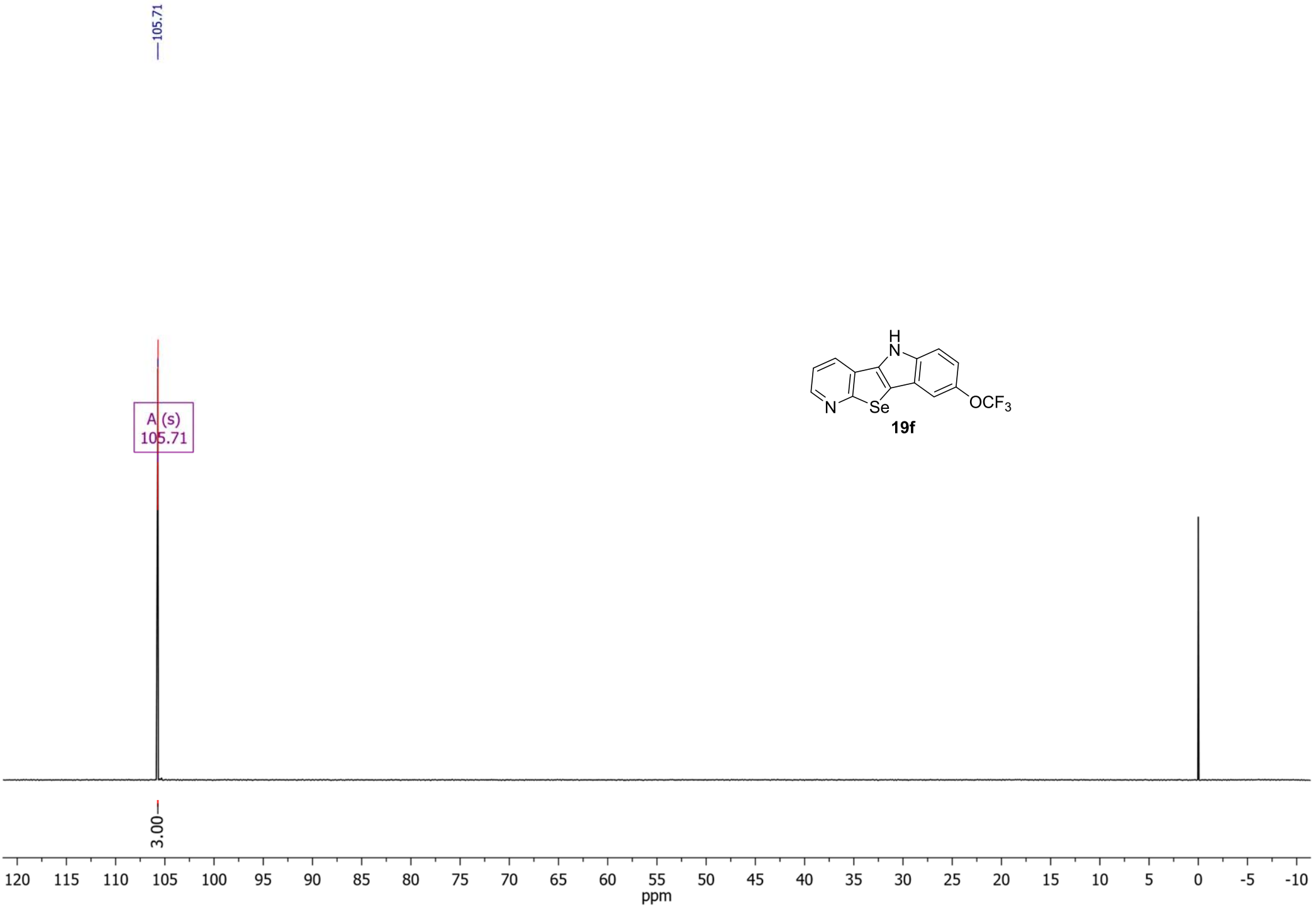
^{13}C NMR (solvent: DMSO-d_6)



^{1}H NMR (solvent: DMSO-d_6)

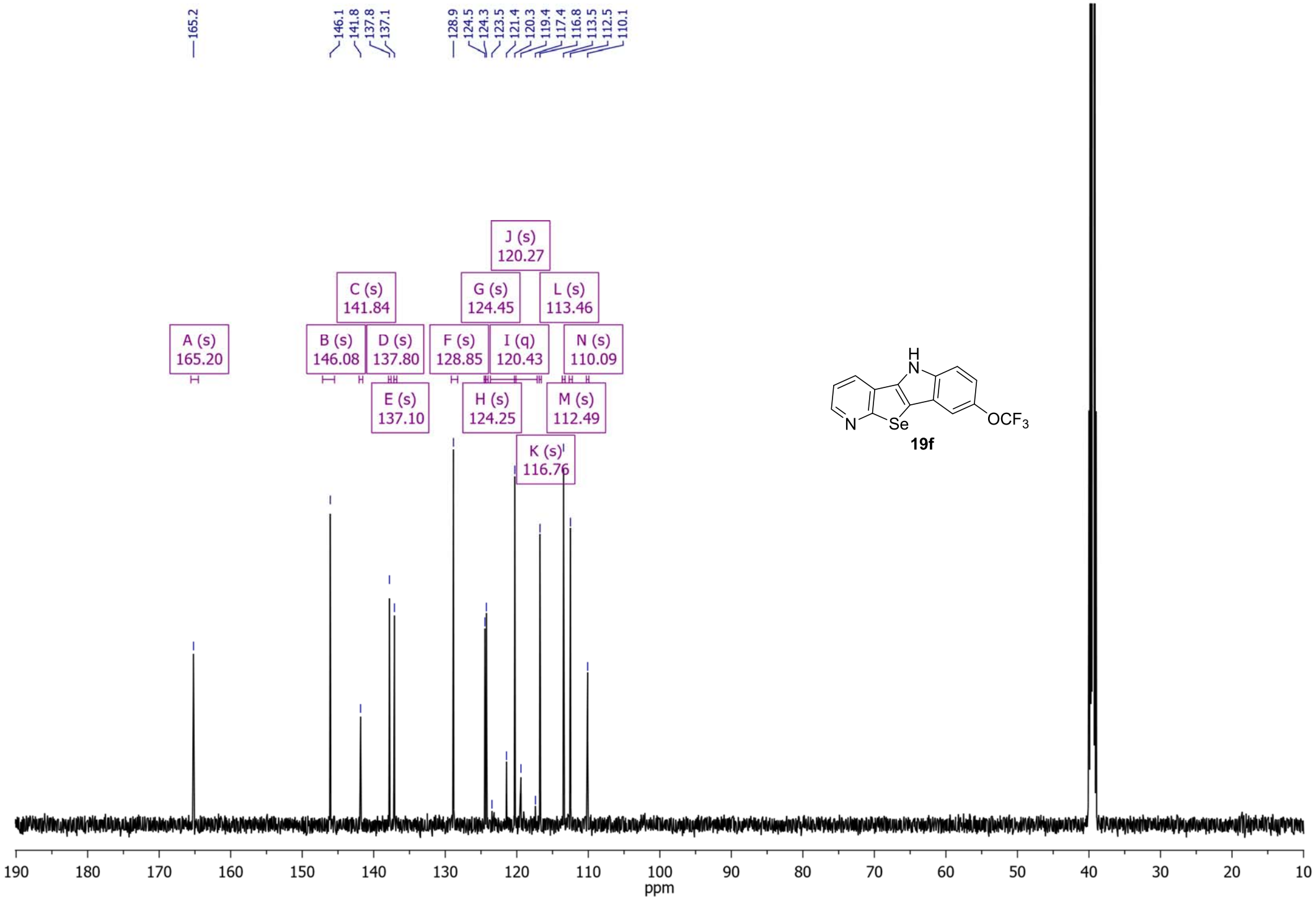


^{19}F NMR (solvent: DMSO-d_6)

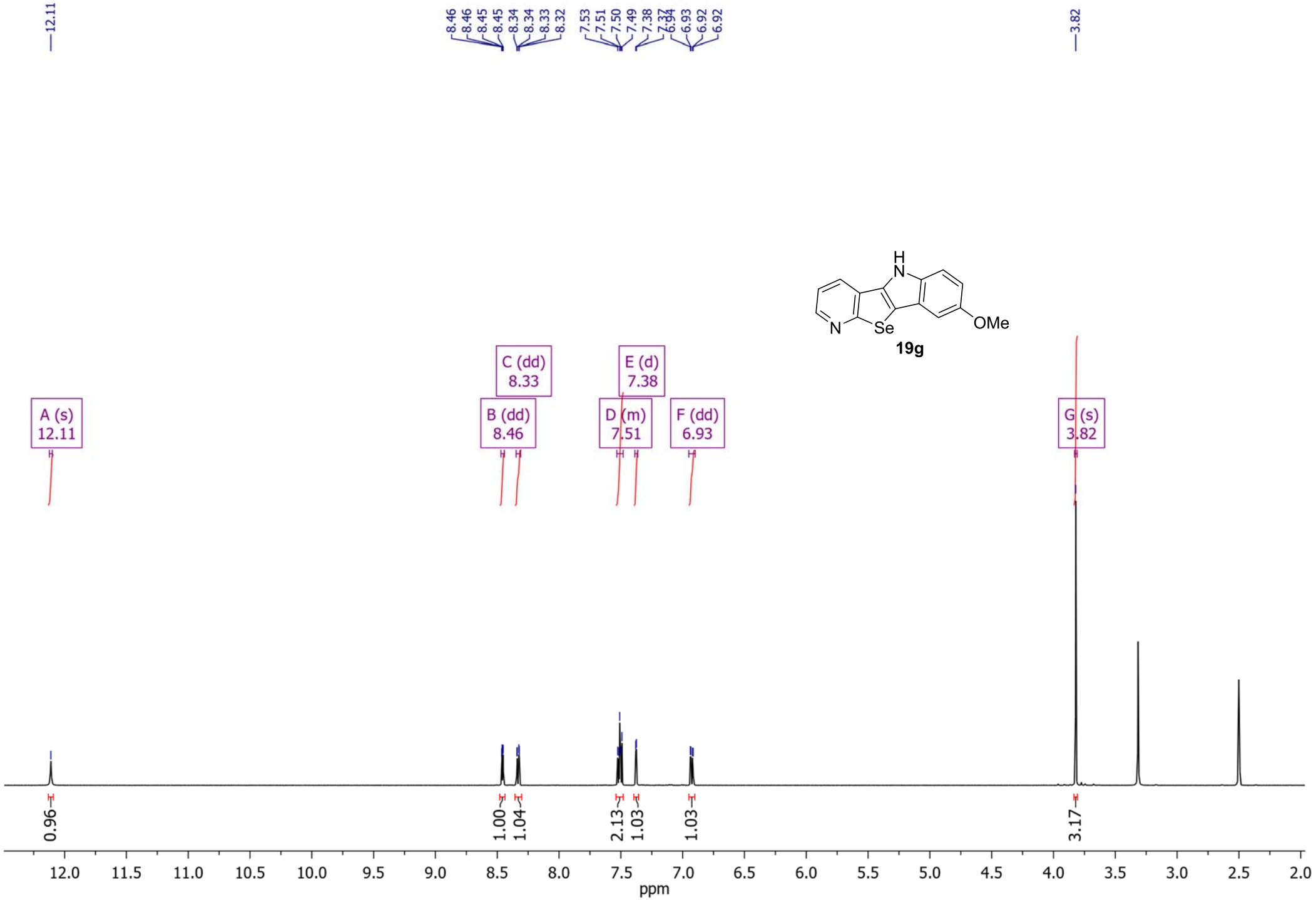


19f

^{13}C NMR (solvent: DMSO-d_6)

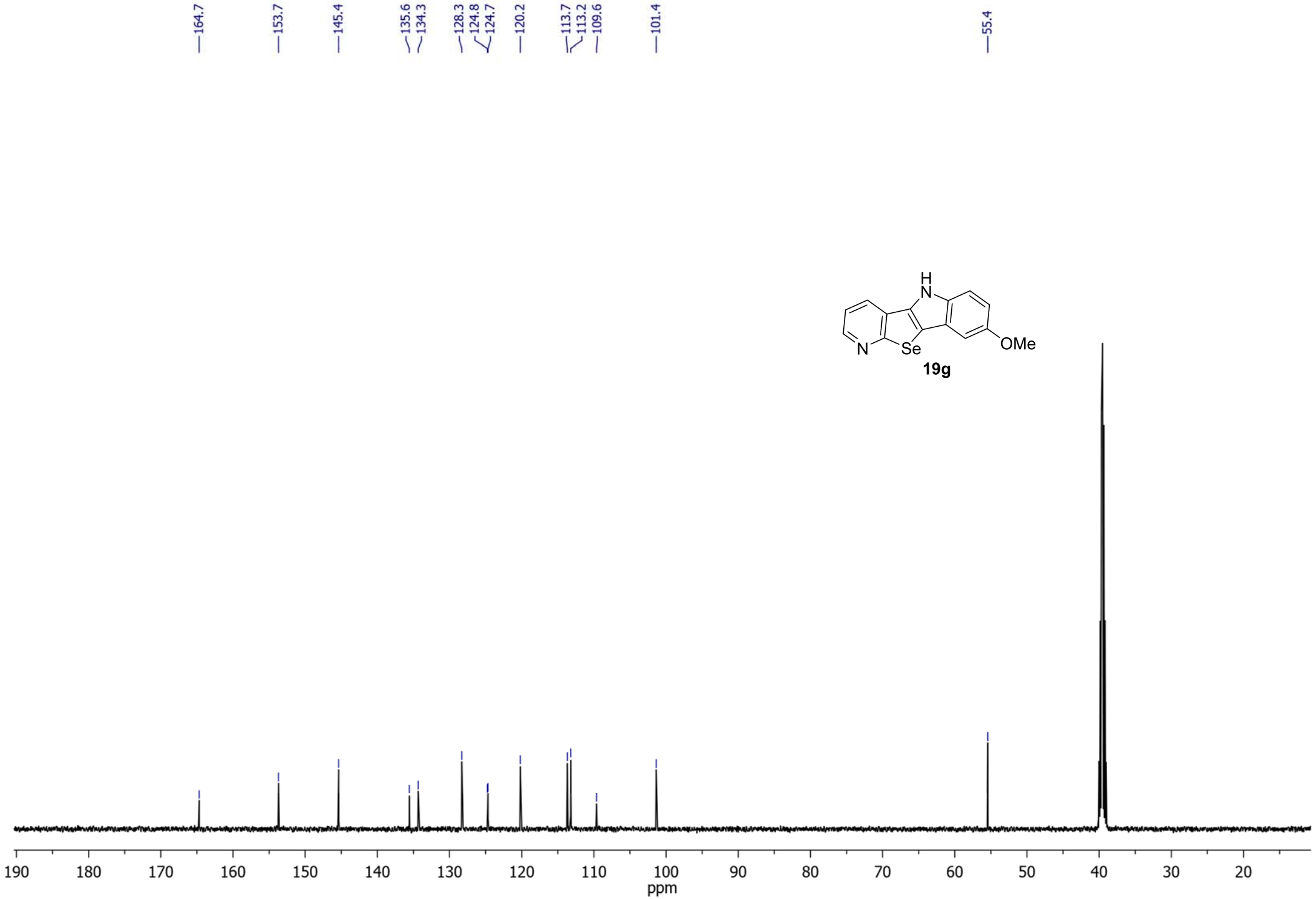


^{1}H NMR (solvent: DMSO-d_6)

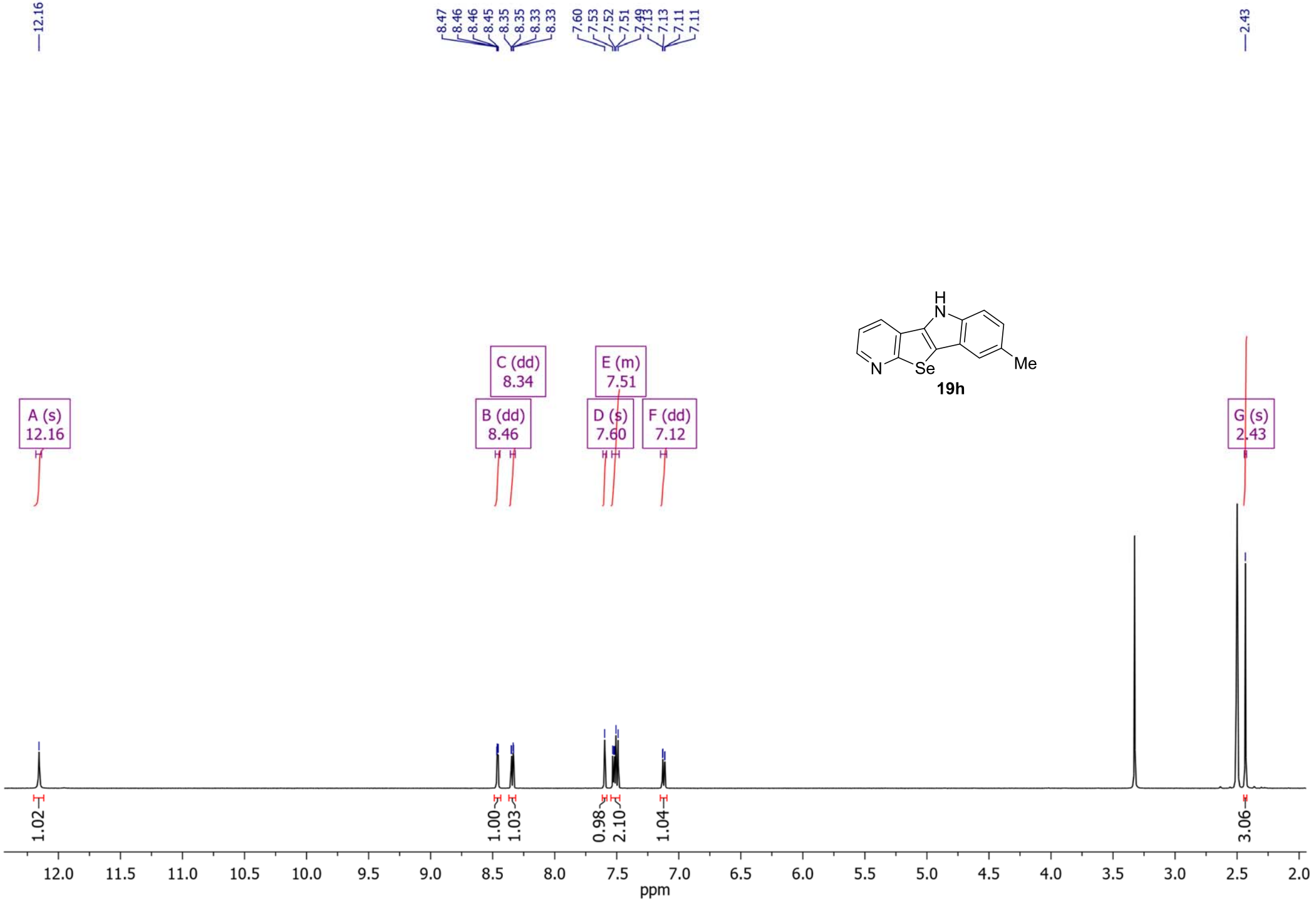


19g

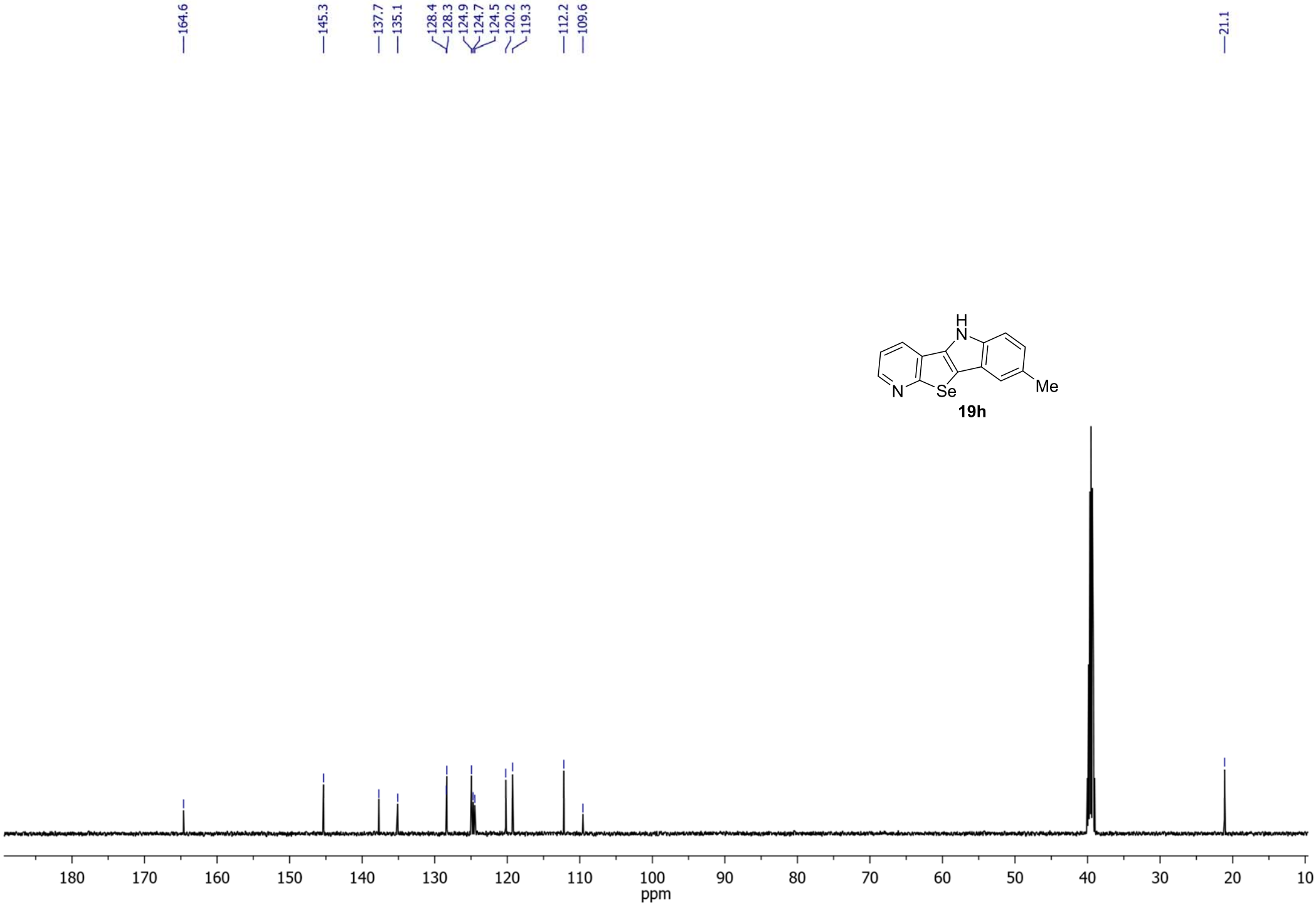
^{13}C NMR (solvent: DMSO-d_6)



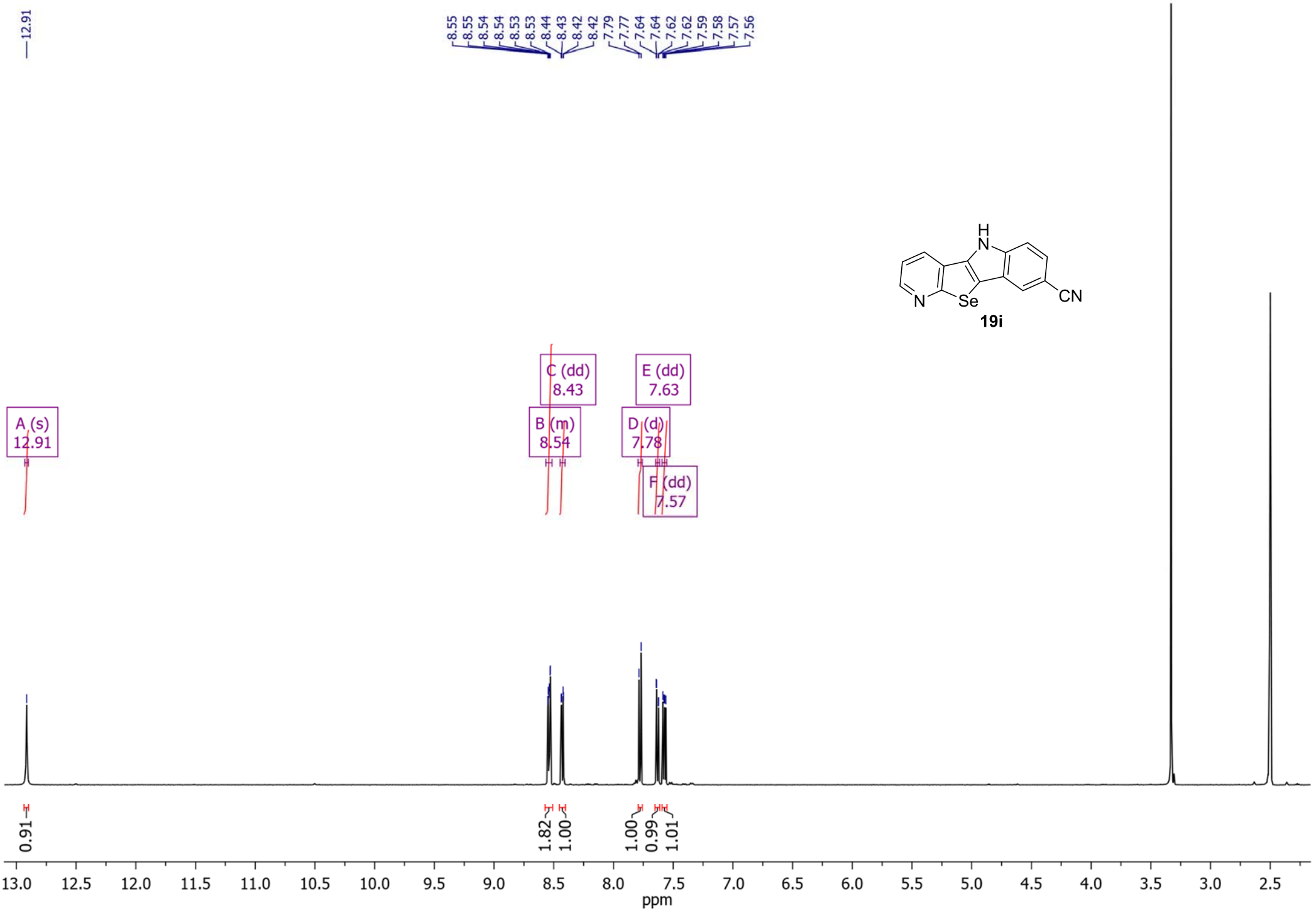
^{1}H NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)

