

Supporting Information

**Electrochemical Multicomponent Synthesis of
4-Selanylpirazoles under Catalyst- and Chemical
Oxidant-free Conditions**

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1. General Information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anode electrode is reticulated vitreous carbon (RVC) (5 mm×5 mm) and cathode electrode is netted platinum electrode (Pd net, 15 mm ×15 mm ×0.3 mm), and all electrodes were purchased from Beijing instrument electric technology co., LTD and used directly. All reagents were purchased from Energy Chemical (China) and used directly. The instrument for cyclic voltammetry is ElectroSyn 2.0 (IKA, made in Germany), and the conditions are as follow: 3 mm diameter glassy carbon disc working electrode, Pt plate electrode, Ag wire reference electrode. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel. ^1H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra were recorded at 100 MHz by using a Bruker Avance 400 spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference (^1H NMR: CDCl_3 7.26 ppm, ^{13}C NMR: CDCl_3 77.0 ppm), the chemical shifts (δ) were expressed in ppm and J values were given in Hz. Mass spectra were performed on a spectrometer operating on ESI-TOF.

Photographic depiction of the reaction setup:



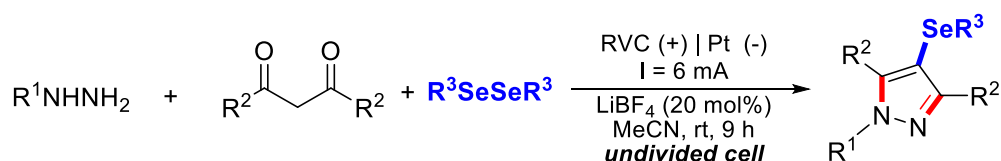
Figure S1 Photographic depiction of the reaction setup



Figure S2 Photographs of electrodes

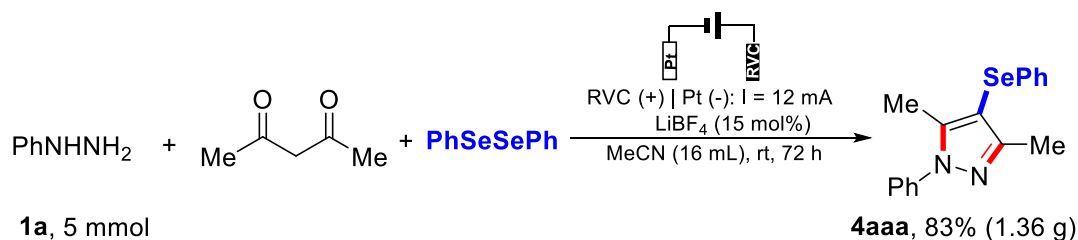
2. Experimental Section

2.1 General experimental procedures for Compound 4



In an undivided three-necked flask (25 mL) equipped with a stir bar, aromatic hydrazine (0.5 mmol), diacetone (0.5 mmol) and various dialkyl diselenides (diaryldiselenides) (0.375 mmol), LiBF₄ (0.1 mmol) and MeCN (8 mL) were added. The flask was equipped with reticulated vitreous carbon (RVC) (5 mm×5 mm) as anode and netted platinum electrode (15 mm ×15 mm × 0.3 mm) as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 6 mA under room temperature for 9 h. After completion, the reaction mixture was concentrated under reduced pressure. The pure products **4** were obtained by flash chromatography on silica gel (elute: petroleum ether/ethyl acetate).

2.2 Larger-scale synthesis of 4aaa



In an undivided three-necked flask (25 mL) equipped with a stir bar, aromatic hydrazine (5.0 mmol), diacetone (5.0 mmol) and diphenyldiselenides (3.75 mmol), LiBF₄ (1.0 mmol) and MeCN (16 mL) were added. The flask was equipped with reticulated vitreous carbon (RVC) (5 mm×5 mm) as anode and netted platinum electrode (15 mm ×15 mm × 0.3 mm) as cathode. The reaction mixture was stirred and electrolyzed at a constant current of 12 mA under room temperature for 72 h. After completion, the reaction mixture was concentrated under reduced pressure. The pure products **4aaa** were obtained by flash chromatography on silica gel (elute: petroleum ether/ethyl acetate).

2.3 Cyclic voltammetry experiment:

CV measurements were performed on an ElectroSyn 2.0 (IKA, made in Germany), and the conditions are as follow: 3 mm diameter glassy carbon disc working electrode, Pt plate electrode, Ag wire reference electrode, scan rate = 0.10 v/s (0-3.0 v), and 0.2 M of LiBF₄ as supporting electrolyte. The measurements were carried out as follows: a) 0.2 M solution of LiBF₄ in CH₃CN was added to the measuring cell. After recording the baseline, the

electroactive compound **3a**, **5a** (0.2 M) or the mixture of **1a**, **2a** and **3a** (0.2 M) in DMSO was added respectively. The cyclic voltammogram was recorded with one to three scans.

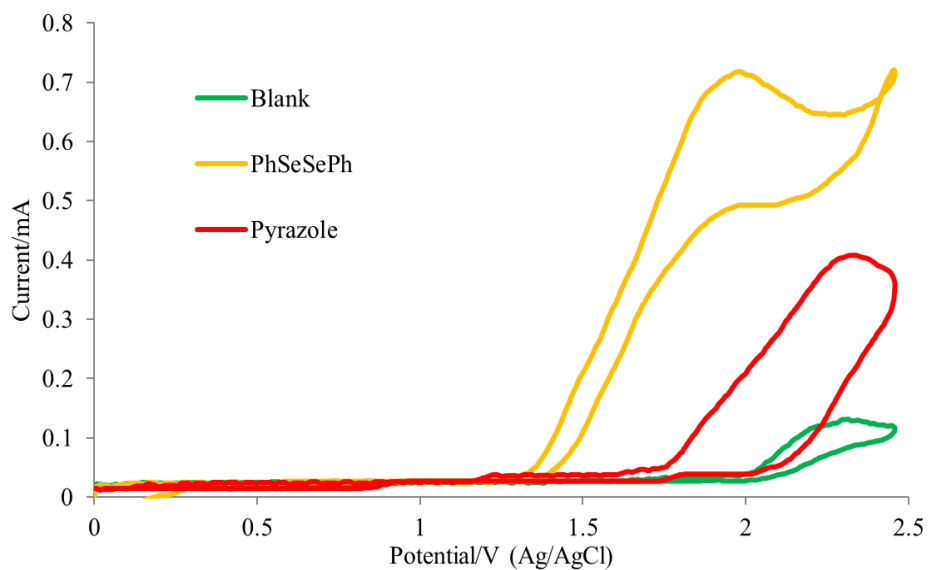
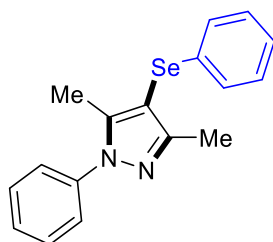
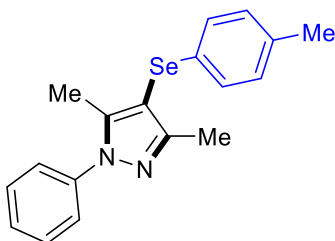


Figure S3 Cyclic voltammetry experiment

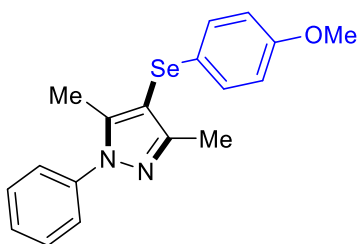
3. Characterization data of products



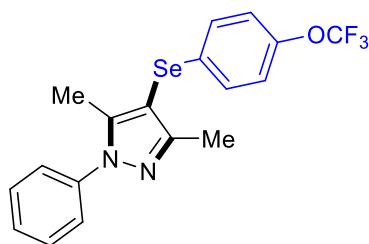
3,5-dimethyl-1-phenyl-4-(phenylselanyl)-1H-pyrazole (4aaa)^[1]: (92%). ¹H NMR (400 MHz, CDCl₃) δ 7.46 (d, *J* = 4.0 Hz, 4H), 7.39-7.35 (m, 1H), 7.20-7.17 (m, 4H), 7.16-7.12 (m, 1H), 3.38 (s, 3H), 3.33 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.32, 144.13, 139.90, 133.02, 129.21, 129.19, 128.37, 127.82, 125.82, 124.81, 102.63, 13.02, 12.53.



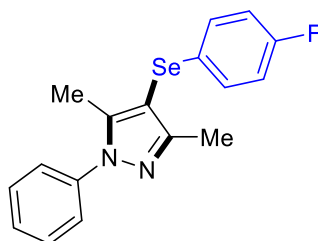
3,5-dimethyl-1-phenyl-4-(p-tolylselanyl)-1H-pyrazole (4aab)^[1]: (91%). ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, *J* = 4.0 Hz, 4H), 7.50-7.26 (m, 1H), 7.04-7.01 (m, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 2.29 (s, 3H), 2.25 (s, 3H), 2.19 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.24, 143.96, 139.93, 135.73, 130.02, 129.17, 129.07, 128.80, 127.77, 124.79, 103.07, 21.01, 13.05, 12.56.



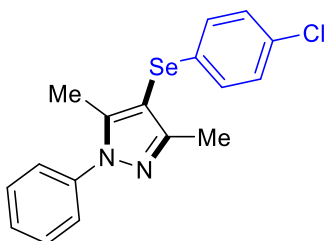
4-((4-methoxyphenyl)selanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aac)^[1]: (89%). ¹H NMR (400 MHz, CDCl₃) δ 7.49-7.48 (m, 4H), 7.42-7.38 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 3.79 (s, 3H), 2.42 (s, 3H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 158.50, 153.00, 143.68, 139.89, 131.11, 129.15, 127.75, 124.78, 122.70, 114.94, 103.90, 55.33, 12.55.



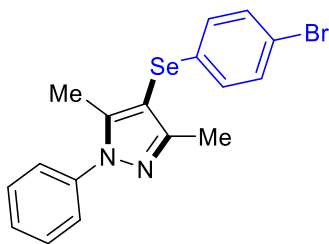
3,5-dimethyl-1-phenyl-4-((4-(trifluoromethoxy)phenyl)selanyl)-1H-pyrazole (4aad): (87%). ^1H NMR (400 MHz, CDCl_3) δ 7.39-7.38 (m, 4H), 7.32-7.28 (m, 1H), 7.11 (d, J = 8.0 Hz, 2H), 6.98 (d, J = 8.0 Hz, 2H), 2.29 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.21, 147.57, 147.55, 147.53, 147.51, 144.21, 139.77, 131.51, 129.49, 129.22, 127.94, 124.80, 121.92, 119.16, 102.32, 12.95, 12.46; HRMS: calcd for $\text{C}_{18}\text{H}_{16}\text{F}_3\text{N}_2\text{OSe}$ $[\text{M}+\text{H}]^+$ 413.0304, found 413.0306.



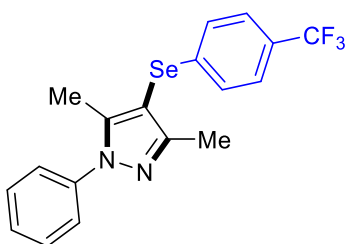
4-((4-fluorophenyl)selanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aae)^[2]: (91%) ^1H NMR (400 MHz, CDCl_3) δ 7.49 (t, J = 8.0 Hz, 4H), 7.40 (m, 1H), 7.21 (d, J = 8.0 Hz, 2H), 6.94 (t, J = 8.0 Hz, 2H), 2.41 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.86, 160.43, 153.07, 143.95, 139.83, 130.56, 130.49, 129.20, 127.86, 127.27, 127.24, 124.78, 116.43, 116.21, 103.12, 13.01, 12.50.



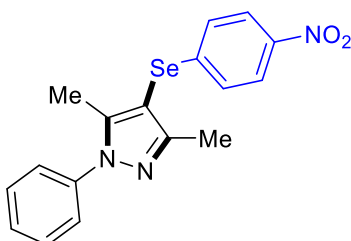
4-((4-chlorophenyl)selanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aaf)^[1]: (80%) ^1H NMR (400 MHz, CDCl_3) δ 7.41 (d, J = 8.0 Hz, 4H), 7.32 (t, J = 8.0 Hz, 1H), 7.11 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 2.30 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.19, 144.14, 139.77, 131.83, 131.27, 129.65, 129.28, 129.21, 127.93, 124.80, 102.36, 12.96, 12.48.



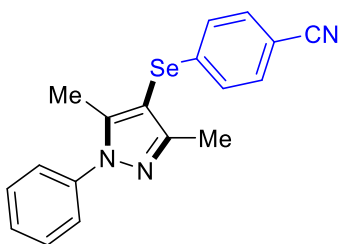
4-((4-bromophenyl)selanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aag): (87%) ^1H NMR (400 MHz, CDCl_3) δ 7.40 (d, J = 8.0 Hz, 4H), 7.33 (d, J = 4.0 Hz, 1H), 7.24 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 2.29 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.20, 144.16, 139.77, 132.17, 132.07, 129.92, 129.22, 127.94, 124.80, 119.69, 102.23, 12.97, 12.49; HRMS: calcd for $\text{C}_{17}\text{H}_{16}\text{BrN}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 406.9662, found 406.9656.



3,5-dimethyl-1-phenyl-4-((4-(trifluoromethyl)phenyl)selanyl)-1H-pyrazole (4aah)^[1]: (86%) ^1H NMR (400 MHz, CDCl_3) δ 7.52 (d, J = 4.0 Hz, 4H), 7.47 (d, J = 8.0 Hz, 3H), 7.28 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.32, 144.41, 139.73, 138.71, 129.25, 128.03, 127.78, 125.94, 125.90, 125.86, 125.83, 124.82, 101.42, 12.92, 12.43.

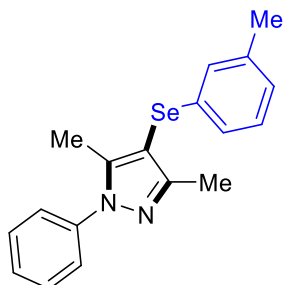


3,5-dimethyl-4-((4-nitrophenyl)selanyl)-1-phenyl-1H-pyrazole (4aai): (85%) ^1H NMR (400 MHz, CDCl_3) δ 8.06 (d, J = 8.0 Hz, 2H), 7.52 (t, J = 8.0 Hz, 4H), 7.44 (m, 1H), 7.29 (d, J = 8.0 Hz, 2H), 2.39 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.20, 145.96, 144.56, 144.20, 139.59, 129.30, 128.17, 127.60, 124.83, 124.05, 100.83, 12.89, 12.42; HRMS: calcd for $\text{C}_{17}\text{H}_{16}\text{N}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 374.0325, found 374.0328.

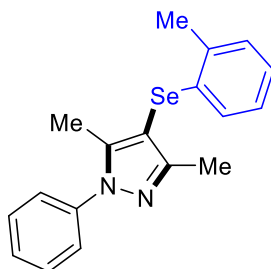


4-((3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)selanyl)benzonitrile (4aaj): (85%) ^1H NMR

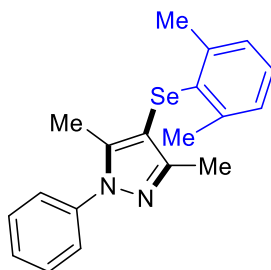
(400 MHz, CDCl₃) δ 7.48 (m, 6H), 7.42 (m, 1H), 7.24 (d, J = 8.0 Hz, 2H), 2.37 (s, 3H), 2.31 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.22, 144.52, 141.33, 139.62, 132.44, 129.28, 128.12, 127.91, 124.80, 118.95, 108.97, 100.87, 12.90, 12.43; HRMS: calcd for C₁₈H₁₆N₃Se [M+H]⁺ 354.0431, found 351.0428.



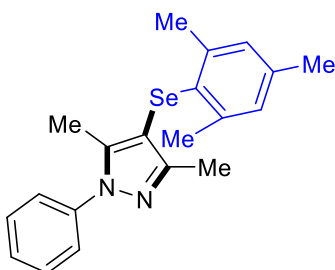
3,5-dimethyl-1-phenyl-4-(*m*-tolylselanyl)-1H-pyrazole (4aak): (86%) ¹H NMR (400 MHz, CDCl₃) δ 7.50 (d, J = 4.0 Hz, 4H), 7.42 (d, J = 8.0 Hz, 1H), 7.13 (t, J = 8.0 Hz, 2H), 7.00 (d, J = 4.0 Hz, 2H), 2.42 (s, 3H), 2.37 (s, 3H), 2.32 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.35, 144.11, 139.90, 139.00, 132.76, 129.19, 129.04, 128.96, 127.81, 126.76, 125.38, 124.80, 102.67, 21.45, 13.05, 12.57; HRMS: calcd for C₁₈H₁₉N₂Se [M+H]⁺ 343.0708, found 343.0699.



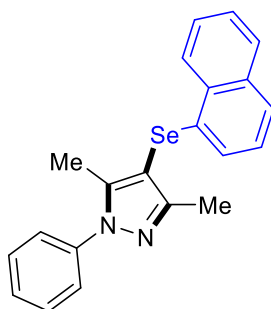
3,5-dimethyl-1-phenyl-4-(*o*-tolylselanyl)-1H-pyrazole (4aal): (90%). ¹H NMR (400 MHz, CDCl₃) δ 7.52 (d, J = 8.0 Hz, 4H), 7.44-7.41 (m, 1H), 7.17 (d, J = 8.0 Hz, 1H), 7.10 (t, J = 8.0 Hz, 1H), 7.03 (t, J = 4.0 Hz, 1H), 6.83 (d, J = 4.0 Hz, 1H), 2.46 (s, 3H), 2.39 (s, 3H), 2.34 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.63, 144.42, 139.85, 136.18, 133.49, 130.11, 129.20, 127.86, 126.90, 126.64, 125.51, 124.82, 101.63, 21.21, 12.96, 12.50; HRMS: calcd for C₁₈H₁₉N₂Se [M+H]⁺ 343.0708, found 343.0702.



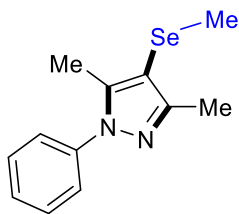
4-((2,6-dimethylphenyl)selanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aam): (83%) ^1H NMR (400 MHz, CDCl_3) δ 7.46 (t, J = 8.0 Hz, 2H), 7.40 (t, J = 8.0 Hz, 3H), 7.14-7.07 (m, 3H), 2.50 (s, 6H), 2.28 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 151.84, 141.96, 141.68, 139.84, 131.47, 129.09, 127.98, 127.87, 127.59, 124.75, 104.08, 24.20, 12.95, 12.31; HRMS: calcd for $\text{C}_{19}\text{H}_{21}\text{N}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 357.0870, found 357.0853.



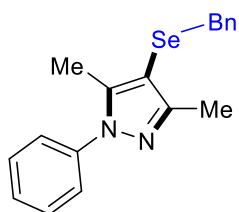
4-(mesitylselanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aan)^[3]: (81%) ^1H NMR (400 MHz, CDCl_3) δ 7.48-7.38 (m, 5H), 6.91 (s, 2H), 2.47 (s, 6H), 2.29 (s, 3H), 2.28 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 151.83, 141.82, 141.63, 139.87, 137.61, 129.07, 128.86, 127.90, 127.54, 124.75, 104.26, 24.08, 20.90, 12.98, 12.32.



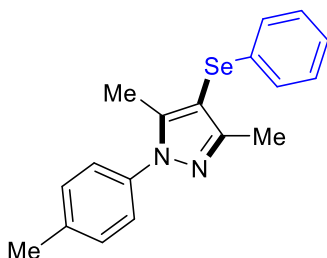
3,5-dimethyl-4-(naphthalen-1-ylselanyl)-1-phenyl-1H-pyrazole (4aao): (87%) ^1H NMR (400 MHz, CDCl_3) δ 8.25 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.54 (m, 4H), 7.44 (d, J = 8.0 Hz, 1H), 7.31 (t, J = 4.0 Hz, 1H), 7.12 (d, J = 4.0 Hz, 1H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.67, 144.49, 139.90, 134.00, 132.17, 131.80, 129.22, 128.65, 127.87, 126.32, 126.29, 126.24, 126.10, 125.50, 125.42, 124.83, 101.61, 13.04, 12.56; HRMS: calcd for $\text{C}_{21}\text{H}_{19}\text{N}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 379.0635, found 379.0641.



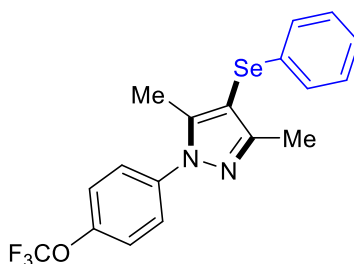
3,5-dimethyl-4-(methylselanyl)-1-phenyl-1H-pyrazole (4aap): (91%). ^1H NMR (400 MHz, CDCl_3) δ 7.50-7.43 (m, 4H), 7.41-7.36 (m, 1H), 2.43 (s, 3H), 2.42 (s, 3H), 2.09 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 152.48, 142.87, 139.93, 129.11, 127.62, 124.75, 104.31, 13.06, 12.51, 8.87; HRMS: calcd for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 267.0435, found 267.0432.



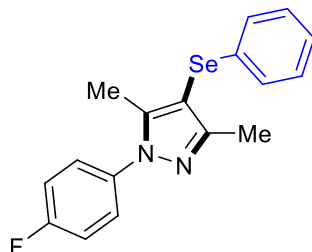
4-(benzylselanyl)-3,5-dimethyl-1-phenyl-1H-pyrazole (4aaq)^[4]: (88%). ^1H NMR (400 MHz, CDCl_3) δ 7.33 (t, J = 8.0 Hz, 2H), 7.25 (t, J = 8.0 Hz, 3H), 7.10-7.08 (m, 3H), 6.89-6.87 (m, 2H), 3.60 (s, 2H), 2.17 (s, 3H), 1.77 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.24, 144.52, 139.99, 139.29, 129.09, 128.96, 128.20, 127.64, 126.61, 124.81, 102.59, 31.72, 12.91, 11.83.



