

Copper-catalyzed direct C-H arylselenation of 4-nitro-pyrazoles and other heterocycles with selenium powder and aryl iodides. Access to unsymmetrical heteroaryl selenides.

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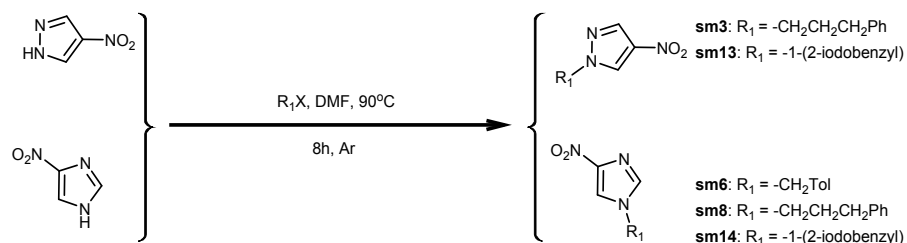
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(A) Experimental section.

Known starting materials: 1-[(4-methylphenyl)methyl]-4-nitro-1*H*-pyrazole (**sm1**), 4-nitro-1-phenethyl-1*H*-pyrazole (**sm2**), 4-nitro-1-butyl-1*H*-pyrazole (**sm4**), 3-methyl-1-phenyl-1*H*-pyrazol-5-amine (**sm5**), 4-nitro-1-phenethyl-1*H*-imidazole (**sm7**), 2-methyl-4-nitro-1-phenethyl-1*H*-imidazole (**sm9**), 1-[(4-methylphenyl)methyl]-1*H*-benzimidazole (**sm10**), 1-phenethyl-1*H*-1,2,4-triazole (**sm11**), 4*H*-chromen-4-one (**sm12**), 1-(2-iodobenzyl)-1*H*-benzo[*d*]imidazole (**sm15**) - were prepared according to literature procedures.¹⁻⁷ Triazole **sm9** was obtained as a 1 : 8.5 molar ratio mixture of 4*H*- and 1*H*- 1,2,4-triazole *N*-alkylation products, respectively. However, only the 1*H*-isomer underwent the selenylation giving the expected C(5)-substituted product after chromatographic separation from impurities and both starting materials (**Table 4**, Entry 46). Starting materials **sm3**, **sm6**, **sm8**, **sm13** and **sm14** (**Scheme 1**) were prepared according to the general procedure described below. Commercially available reagents, catalysts and anhydrous and degassed solvents were used without further purification. Flash column chromatography was performed with Merck silica gel 60 (230-400 mesh). The solvents for column chromatography were distilled before use. Thin layer chromatography was carried out using Merck TLC Silica gel 60 F254 and visualized by short-wavelength ultraviolet light or by treatment with iodine or potassium permanganate (KMnO₄) stain. Melting points are uncorrected. ¹H, ¹³C and ¹⁹F NMR spectra were recorded on a Bruker 200 and 500 MHz at 20°C. All ¹H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals for CHCl₃ (7.26 ppm) and DMSO (2.50 ppm). All ¹³C NMR spectra were reported in ppm relative to residual CHCl₃ (77.00 ppm) or DMSO (39.70 ppm) and were obtained with ¹H decoupling. Coupling constants, *J*, are reported in Hertz (Hz). Gas chromatographic analyses was performed on Gas Chromatograph Mass Spectrometer GCMS-QP2010 Ultra instrument. Isolation of obtained compounds was achieved by column chromatography on Silica gel.



Scheme 1: Preparation of previously unknown starting materials.

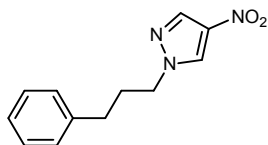
General procedure for the *N*-alkylation of pyrazol and imidazole derivatives (starting materials **sm3**, **sm6**, **sm8**, **sm13**, **sm14**): Corresponding 4-nitro-1*H*-pyrazole (1eq.) and K₂CO₃ (2.3eq.) successively were weighed to air and placed in a Schlenk flask, equipped with a magnetic stir bar, which then was capped with a rubber septum. The reaction

vessel was evacuated and backfilled with argon. The DMF (8mL for 1g of 4-nitro-1*H*-pyrazole) and corresponding alkyl bromide (1.3eq.) were added via a syringe, and the reaction was heated to 90 °C for 8 h. Upon completion, the reaction was cooled to room temperature and concentrated under vacuum. The crude mass was washed with water, which was extracted with chloroform afterward. Finally, the organic phase was dried (Na₂SO₄), filtered, and evaporated to dryness, or (if necessary) the residue was purified by column chromatography typically using hexane/ethyl acetate mixtures to provide the desired alkylated product.