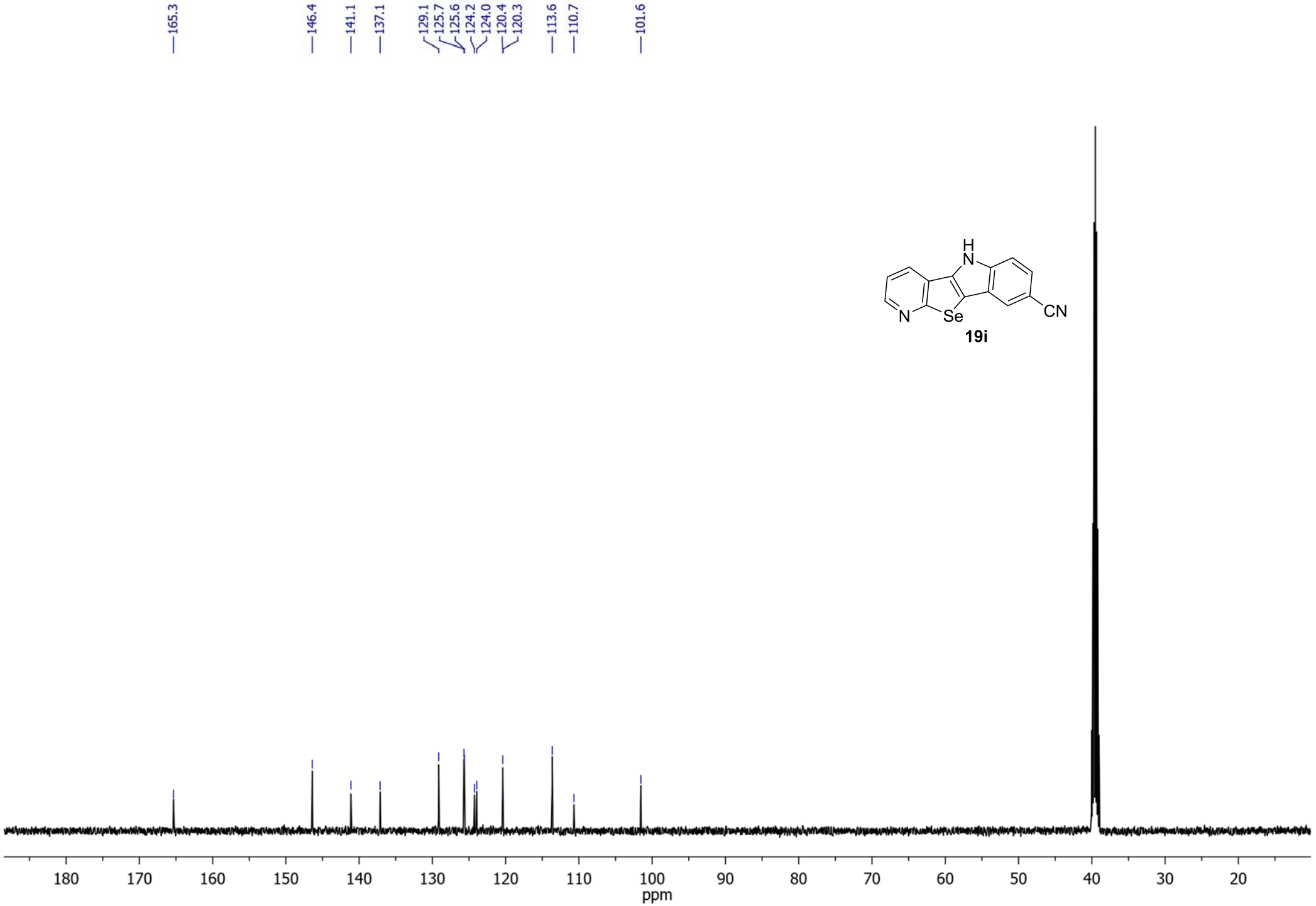


^{1}H NMR (solvent: DMSO-d_6)

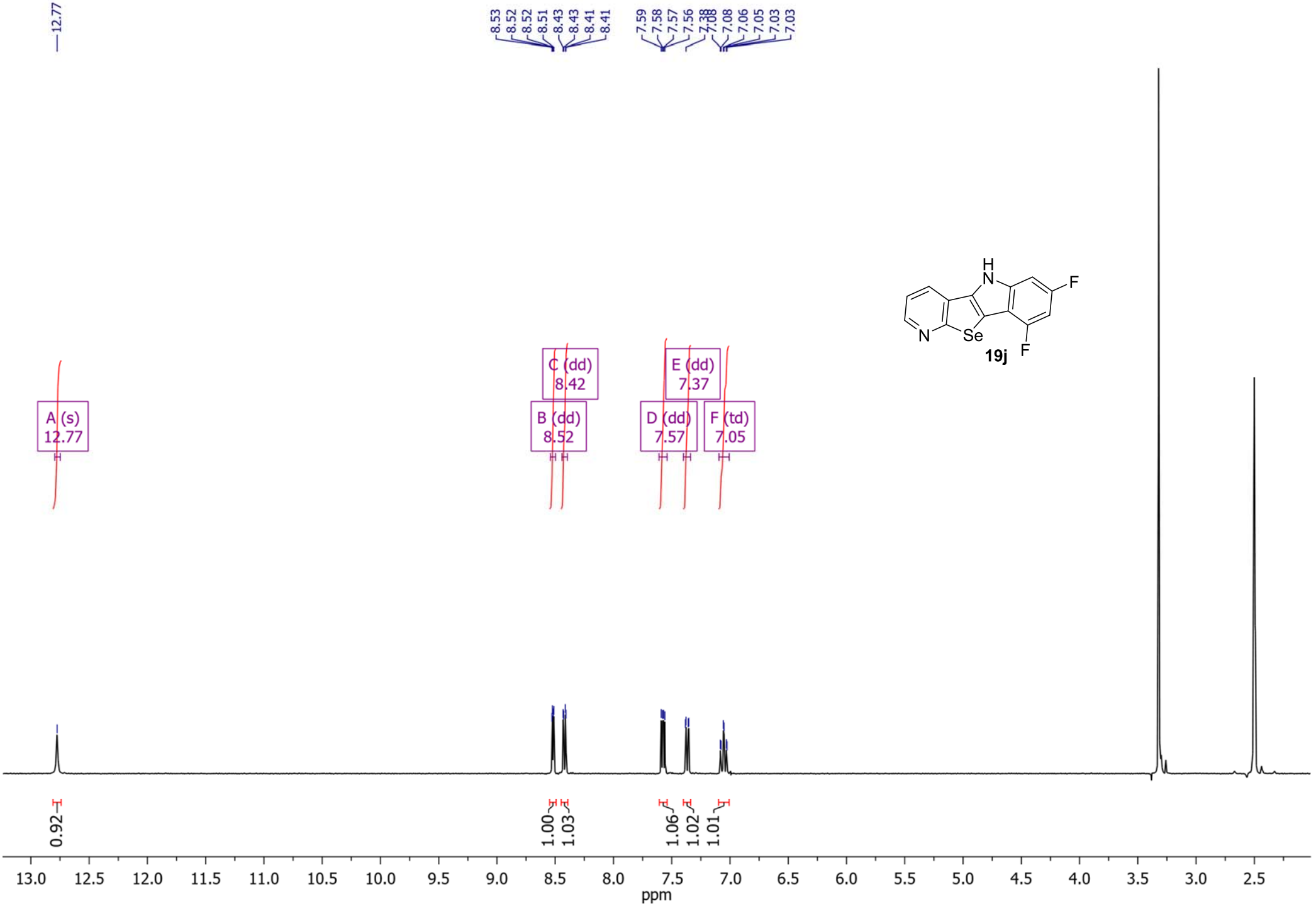


19i

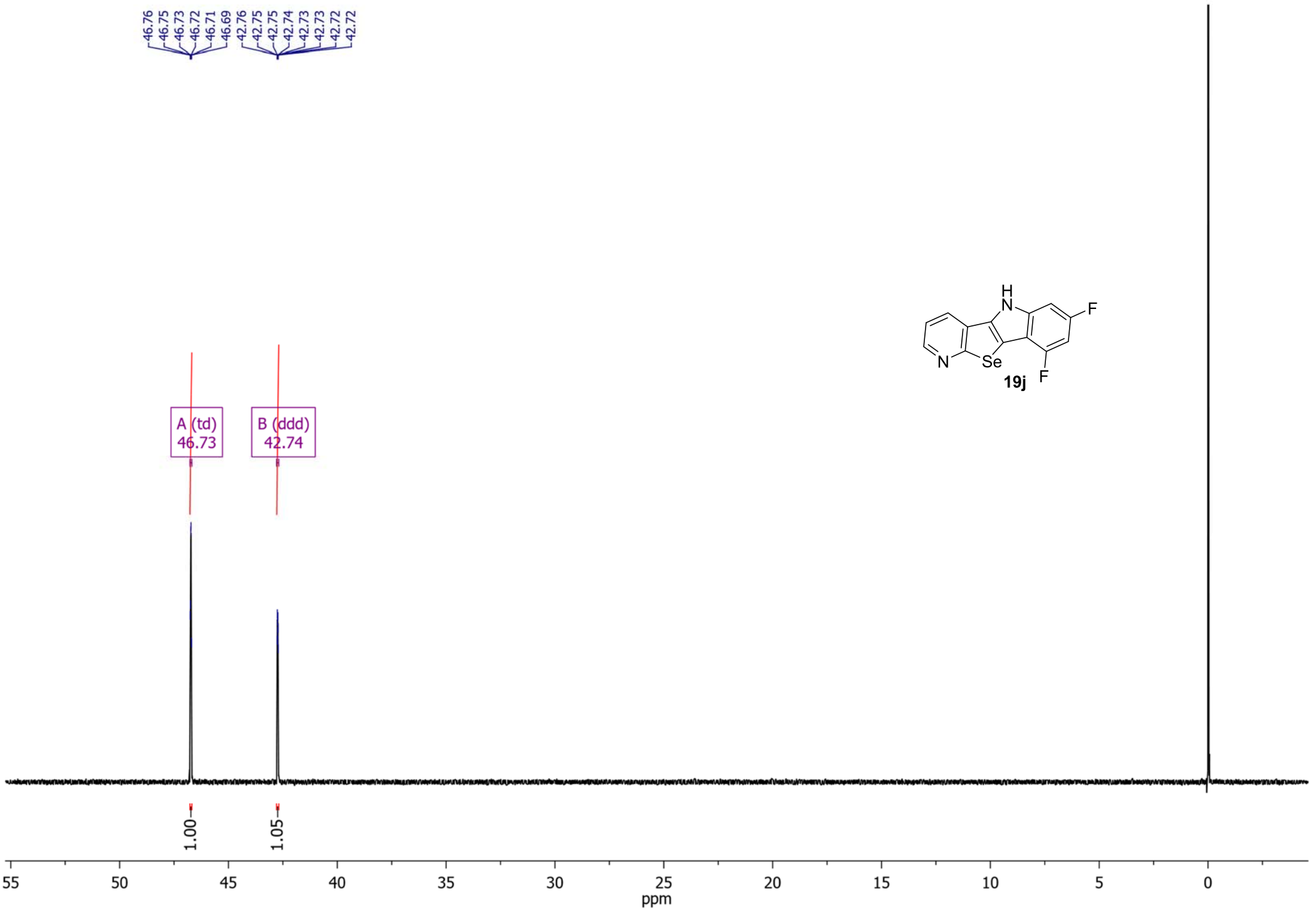
^{13}C NMR (solvent: DMSO-d_6)



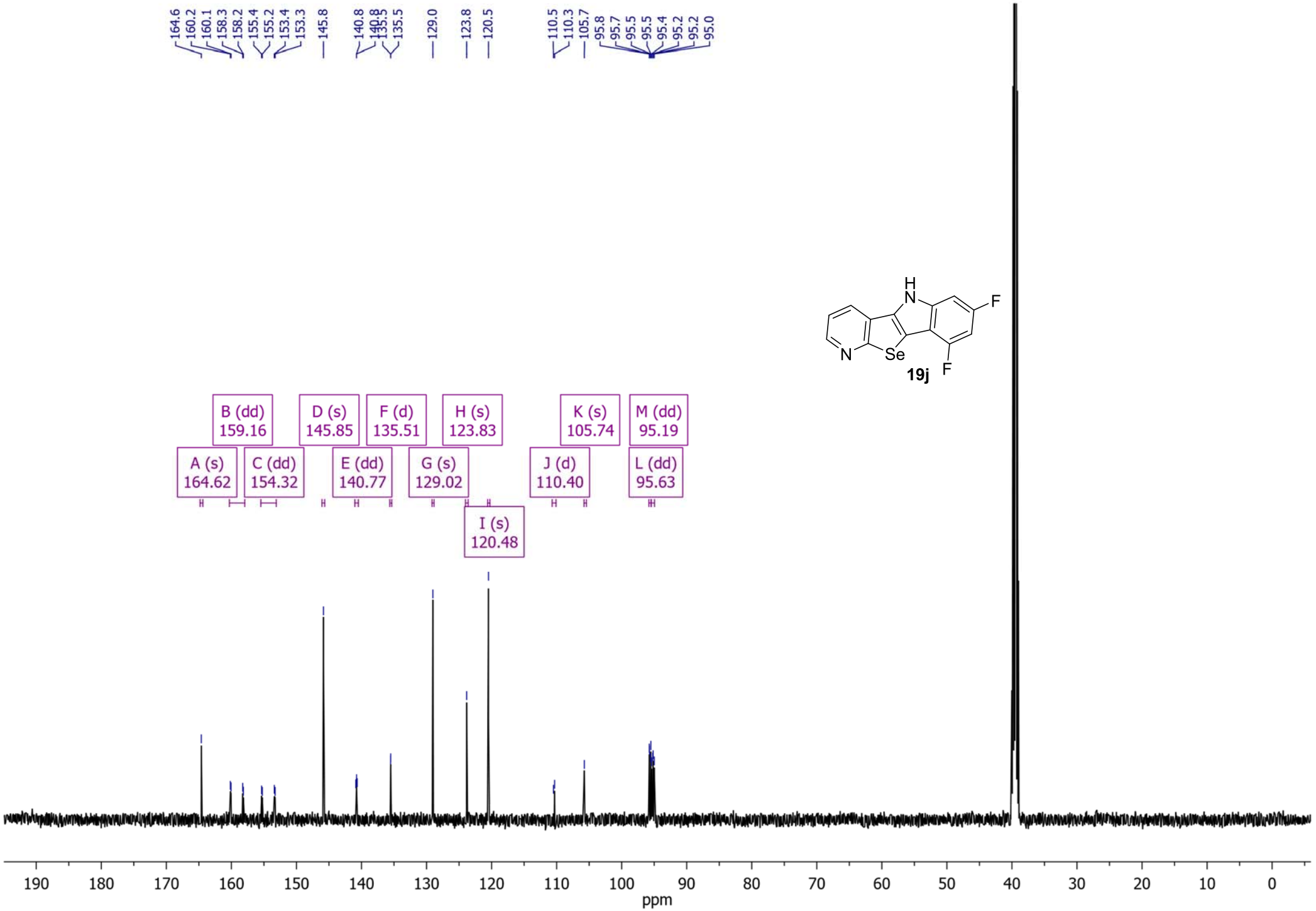
^{1}H NMR (solvent: DMSO-d_6)



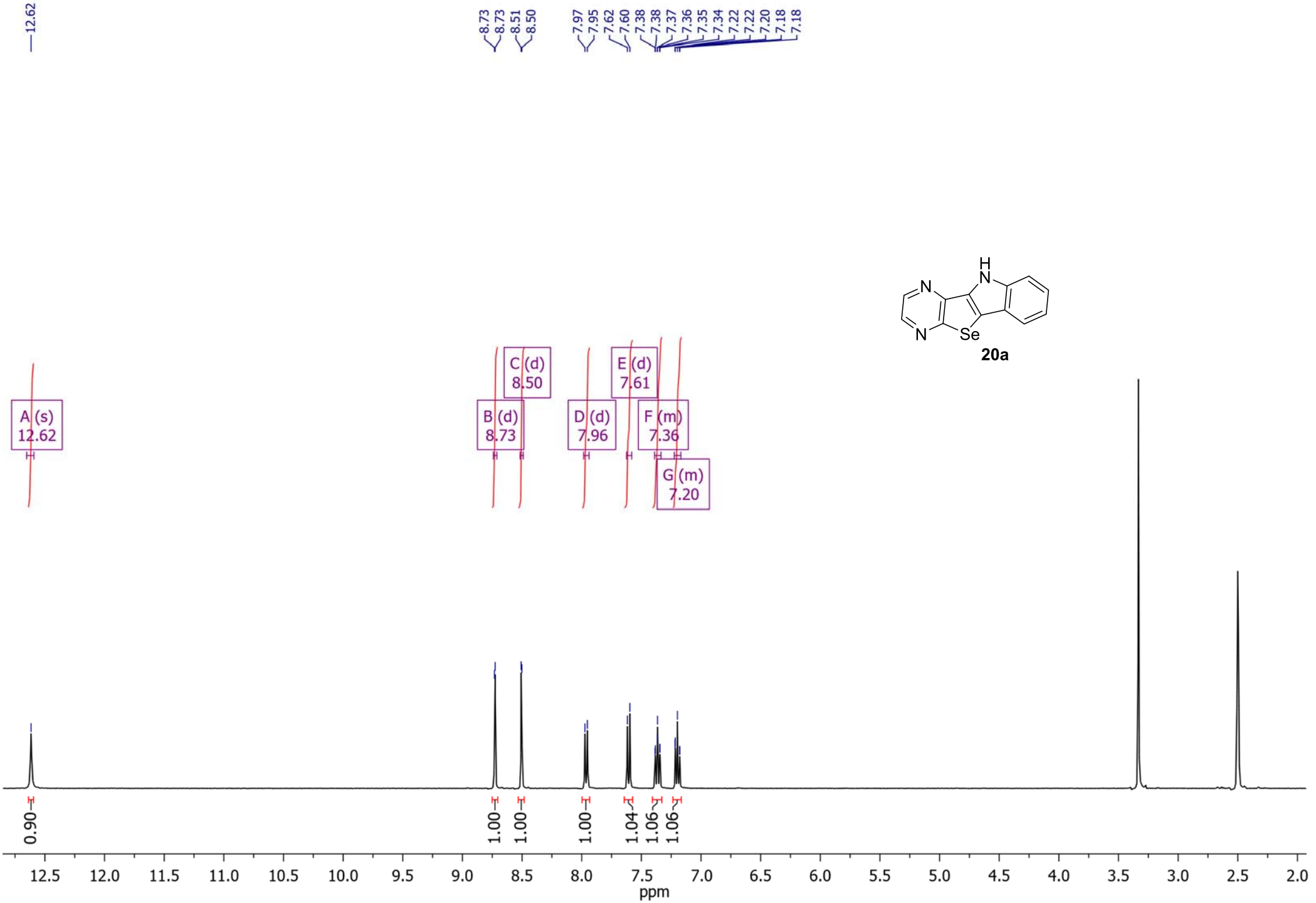
^{19}F NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)

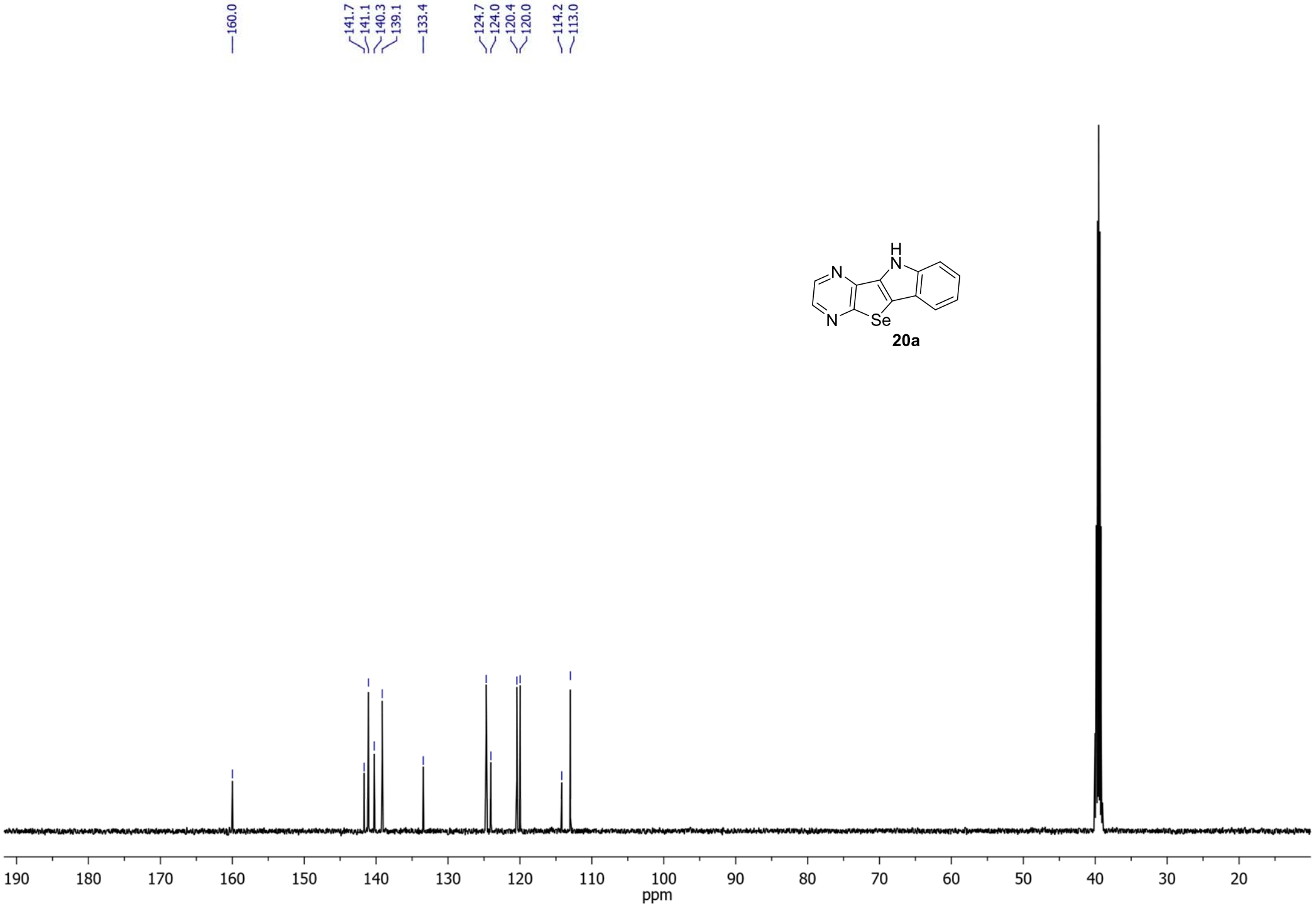


^{1}H NMR (solvent: DMSO-d_6)

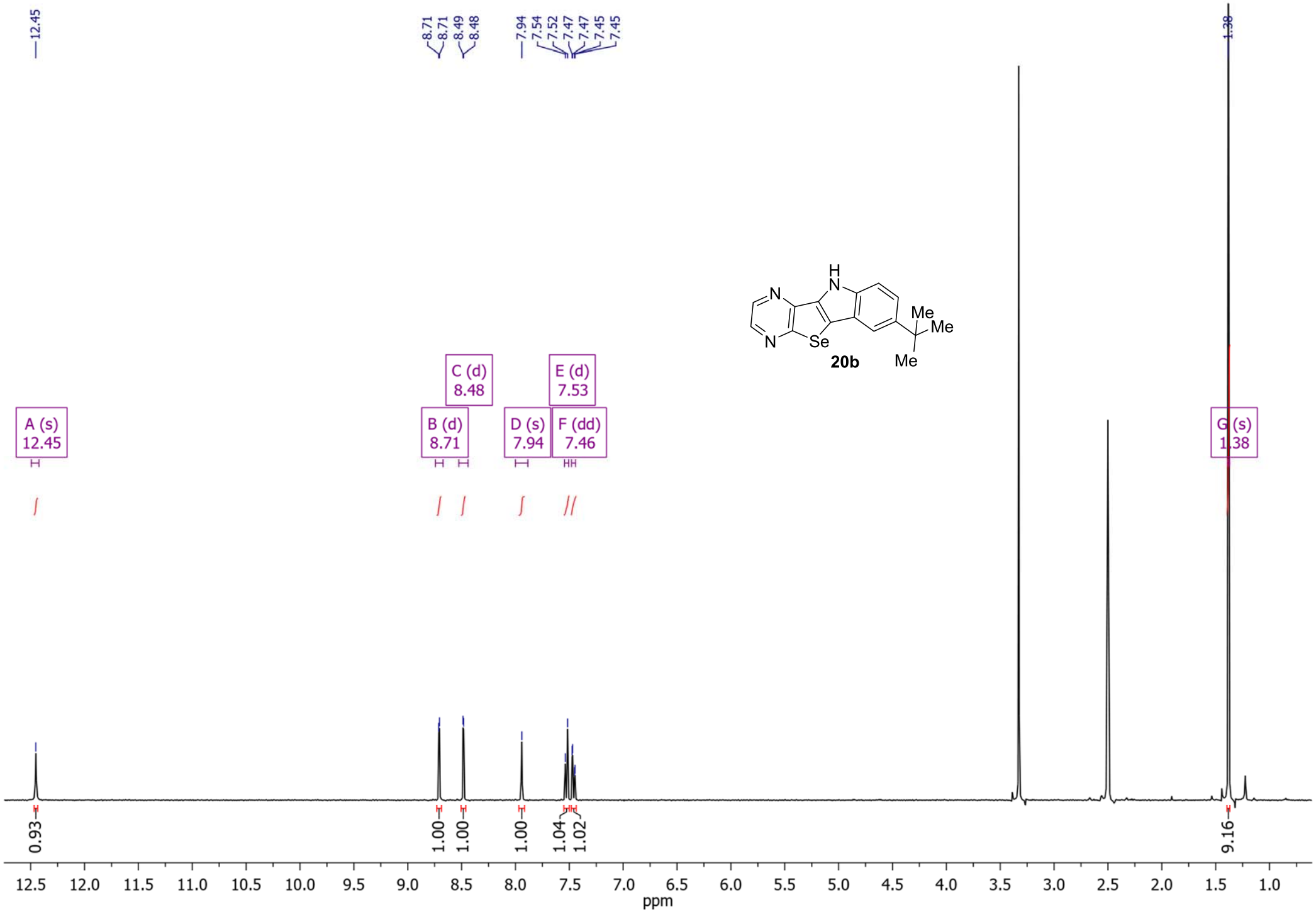


20a

^{13}C NMR (solvent: DMSO-d_6)