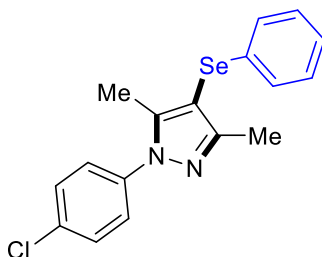
3,5-dimethyl-4-(phenylselanyl)-1-(p-tolyl)-1H-pyrazole (4baa)^[4]: (89%) ^1H NMR (400 MHz, CDCl_3) δ 7.37 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 7.22 (s, 4H), 7.19 (d, J = 4.0 Hz, 1H), 2.44 (s, 3H), 2.38 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.09, 144.12, 137.80, 137.44, 133.10, 129.72, 129.18, 128.31, 125.76, 124.72, 102.20, 21.17, 13.00, 12.44.



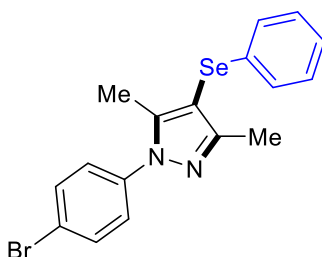
3,5-dimethyl-4-(phenylselanyl)-1-(4-(trifluoromethoxy)phenyl)-1H-pyrazole (4caa): (86%). ¹H NMR (400 MHz, CDCl₃) δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.36 (t, *J* = 8.0 Hz, 2H), 7.26-7.17 (m, 5H), 2.43 (s, 3H), 2.35 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.76, 148.24, 148.21, 144.17, 138.38, 132.74, 129.24, 128.47, 126.03, 125.94, 119.15, 103.31, 12.98, 12.56; HRMS: calcd for C₁₈H₁₆F₃N₂OSe [M+H]⁺ 413.0304, found 413.0302.



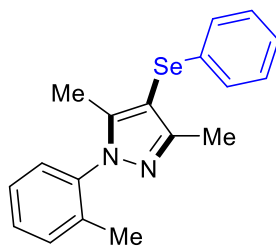
1-(4-fluorophenyl)-3,5-dimethyl-4-(phenylselanyl)-1H-pyrazole (4daa)^[5]: (94%). ¹H NMR (400 MHz, CDCl₃) δ 7.49-7.46 (m, 2H), 7.24-7.17 (m, 7H), 2.38-2.35 (m, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 163.12, 160.66, 153.42, 144.23, 136.03, 132.88, 129.22, 128.42, 126.75, 126.66, 125.88, 116.22, 115.99, 102.68, 12.98, 12.40.



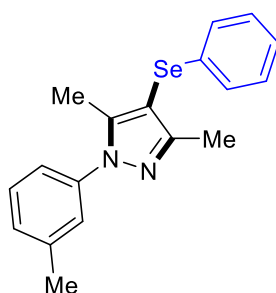
1-(4-chlorophenyl)-3,5-dimethyl-4-(phenylselanyl)-1H-pyrazole (4eaa)^[5]: (88%). ¹H NMR (400 MHz, CDCl₃) δ 7.49-7.44 (m, 4H), 7.24-7.18 (m, 5H), 2.41 (s, 3H), 2.35 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.66, 144.12, 138.41, 133.46, 132.80, 129.35, 129.25, 128.45, 125.92, 125.86, 103.22, 13.03, 12.60.



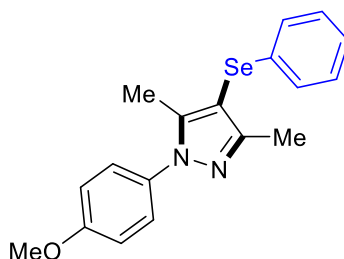
1-(4-bromophenyl)-3,5-dimethyl-4-(phenylselanyl)-1H-pyrazole (4faa)^[5]: (90%). ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.24-7.22 (m, 4H), 7.20-7.16 (m, 1H), 2.41 (s, 3H), 2.35(s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.71, 144.08, 138.91, 132.78, 132.32, 129.26, 128.48, 126.12, 125.94, 121.39, 103.34, 13.05, 12.64.



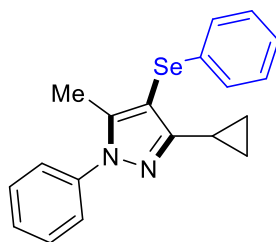
3,5-dimethyl-4-(phenylselanyl)-1-(o-tolyl)-1H-pyrazole (4gaa)^[1]: (88%). ¹H NMR (400 MHz, CDCl₃) δ 7.41-7.33 (m, 2H), 7.31 (t, *J* = 8.0 Hz, 2H), 7.26-7.15 (m, 5H), 2.36 (s, 3H), 2.16 (s, 3H), 2.12 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 152.95, 145.20, 138.77, 136.03, 133.33, 131.04, 129.42, 129.20, 128.04, 127.74, 126.72, 125.69, 100.58, 17.29, 13.05, 11.39.



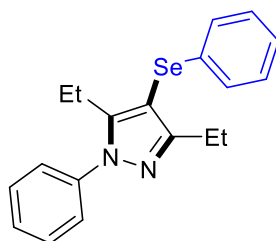
3,5-dimethyl-4-(phenylselanyl)-1-(m-tolyl)-1H-pyrazole (4haa)^[1]: (90%) ¹H NMR (400 MHz, CDCl₃) δ 7.37 (d, *J* = 8.0 Hz, 2H), 7.24 (m, 6H), 7.18 (d, *J* = 8.0 Hz, 1H), 2.45 (s, 3H), 2.41 (s, 3H), 2.37 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.18, 144.13, 139.80, 139.38, 133.07, 129.20, 128.87, 128.63, 128.33, 125.79, 125.58, 121.77, 102.42, 21.42, 13.02, 12.53.



1-(4-methoxyphenyl)-3,5-dimethyl-4-(phenylselanyl)-1H-pyrazole (4iaa)^[4]: (84%). ¹H NMR (400 MHz, CDCl₃) δ 7.39 (d, *J* = 8.0 Hz, 2H), 7.23-7.22 (m, 4H), 7.19-7.17 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 3H), 2.35 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 159.13, 152.94, 144.25, 136.38, 133.12, 129.18, 128.31, 126.38, 125.76, 114.27, 101.86, 55.60, 12.98, 12.29.



3-cyclopropyl-5-methyl-1-phenyl-4-(phenylselanyl)-1H-pyrazole (4aba): (82%) ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.50 (t, J = 8.0 Hz, 2H), 7.40 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 4.0 Hz, 4H), 7.17 (m, 1H), 2.32 (s, 3H), 1.84 (m, 1H), 0.85 (t, J = 4.0 Hz, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.56, 147.11, 139.96, 133.62, 129.23, 128.93, 128.12, 127.68, 125.69, 125.16, 101.48, 12.88, 8.12, 7.76; HRMS: calcd for $\text{C}_{19}\text{H}_{19}\text{N}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 355.0713, found 355.0717.



3,5-diethyl-1-phenyl-4-(phenylselanyl)-1H-pyrazole (4aca)^[1]: (62%). ^1H NMR (400 MHz, CDCl_3) δ 7.52-7.50 (m, 4H), 7.44 (d, J = 8.0 Hz, 1H), 7.29-7.23 (m, 4H), 7.17 (t, J = 8.0 Hz, 1H), 2.84-2.80 (m, 2H), 2.75 (t, J = 8.0 Hz, 2H), 1.26 (t, J = 8.0 Hz, 3H), 1.03 (t, J = 8.0 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.38, 149.87, 140.04, 133.72, 129.24, 129.11, 128.17, 128.07, 125.65, 125.45, 100.33, 20.93, 19.25, 14.01, 13.82.

4. References

- [1] D. H. Oliveira, T. B. Aquino, J. E. R. Nascimento, G. Perin, R. G. Jacob, D. Alves, *Adv. Synth. Catal.*, **2015**, 357, 4041–4049.
- [2] R. G. Jacob, D. H. de Oliveira, T. J. Peglow, J. E. R. Nascimento, R. H. Bartz, *J. Braz. Chem. Soc.*, **2019**, 30, 2144-2152.
- [3] J. F. Souza, T. F. B. de Aquino, J. E. R. Nascimento, R. G. Jacob, A. R. Fajardo, *Catal. Sci. Technol.*, **2020**, 10, 3918-3930.
- [4] J. Wang, Y. Liu, J. Yan, *New J. Chem.*, **2018**, 42, 13684-13688.
- [5] Y. Fang, J. Wang, Y. Liu, J. Yan, *Appl Organometal Chem.*, **2019**, 33, 4921-4929.

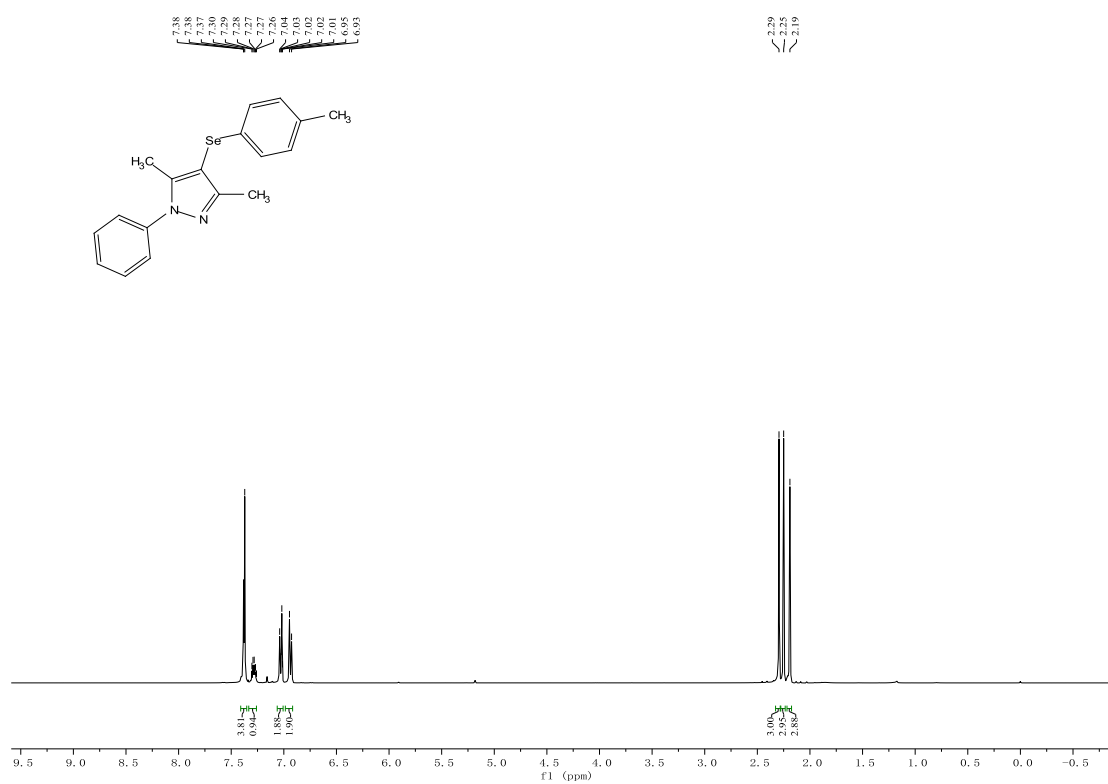
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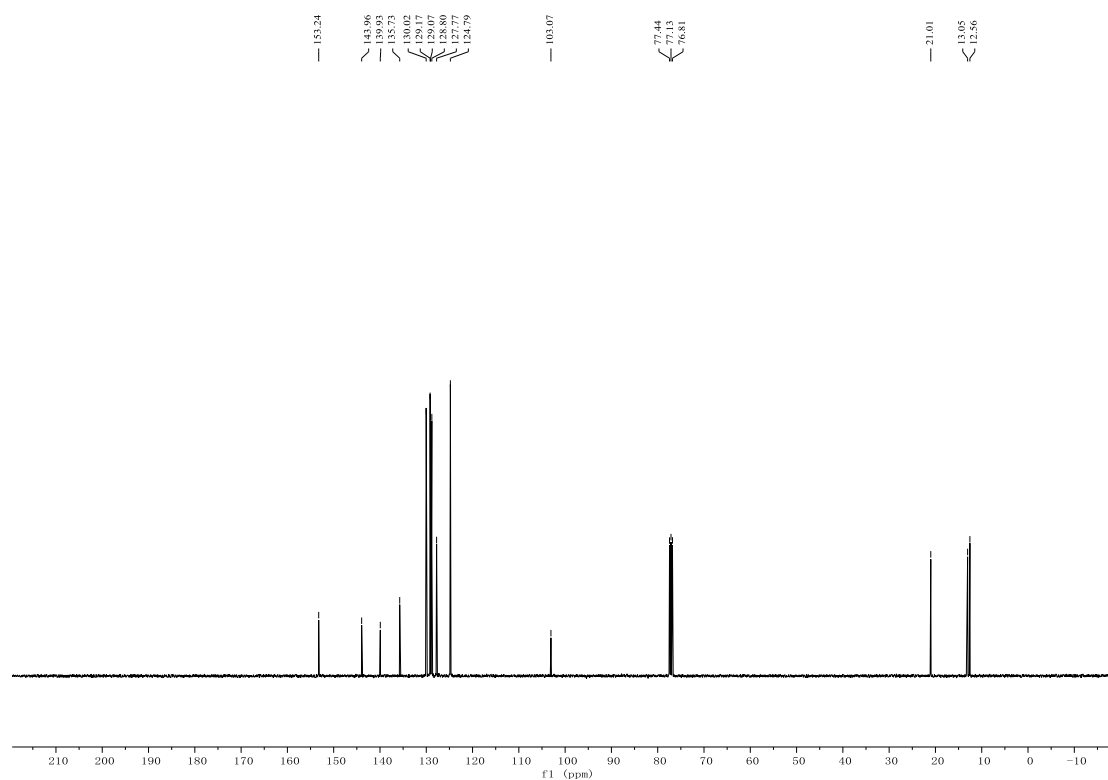
153.32
144.13
138.90
133.02
129.21
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76.80
13.00
12.53

f1 (ppm)