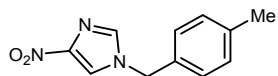
General procedure for the synthesis of diorganyl selenides (compounds 1a-1i, 2a-2f, 3a-3c, 4a-4d, 5a-5m, 6, 7a-7d, 8, 9a, 9b, 10a, 10b, 11, 12a, 12b): An Ace Glass Pressure Tube was equipped with a suitable stirring pellet and loaded with 250mg (1.15mmol, 1eq.) of 1-[(4-methylphenyl)methyl]-4-nitro-1*H*-pyrazole, 502mg (2.30mmol, 2eq.) of 3-iodotoluene, 273mg (3.45mmol, 3.5eq.) of selenium (100 mesh), 26mg (0.11mmol, 0.1eq.) of CuBr₂ and 636mg (4.60mmol, 4eq.) of K₂CO₃. 1mL of dry DMSO was added and the tube was carefully closed with an original Ace Glass Tube (Teflon) plug. The vessel was placed in an aluminium heating-block on a hotplate. The reaction was kept in 115°C for 24h. After cooling down - the pressure tube was carefully opened under venting hood and the mixture was washed to a flask with MeOH. The volatiles were removed using a rotary evaporator and DMSO was removed by heating to about 60 °C under vacuum (oil vacuum pump). The solid crude mixture was purified by column chromatography typically using hexane/ethyl acetate gradient to provide the desired selenide.

General procedure for the synthesis of benzoselenazines (compounds 13a, 13b and 13c): An Ace Glass Pressure Tube was equipped with a suitable stirring pellet and loaded with 360mg (1.07mmol, 1eq.) of 1-(2-iodobenzyl)-1*H*-benzo[*d*]imidazole (**sm15**), 196mg (2.47mmol, 2.3eq.) of selenium (100 mesh), 24mg (0.10mmol, 0.1eq.) of CuBr₂ and 596mg (4.30mmol, 4eq.) of K₂CO₃. 1mL of dry DMSO was added and the tube was carefully closed with an original Ace Glass Tube (Teflon) plug. The vessel was placed in an aluminium heating-block on a hotplate. The reaction was kept in 115 °C for 24h. After cooling down - the pressure tube was carefully opened under venting hood and the mixture was washed to a flask with MeOH. The volatiles were removed using a rotary evaporator and DMSO was removed by heating to about 60 °C under vacuum (oil vacuum pump). The solid crude mixture was purified by column chromatography typically using hexane/ethyl acetate gradient to provide the desired benzoselenazine.

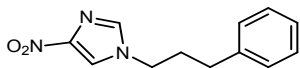
(B) Characterization of products.



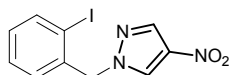
4-nitro-1-(3-phenylpropyl)-1H-pyrazole (sm3): white powder, mp. 55-56 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.08 (s, 2H, C(3) and C(5)-pyrazole), 7.31 (t, 2H, $^3J = 7.4$ Hz, CH_{Ar}), 7.22 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.17 (d, 2H, $^3J = 7.0$ Hz, CH_{Ar}), 4.14 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.65 (t, 2H, $^3J = 7.5$ Hz, CH_2), 2.33 - 2.18 (m, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.98, 135.94, 128.80, 128.56, 128.47, 126.58, 52.72, 32.47, 31.08, MS (GC, 70 eV): $m/z = 231$ (M^+ , 19%), 126 (29), 118 (100), 91 (31), 65 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{12}\text{H}_{14}\text{N}_3\text{O}_2$ ($\text{M} + \text{H}$) $^+$ 232.1086, found 232.1088.



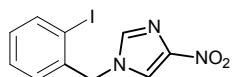
1-[(4-methylphenyl)methyl]-4-nitro-1H-imidazole (sm6): white powder, 103-104 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.70 (s, 1H, C(2)-imidazole), 7.47 (s, 1H, C(5)-imidazole), 7.22 (d, 2H, $^3J = 7.8$ Hz, CH_{Ar}), 7.13 (d, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 5.12 (s, 2H, CH_2), 2.37 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.55, 136.03, 130.65, 130.29, 128.12, 119.38, 52.17, 21.31, MS (GC, 70 eV): $m/z = 217$ (M^+ , 11%), 105 (100), 77 (13), HRMS (TOF MS ES+): calcd for $\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}_2\text{Na}$ ($\text{M} + \text{Na}$) $^+$ 240.0749, found 240.0754.