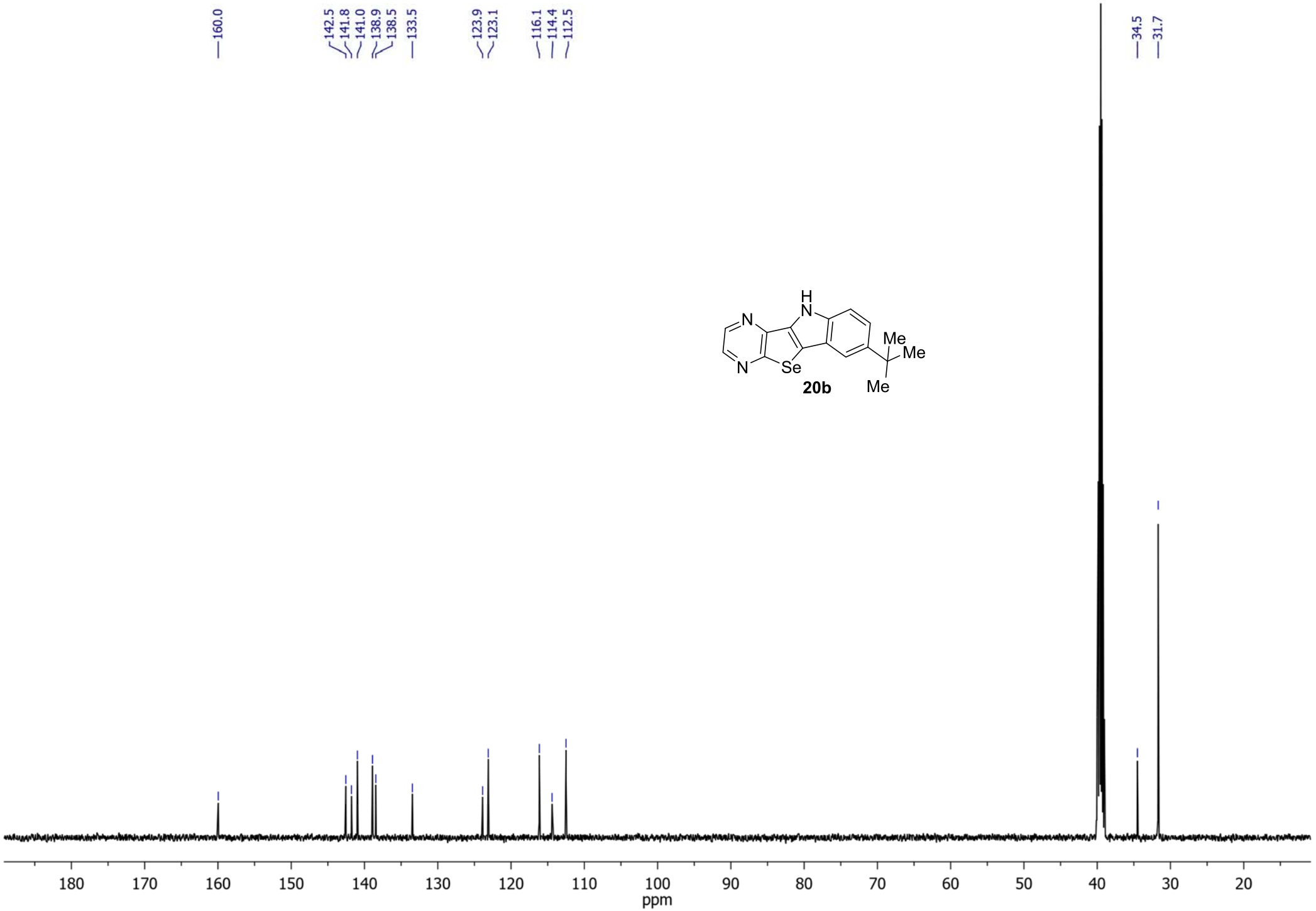


^{1}H NMR (solvent: DMSO-d_6)

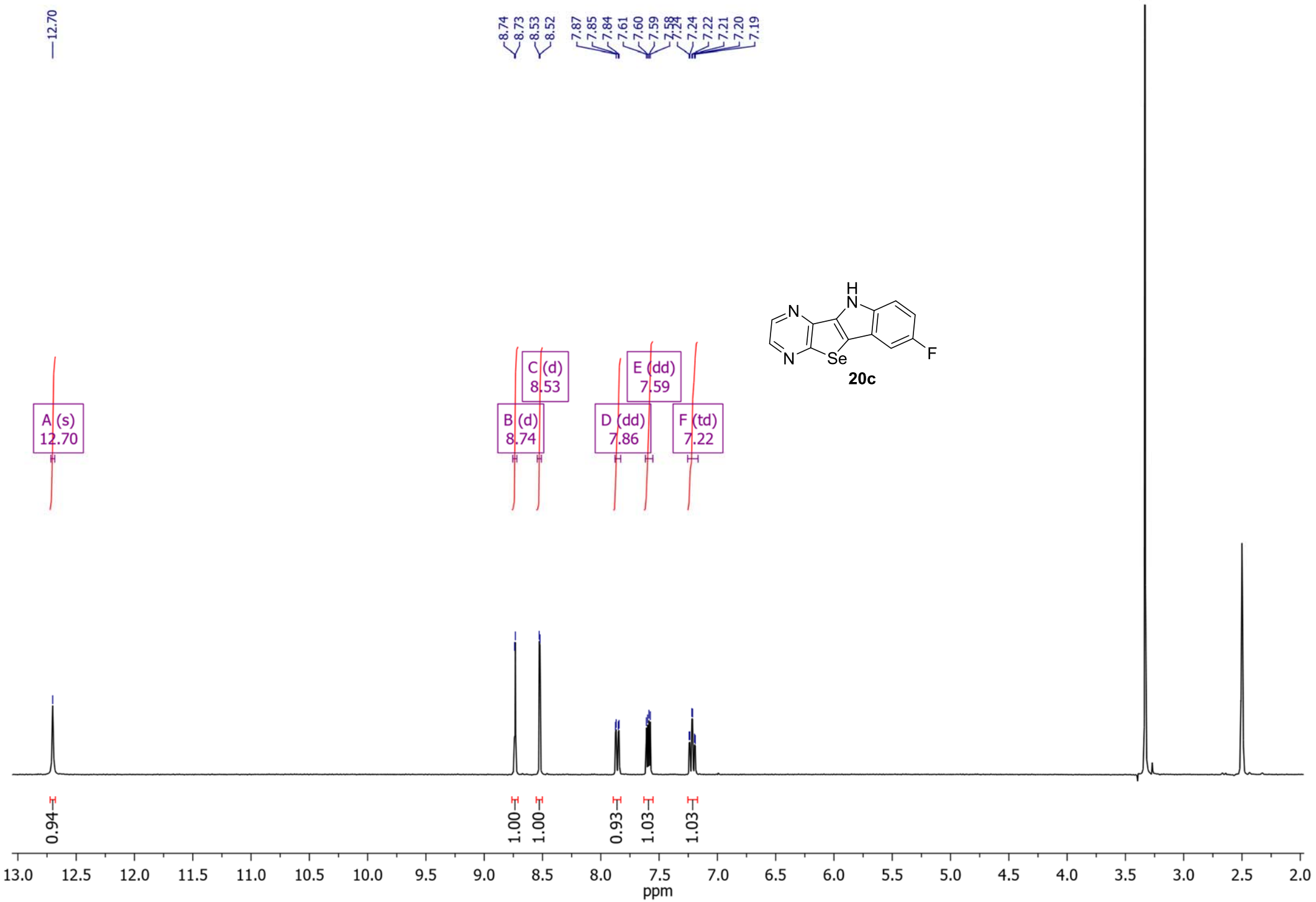


20b

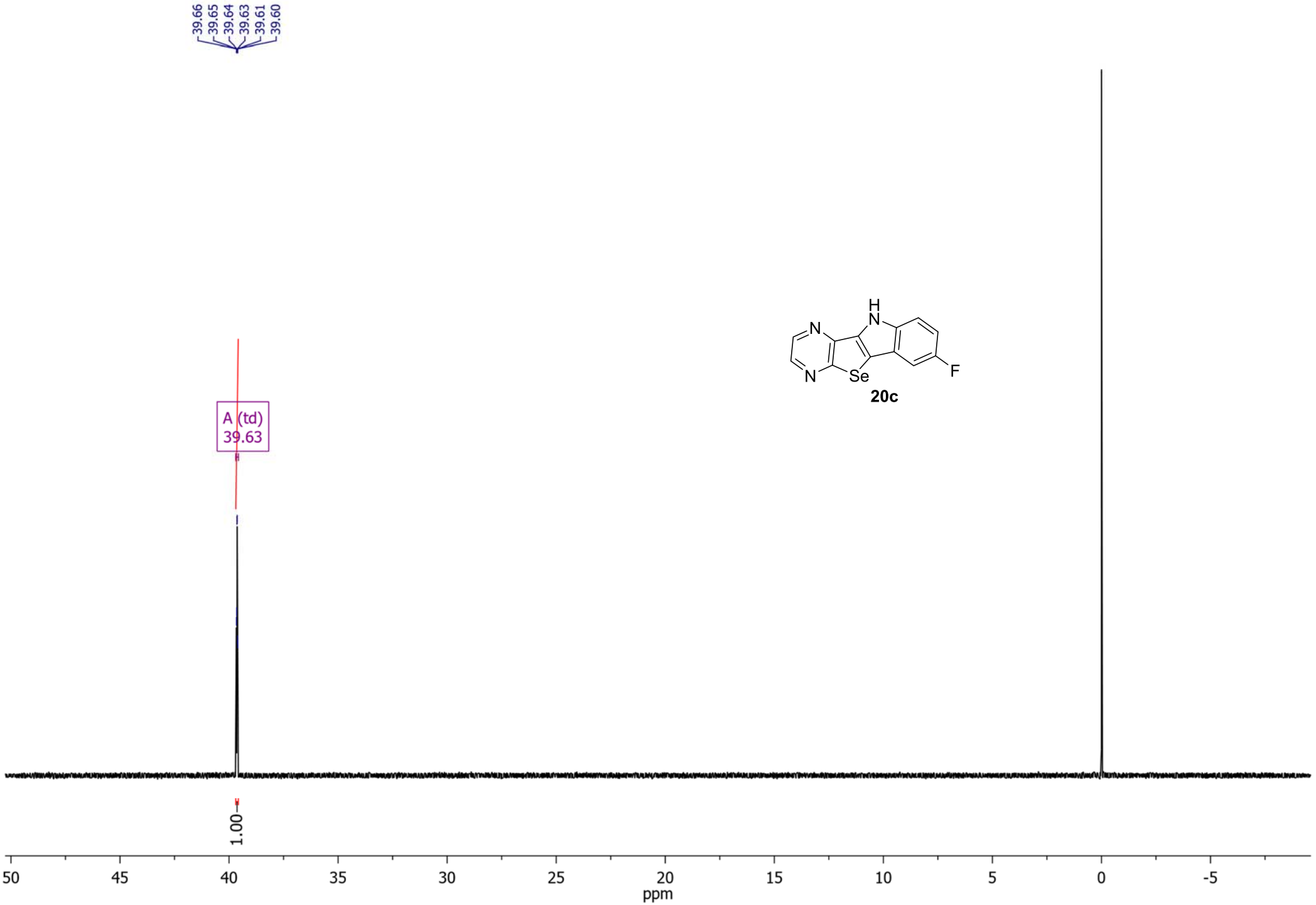
^{13}C NMR (solvent: DMSO-d_6)



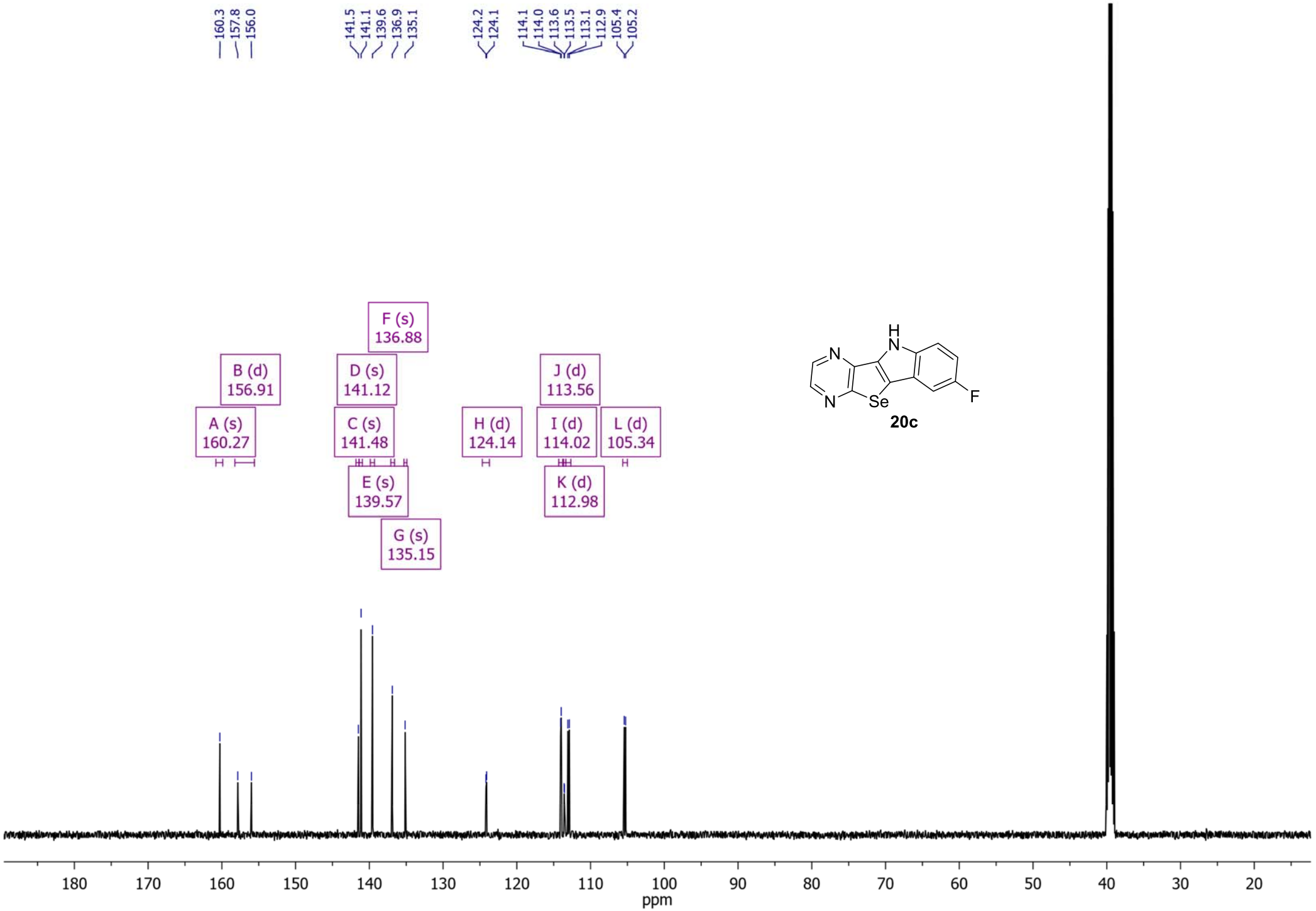
^{1}H NMR (solvent: DMSO-d_6)



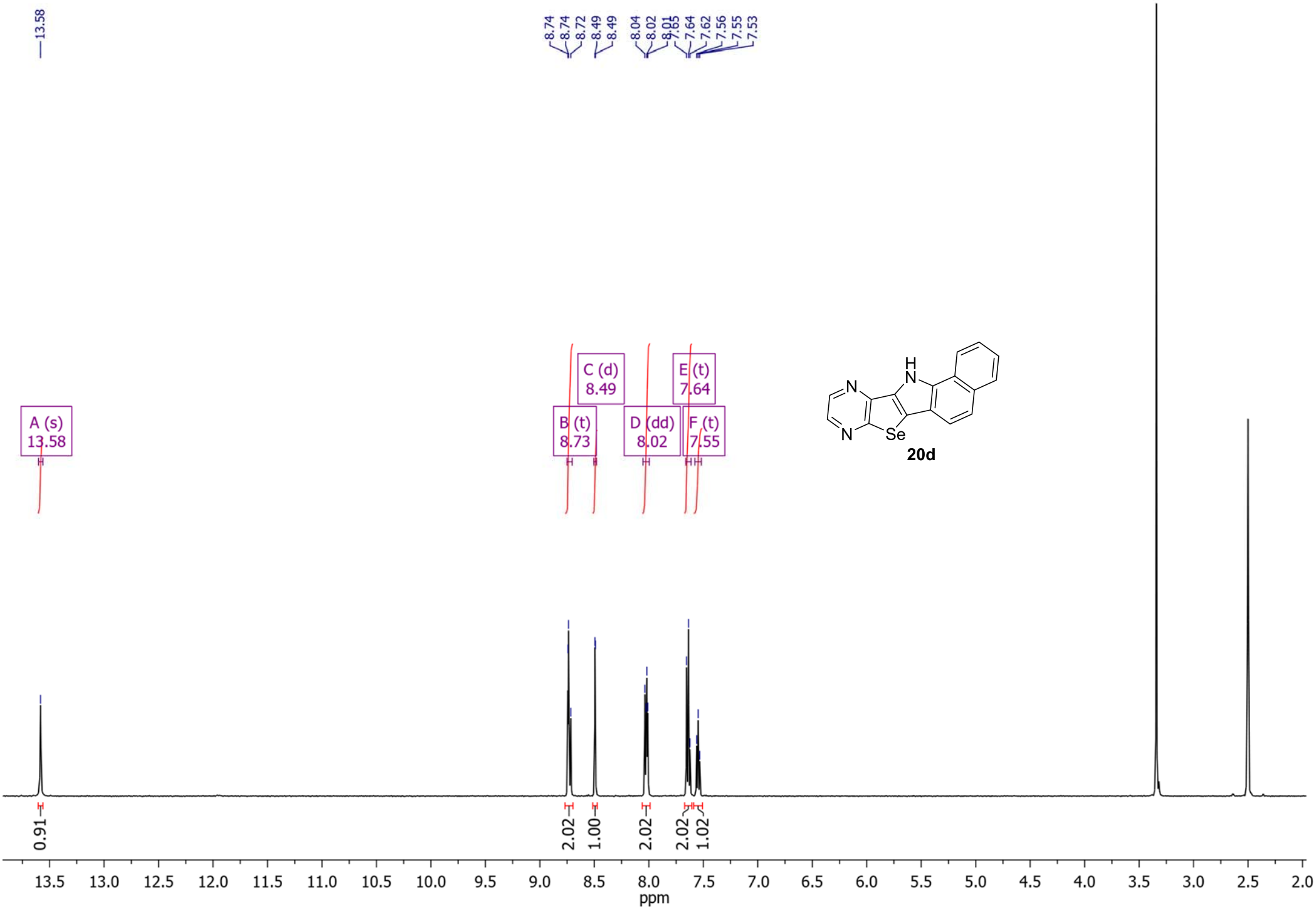
^{19}F NMR (solvent: DMSO-d_6)



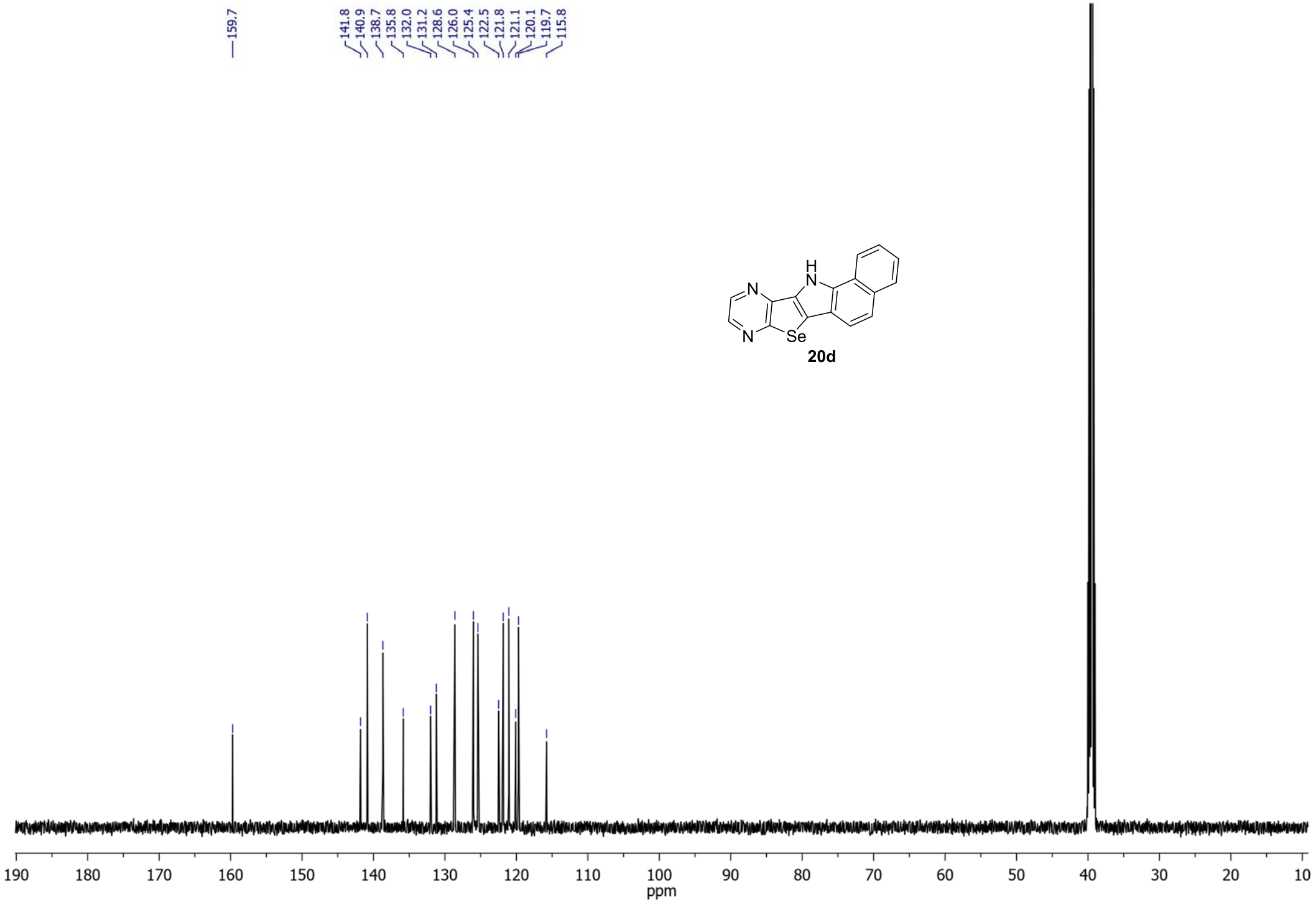
^{13}C NMR (solvent: DMSO-d_6)



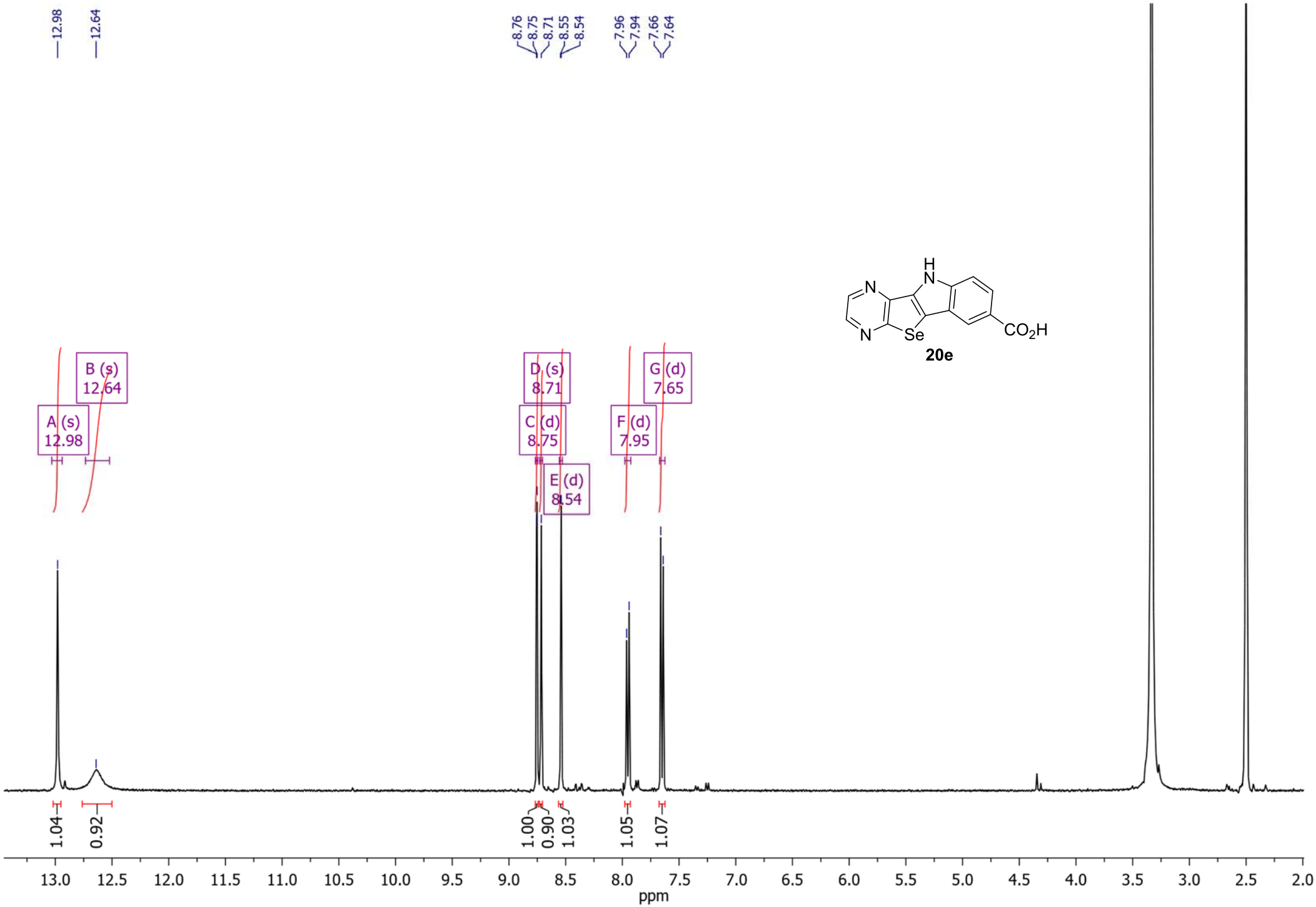
^{1}H NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)