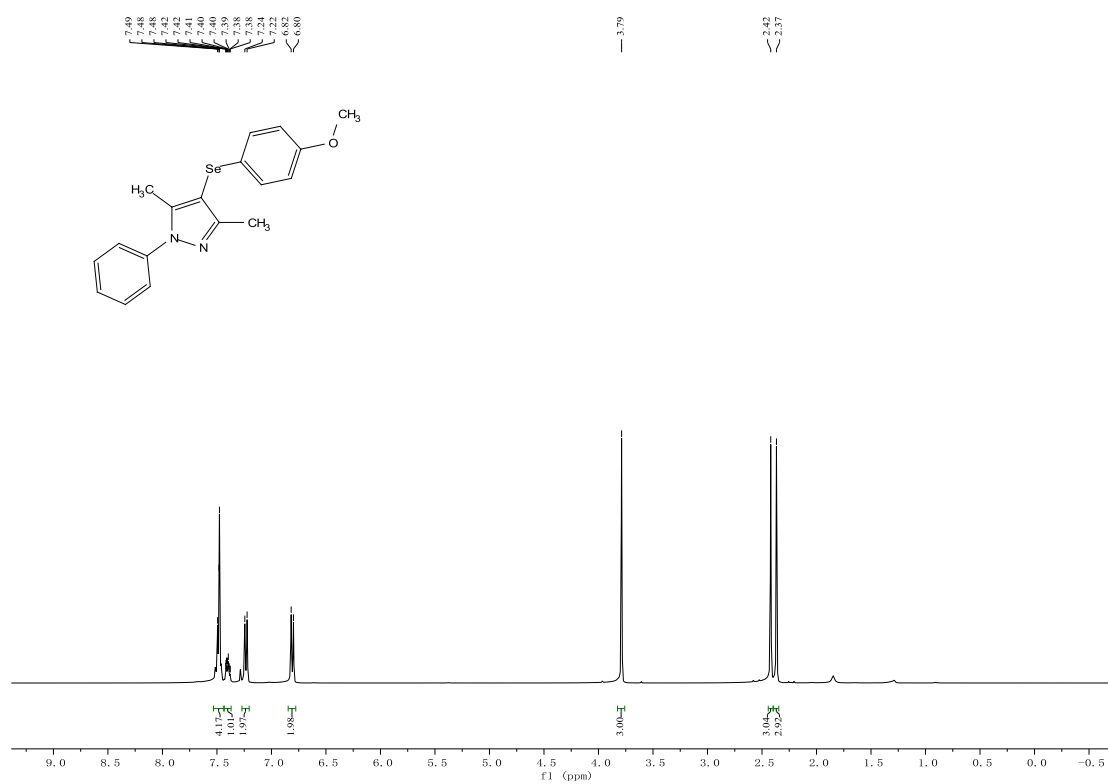
S16



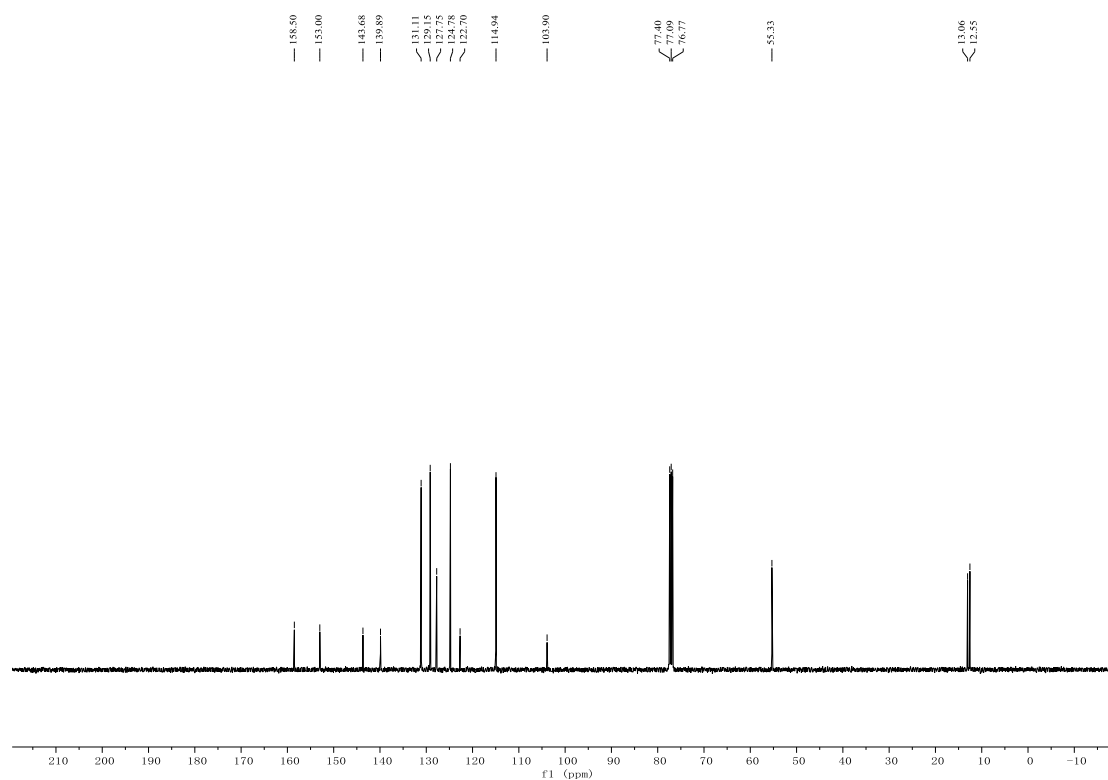
¹H NMR of compound 4aab



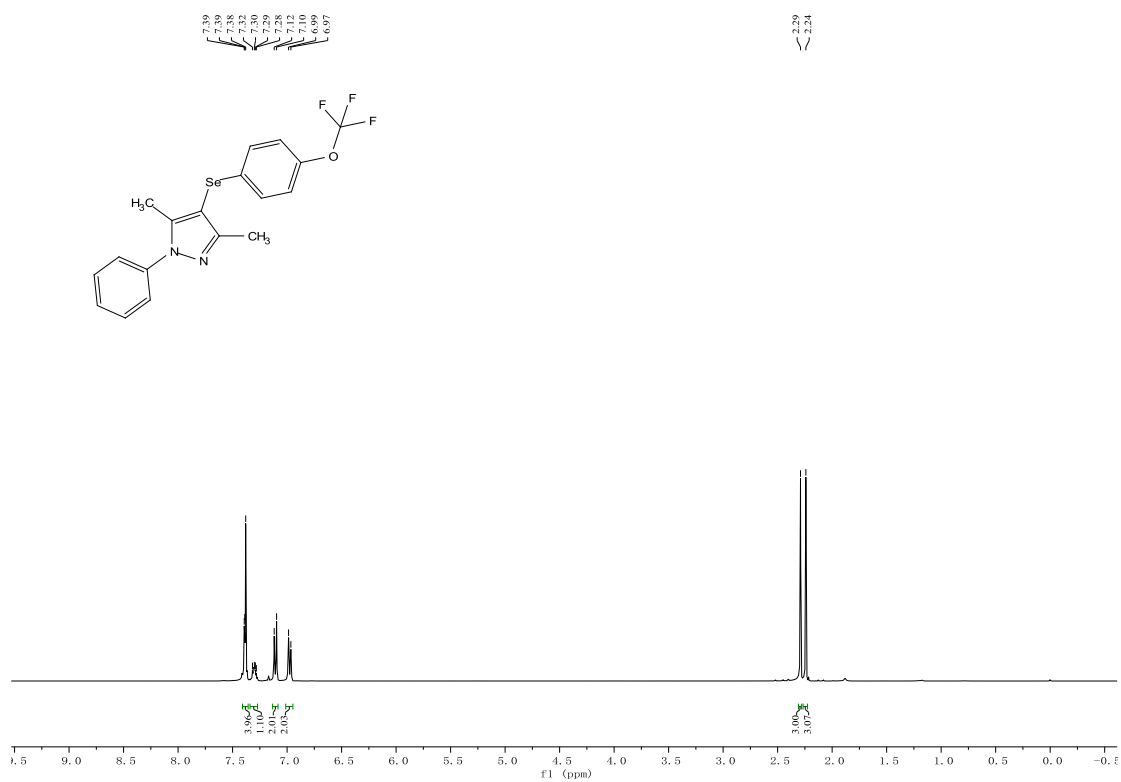
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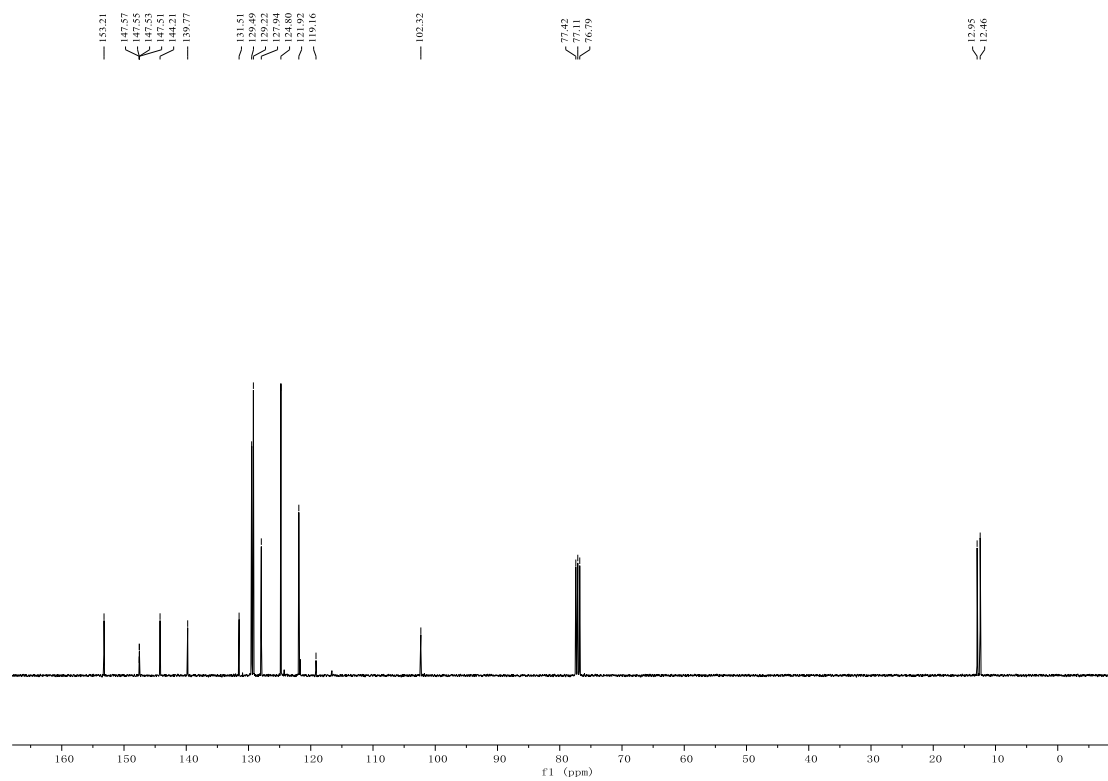
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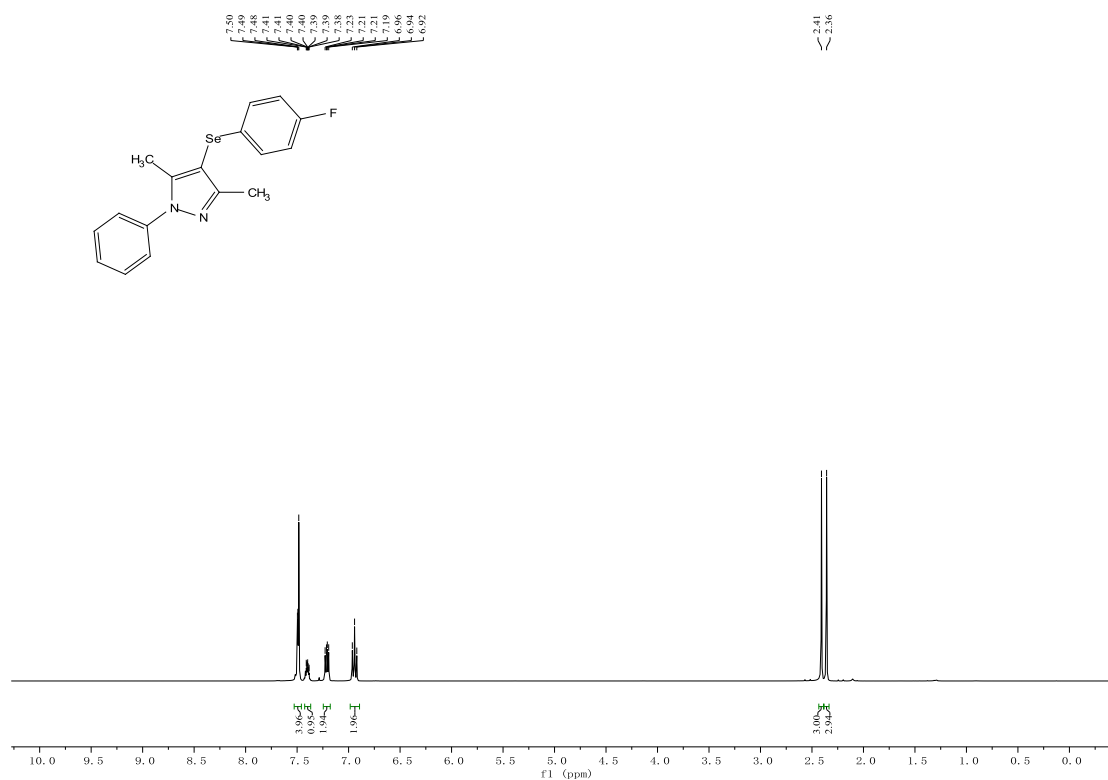
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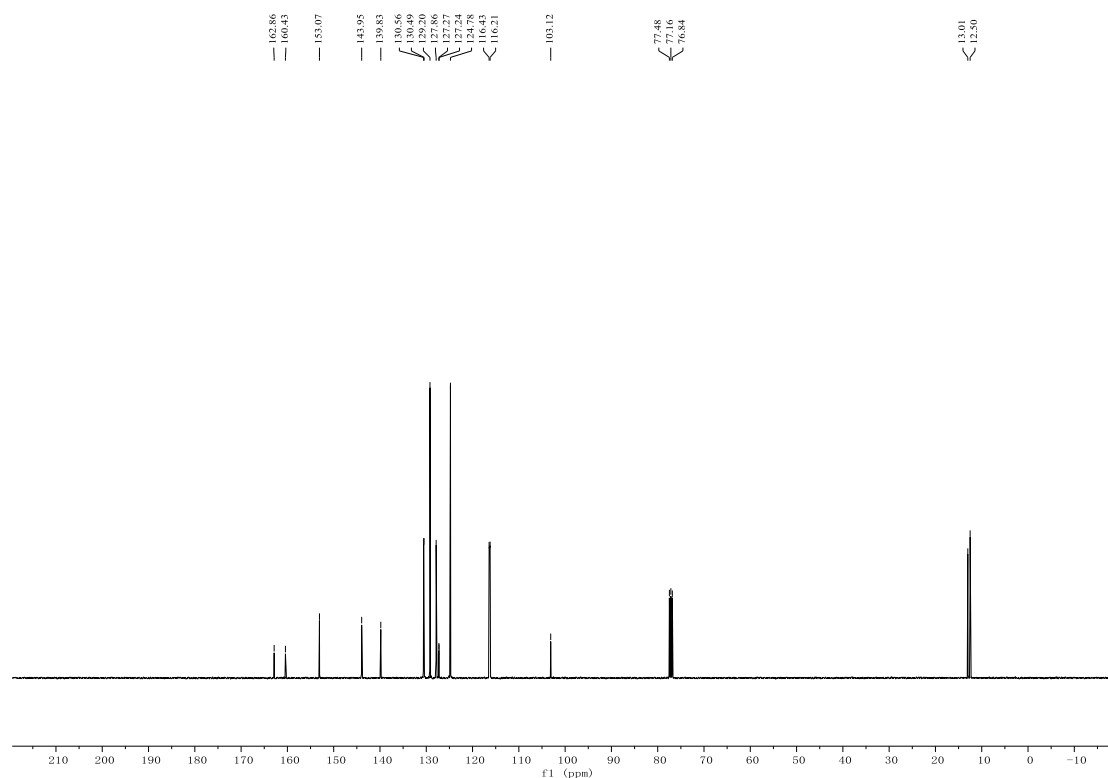
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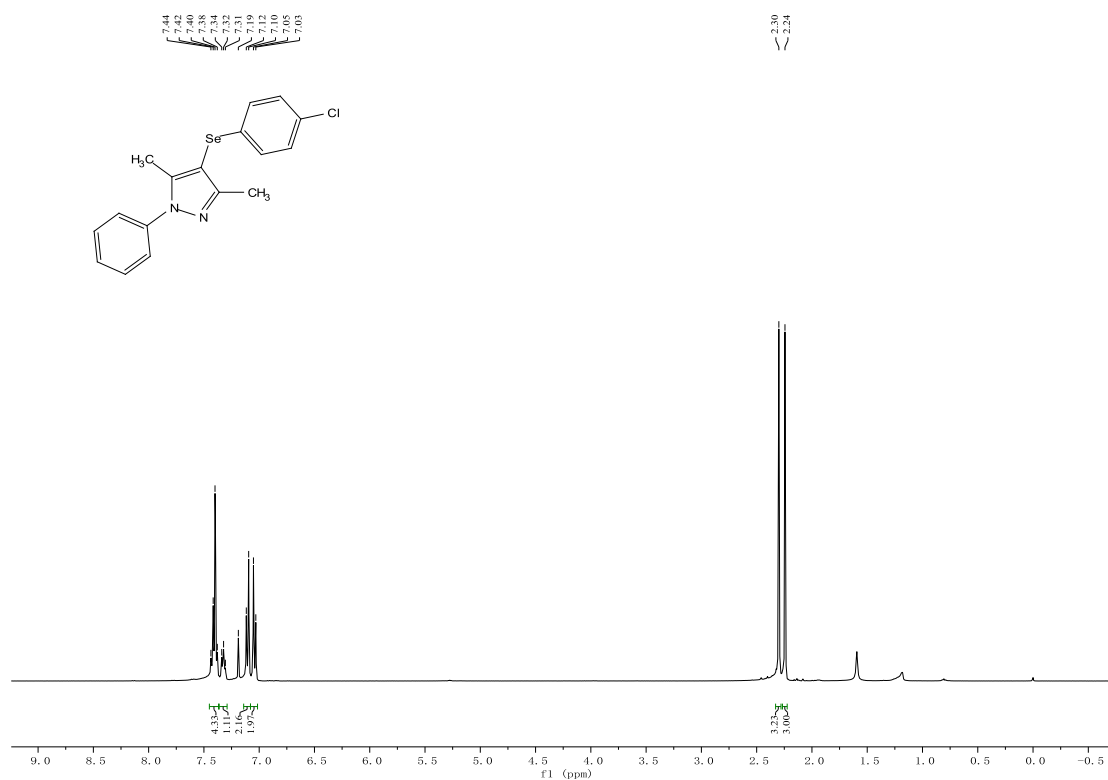
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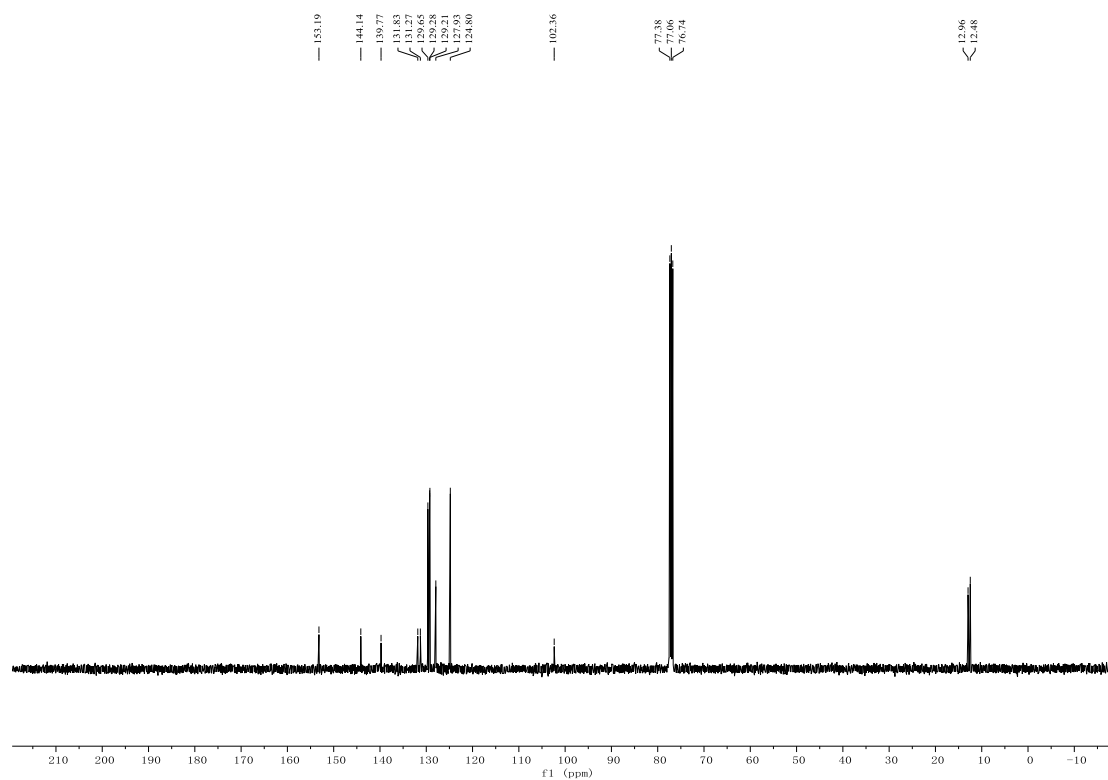
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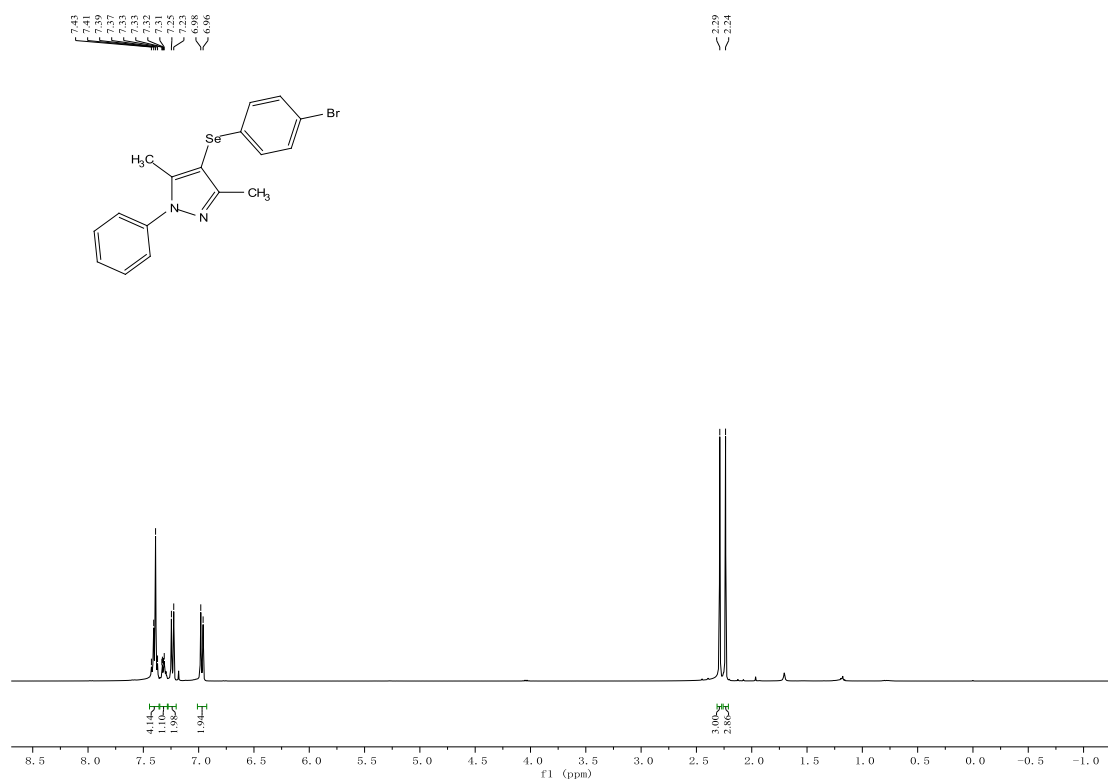
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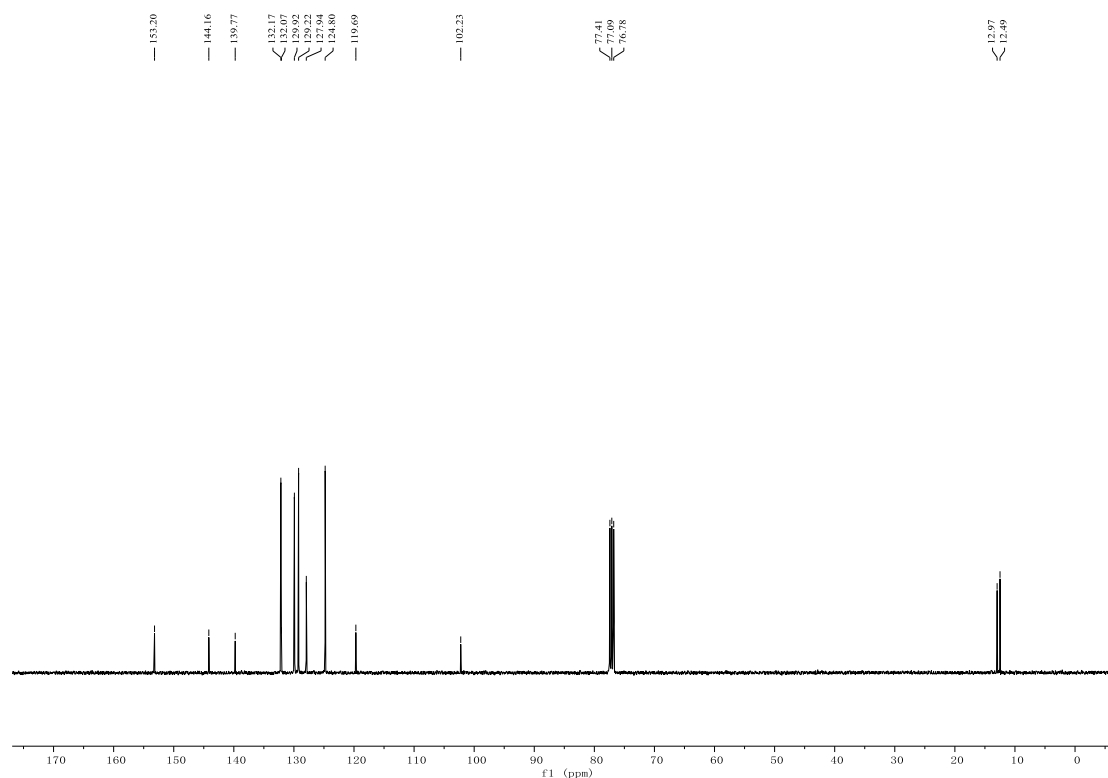