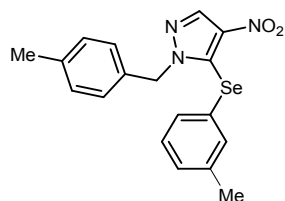
4-nitro-1-(3-phenylpropyl)-1H-imidazole (sm8): white powder, mp. 79-80 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.75 (s, 1H, C(2)-imidazole), 7.40 (s, 1H, C(5)-imidazole), 7.32 (t, 2H, $^3J = 7.5$ Hz, CH_{Ar}), 7.24 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.15 (d, 2H, $^3J = 7.2$ Hz, CH_{Ar}), 4.01 (t, 2H, $^3J = 7.2$ Hz, CH_2), 2.67 (t, 2H, $^3J = 7.4$ Hz, CH_2), 2.21 (quint, 2H, $^3J = 7.3$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.36, 136.08, 128.96, 128.40, 126.84, 119.13, 47.57, 32.35, 31.88, MS (GC, 70 eV): $m/z = 231$ (M^+ , 29%), 127 (100), 118 (57), 91 (82), 77 (13), 65 (24), HRMS (TOF MS ES+): calcd for $\text{C}_{12}\text{H}_{13}\text{N}_3\text{O}_2\text{Na}$ ($\text{M} + \text{Na}$) $^+$ 254.0905, found 254.0906.



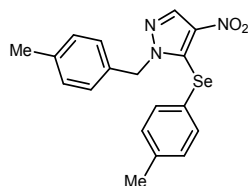
1-(2-iodobenzyl)-4-nitro-1H-pyrazole (sm13): light yellow crystals, mp. 100 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.12 (s, 1H, C(3)-pyrazole), 8.11 (s, 1H, C(5)-pyrazole), 7.91 (dd, 1H, $^3J = 7.9$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.39 (td, 1H, $^3J = 7.6$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.23 (dd, 1H, $^3J = 7.7$ Hz, $^4J = 1.4$ Hz, CH_{Ar}), 7.10 (td, 1H, $^3J = 7.8$ Hz, $^4J = 1.6$ Hz, CH_{Ar}), 5.40 (s, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 140.29, 136.58, 136.23, 136.14, 130.98, 130.49, 129.26, 129.04, 99.40, 61.55, MS (GC, 70 eV): $m/z = 217$ (2-iodobenzene- CH_2^+ , 14%), minus iodide 202 (100), 156 (35), 129 (10), 90 (43), HRMS (TOF MS ES+): calcd for $\text{C}_{10}\text{H}_9\text{IN}_3\text{O}_2$ ($\text{M} + \text{H}$) $^+$ 329.9739, found 329.9742.



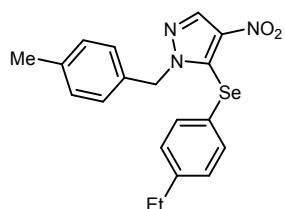
1-(2-iodobenzyl)-4-nitro-1H-imidazole (sm14): white powder, mp. 76-77 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.84 - 7.80 (m, 1H, CH_{Ar}), 7.73 (s, 1H, C(2)-imidazole), 7.51 (s, 1H, C(5)-imidazole), 7.36 - 7.30 (m, 1H, CH_{Ar}), 7.19 (d, 1H, $^3J = 6.5$ Hz, CH_{Ar}), 7.06 - 7.01 (m, 1H, CH_{Ar}), 5.23 (s, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 147.87, 140.22, 136.53, 136.21, 130.94, 130.02, 129.26, 119.69, 99.16, 56.34, MS (GC, 70 eV): $m/z = 329$ (M^+ , 22%), 217 (100), 202 (28), 156 (84), 90 (65), HRMS (TOF MS ES+): calcd for $\text{C}_{10}\text{H}_8\text{IN}_3\text{O}_2$ ($\text{M} + \text{H}$) $^+$ 329.9739, found 329.9744.



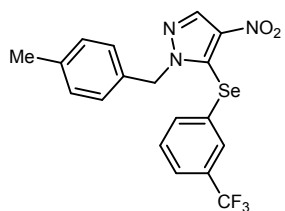
1-[(4-methylphenyl)methyl]-5-[(3-methylphenyl)selenanyl]-4-nitro-1H-pyrazole (1a): light yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.25 (s, 1H, C(3)-pyrazole), 7.19 - 7.03 (m, 8H, CH_{Ar}), 5.41 (s, 2H, CH_2), 2.33 (s, 3H, CH_3), 2.24 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.88, 138.21, 137.88, 137.47, 133.11, 132.15, 129.63, 129.61, 129.54, 129.52, 128.30, 127.80, 127.76, 55.40, 21.29, 21.20, MS (GC, 70 eV): $m/z = 387$ (M^+ , 5%), 280 (6), 222 (12), 195 (4), 105 (100), 91 (6), 77 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 388.0564, found 388.0566.