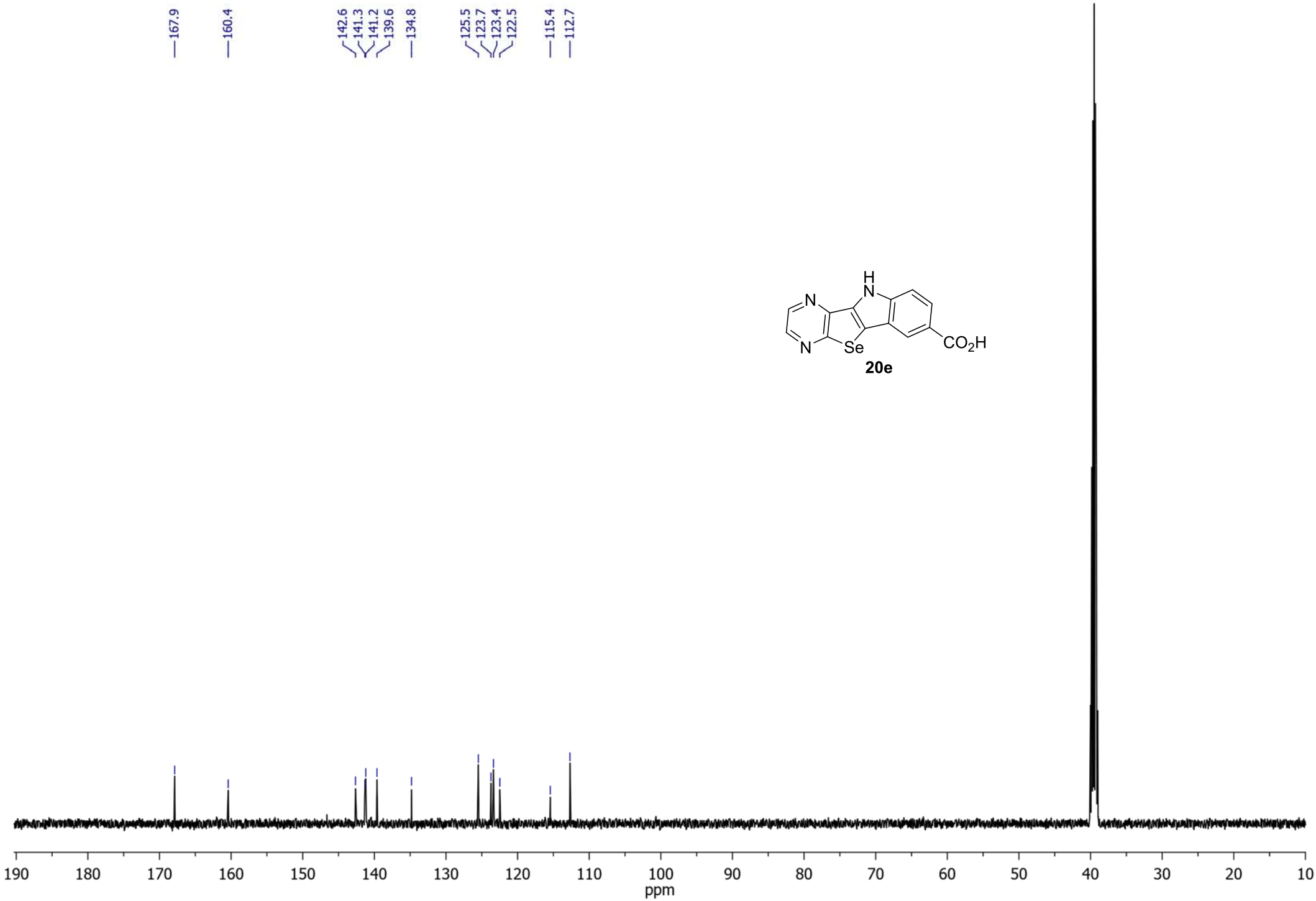


^{1}H NMR (solvent: DMSO-d_6)

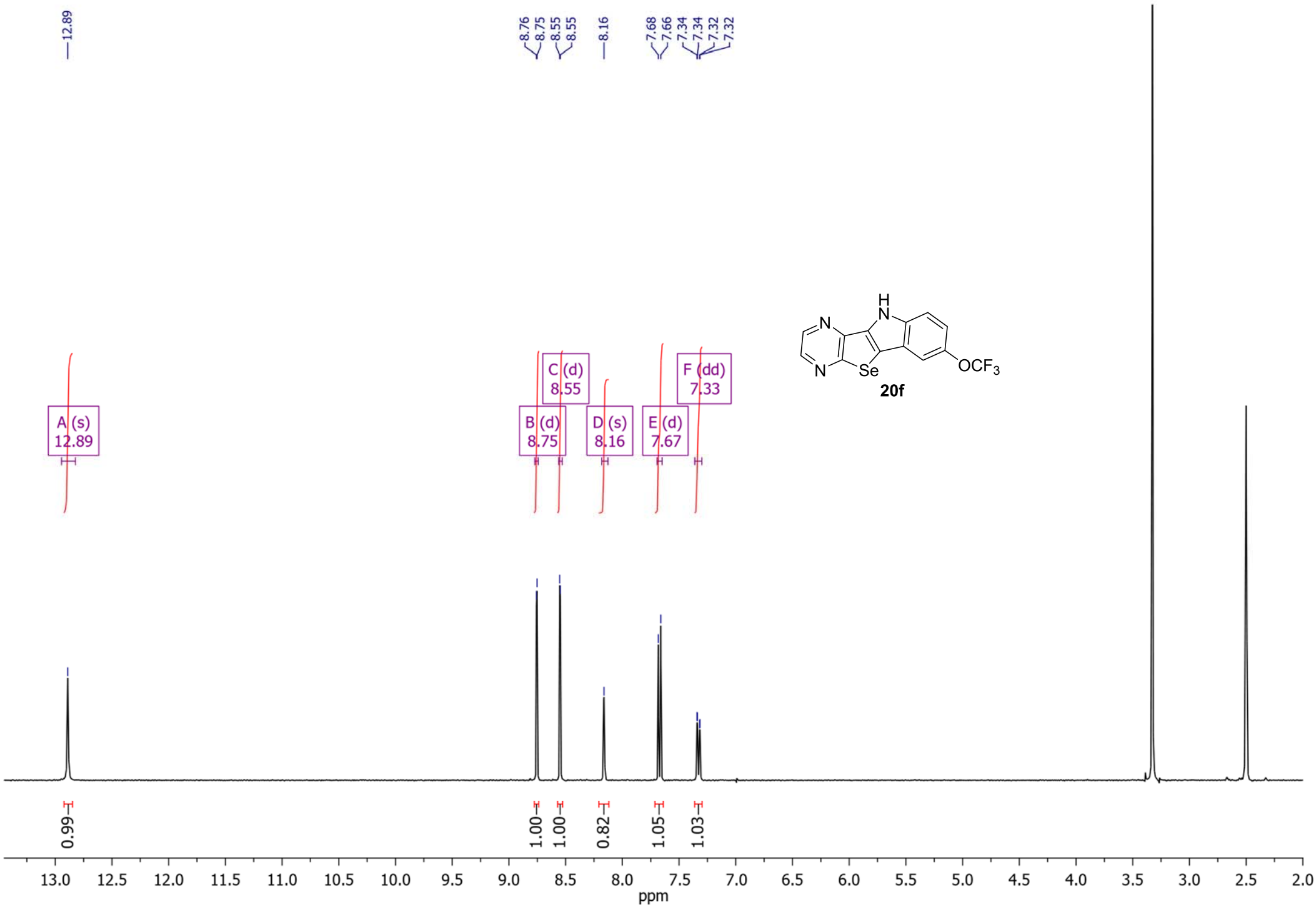


20e

^{13}C NMR (solvent: DMSO-d_6)

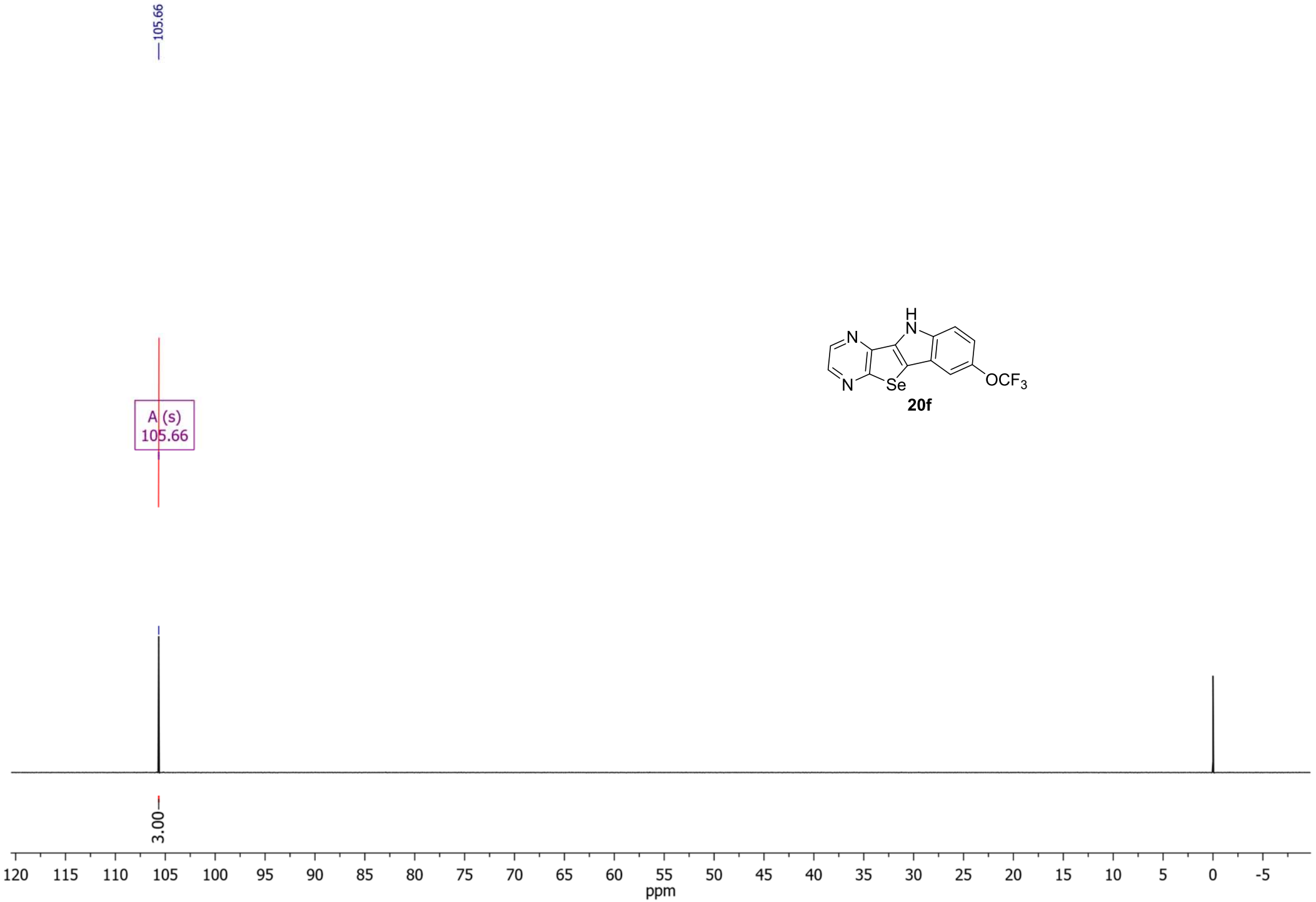


^{1}H NMR (solvent: DMSO-d_6)



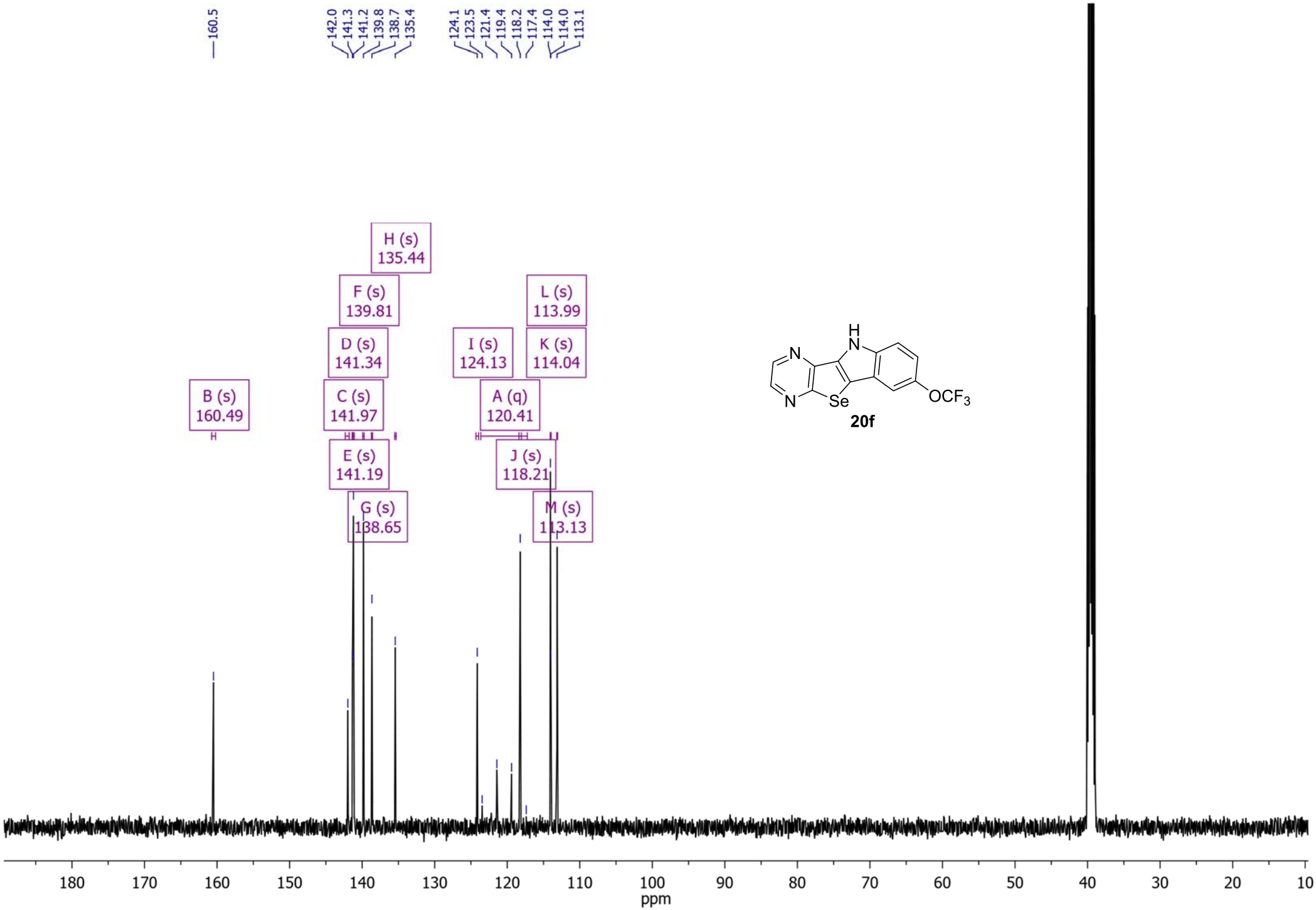
20f

^{19}F NMR (solvent: DMSO-d_6)

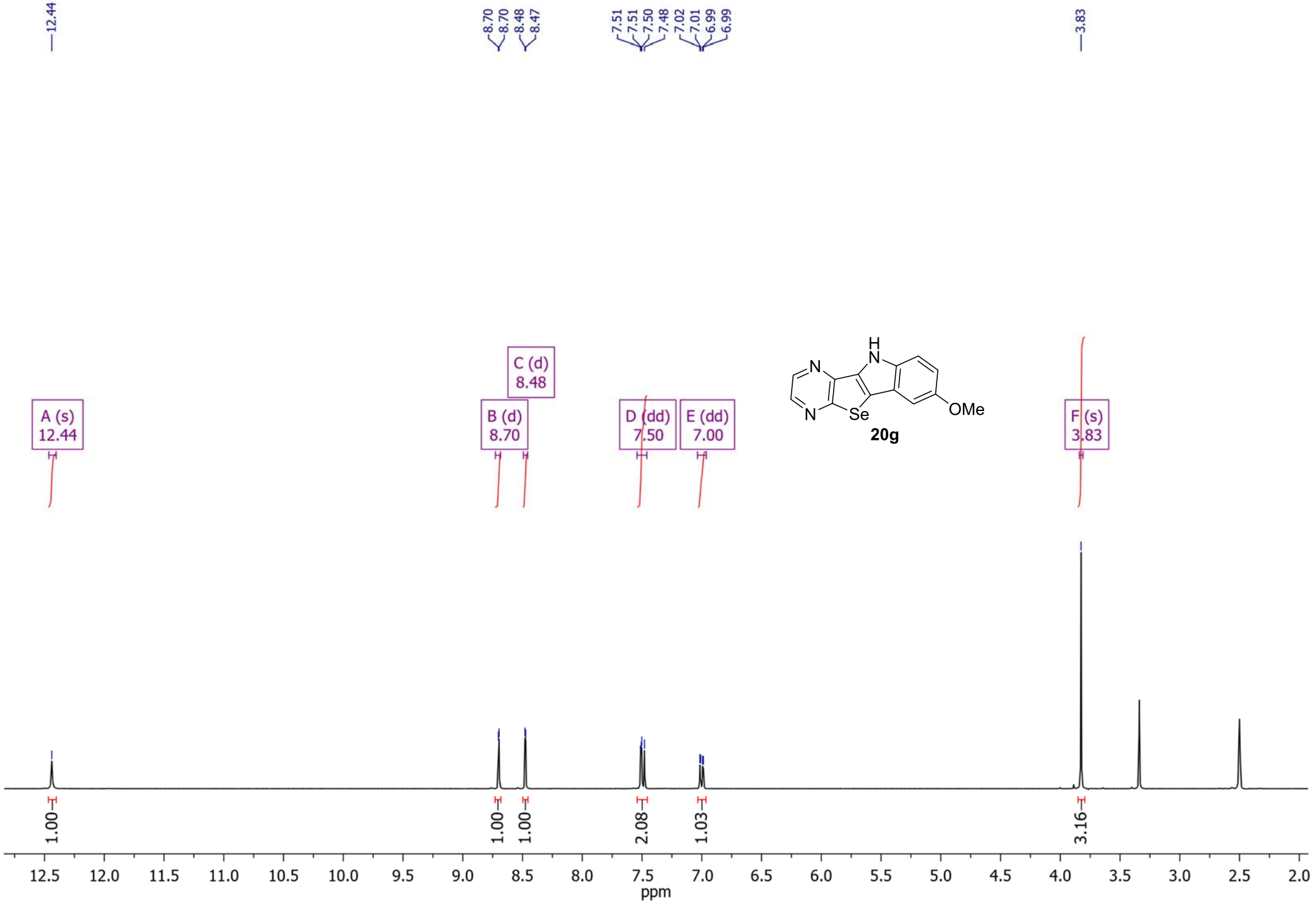


20f

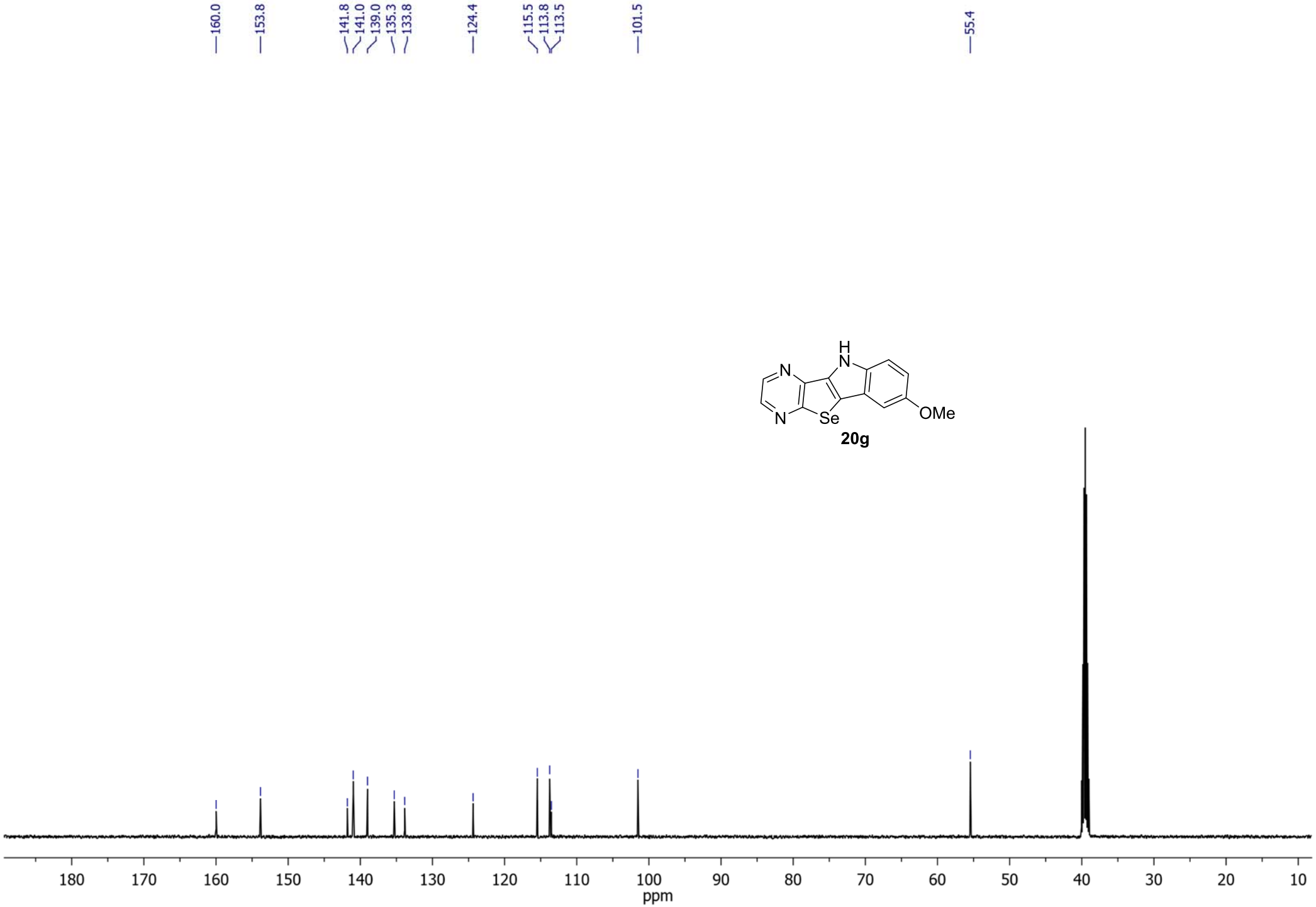
^{13}C NMR (solvent: DMSO-d_6)



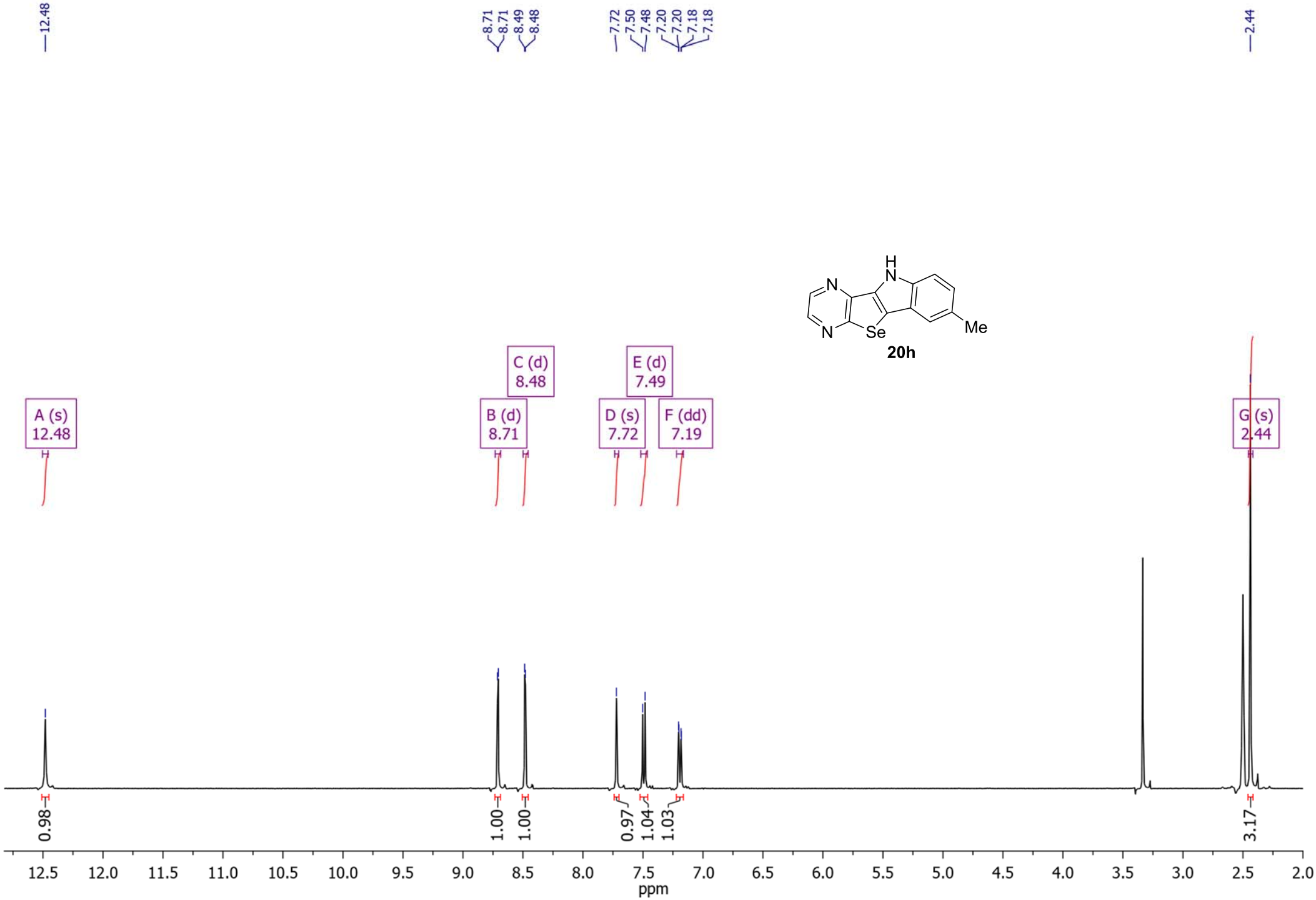
^{1}H NMR (solvent: DMSO-d_6)