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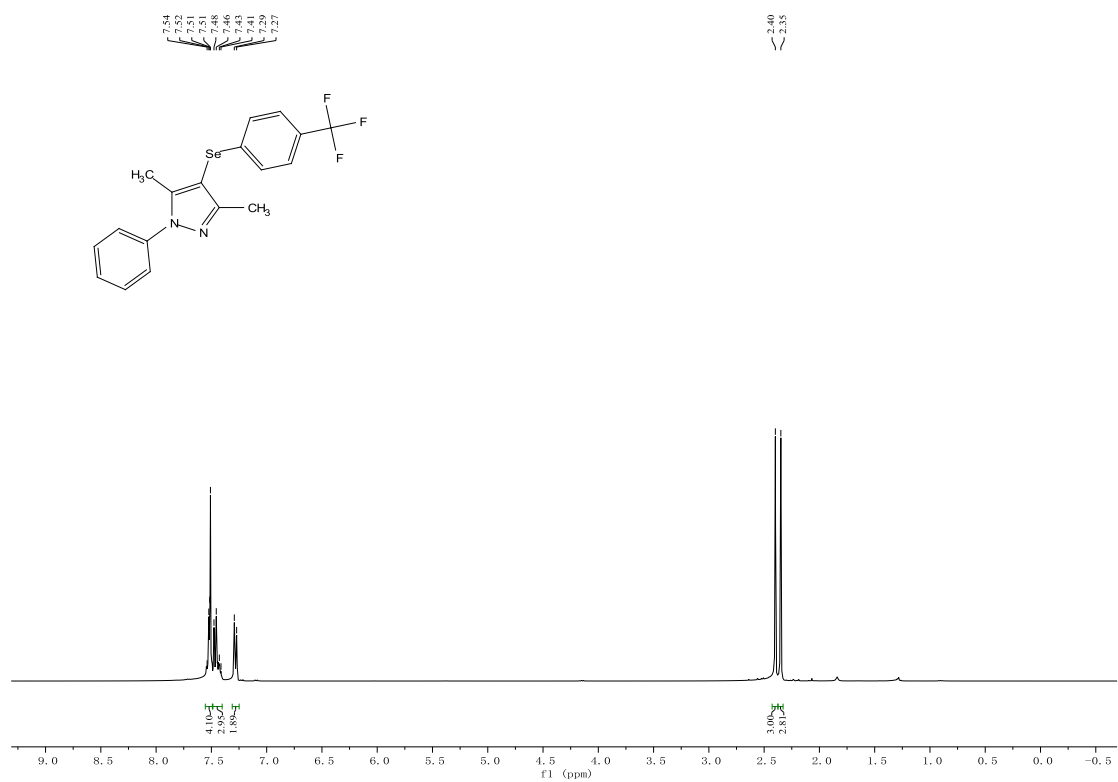
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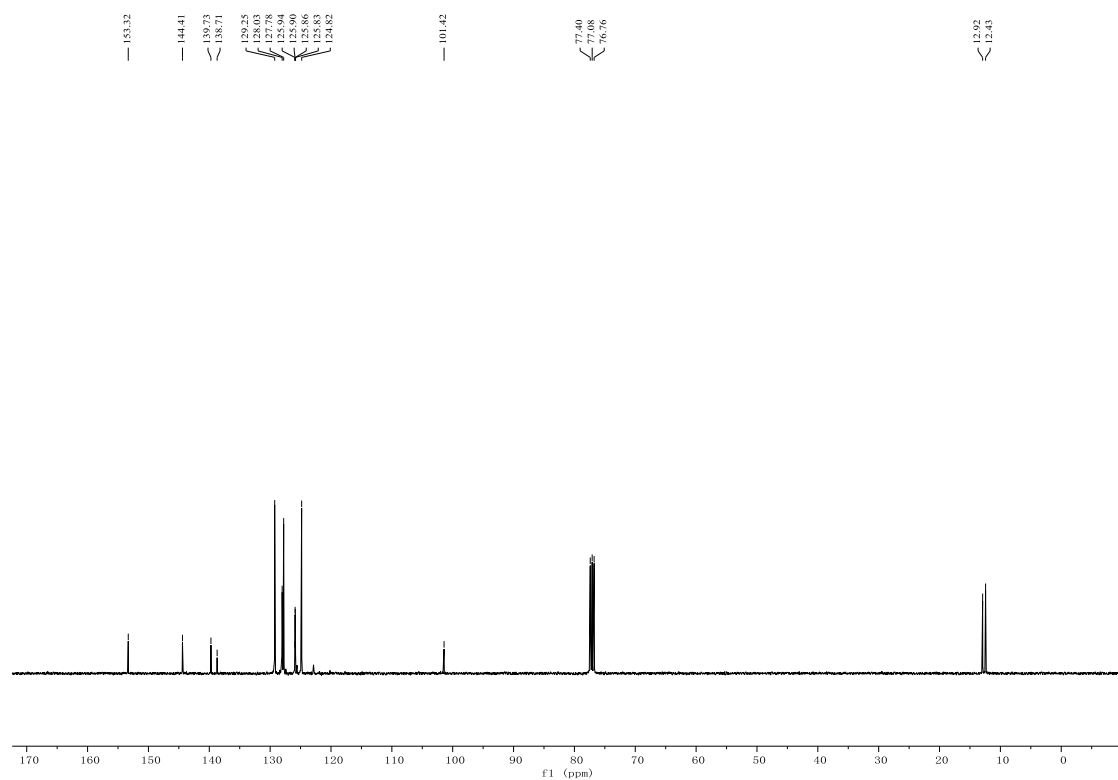
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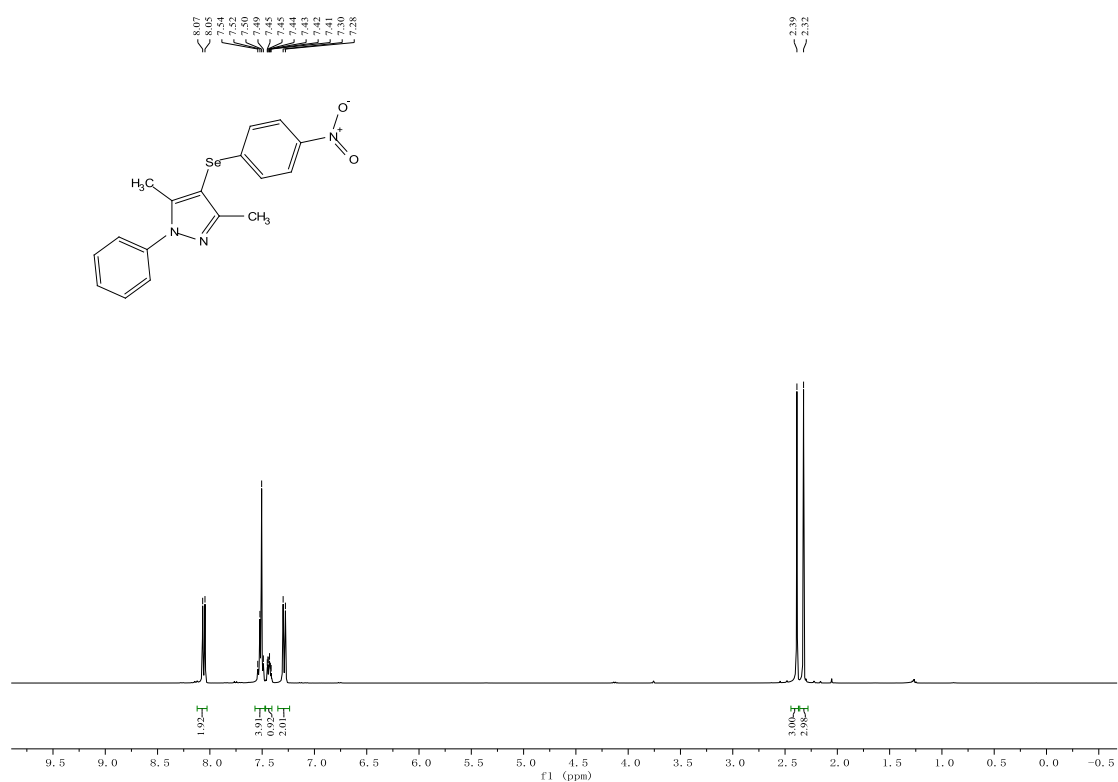
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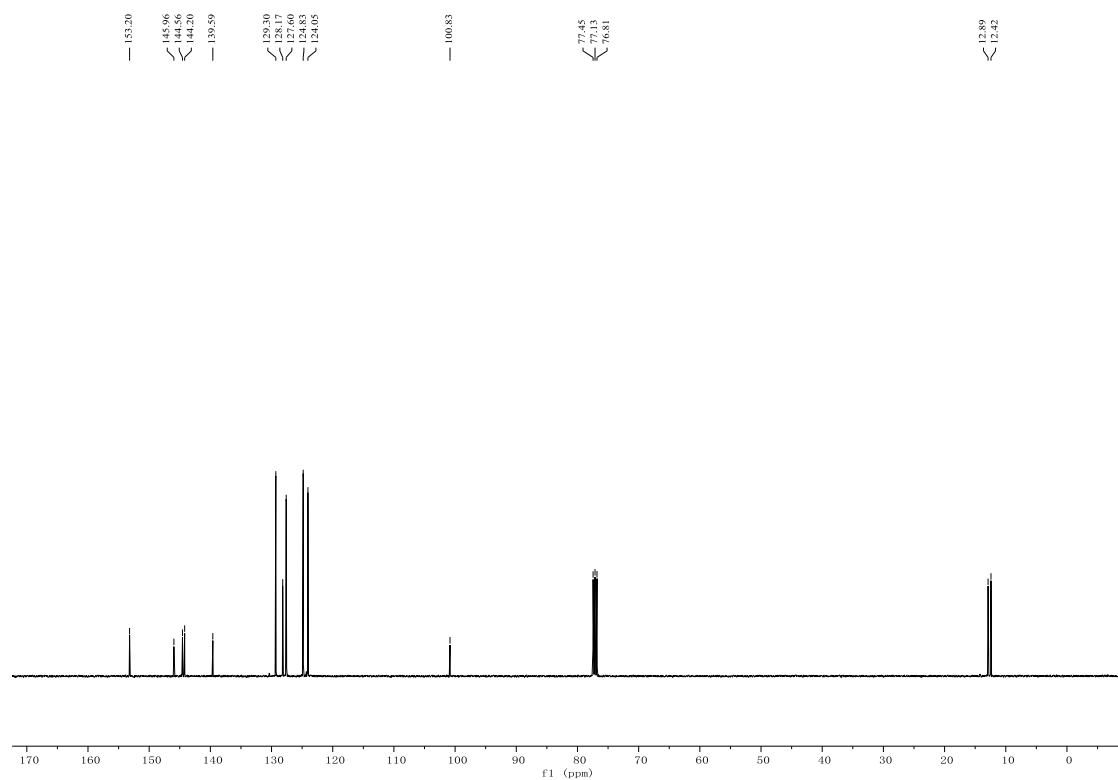
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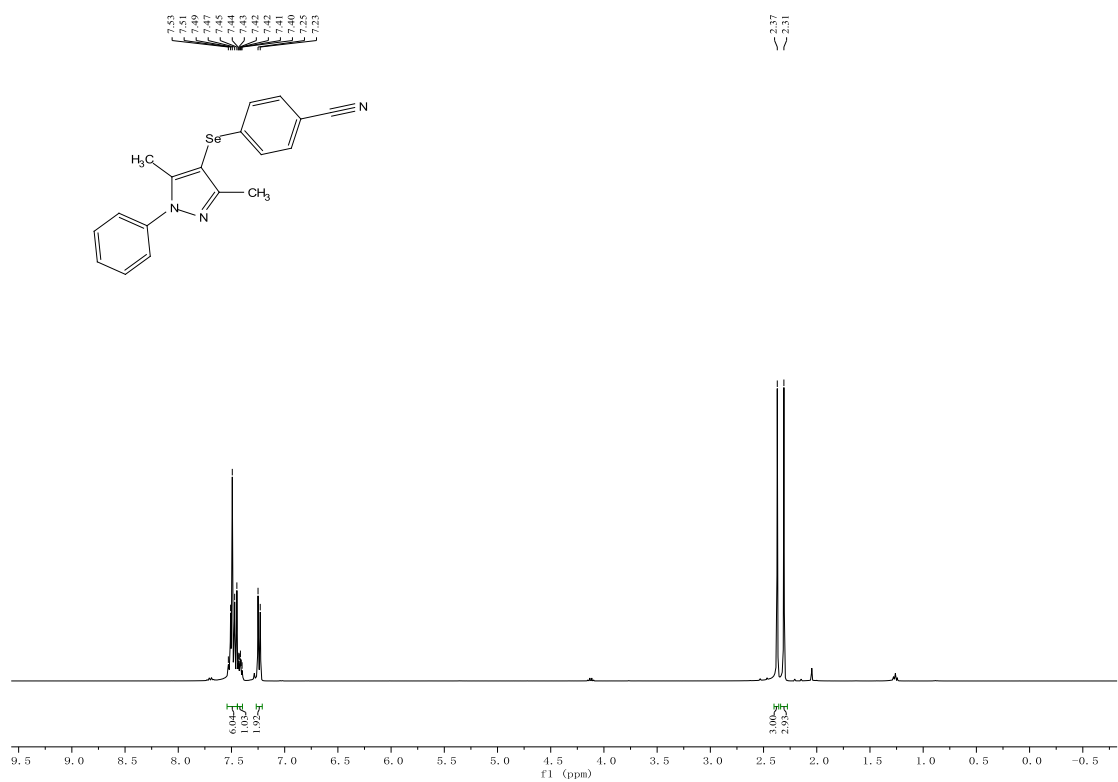
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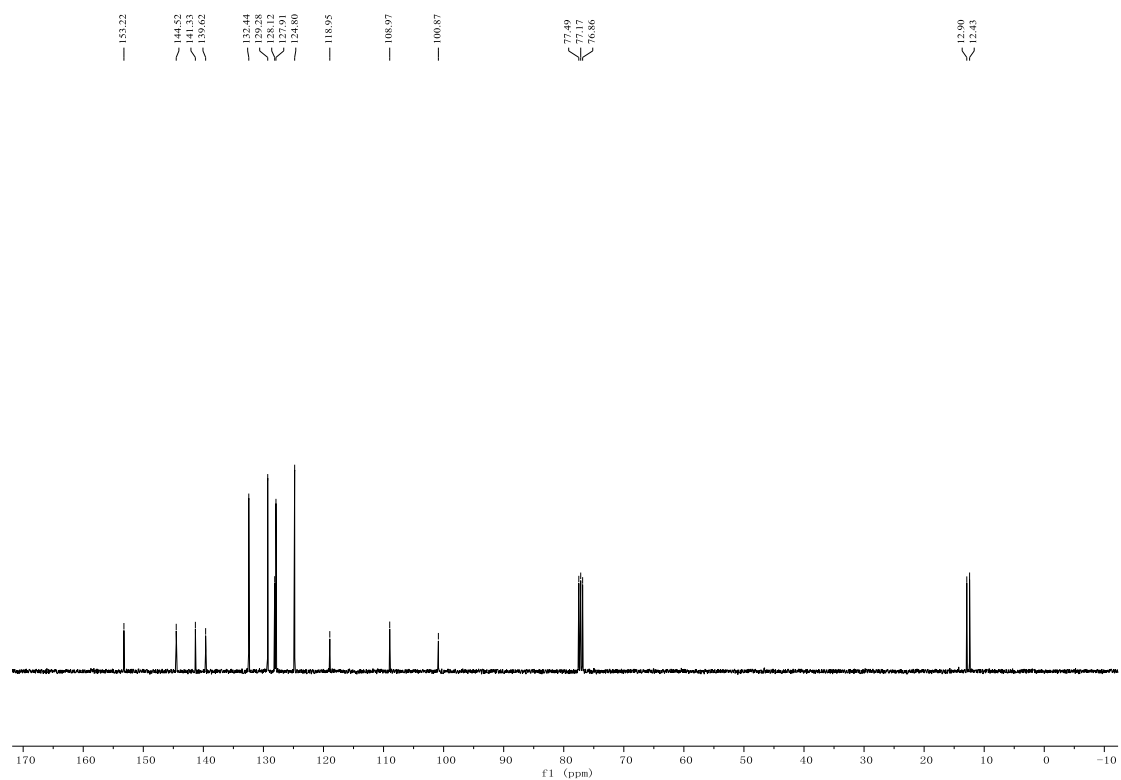
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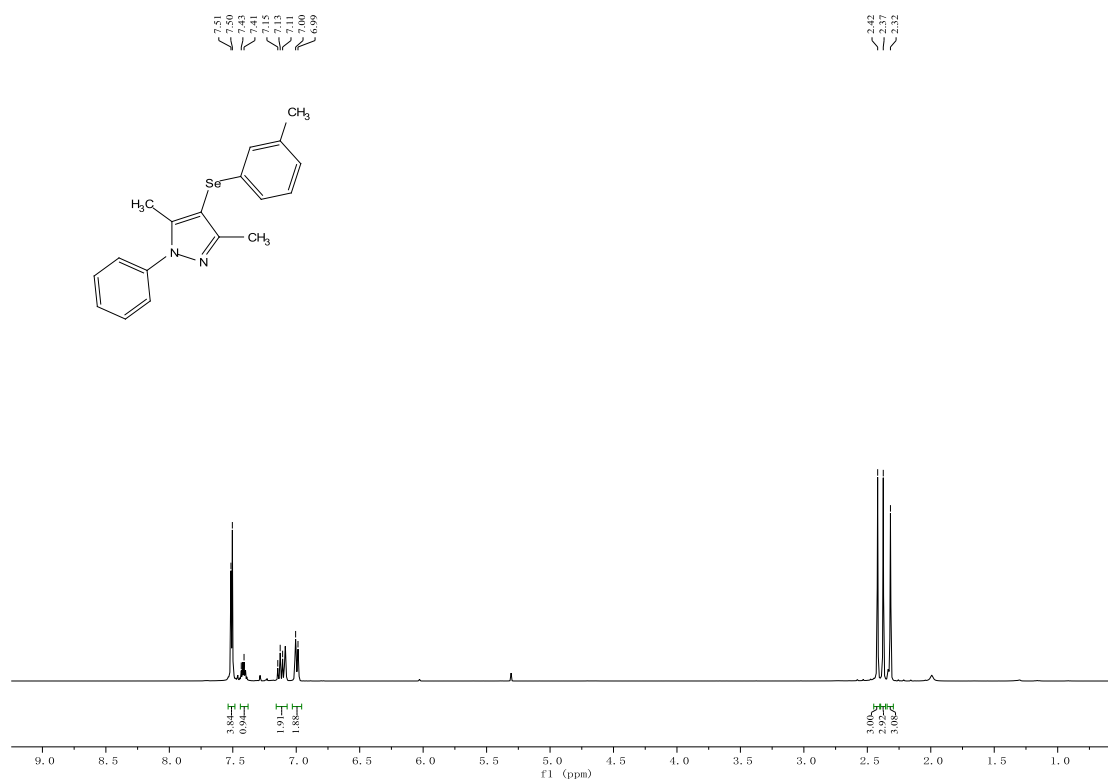
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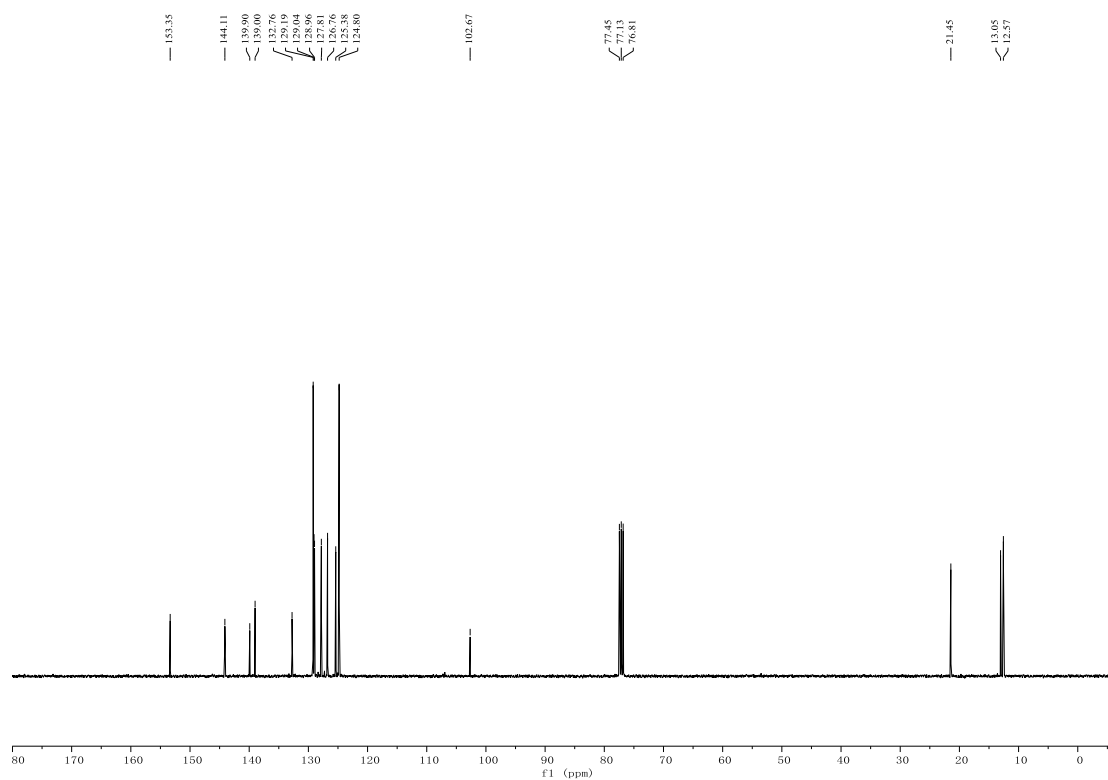