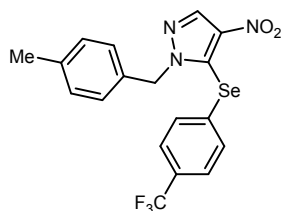
1-[(4-methylphenyl)methyl]-5-[(4-methylphenyl)selanyl]-4-nitro-1H-pyrazole (1b): white powder, mp. 55-56 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.23 (s, 1H, C(3)-pyrazole), 7.26 (d, 2H, $^3J = 8.1$ Hz, CH_{Ar}), 7.11 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 7.04 (dd, 4H, $^3J = 8.1$ Hz, $^4J = 4.7$ Hz, CH_{Ar}), 5.39 (s, 2H, CH_2), 2.33 (s, 3H, CH_3), 2.31 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.12, 138.21, 137.73, 137.45, 133.08, 132.17, 130.65, 129.52, 128.78, 127.72, 124.25, 55.33, 21.21, MS (GC, 70 eV): $m/z = 387$ (M^+ , 5%), 280 (7), 195 (3), 119 (2), 105 (100), 91 (6), 77 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 388.0564, found 388.0562.



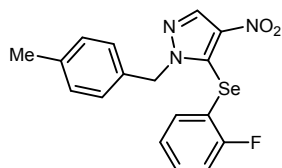
1-[(4-methylphenyl)methyl]-5-[(4-ethylphenyl)selanyl]-4-nitro-1H-pyrazole (1c): yellow powder, mp. 58 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.24 (s, 1H, C(3)-pyrazole), 7.29 (d, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 7.10 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 7.07 (d, 2H, $^3J = 8.1$ Hz, CH_{Ar}), 7.04 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 5.41 (s, 2H, CH_2), 2.61 (q, 2H, $^3J = 7.6$ Hz, CH_2), 2.33 (s, 3H, CH_3), 1.21 (t, 3H, $^3J = 7.6$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 145.36, 138.18, 137.75, 137.45, 133.15, 132.16, 129.51, 129.47, 128.73, 127.72, 124.47, 55.30, 28.54, 21.21, 15.39, MS (GC, 70 eV): $m/z = 401$ (M^+ , 5%), 280 (8), 209 (3), 105 (100), 77 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{19}\text{H}_{20}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 402.0721, found 402.0721.



1-[[4-methylphenyl)methyl]-5-[[3-(trifluoromethyl)phenyl]selanyl]-4-nitro-1H-pyrazole (1d): light yellow powder, mp. 68-70 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.28 (s, 1H, C(3)-pyrazole), 7.50 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 7.45 - 7.40 (m, 2H, CH_{Ar}), 7.31 (t, 1H, $^3J = 8.0$ Hz, CH_{Ar}), 7.07 (q, 4H, $^3J = 8.3$ Hz, CH_{Ar}), 5.51 (s, 2H, CH_2), 2.30 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 138.56, 138.28, 137.63, 135.44, 131.99 (q, $^2J_{\text{CF}} = 32.7$ Hz, $\text{C}_{\text{ipso}}\text{-CF}_3$), 131.85, 130.11, 129.68, 129.35, 128.64 (dd, $J_{\text{CF}} = 7.5$ Hz, $J_{\text{CF}} = 3.7$ Hz), 127.63, 126.66, 125.32 (dd, $J_{\text{CF}} = 6.9$ Hz, $J_{\text{CF}} = 3.3$ Hz), 123.34 (q, $^1J_{\text{CF}} = 273.0$ Hz, CF_3), 55.87, 21.16, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -62.15 (CF_3), MS (GC, 70 eV): $m/z = 441$ (M^+ , 5%), 280 (3), 105 (100), 77 (10), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 442.0282, found 442.0277.