^{13}C NMR (solvent: DMSO-d_6)

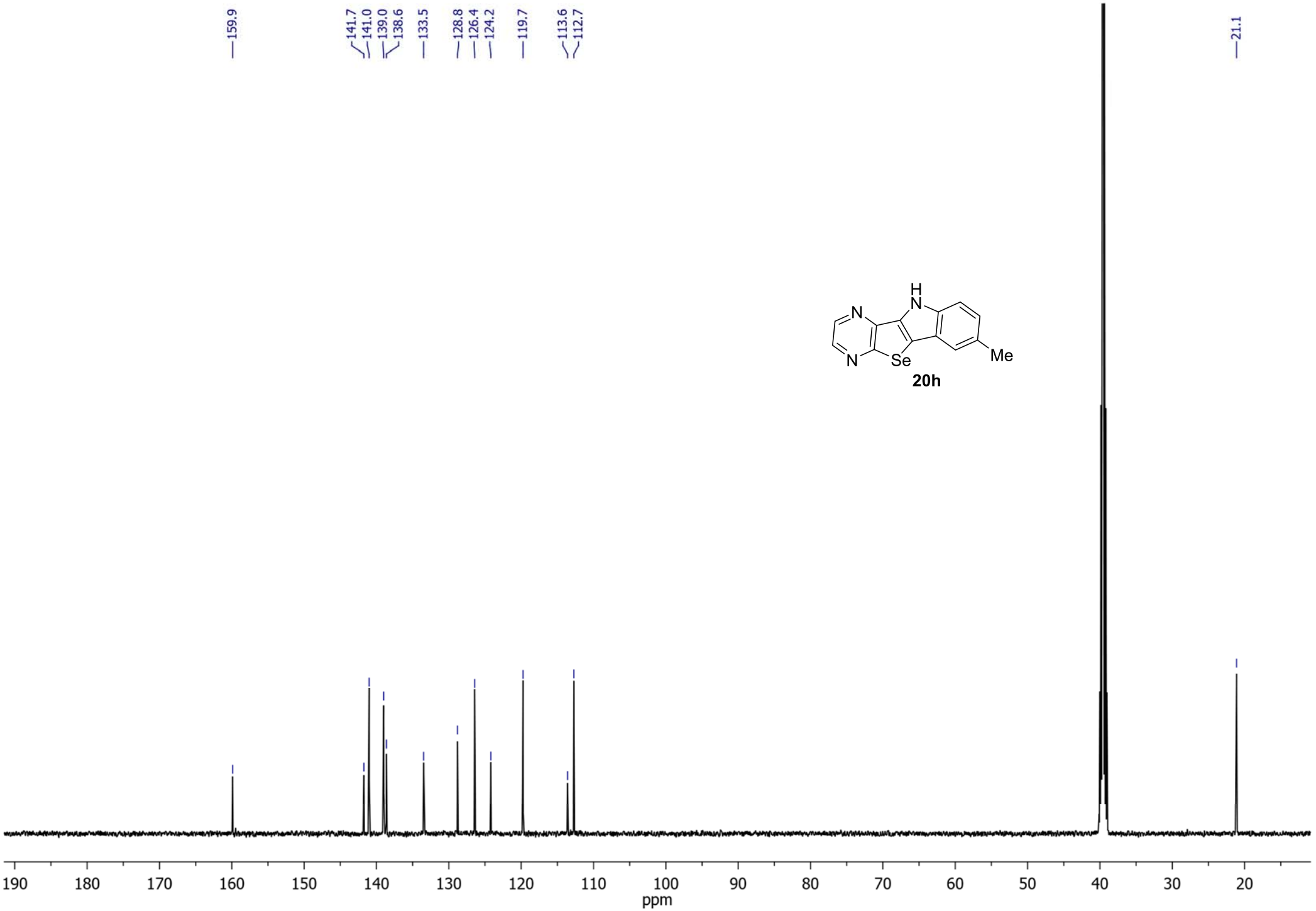


^{1}H NMR (solvent: DMSO-d_6)

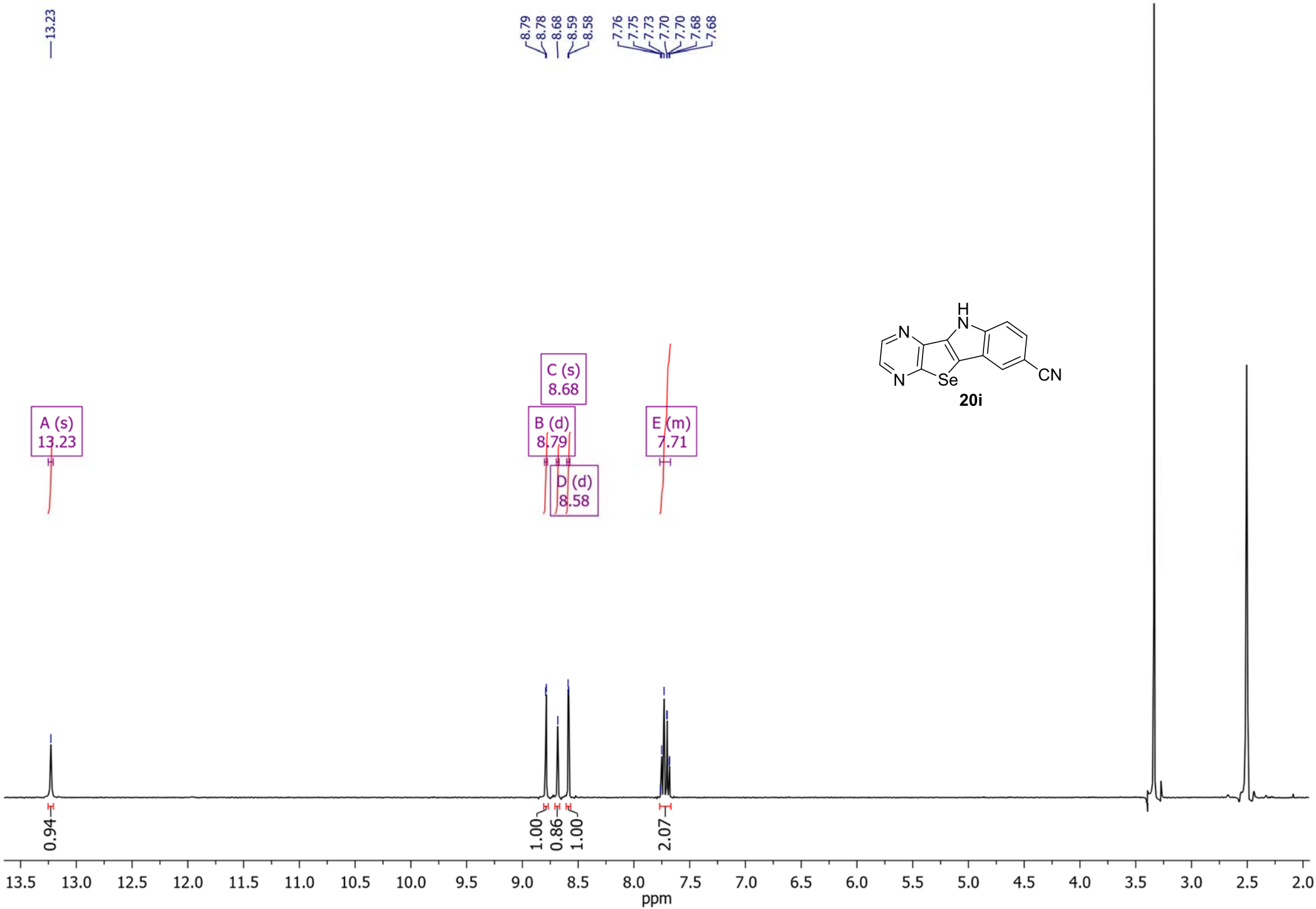


20h

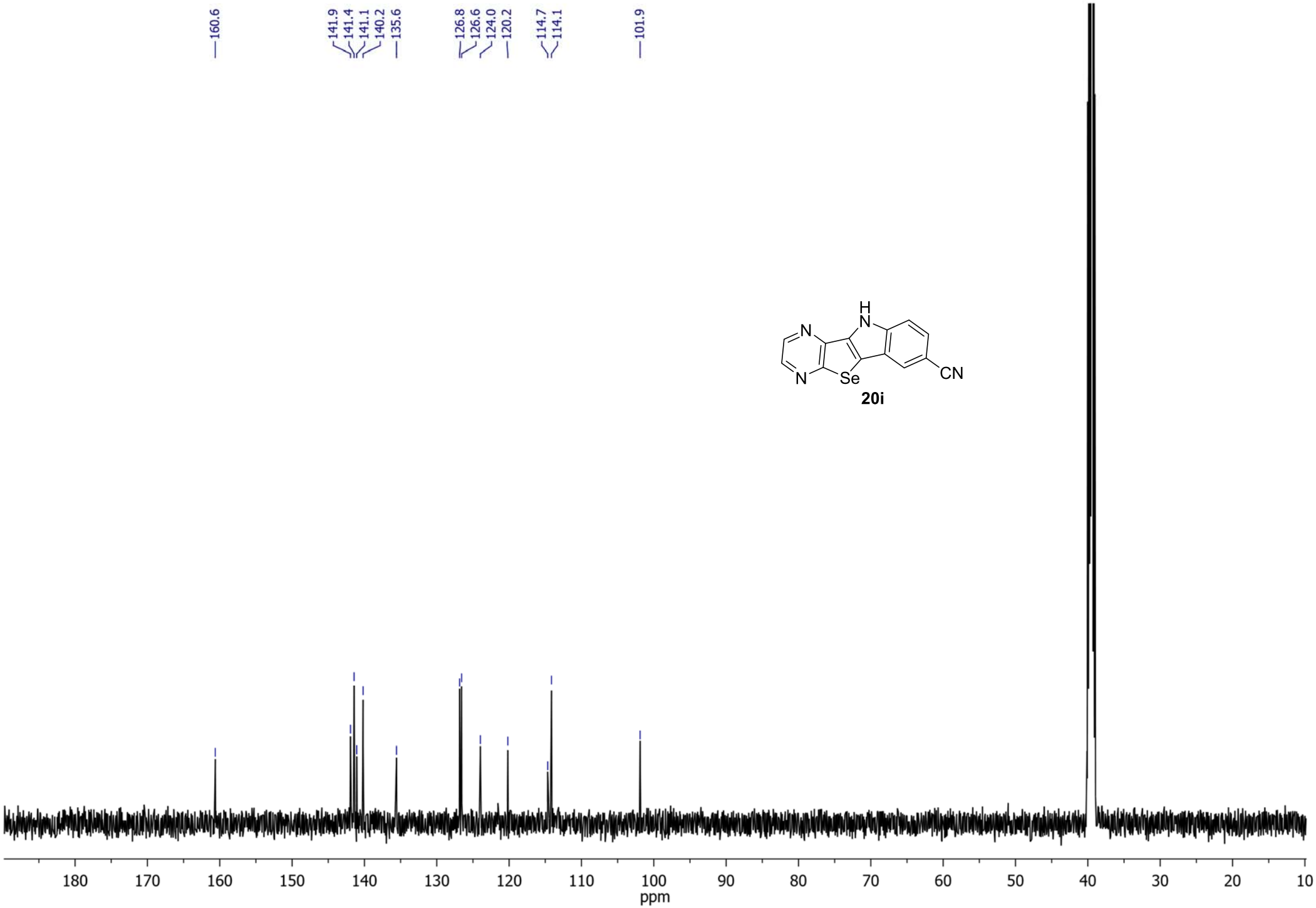
^{13}C NMR (solvent: DMSO-d_6)



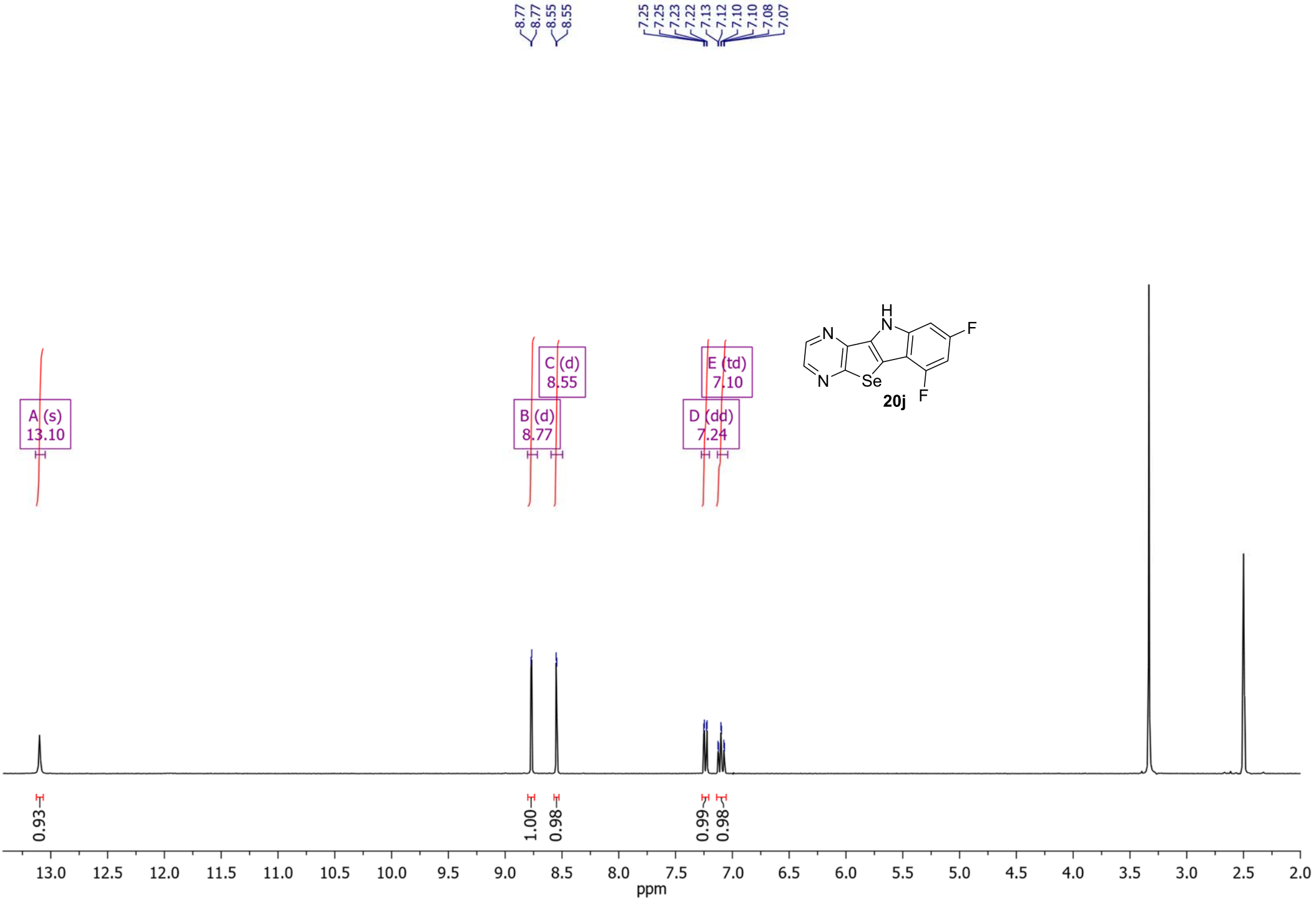
^{1}H NMR (solvent: DMSO-d_6)



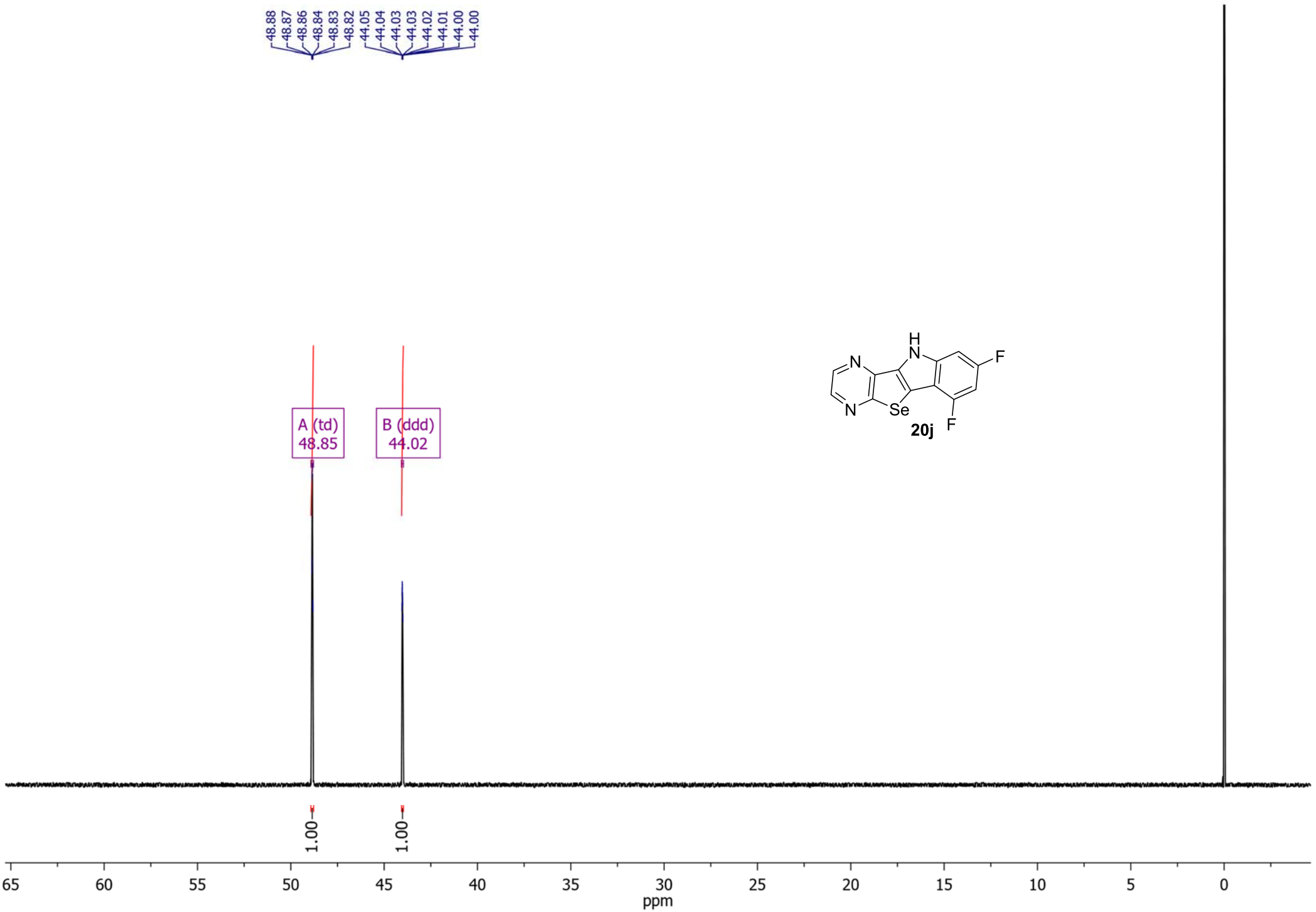
^{13}C NMR (solvent: DMSO-d_6)



^{1}H NMR (solvent: DMSO-d_6)

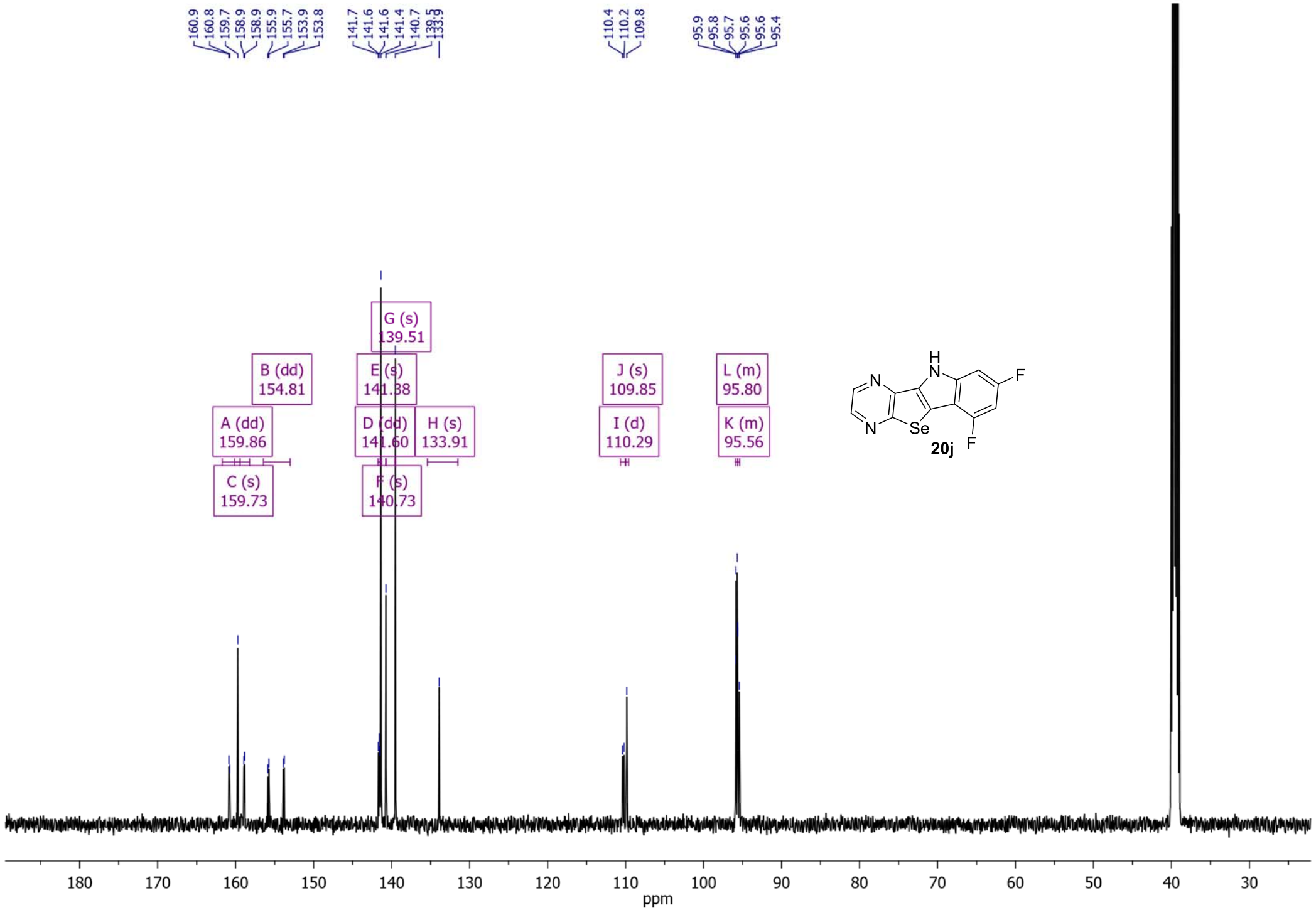


^{19}F NMR (solvent: DMSO-d_6)