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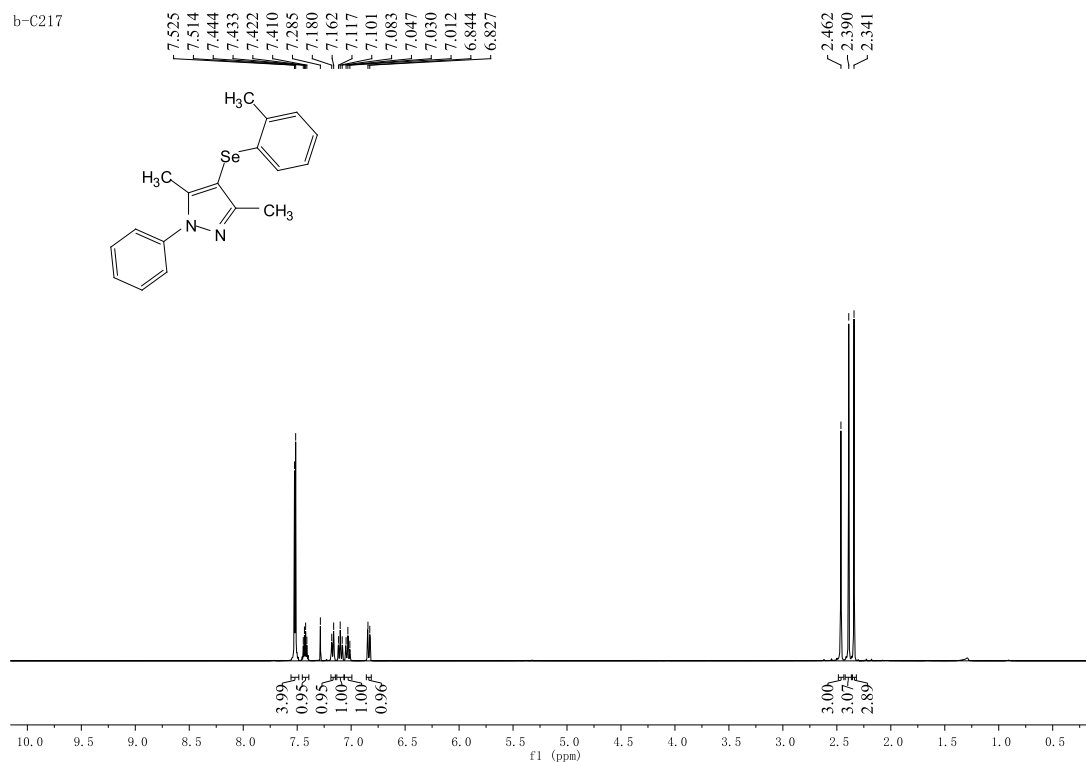
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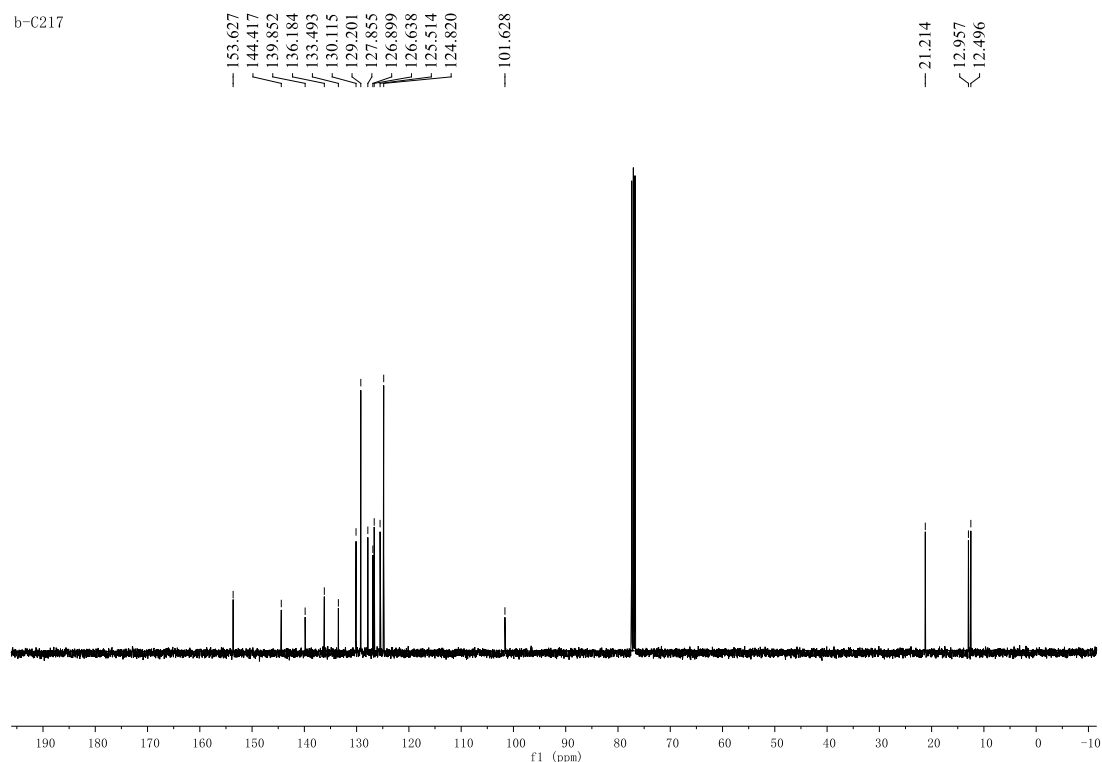
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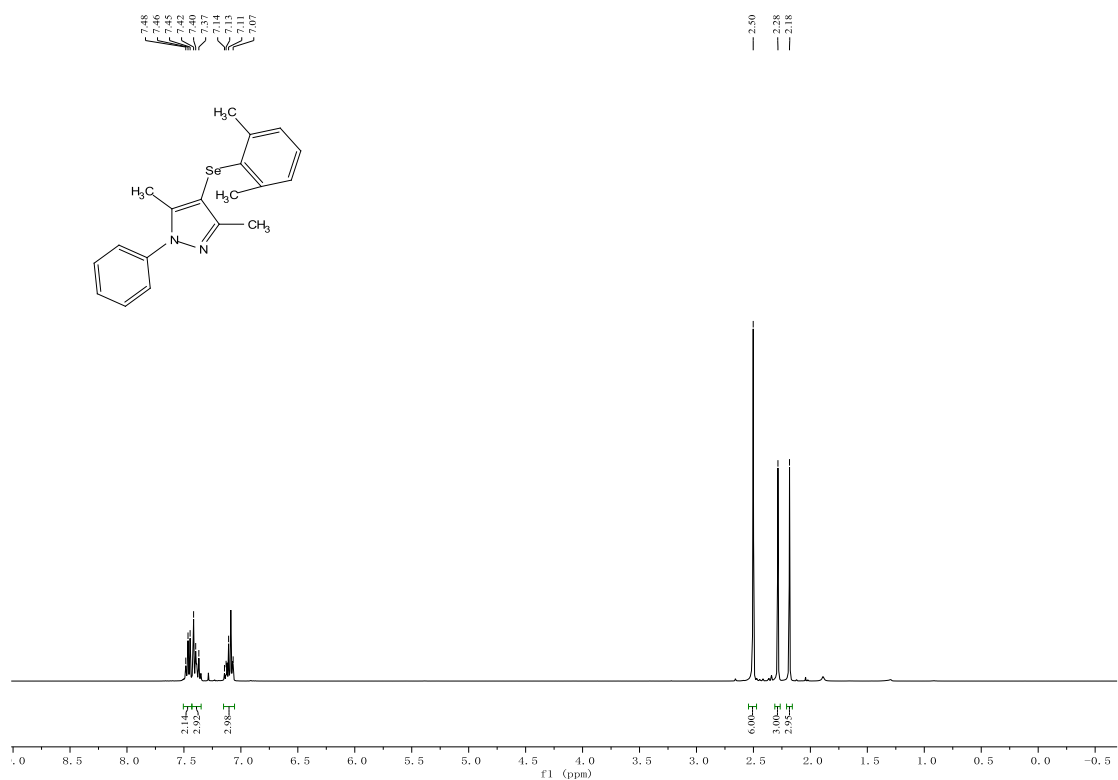
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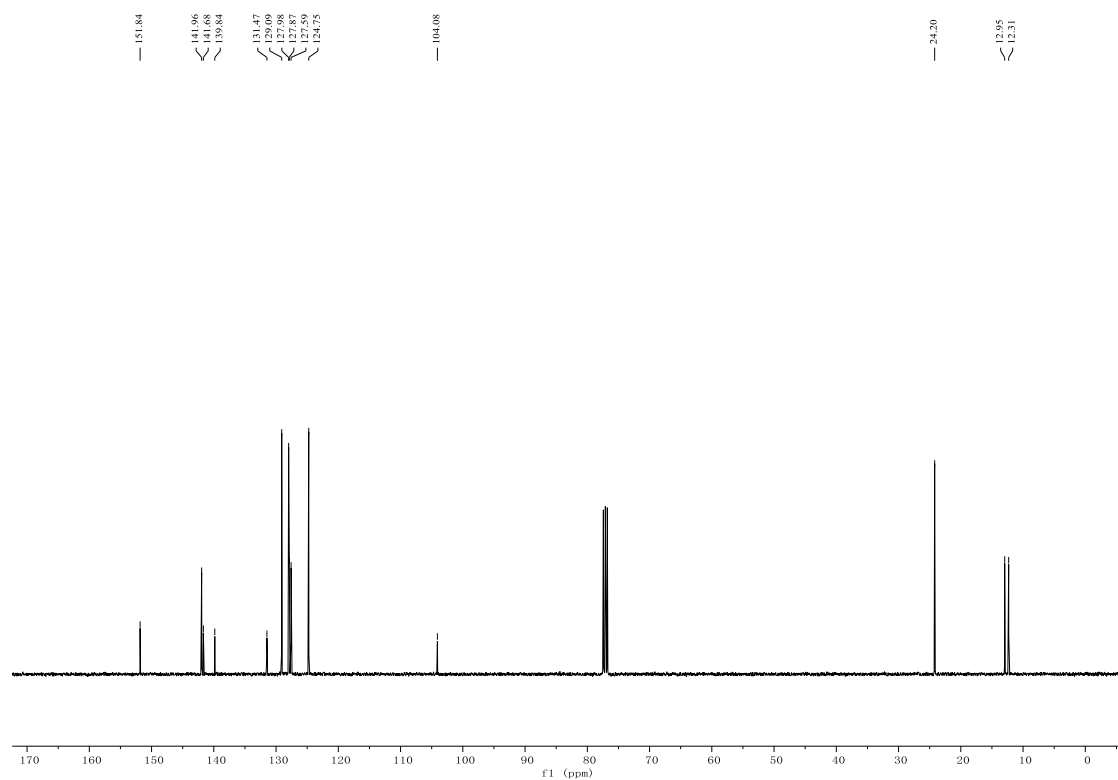
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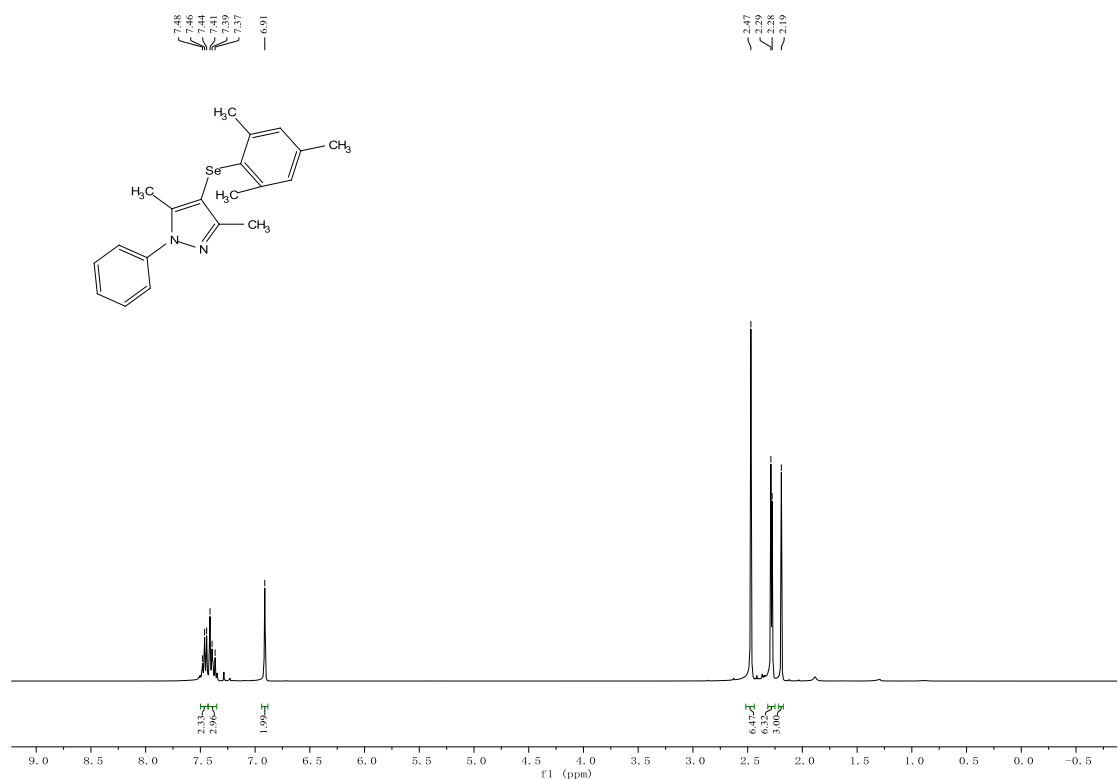
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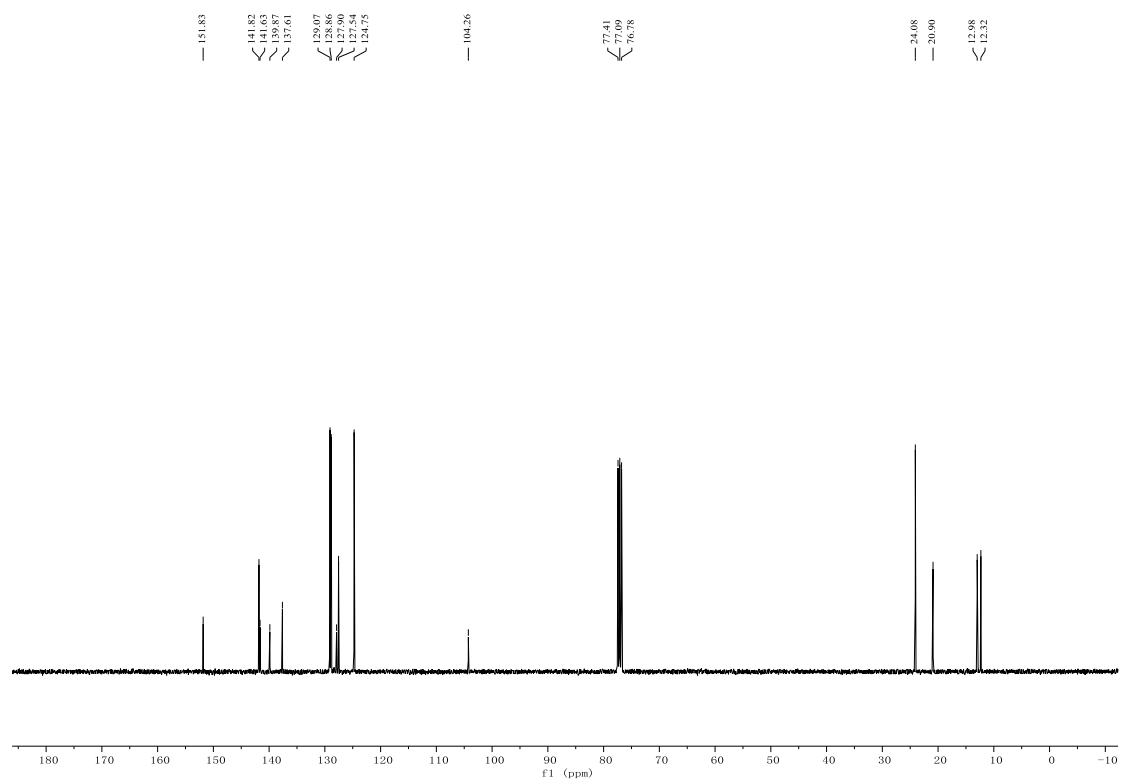
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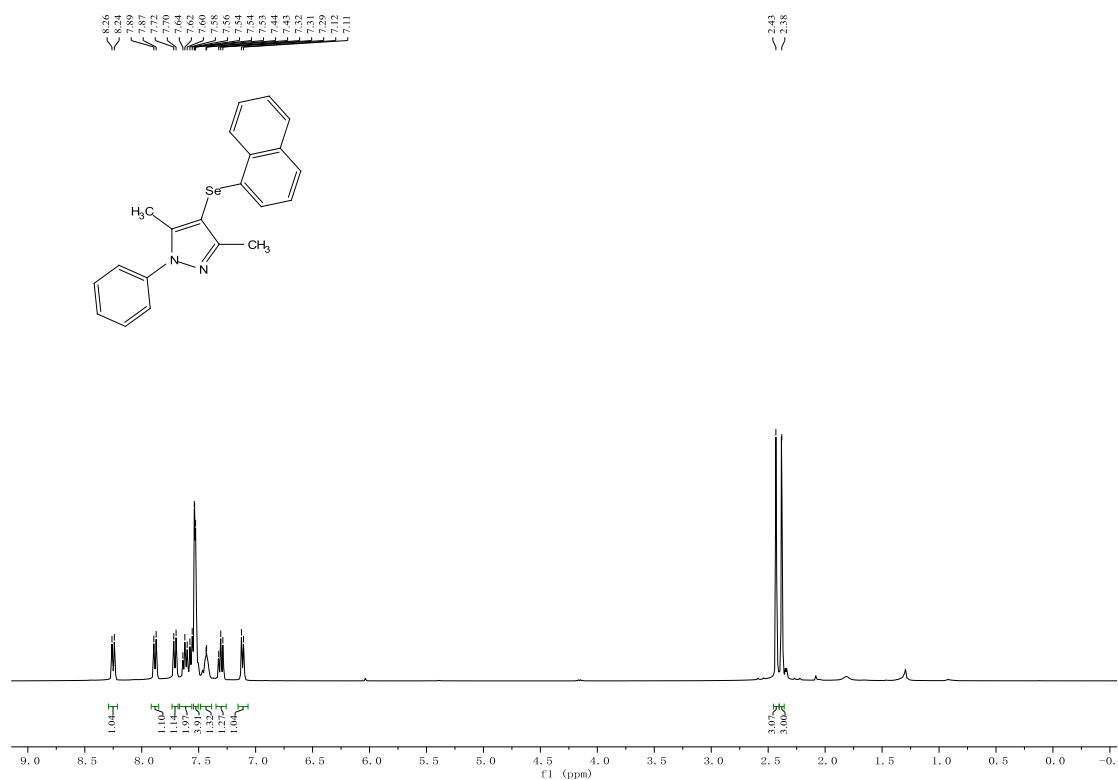
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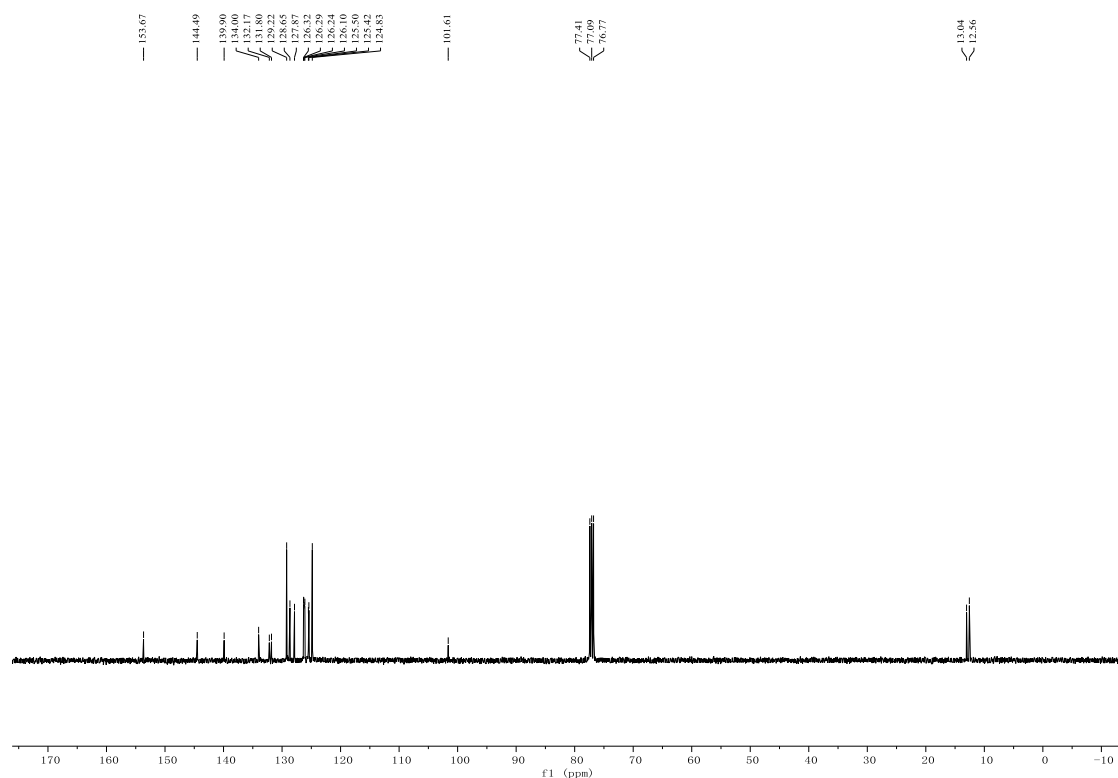