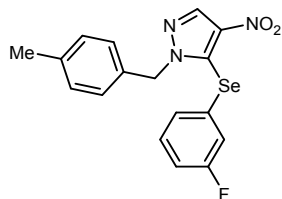


1-[[4-methylphenyl)methyl]-5-[[4-(trifluoromethyl)phenyl]selanyl]-4-nitro-1H-pyrazole (1e): white powder, mp. 75-76 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.30 (s, 1H, C(3)-pyrazole), 7.40 (d, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 7.27 - 7.24 (m, 2H, CH_{Ar}), 7.03 (q, 4H, $^3J = 8.2$ Hz, CH_{Ar}), 5.49 (s, 2H, CH_2), 2.29 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): δ 138.59, 138.53, 137.69, 133.4 (d, $^2J_{\text{CF}} = 11.8$ Hz, $\text{C}_{\text{ipso}}\text{-CF}_3$), 131.97, 131.82, 131.34, 129.66, 127.73, 126.52 (dd, $J_{\text{CF}} = 7.1$ Hz, $J_{\text{CF}} = 3.3$ Hz), 126.23, 125.08 (q, $^1J_{\text{CF}} = 288.3$ Hz, CF_3), 55.89, 21.19, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -62.20 (CF_3), MS (GC, 70 eV): $m/z = 441$ (M^+ , 7%), 280 (6), 105 (100), 77 (13), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{14}\text{F}_3\text{N}_3\text{O}_2\text{SeNa}$ ($\text{M} + \text{Na}$) $^+$ 464.0101, found 464.0104.

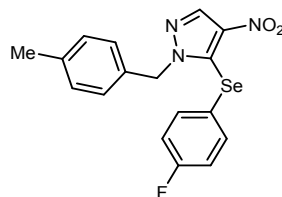


1-[[4-methylphenyl)methyl]-5-[[2-fluorophenyl]selanyl]-4-nitro-1H-pyrazole (1f): light yellow powder, mp. 63-65 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.25 (s, 1H, C(3)-pyrazole), 7.33 - 7.23 (m, 2H, CH_{Ar}), 7.13 - 6.99 (m, 6H, CH_{Ar}), 5.51 (s, 2H, CH_2), 2.32 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.10 (d, $^1J_{\text{CF}} = 245.3$ Hz, $\text{C}_{\text{ipso}}\text{-F}$), 138.34, 138.25, 137.52, 134.11 (d, $J = 1.6$ Hz), 132.06, 130.91 (d, $J_{\text{CF}} = 7.8$ Hz), 129.59, 127.82, 126.33 (d, $J = 1.7$ Hz), 125.43 (d, $J_{\text{CF}} = 3.3$ Hz), 116.12 (d, $^2J_{\text{CF}} = 22.6$ Hz), 115.07 (d, $^2J_{\text{CF}} =$

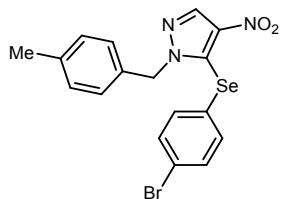
21.4 Hz), 55.57, 21.20, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -103.00 (CF), MS (GC, 70 eV): m/z = 391 (M^+ , 5%), 280 (5), 105 (100), 79 (12), 77 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0317.



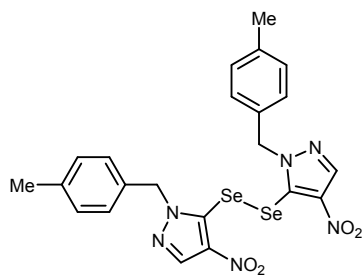
1-[(4-methylphenyl)methyl]-5-[(3-fluorophenyl)selanyl]-4-nitro-1H-pyrazole (1g): yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.27 (s, 1H, C(3)-pyrazole), 7.23 - 7.16 (m, 1H, CH_{Ar}), 7.12 - 7.05 (m, 5H, CH_{Ar}), 6.96 (td, 1H, $^3J = 8.4$ Hz, $^4J = 2.0$ Hz, CH_{Ar}), 6.88 (dd, 1H, $^3J = 8.4$ Hz, $^5J = 1.3$ Hz, CH_{Ar}), 5.47 (s, 2H, CH_2), 2.32 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 162.79 (d, $^1J_{\text{CF}} = 251.4$ Hz, $\text{C}_{\text{ipso-F}}$), 138.47, 138.19, 137.56, 131.96, 131.02 (d, $J_{\text{CF}} = 8.1$ Hz), 129.74 (d, $J_{\text{CF}} = 7.1$ Hz), 129.61, 127.74, 127.55 (d, $J_{\text{CF}} = 3.1$ Hz), 126.91, 118.93 (d, $^2J_{\text{CF}} = 23.2$ Hz), 115.61 (d, $^2J_{\text{CF}} = 21.1$ Hz), 55.70, 21.18, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -109.57 (CF), MS (GC, 70 eV): m/z = 391 (M^+ , 6%), 280 (6), 105 (100), 79 (12), 77 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0316.