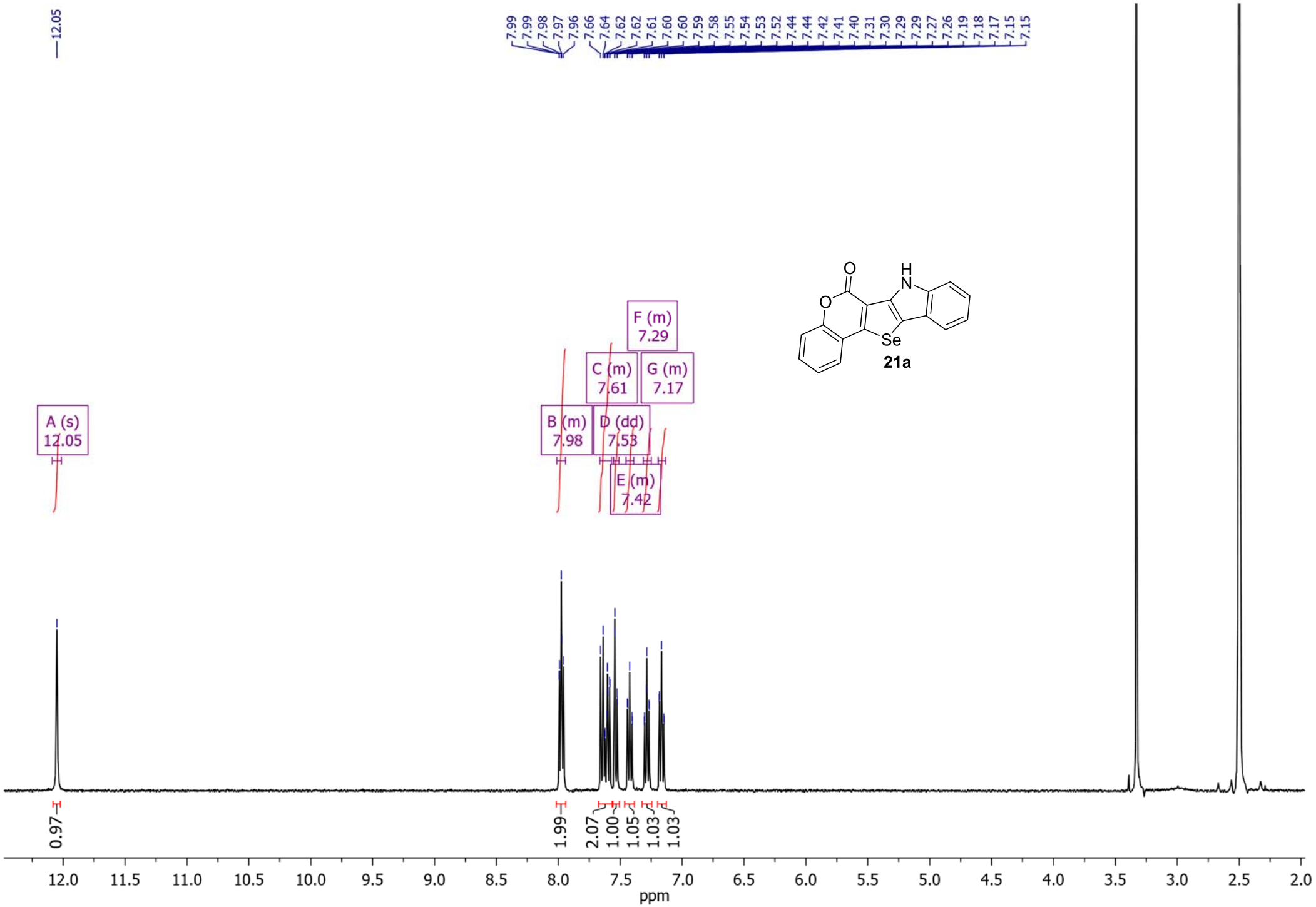


20j

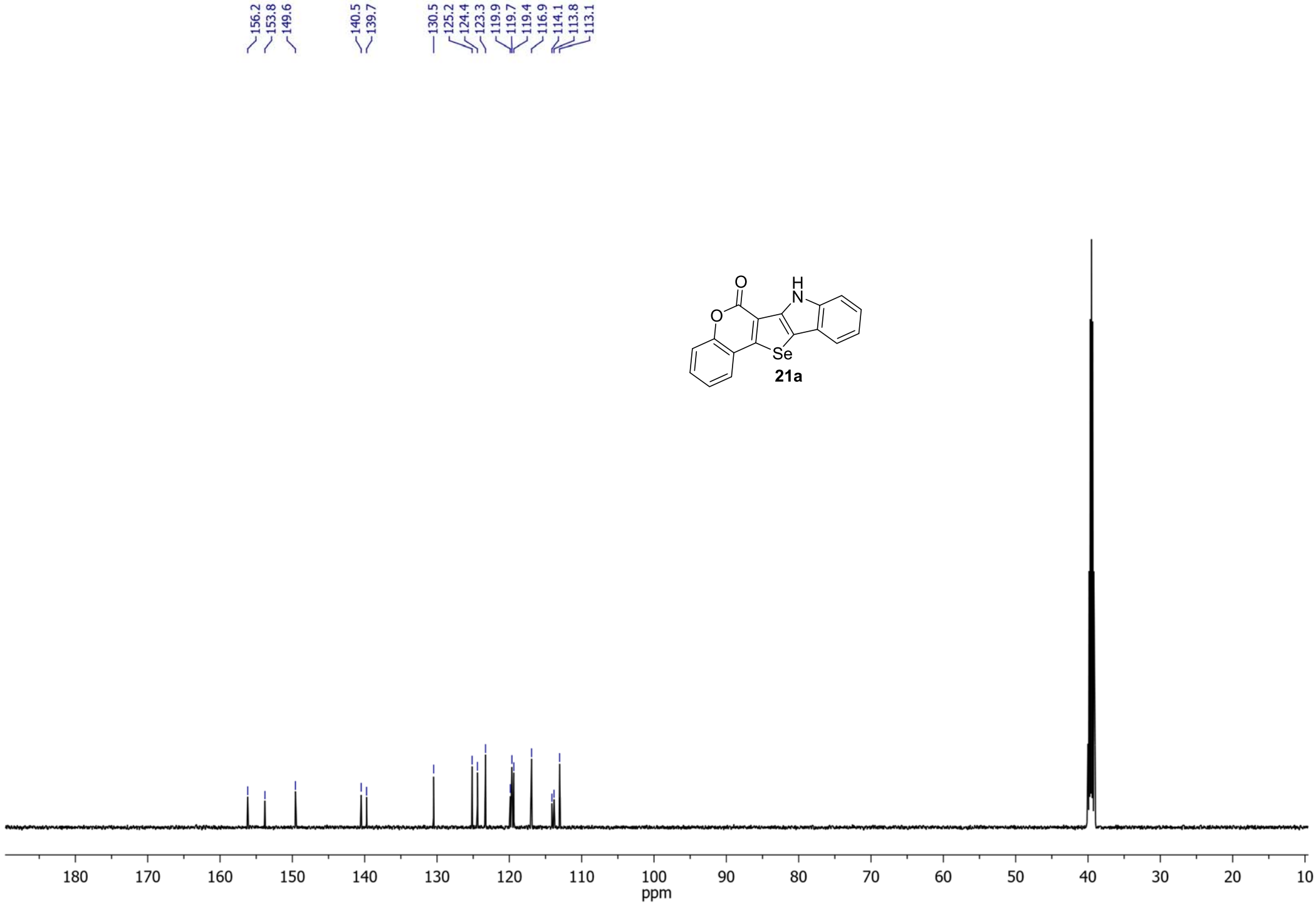
^{13}C NMR (solvent: DMSO-d_6)



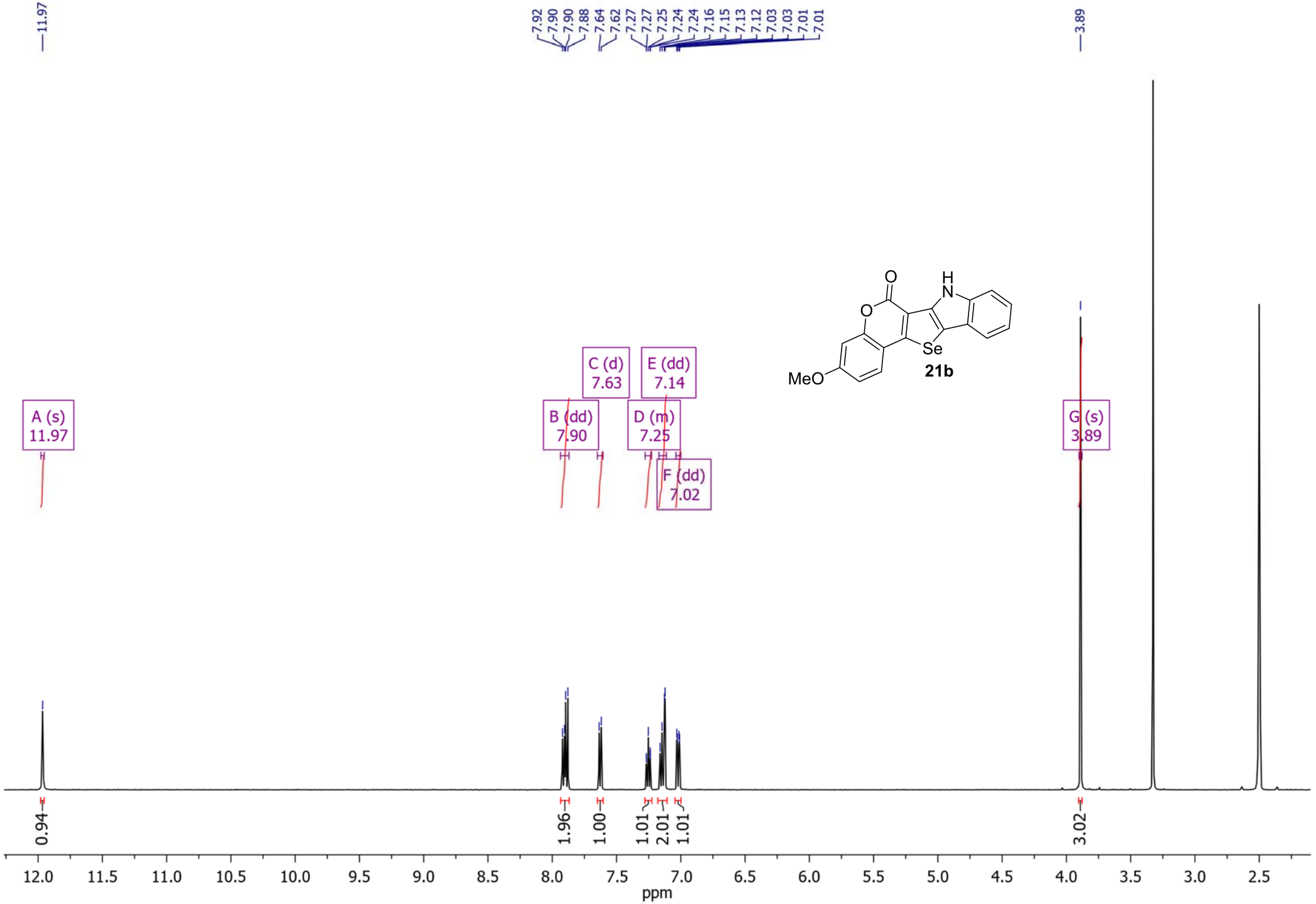
^{1}H NMR (solvent: DMSO-d_6)



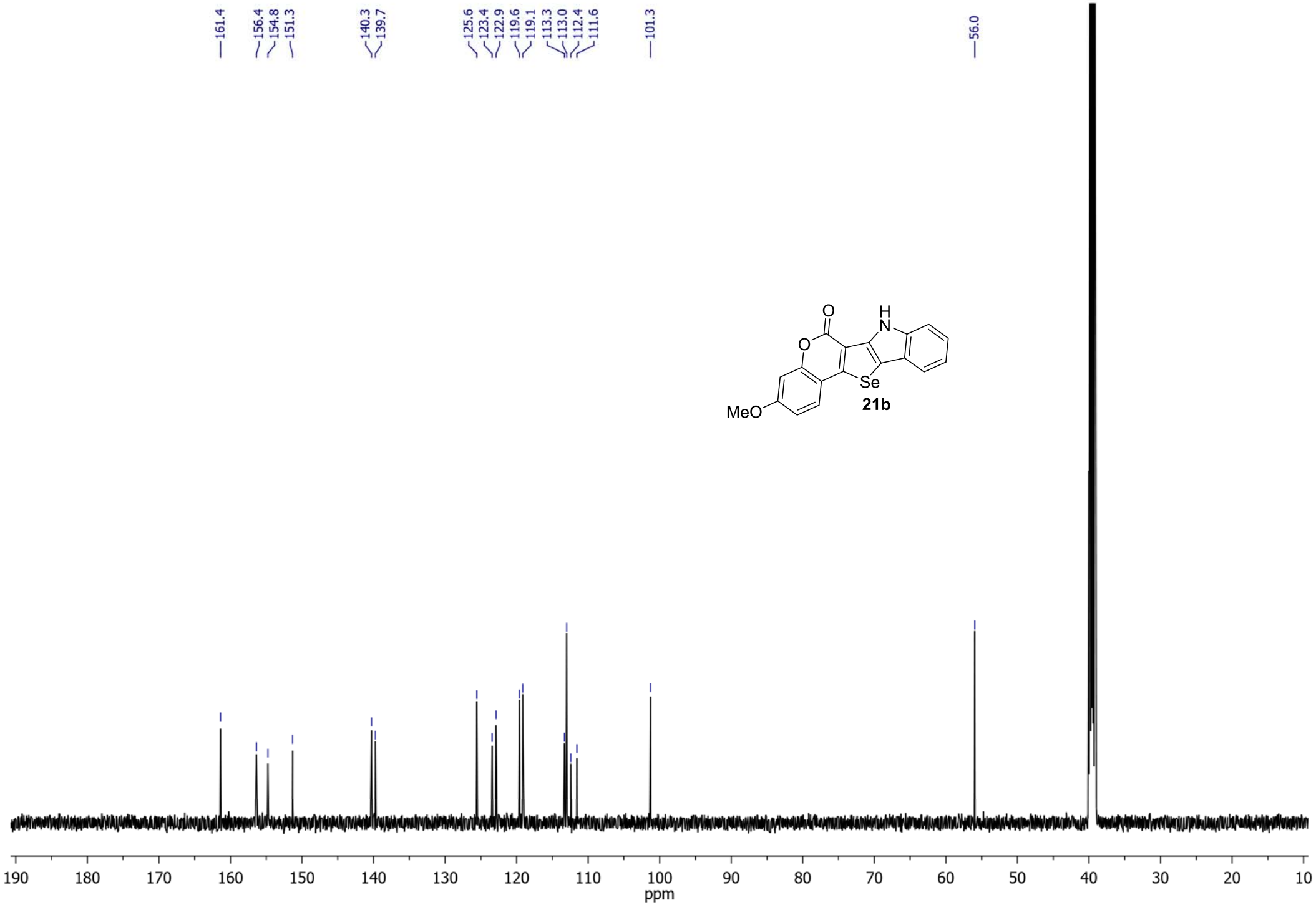
^{13}C NMR (solvent: DMSO-d_6)



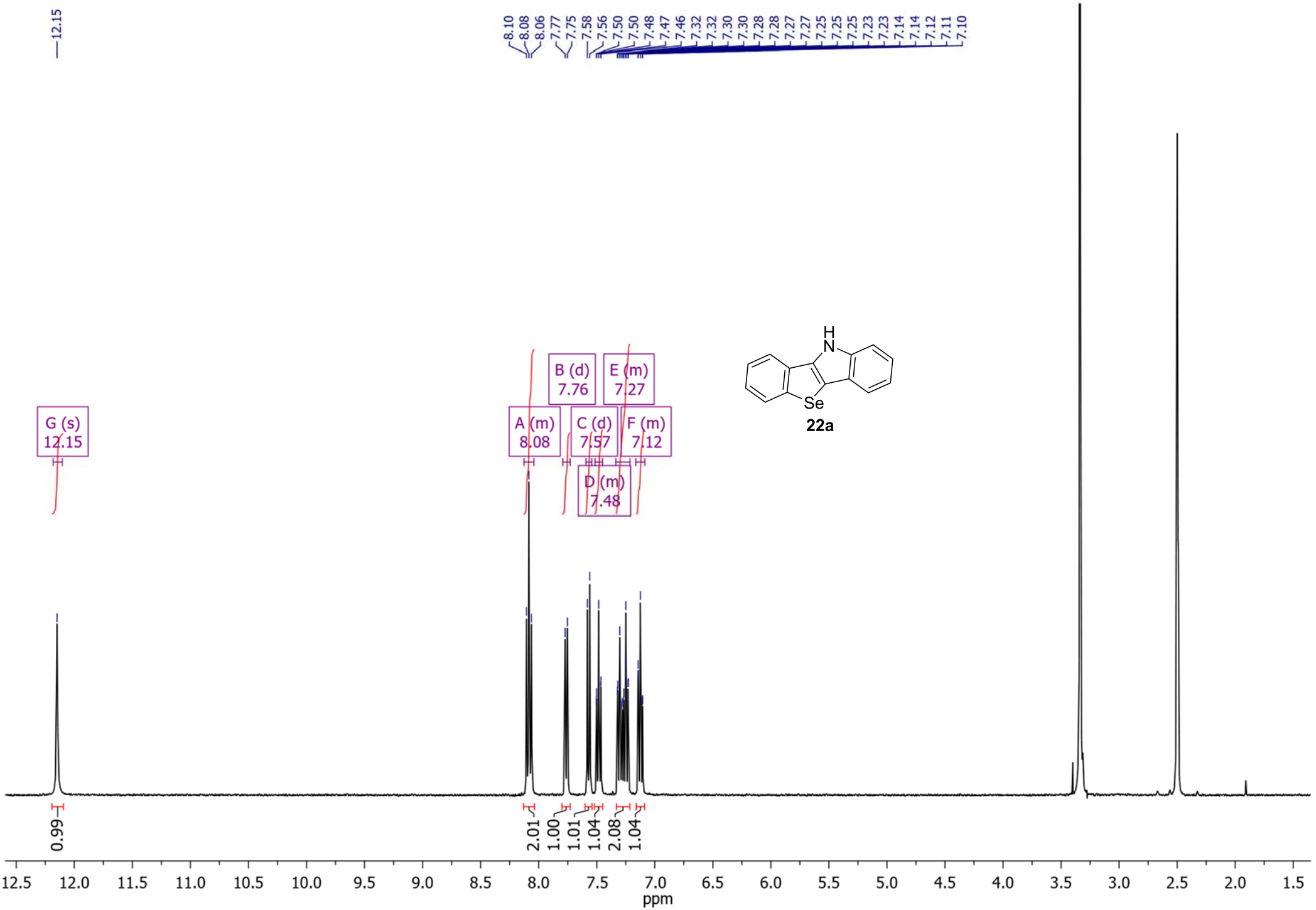
^{1}H NMR (solvent: DMSO-d_6)



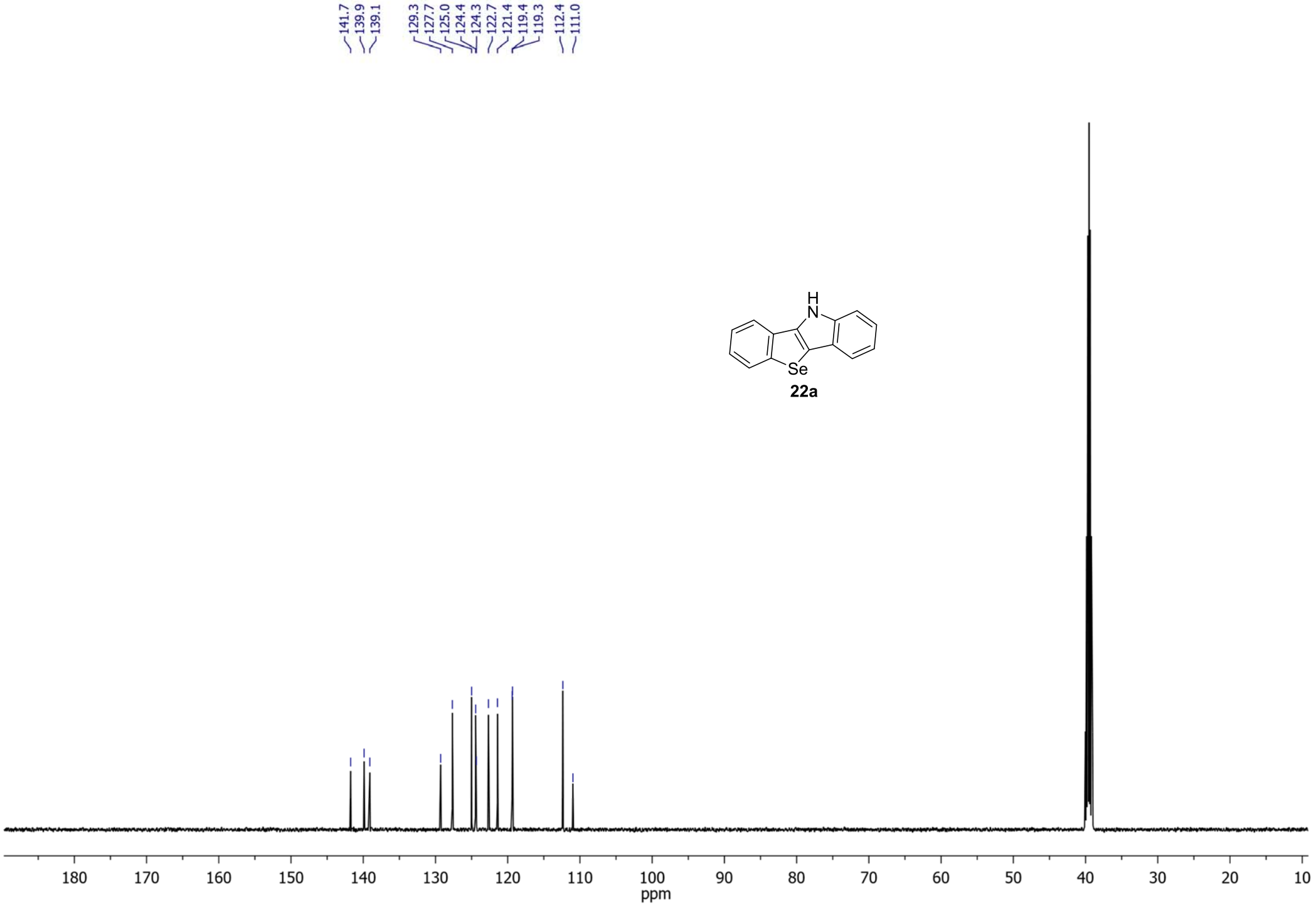
^{13}C NMR (solvent: DMSO-d_6)



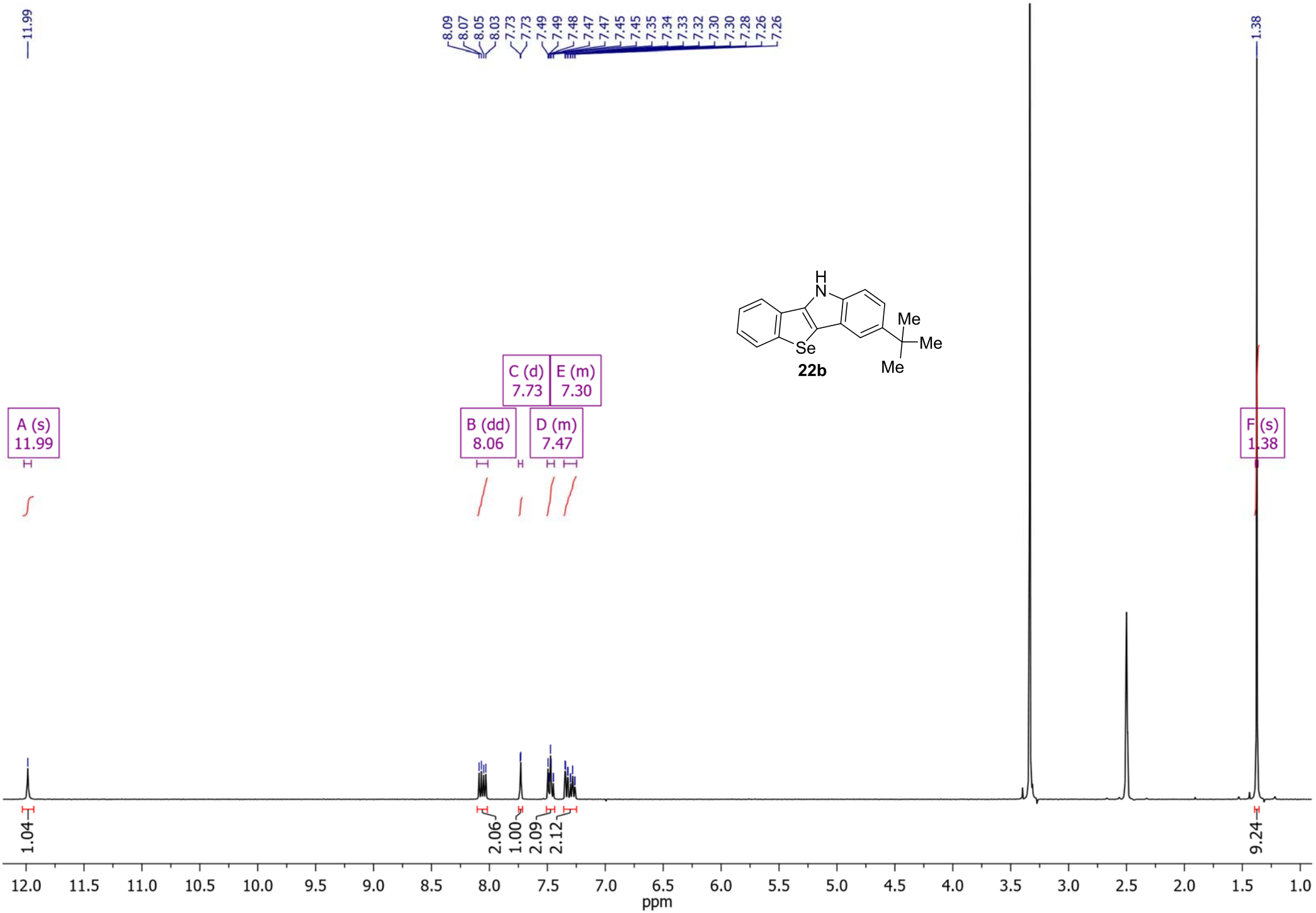
^{1}H NMR (solvent: DMSO-d_6)