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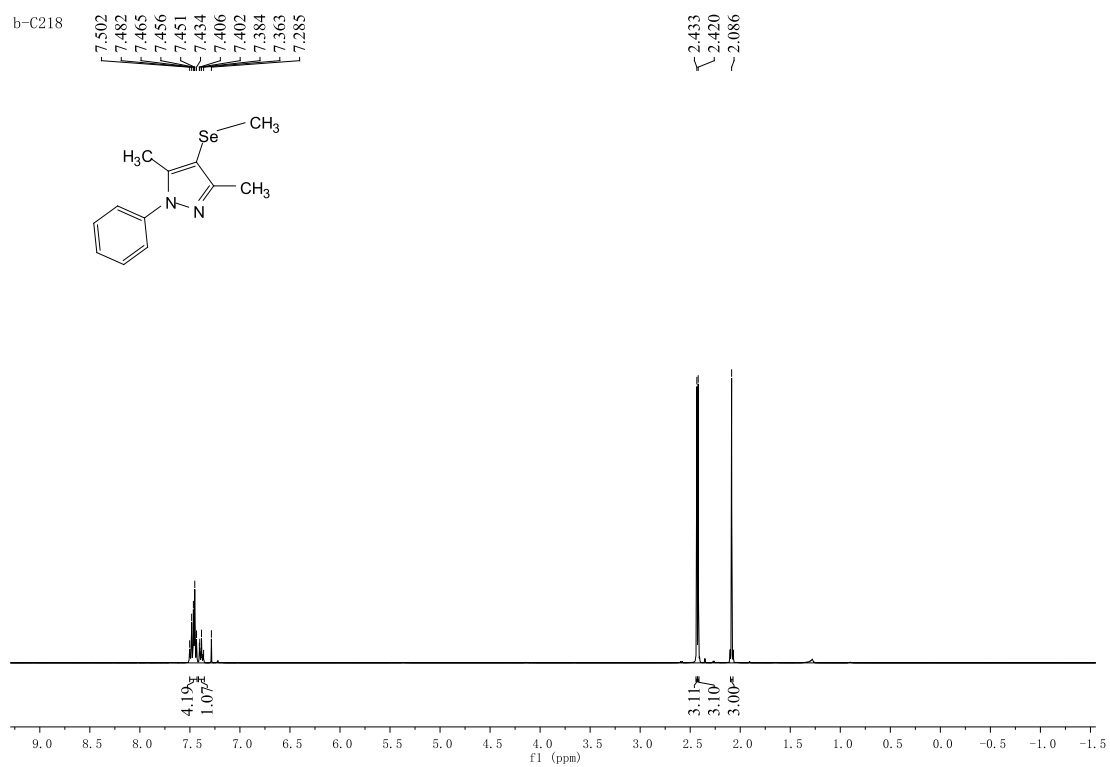
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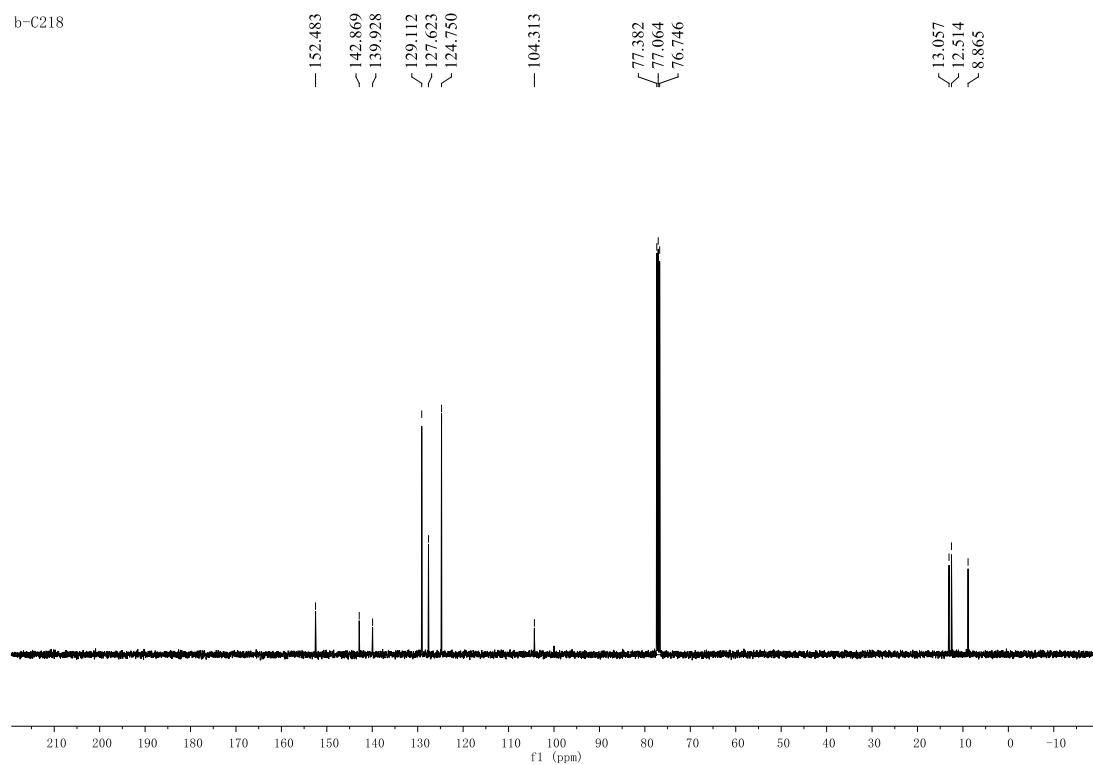
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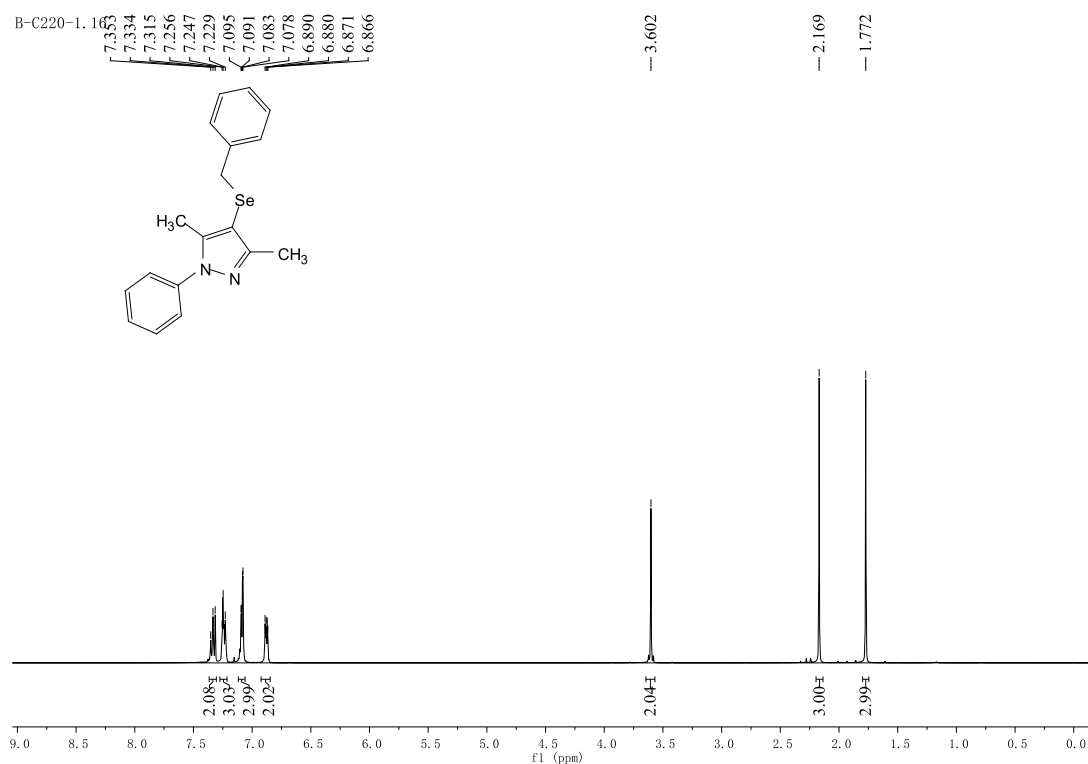
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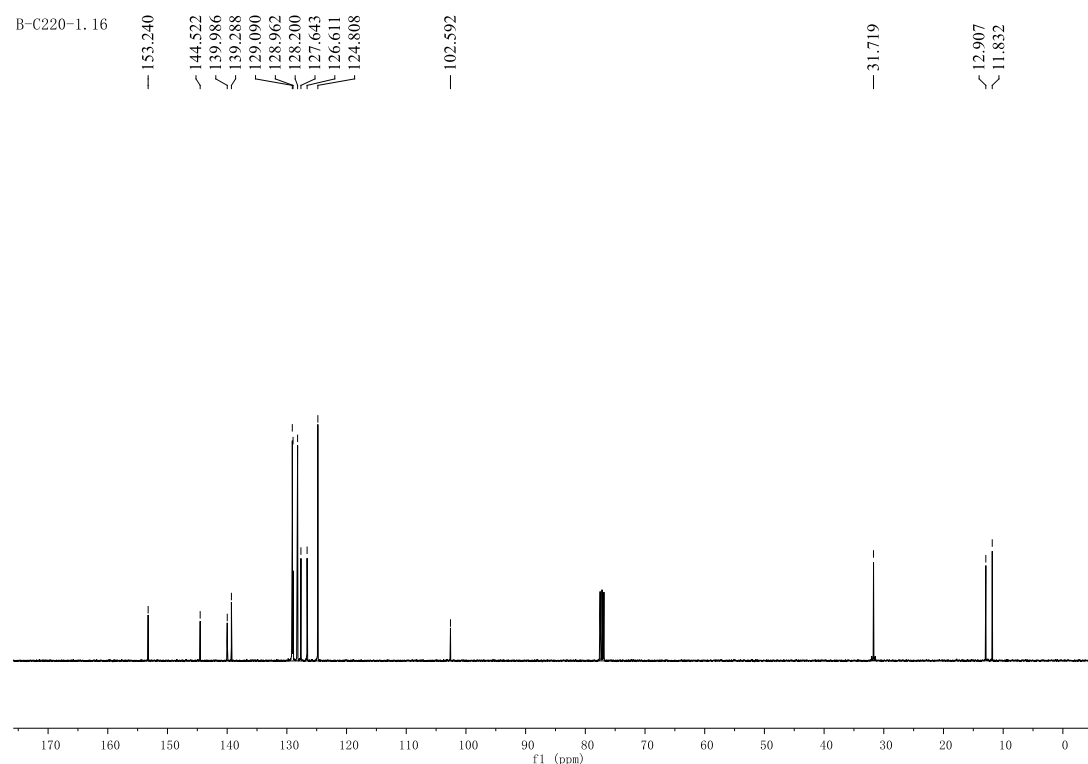
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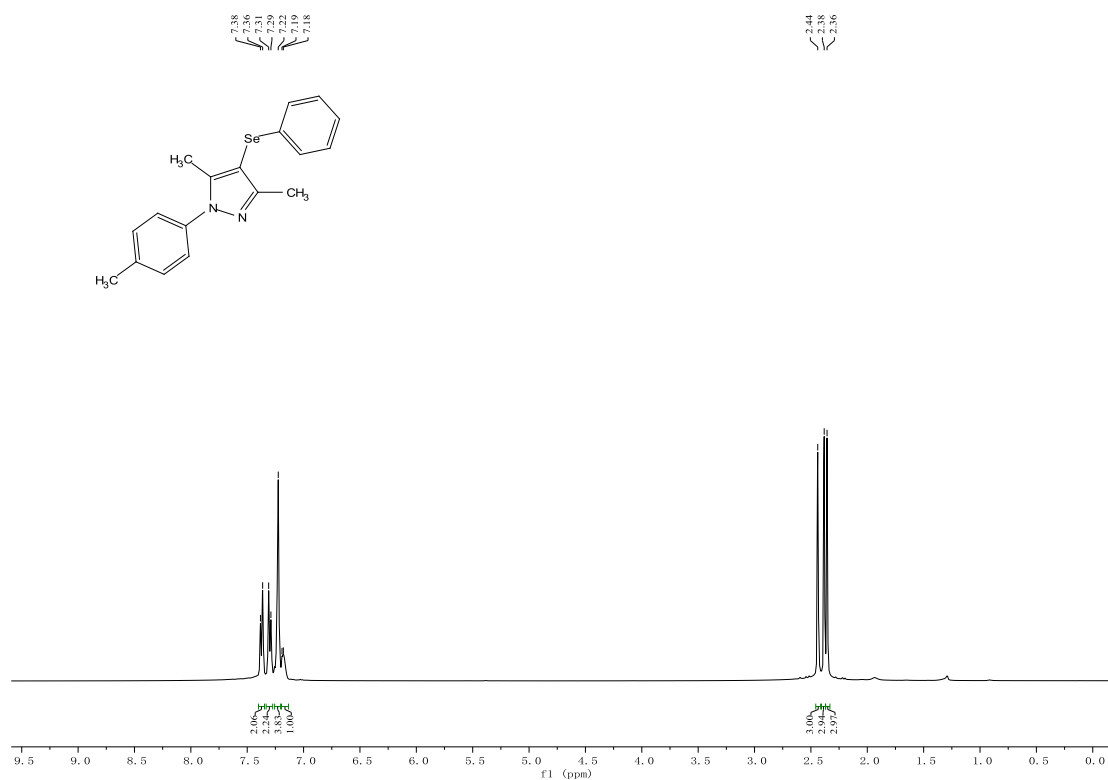
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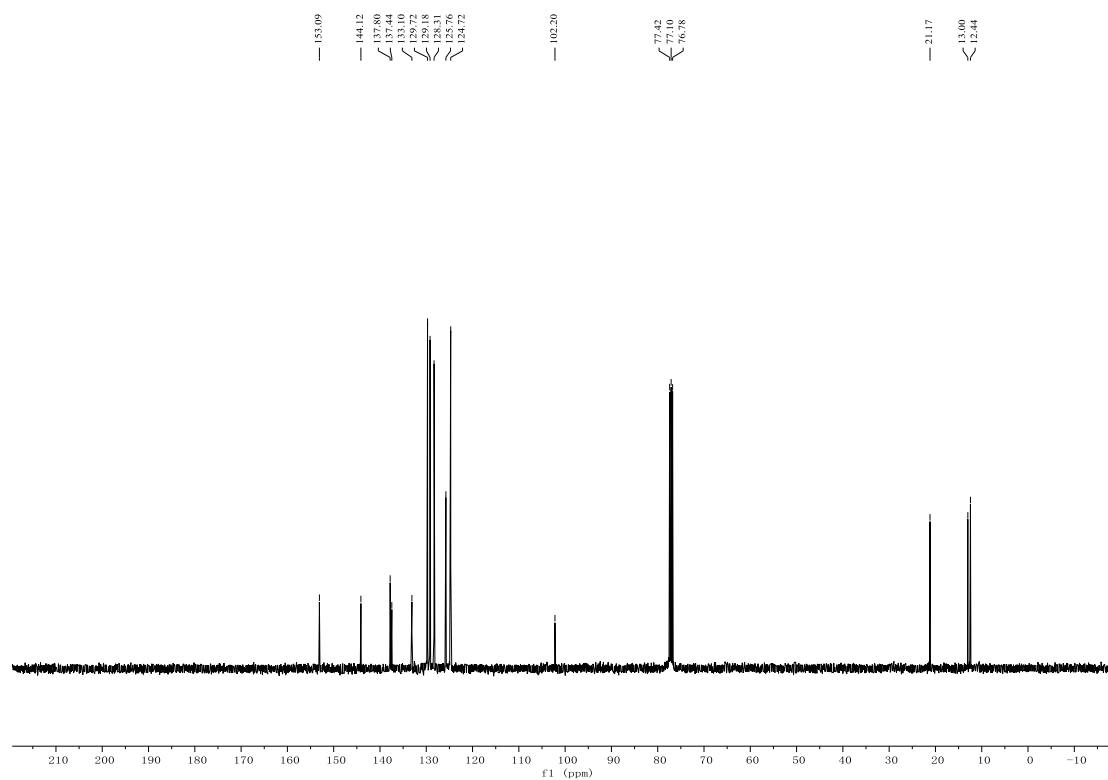
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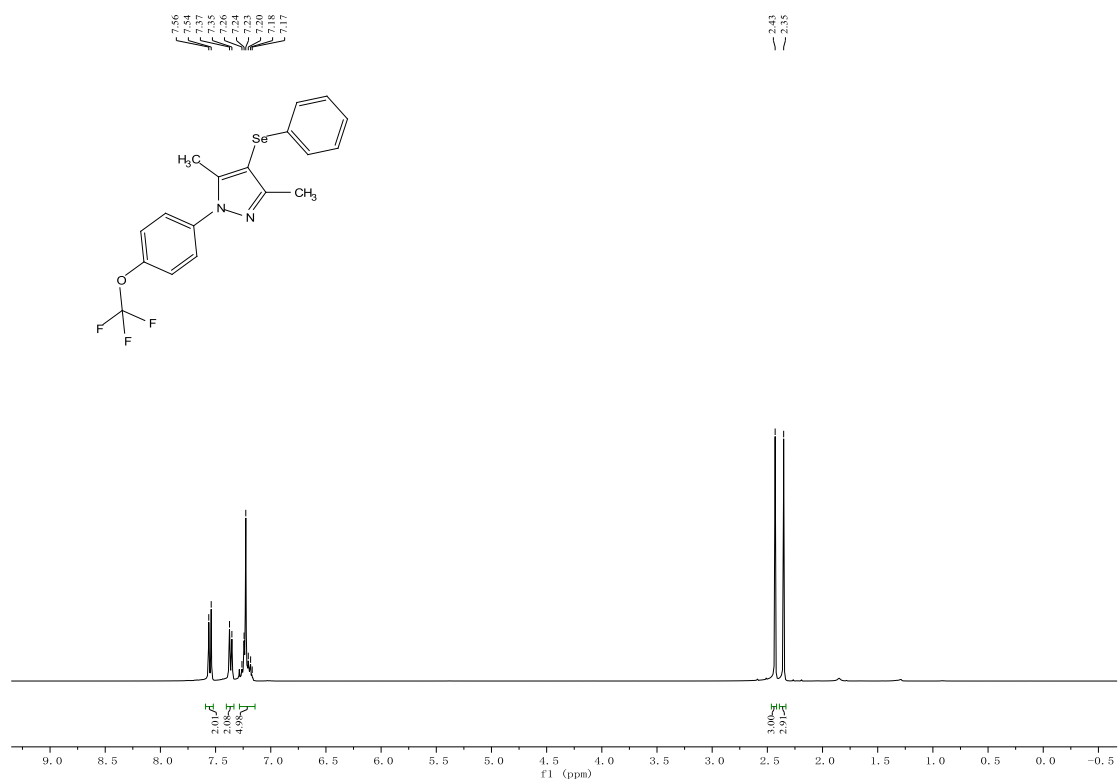
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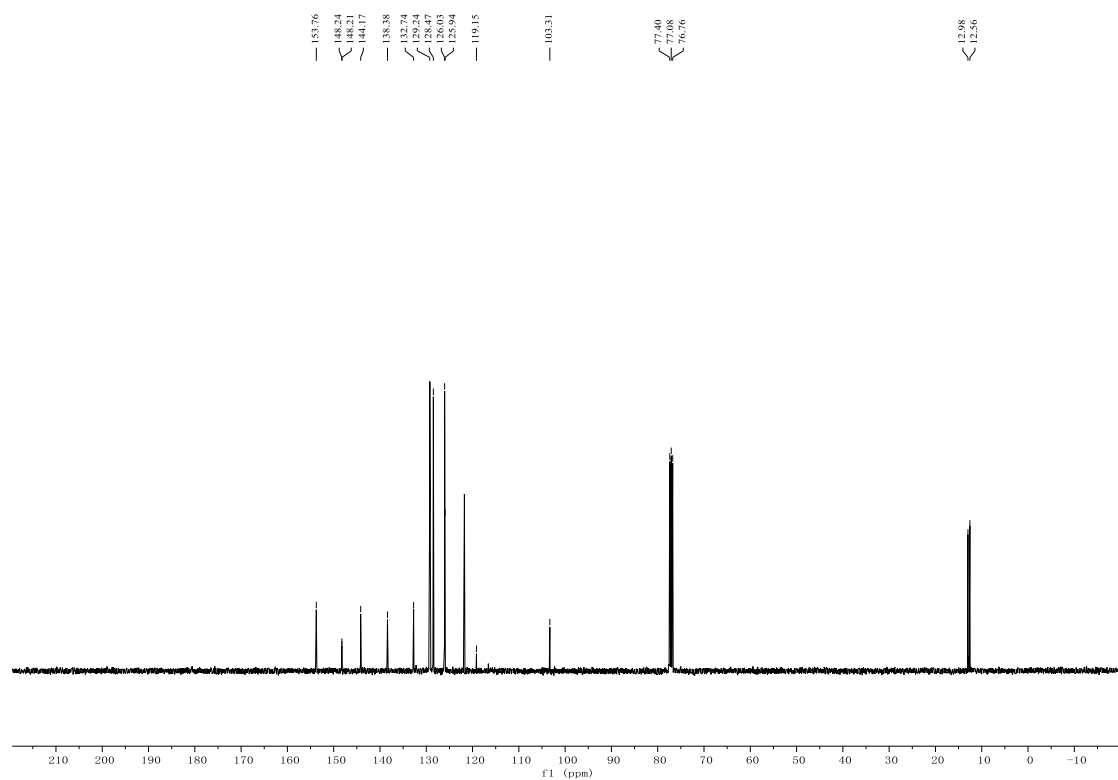
¹H NMR of compound 4baa