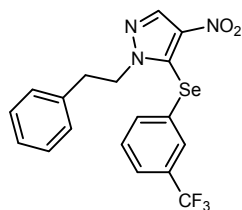
1-[(4-methylphenyl)methyl]-5-[(4-fluorophenyl)selanyl]-4-nitro-1H-pyrazole (1h): light yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.24 (s, 1H, C(3)-pyrazole), 7.35 - 7.29 (m, 2H, CH_{Ar}), 7.1 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 7.0 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 6.95 - 6.88 (m, 2H, CH_{Ar}), 5.46 (s, 2H, CH_2), 2.33 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.21 (d, $^1J_{\text{CF}} = 250.0$ Hz, $\text{C}_{\text{ipso-F}}$), 138.45, 137.86, 137.61, 135.41 (d, $J_{\text{CF}} = 8.2$ Hz), 132.15, 129.67, 128.26, 127.65, 122.48 (d, $J_{\text{CF}} = 3.3$ Hz), 117.10 (d, $^2J_{\text{CF}} = 22.0$ Hz), 55.58, 21.26, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -110.86 (CF), MS (GC, 70 eV): m/z = 391 (M^+ , 5%), 280 (4), 105 (100), 77 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0314.



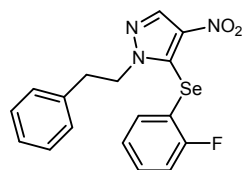
1-[(4-methylphenyl)methyl]-5-[(4-bromophenyl)selenanyl]-4-nitro-1H-pyrazole (1i): white powder, mp. 100-101 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.32 (s, 1H, C(3)-pyrazole), 7.52 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 7.13 - 7.00 (m, 6H, CH_{Ar}), 6.65 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 5.45 (s, 2H, CH_2), 2.28 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 138.90, 138.47, 137.70, 133.31, 132.22, 131.78, 130.39, 129.59, 128.85, 128.57, 128.12, 126.79, 123.28, 55.85, 21.24, MS (GC, 70 eV): $m/z = 451$ (M^+ , 5%), 280 (8), 105 (100), 79 (12), 77 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{BrN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 451.9513, found 451.9510.



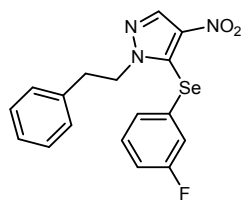
Identification of byproduct 1,2-bis(1-(4-methylbenzyl)-4-nitro-1H-pyrazol-5-yl)diselane (1by): colorless crystals, mp. 59-60 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.22 (s, 2H, C(3)-pyrazole), 7.19 (d, 4H, $^3J = 7.9$ Hz, CH_{Ar}), 7.10 (d, 4H, $^3J = 8.0$ Hz, CH_{Ar}), 5.30 (s, 4H, CH_2), 2.33 (s, 6H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 138.76, 137.47, 131.82, 129.91, 127.75, 125.96, 56.01, 21.33, MS (GC, 70 eV): $m/z = 592$ (M^+ , 3%), 296 (37), 279 (11), 176 (7), 121 (26), 105 (100), 79 (17), 77 (17), HRMS (TOF MS ES+): calcd for $\text{C}_{22}\text{H}_{21}\text{N}_6\text{O}_4\text{Se}_2$ ($\text{M} + \text{H}$) $^+$ 592.9955, found 592.9967.



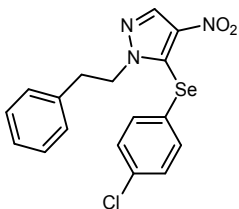
5-(3-(trifluoromethyl)phenylselanyl)-4-nitro-1-phenethyl-1H-pyrazole (2a): light yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.31 (s, 1H, C(3)-pyrazole), 7.60 (s, 1H, CH_{Ar}), 7.53 (d, 1H, $^3J = 7.6$ Hz, CH_{Ar}), 7.38 - 7.28 (m, 2H, CH_{Ar}), 7.27 - 7.20 (m, 3H, CH_{Ar}), 6.99 (dd, 2H, $^3J = 7.4$ Hz, $^4J = 1.9$ Hz, CH_{Ar}), 4.58 (t, 2H, $^3J = 7.1$ Hz, CH_2), 3.13 (t, 2H, $^3J = 7.1$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 137.88, 137.54, 136.70, 135.01, 132.13 (q, $^2J_{\text{CF}} = 33.0$ Hz, $\text{C}_{\text{ipso-CF}_3}$), 130.32, 129.77, 128.98, 128.88, 128.34 (dd, $J_{\text{CF}} = 7.5$ Hz, $J_{\text{CF}} = 3.9$ Hz), 127.51, 127.39, 125.33 (q, $J_{\text{CF}} = 3.6$ Hz), 123.41 (q, $^1J_{\text{CF}} = 272.9$ Hz, CF_3), 53.11, 36.37, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -62.14 (CF_3), MS (GC, 70 eV): $m/z = 441$ (M^+ , 7%), 337 (76), 230 (24), 176 (28), 104 (94), 91 (100), 77 (38), 65 (21), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{15}\text{F}_3\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 442.0282, found 442.0285.