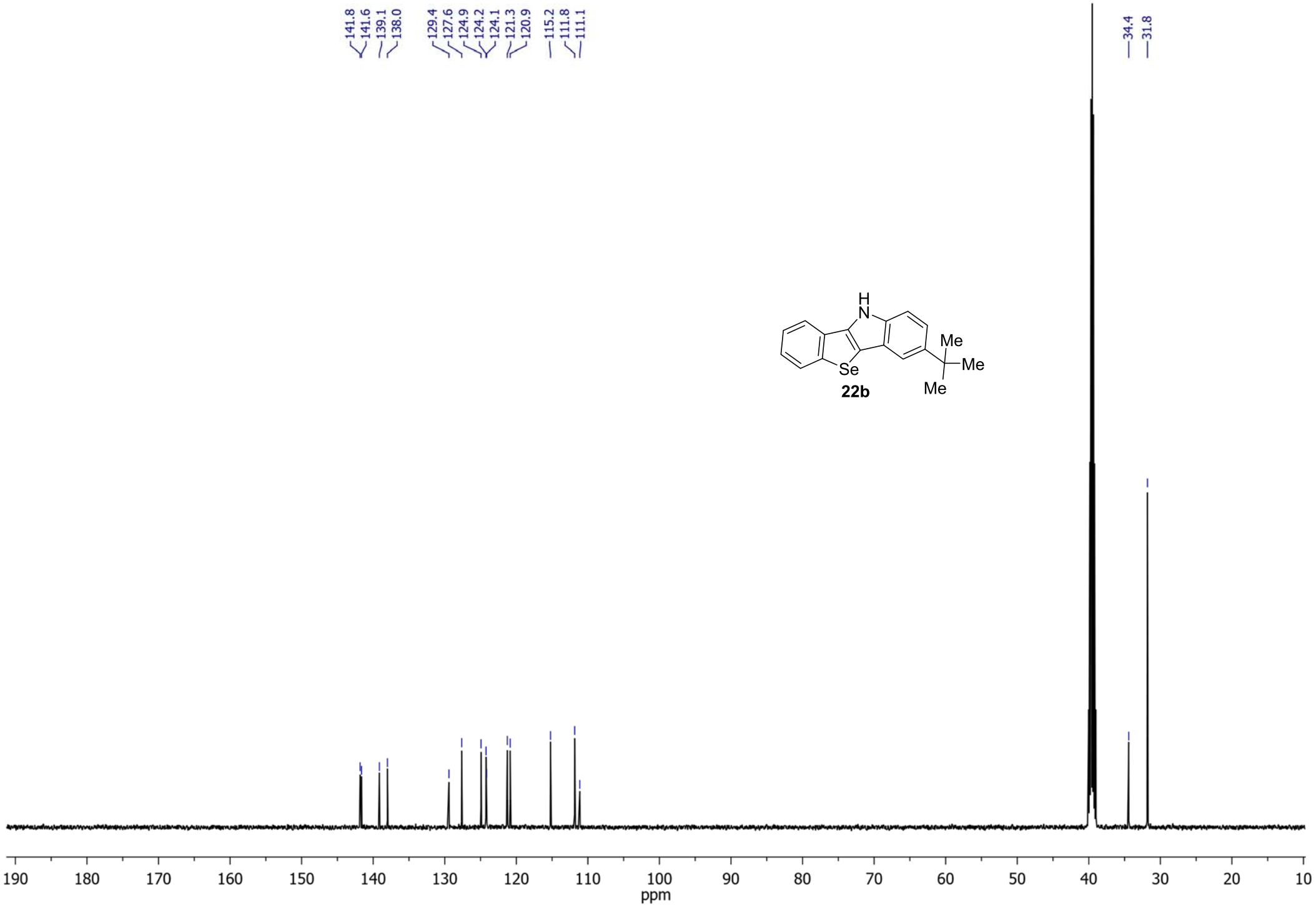
^{13}C NMR (solvent: DMSO-d_6)



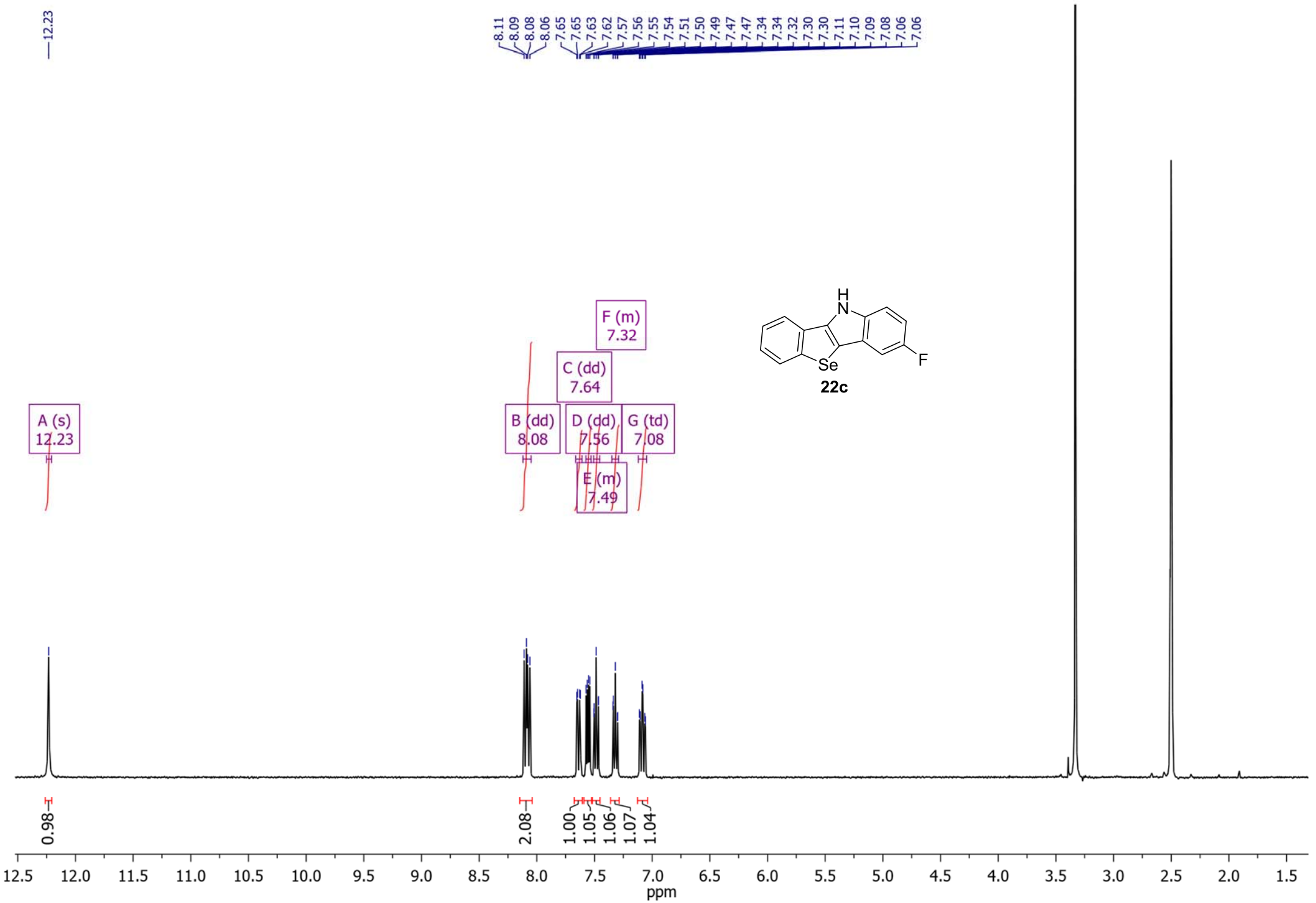
^{1}H NMR (solvent: DMSO-d_6)



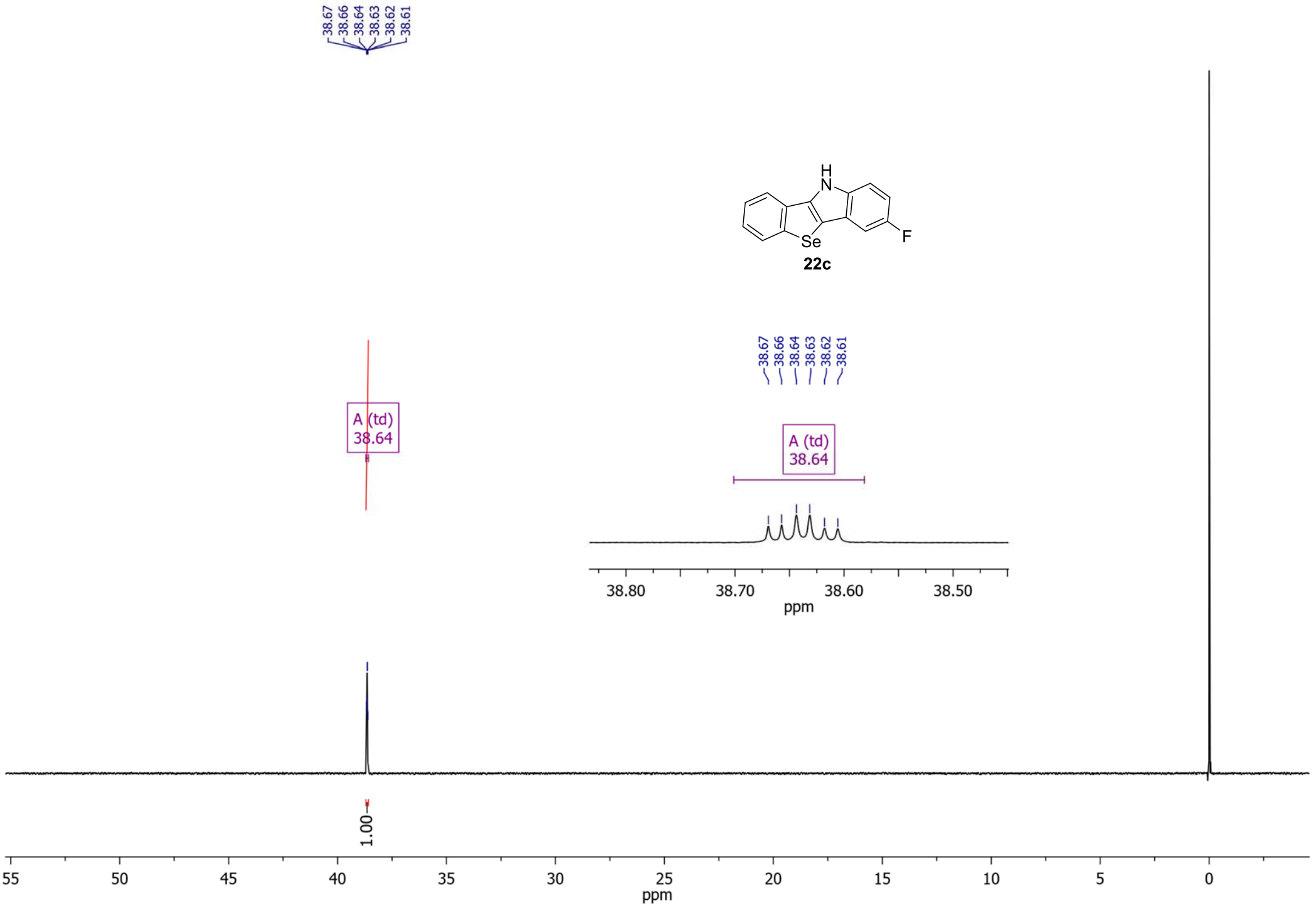
^{13}C NMR (solvent: DMSO-d_6)



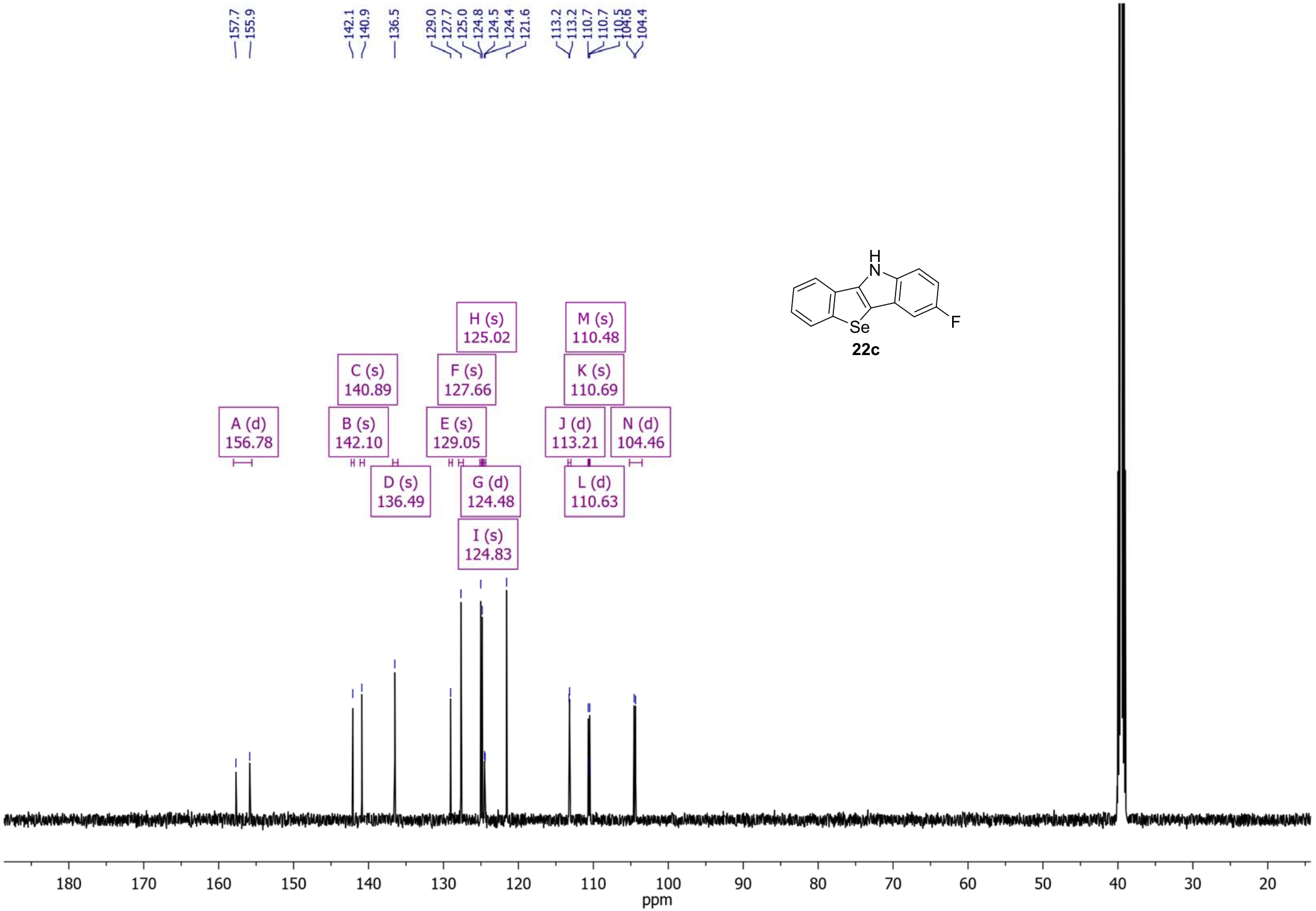
^{1}H NMR (solvent: DMSO-d_6)



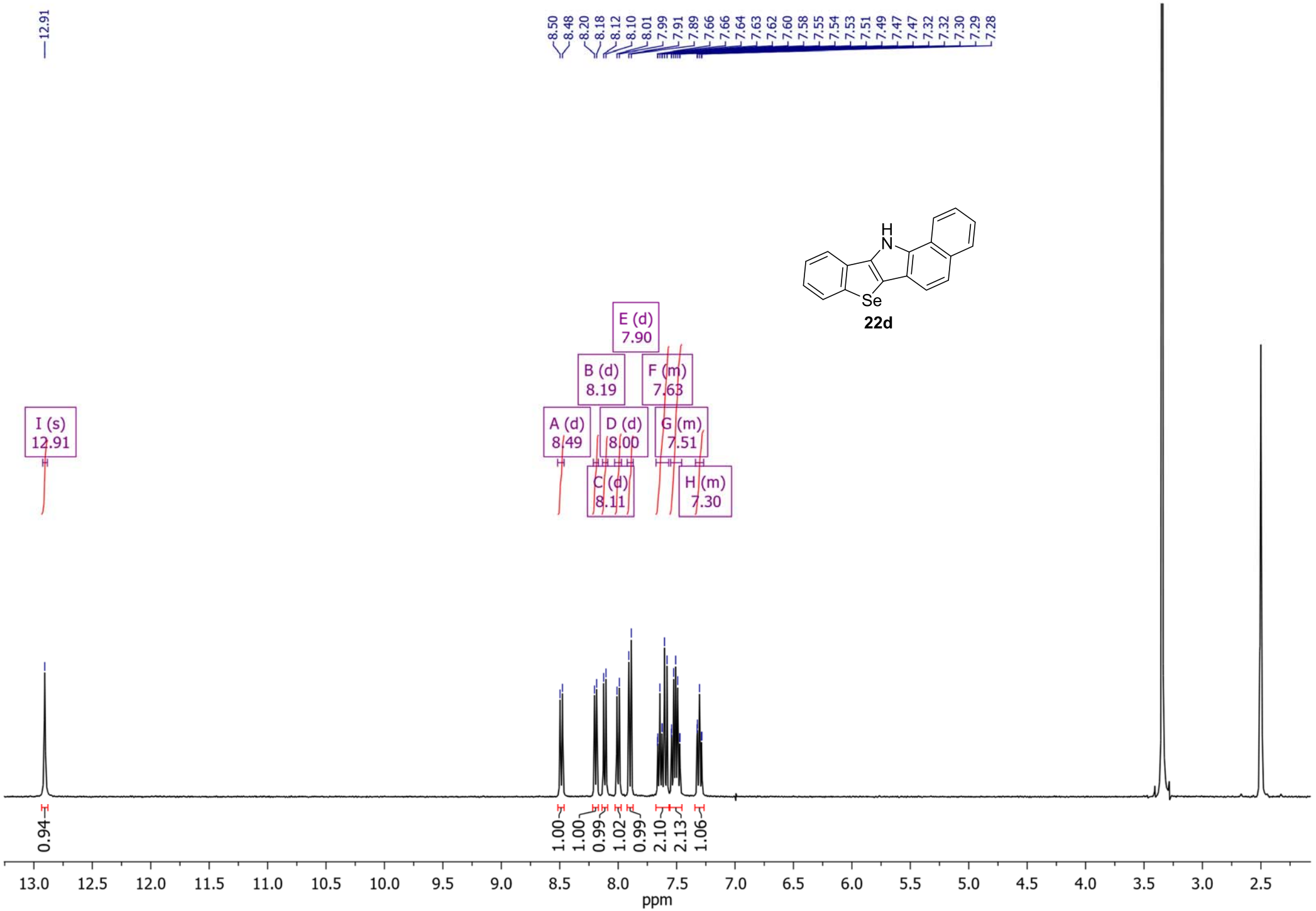
^{19}F NMR (solvent: DMSO-d_6)



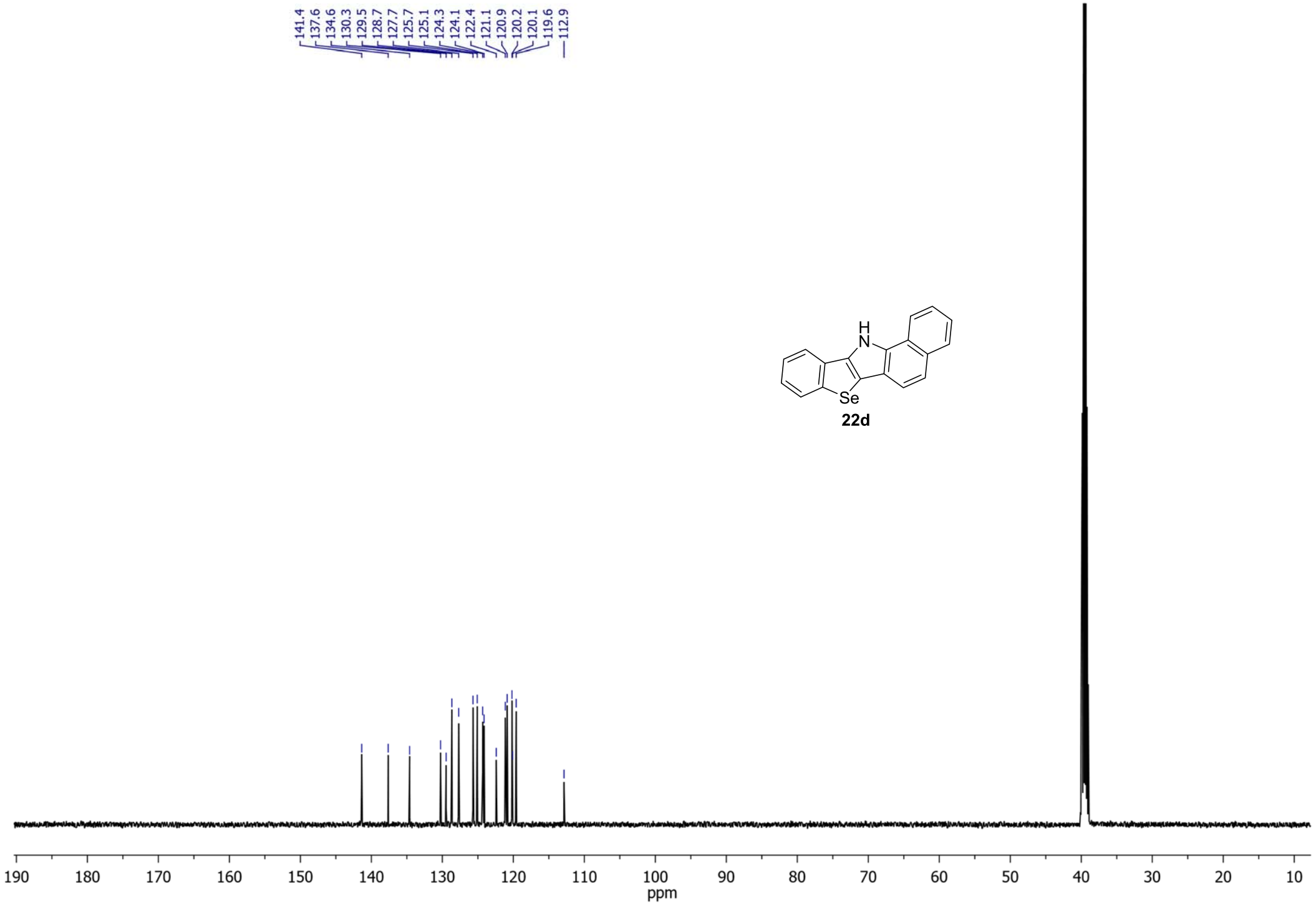
^{13}C NMR (solvent: DMSO-d_6)



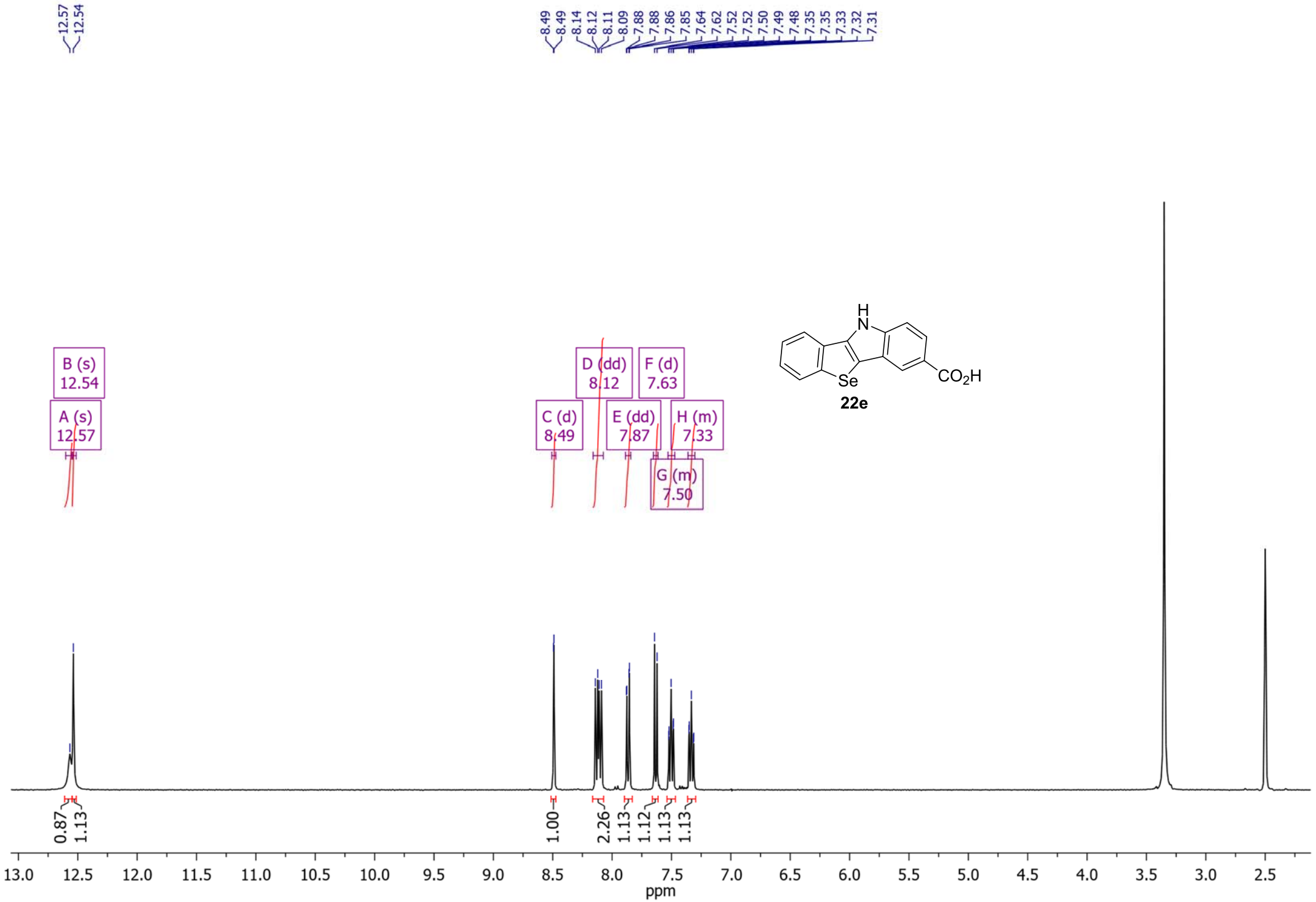
^{1}H NMR (solvent: DMSO-d_6)