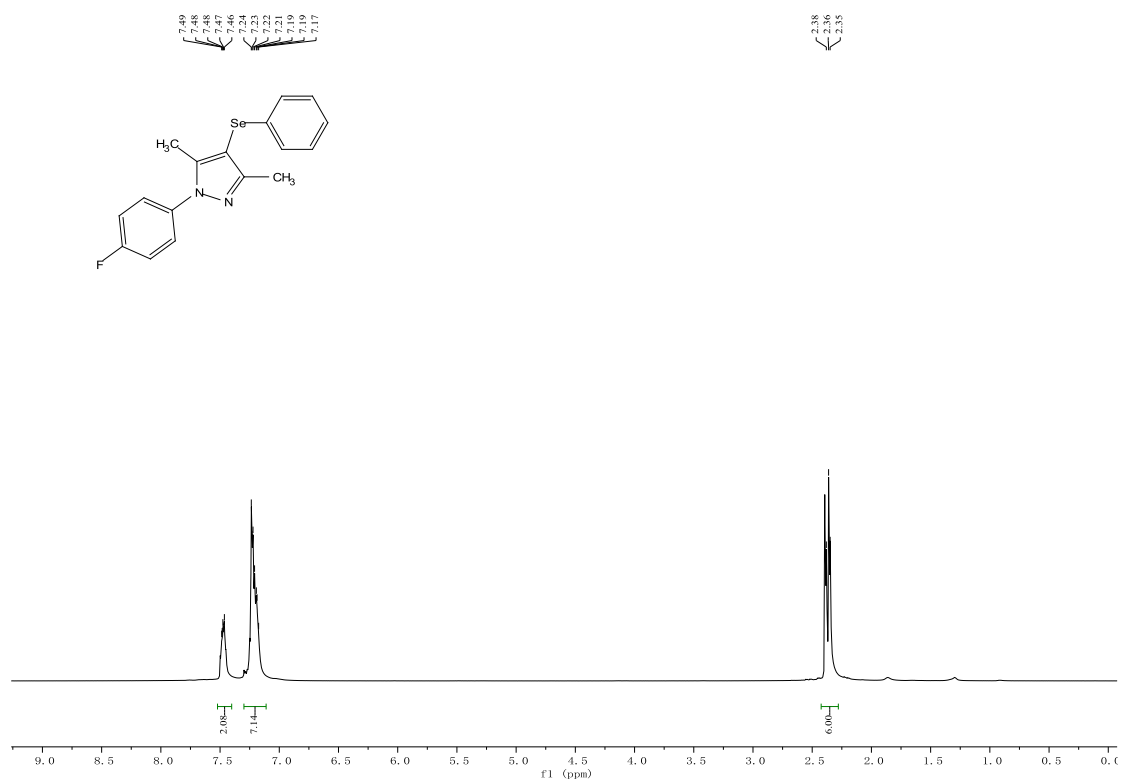
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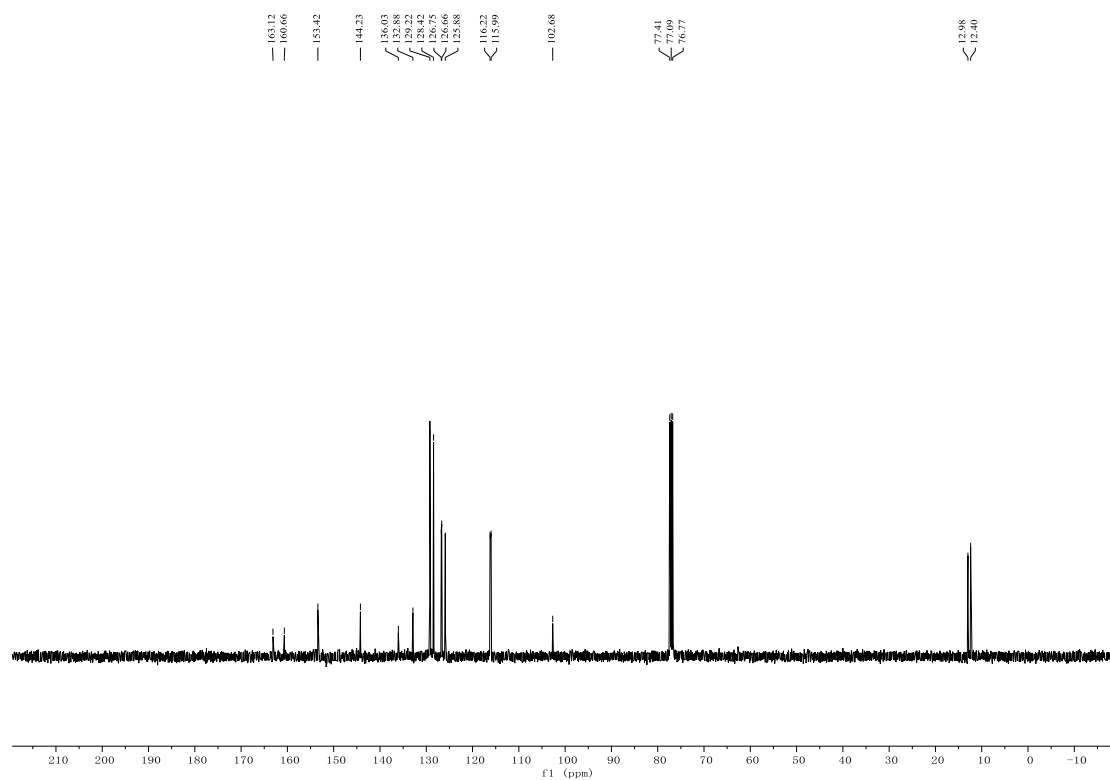
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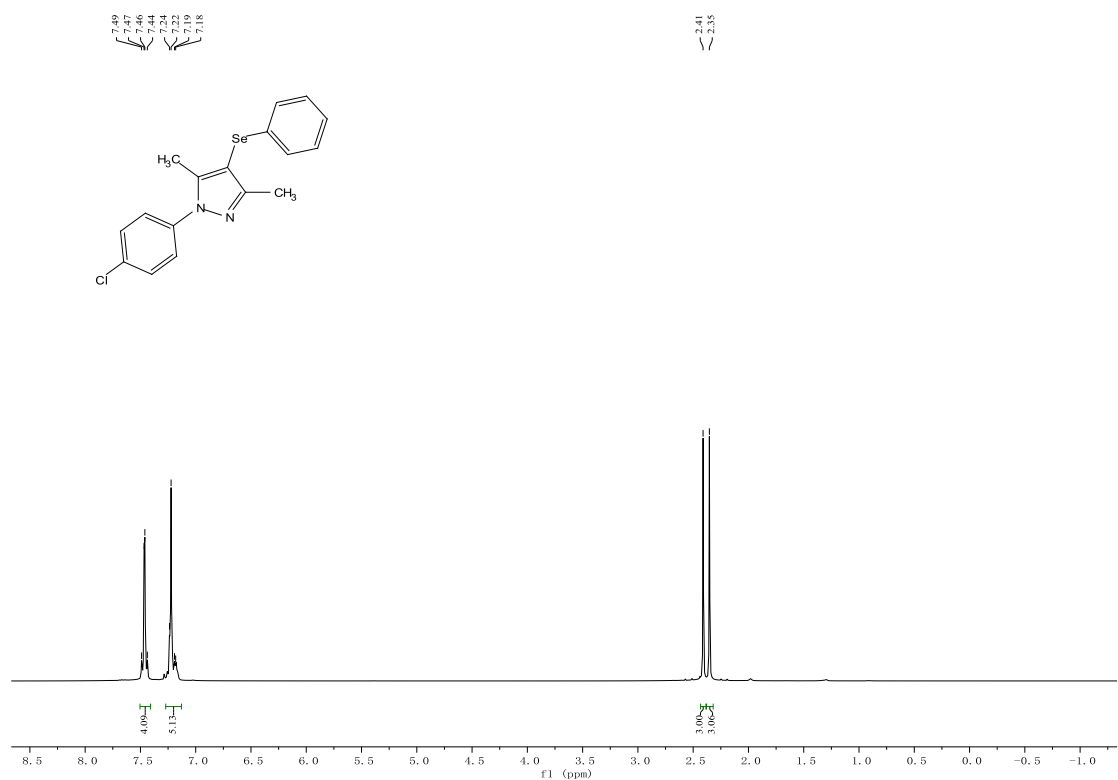
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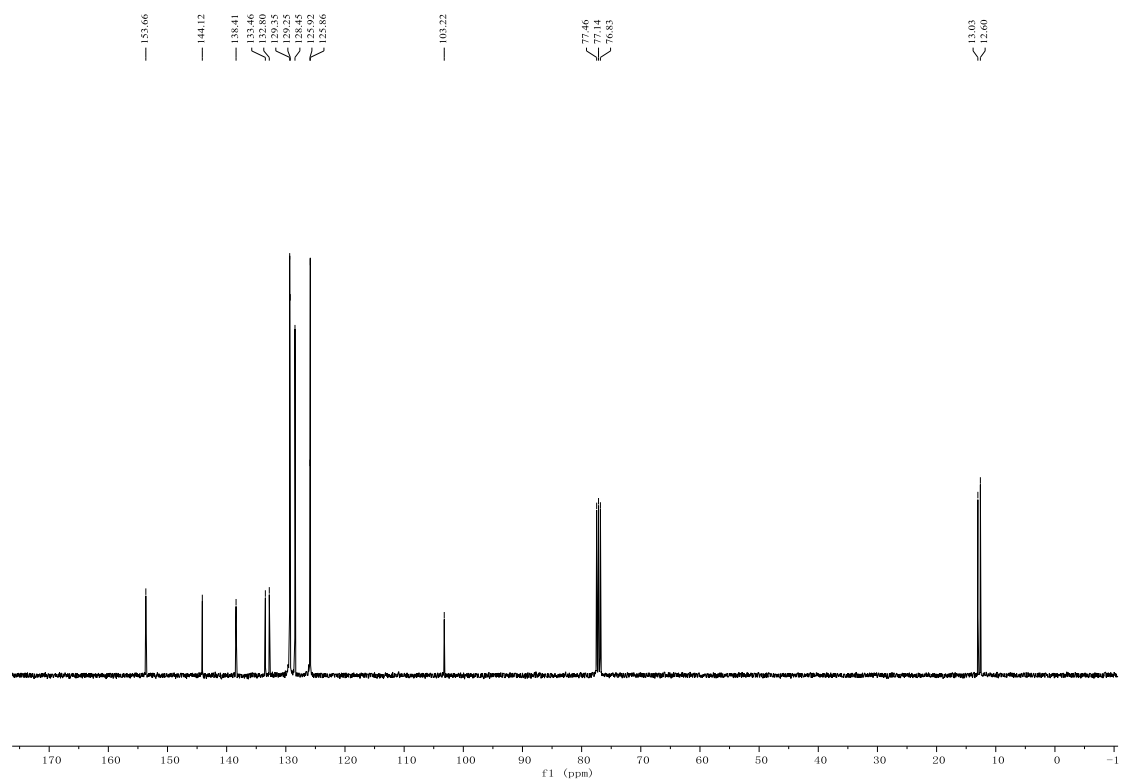
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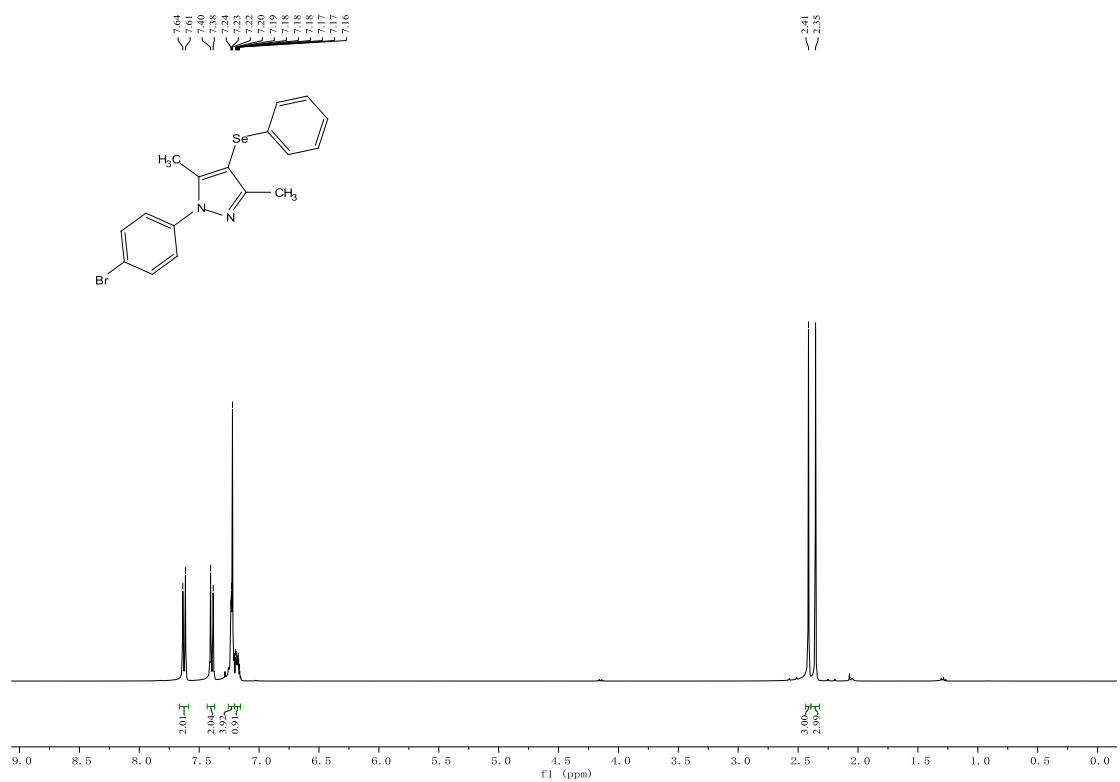
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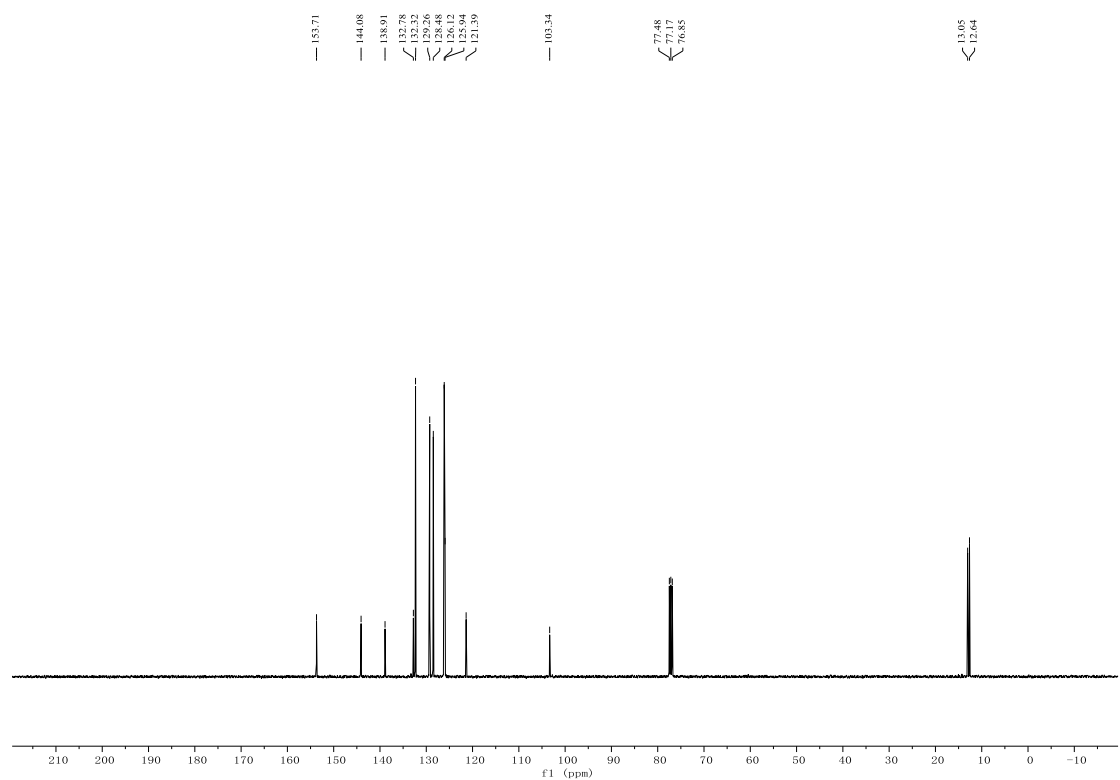
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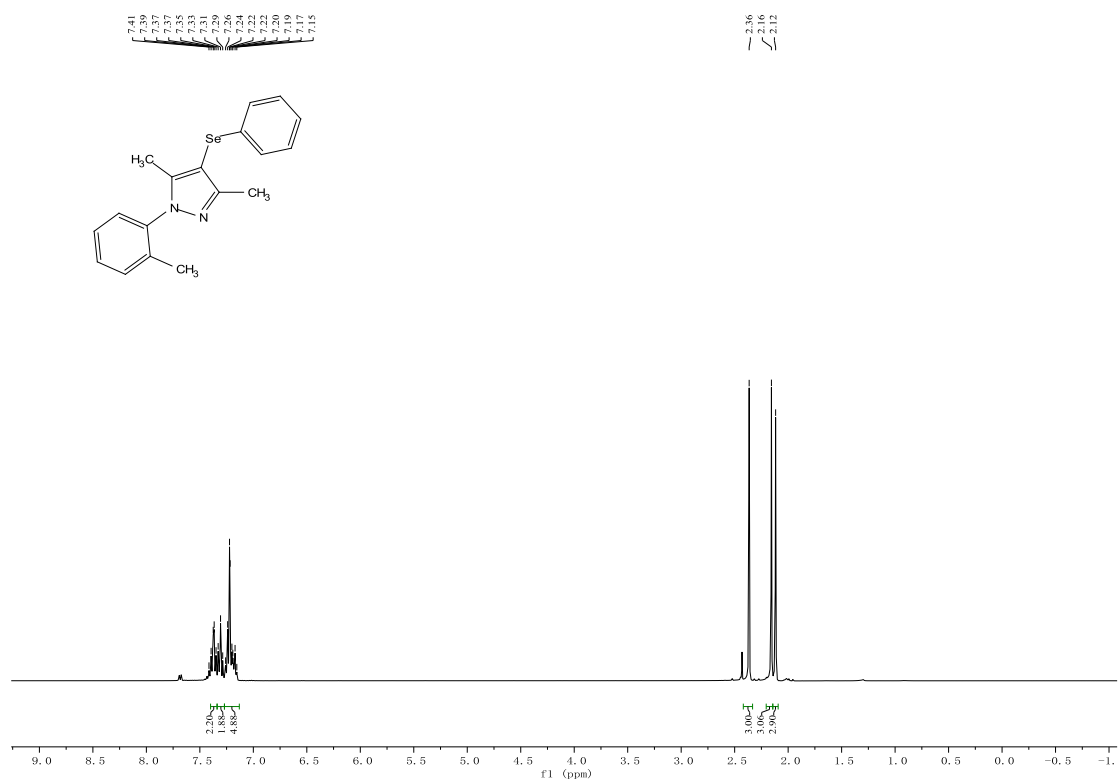
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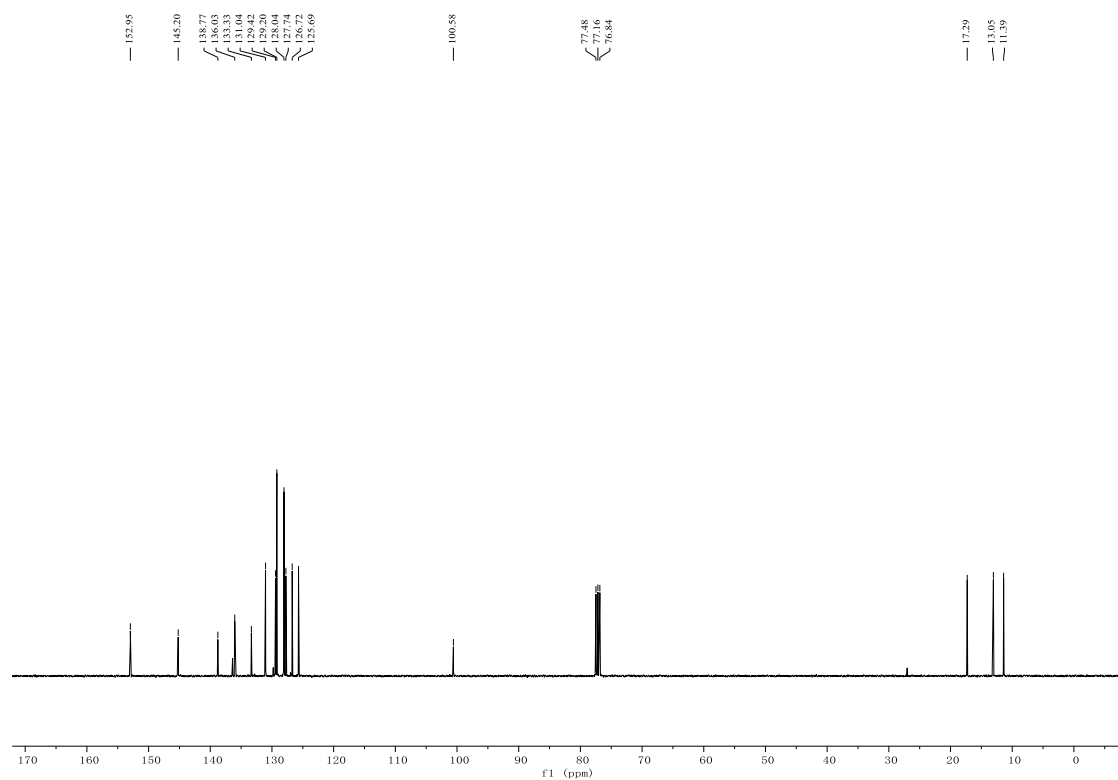
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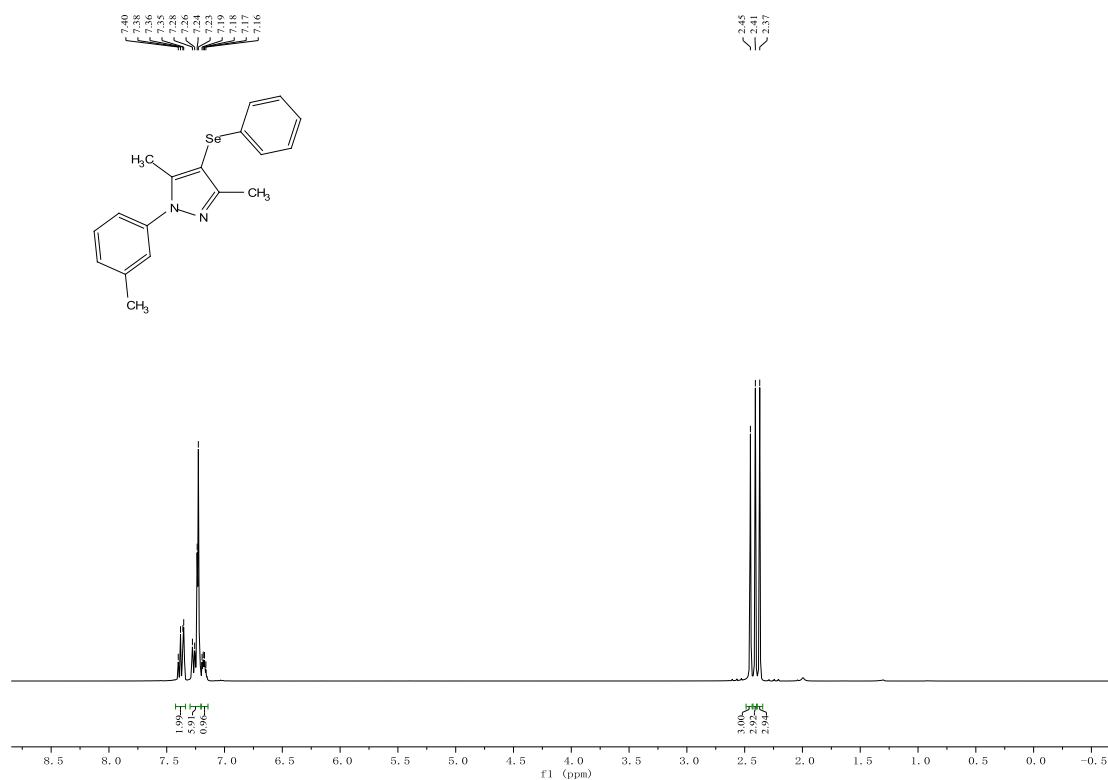