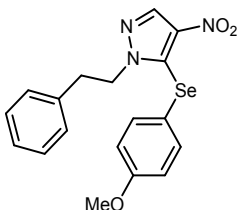
5-(2-fluorophenylselanyl)-4-nitro-1-phenethyl-1H-pyrazole (2b): light yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.26 (s, 1H, C(3)-pyrazole), 7.35 - 7.20 (m, 5H, CH_{Ar}), 7.10 - 6.99 (m, 4H, CH_{Ar}), 4.61 (t, 2H, $^3J = 7.2$ Hz, CH_2), 3.12 (t, 2H, $^3J = 7.2$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.23 (d, $^1J_{\text{CF}} = 245.3$ Hz, $\text{C}_{\text{ipso-F}}$), 137.67, 137.60, 136.87, 134.41, 131.04 (d, $J_{\text{CF}} = 7.8$ Hz), 128.92, 127.29, 127.04, 125.47 (d, $J_{\text{CF}} = 3.3$ Hz), 116.13 (d, $^2J_{\text{CF}} = 22.8$ Hz), 115.14 (d, $^2J_{\text{CF}} = 21.4$ Hz), 53.04, 36.39, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -103.01 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 10%), 287 (88), 176 (39), 109 (44), 104 (55), 91 (100), 77 (45), 65 (23), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0320.



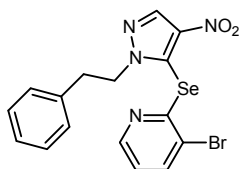
5-(3-fluorophenylselanyl)-4-nitro-1-phenethyl-1H-pyrazole (2c): light yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.30 (s, 1H, C(3)-pyrazole), 7.35 - 7.16 (m, 4H, CH_{Ar}), 7.08 - 6.90 (m, 5H, CH_{Ar}), 4.56 (t, 2H, $^3J = 7.2$ Hz, CH_2), 3.13 (t, 2H, $^3J = 7.2$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 162.85 (d, $^1J_{\text{CF}} = 251.5$ Hz, $\text{C}_{\text{ipso-F}}$), 137.70, 137.49, 136.76, 131.13 (d, $J_{\text{CF}} = 8.0$ Hz), 130.07 (d, $J_{\text{CF}} = 7.0$ Hz), 128.89, 128.83, 127.63, 127.29, 127.26 (d, $J_{\text{CF}} = 3.4$ Hz), 118.65 (d, $^2J_{\text{CF}} = 23.1$ Hz), 115.60 (d, $^2J_{\text{CF}} = 21.0$ Hz), 53.00, 36.24, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -109.39 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 12%), 287 (80), 176 (36), 109 (36), 104 (60), 91 (100), 77 (41), 65 (21), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0319.



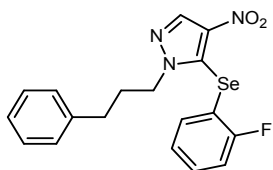
5-(4-chlorophenylselanyl)-4-nitro-1-phenethyl-1H-pyrazole (2d): yellow crystals, mp. 95 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.27 (s, 1H, C(3)-pyrazole), 7.32 - 7.22 (m, 3H, CH_{Ar}), 7.22 - 7.12 (m, 4H, CH_{Ar}), 7.01 (dd, 2H, $^3J = 7.3$ Hz, $^4J = 2.0$ Hz, CH_{Ar}), 4.55 (t, 2H, $^3J = 7.1$ Hz, CH_2), 3.13 (t, 2H, $^3J = 7.1$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 137.73, 137.32, 136.85, 135.03, 133.67, 130.06, 128.95, 128.90, 128.30, 127.30, 126.50, 52.97, 36.23, MS (GC, 70 eV): $m/z = 407$ (M^+ , 12%), 303 (60), 280 (15), 176 (40), 125 (23), 104 (48), 91 (100), 77 (51), 65 (23), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{ClN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 408.0018, found 408.0017.