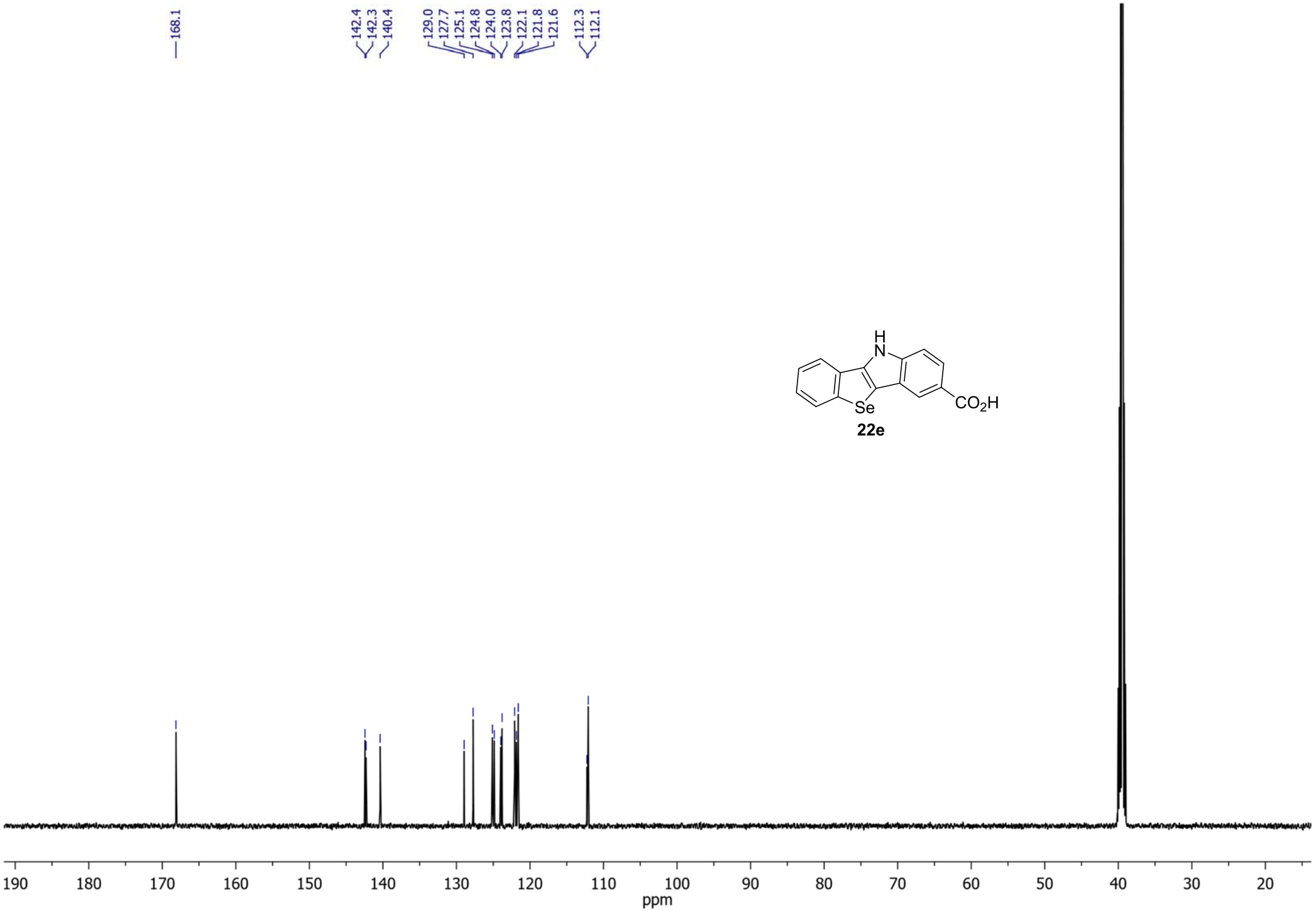
^{13}C NMR (solvent: DMSO-d_6)



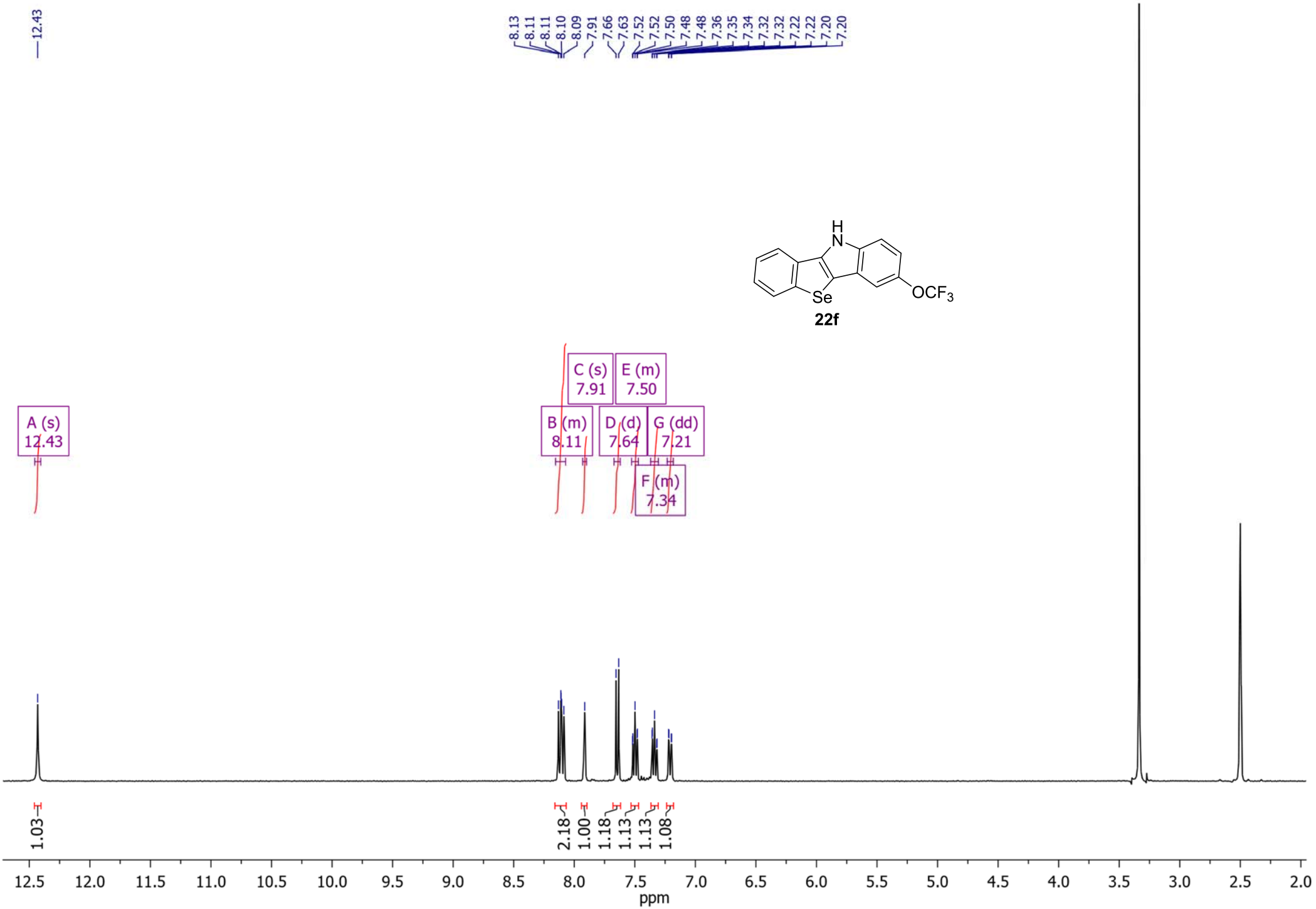
^{1}H NMR (solvent: DMSO-d_6)



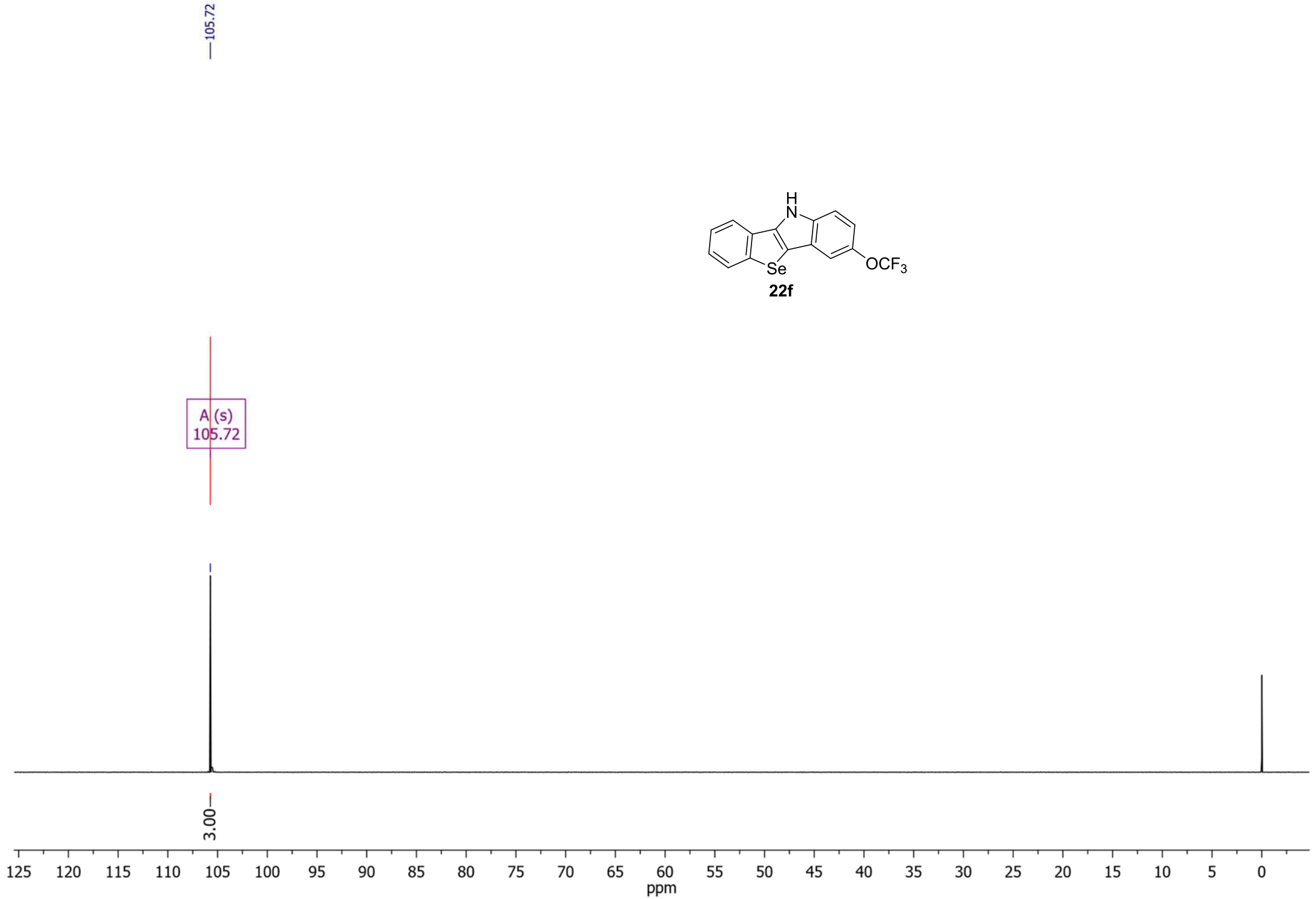
^{13}C NMR (solvent: DMSO-d_6)



^{1}H NMR (solvent: DMSO-d_6)

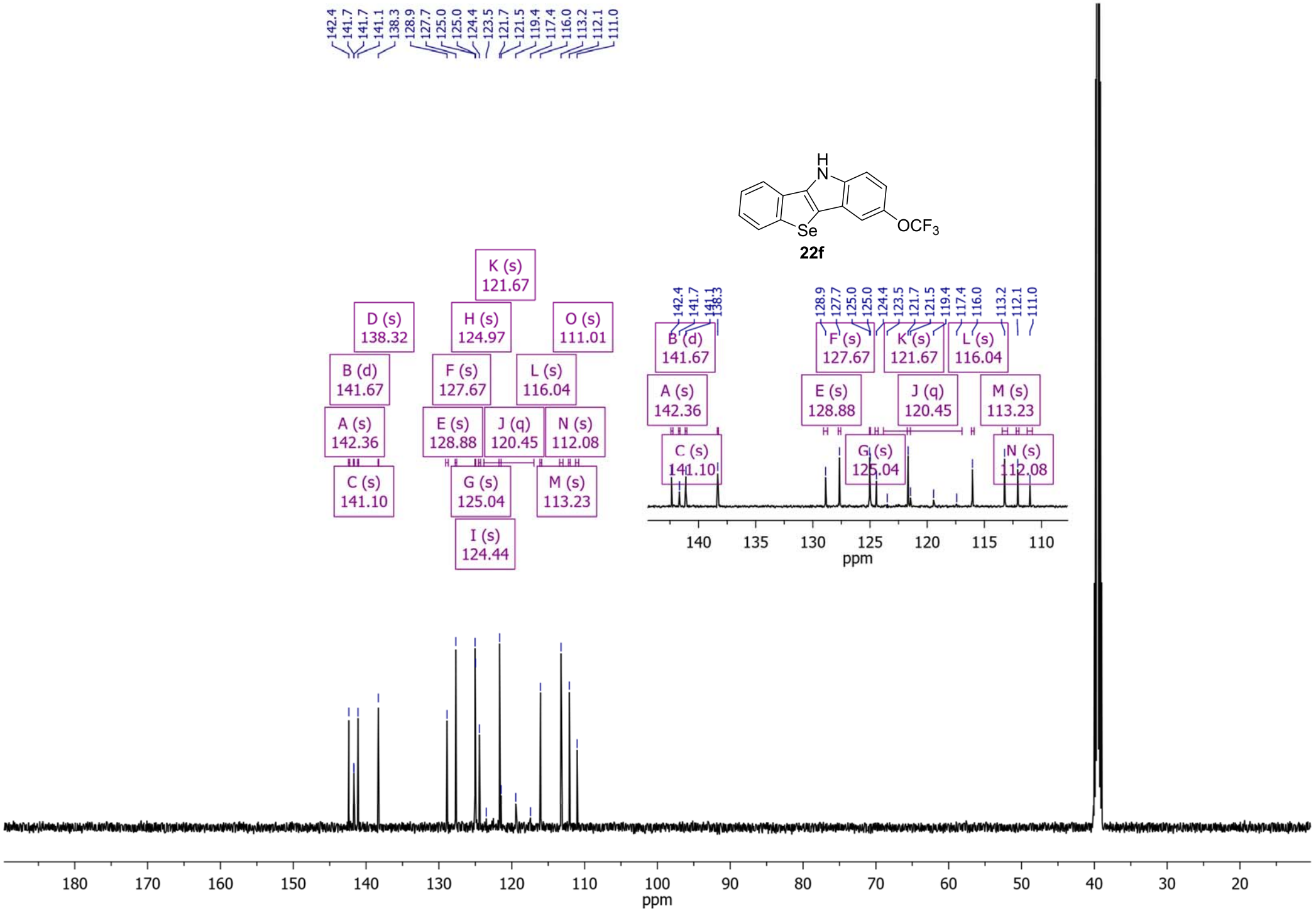


^{19}F NMR (solvent: DMSO-d_6)

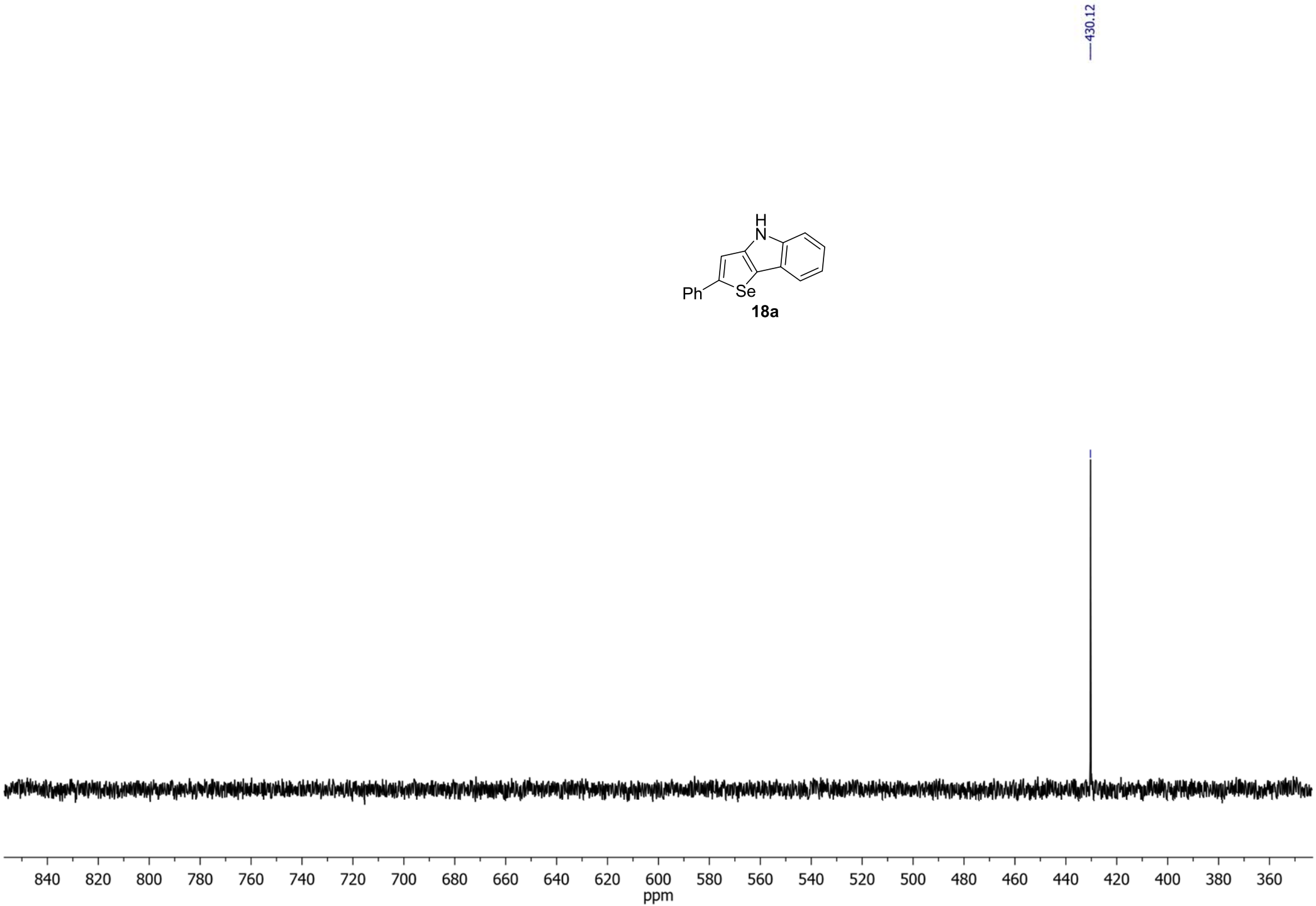


22f

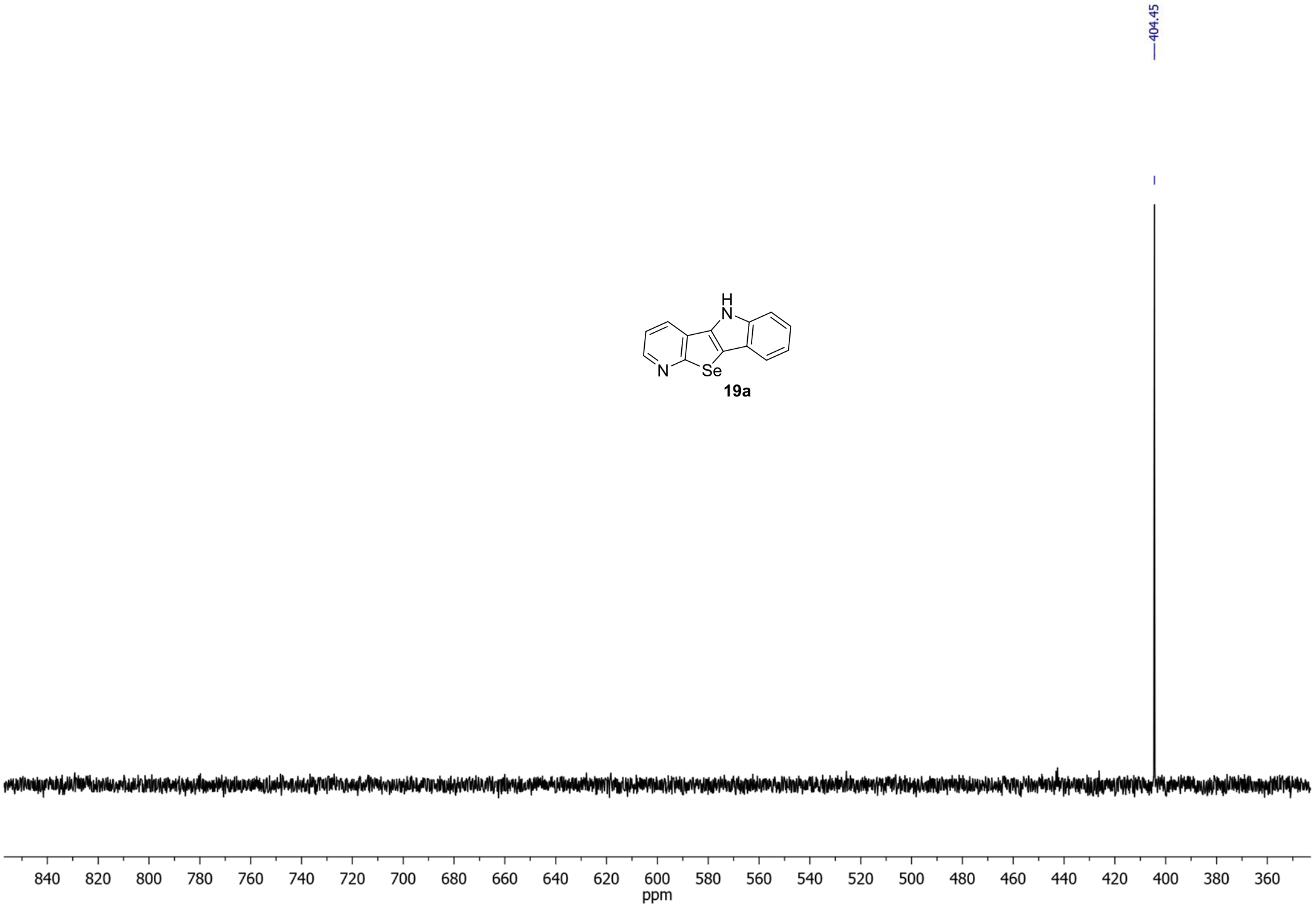
^{13}C NMR (solvent: DMSO-d_6)



^{77}Se NMR (solvent: DMSO-d_6)



^{77}Se NMR (solvent: DMSO-d_6)



^{77}Se NMR (solvent: DMSO-d_6)

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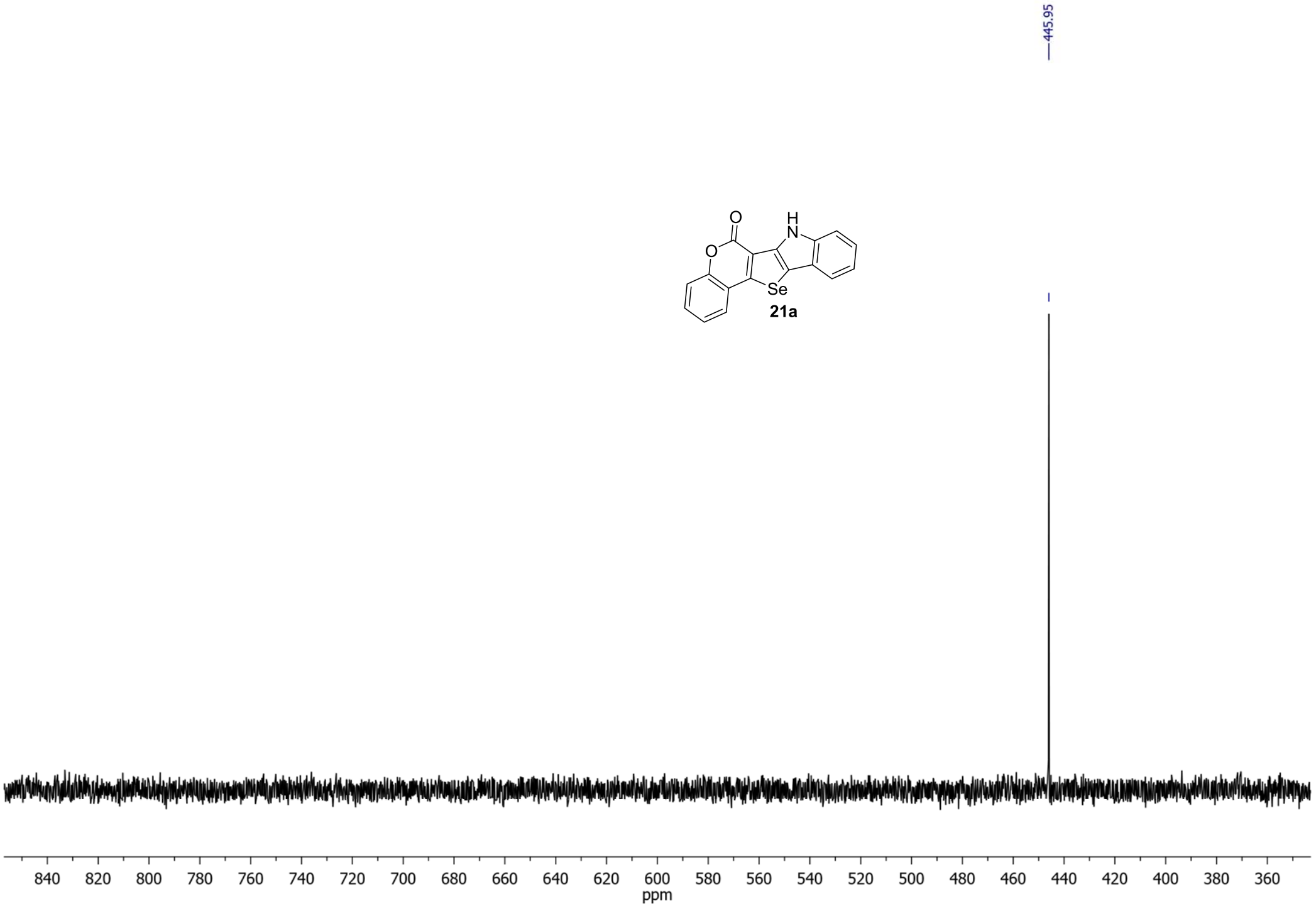

^{77}Se NMR (solvent: DMSO-d_6)