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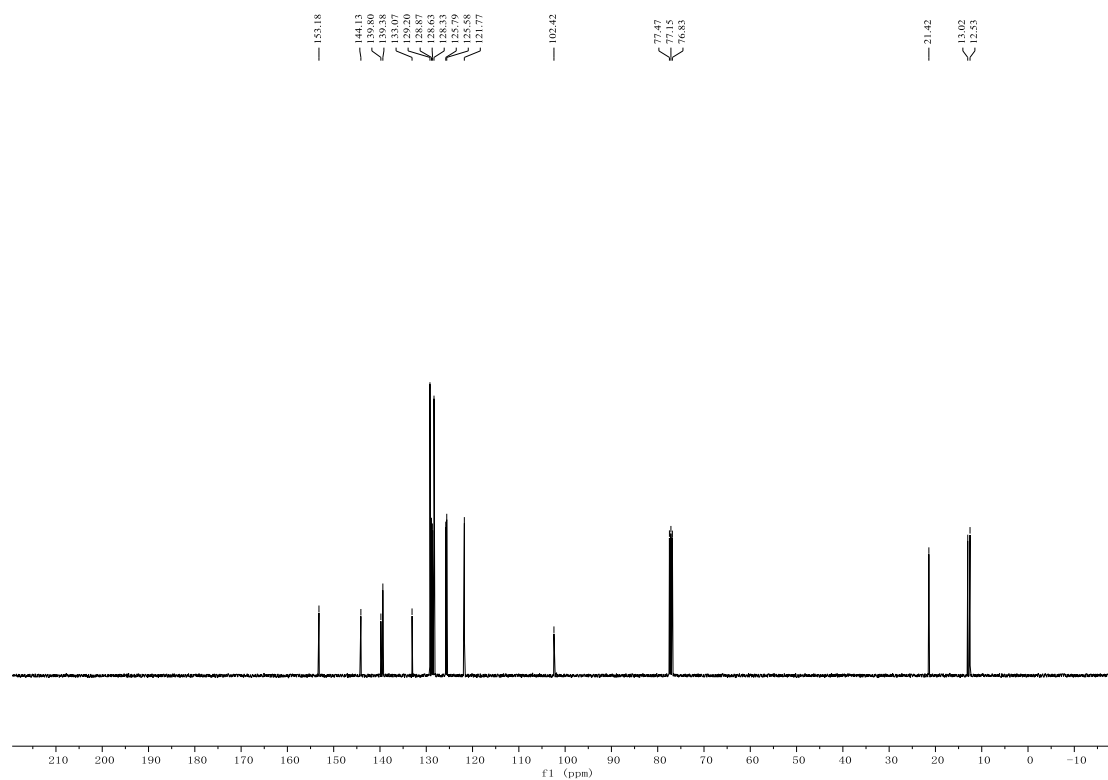
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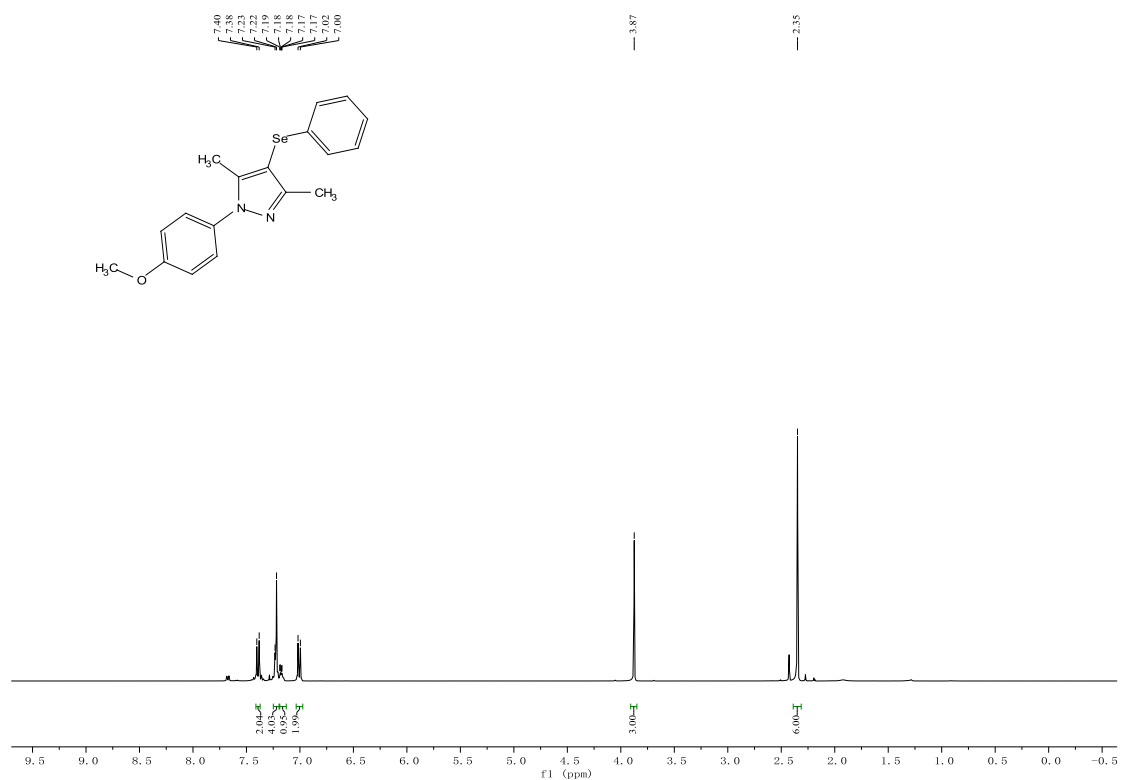
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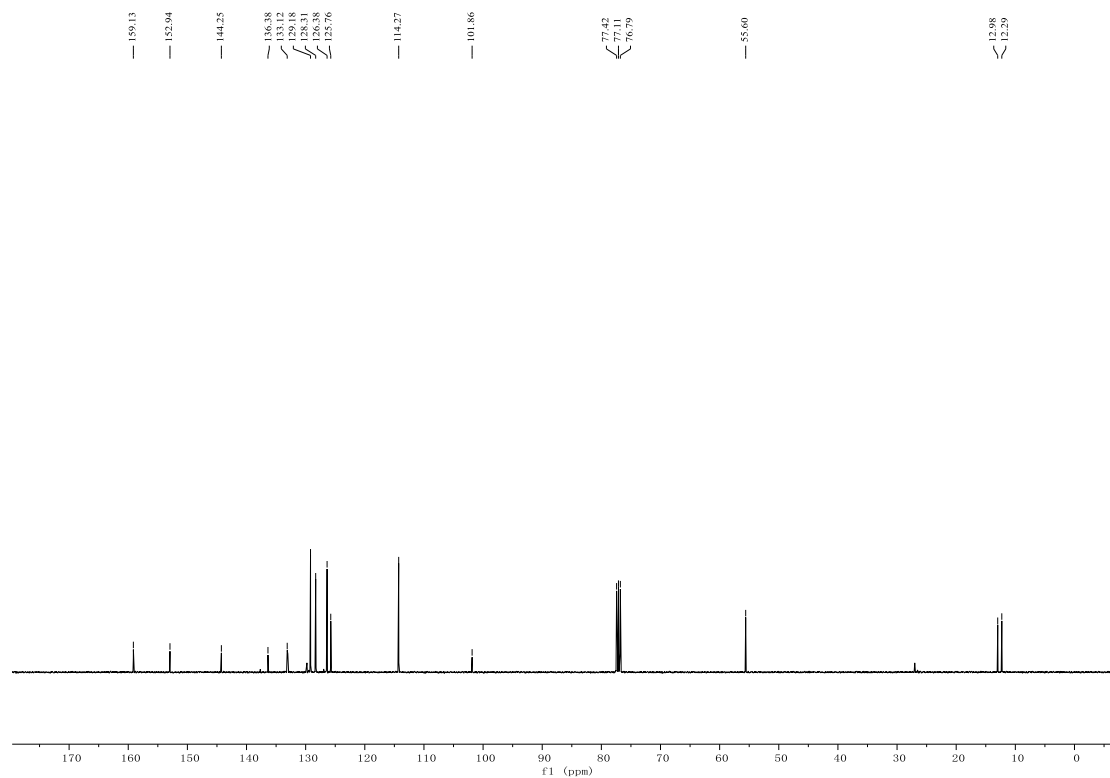
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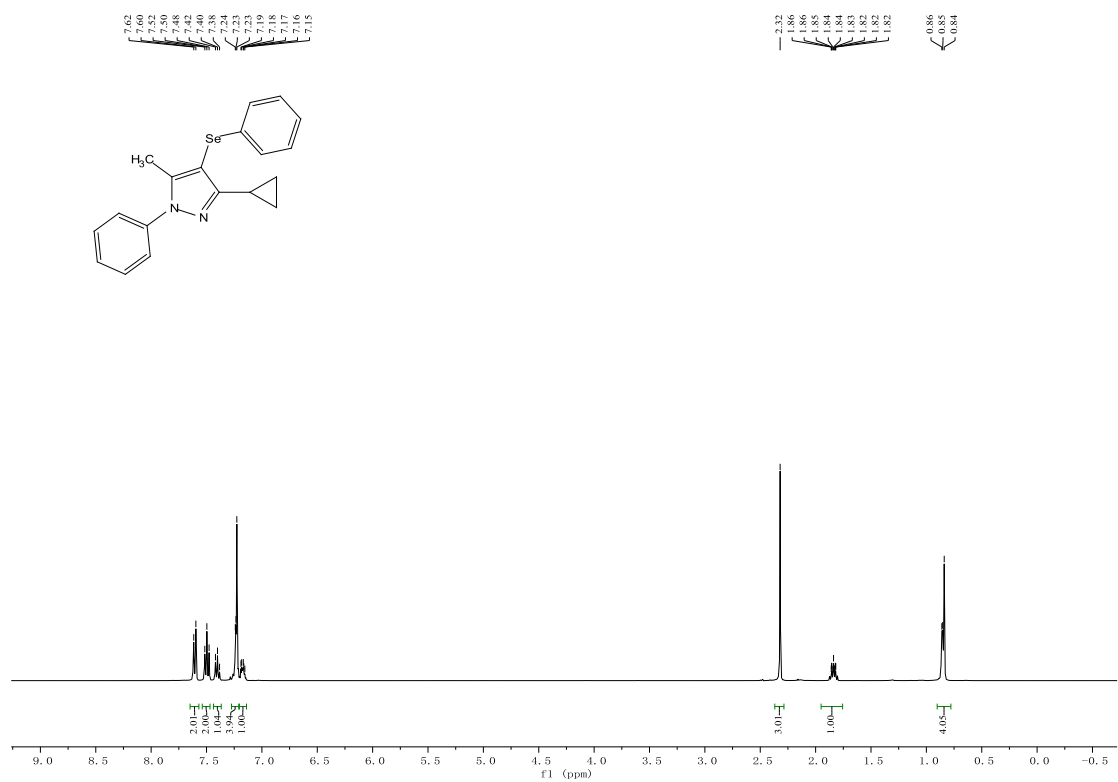
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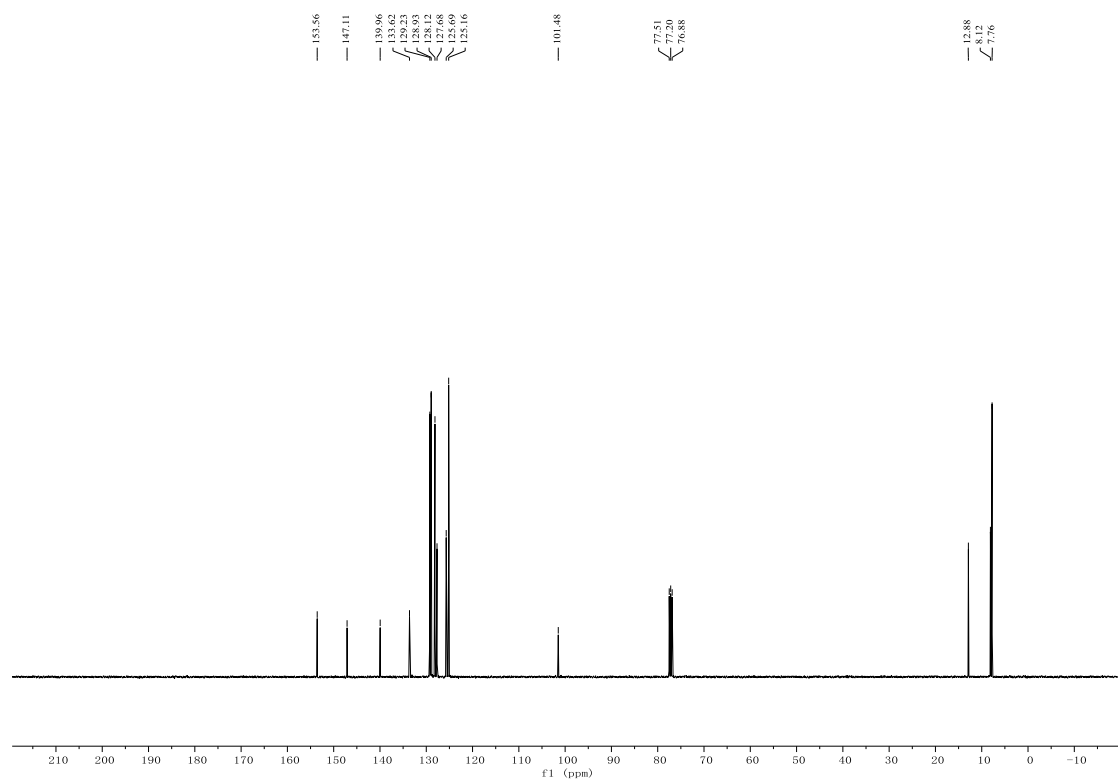
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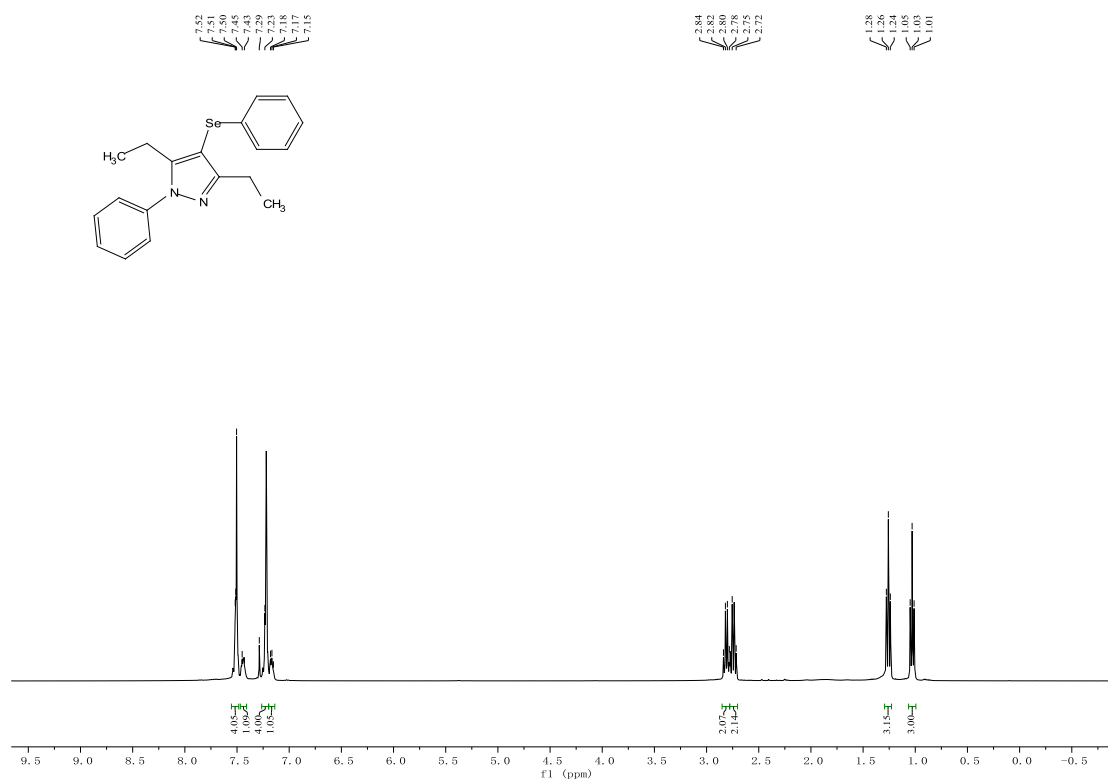
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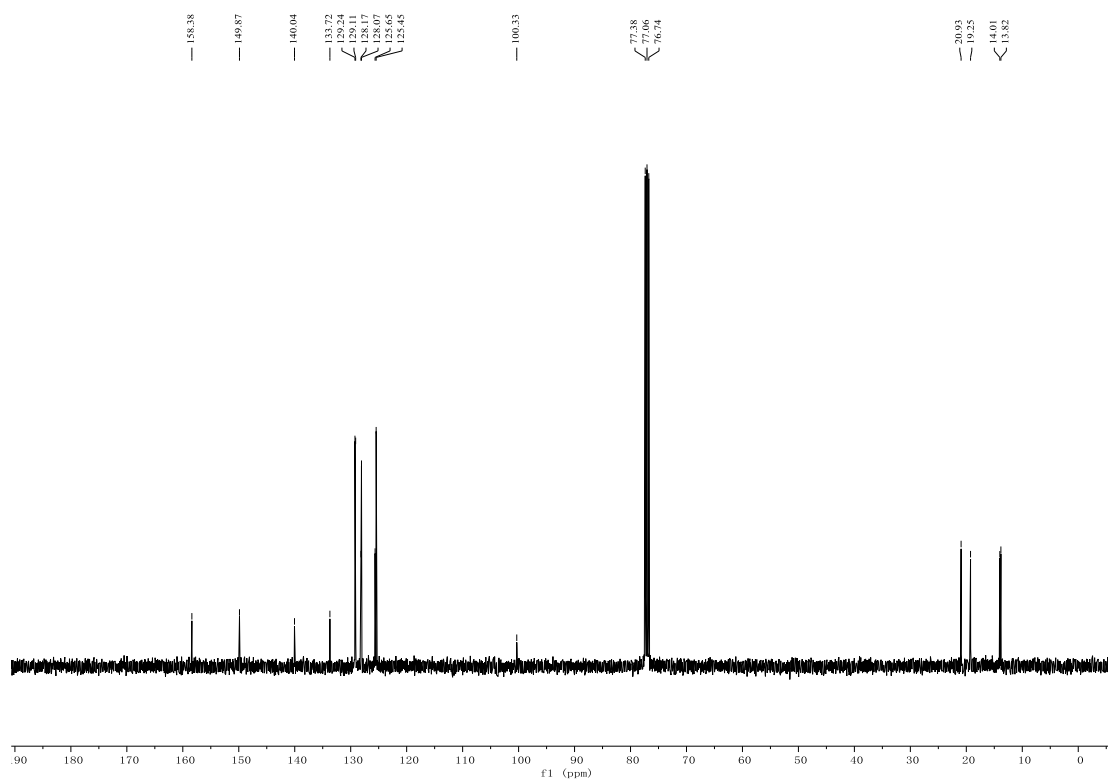
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¹³C NMR of compound **4aba**



^1H NMR of compound **4aca**



^{13}C NMR of compound **4aca**