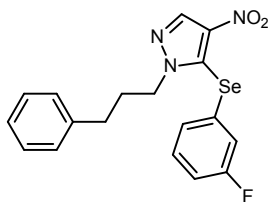
5-(4-methoxyphenylselanyl)-4-nitro-1-phenethyl-1H-pyrazole (2e): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.22 (s, 1H, C(3)-pyrazole), 7.35 (d, 2H, $^3J = 8.9$ Hz, CH_{Ar}), 7.31 - 7.21 (m, 3H, CH_{Ar}), 7.04 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 6.79 (d, 2H, $^3J = 8.9$ Hz, CH_{Ar}), 4.50 - 4.45 (m, 2H, CH_2), 3.77 (s, 3H, OCH_3), 3.11 - 3.03 (m, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 160.48, 137.40, 137.01, 136.97, 135.58, 129.76, 128.85, 128.84, 127.14, 117.73, 115.55, 55.43, 52.79, 36.11, MS (GC, 70 eV): $m/z = 403$ (M^+ , 29%), 299 (17), 280 (22), 123 (100), 105 (25), 91 (37), 77 (24), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{O}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 404.0513, found 404.0521.



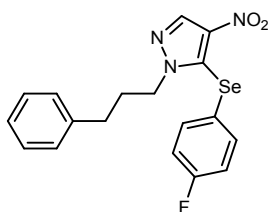
2-(4-nitro-1-phenethyl-1H-pyrazol-5-ylselanyl)-3-bromopyridine (2f): white powder, 120-121 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.34 (s, 1H, C(3)-pyrazole), 8.13 (dd, 1H, $^3J = 4.7$ Hz, $^4J = 1.5$ Hz, CH_{Ar}), 7.71 (dd, 1H, $^3J = 7.9$ Hz, $^4J = 1.5$ Hz, CH_{Ar}), 7.29 - 7.18 (m, 3H, CH_{Ar}), 7.08 - 7.03 (m, 2H, CH_{Ar}), 6.97 (dd, 1H, $^3J = 7.9$, $^3J = 4.7$ Hz, CH_{Ar}), 4.54 (t, 2H, $^3J = 7.3$ Hz, CH_2), 3.17 (t, 2H, $^3J = 7.3$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 154.85, 148.86, 139.71, 138.14, 137.60, 137.06, 128.93, 128.83, 127.18, 122.73, 120.59, 53.29, 36.52, MS (GC, 70 eV): $m/z = 406$ (minus nitro, M^+ , 100%), 355 (13), 302 (42), 287 (7), 236 (8), 195 (13), 156 (23), 104 (74), 91 (79), 77 (84), 65 (35), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{14}\text{BrN}_4\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 452.9465, found 452.9467.



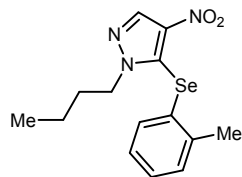
5-(2-fluorophenylselanyl)-4-nitro-1-(3-phenylpropyl)-1H-pyrazole (3a): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.23 (s, 1H, C(3)-pyrazole), 7.35 - 7.27 (m, 4H, CH_{Ar}), 7.21 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.14 - 7.06 (m, 4H, CH_{Ar}), 4.31 (t, 2H, $^3J = 7.3$ Hz, CH_2), 2.60 (t, 2H, $^3J = 7.7$ Hz, CH_2), 2.14 (quint, 2H, $^3J = 7.6$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.19 (d, $^1J_{\text{CF}} = 245.6$ Hz, $\text{C}_{\text{ipso-F}}$), 140.28, 137.85, 137.25, 134.33, 131.12 (d, $J_{\text{CF}} = 7.7$ Hz), 128.61, 128.35, 126.34, 126.31 (d, $J_{\text{CF}} = 8.0$ Hz), 125.54 (d, $J_{\text{CF}} = 3.4$ Hz), 116.22 (d, $^2J_{\text{CF}} = 22.7$ Hz), 115.02 (d, $^2J_{\text{CF}} = 21.5$ Hz), 51.48, 32.61, 31.15, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -102.72 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 1%), 287 (5), 230 (100), 202 (12), 175 (9), 117 (48), 109 (35), 91 (76), 65 (17), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0474.



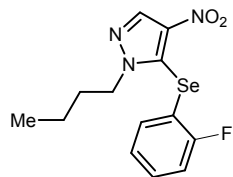
5-(3-fluorophenylselanyl)-4-nitro-1-(3-phenylpropyl)-1H-pyrazole (3b): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.25 (s, 1H, C(3)-pyrazole), 7.36 - 7.26 (m, 4H, CH_{Ar}), 7.19 - 7.14 (m, 3H, CH_{Ar}), 7.11 - 7.04 (m, 2H, CH_{Ar}), 4.23 (t, 2H, $^3J = 7.4$ Hz, CH_2), 2.58 (t, 2H, $^3J = 7.5$ Hz, CH_2), 2.11 (quint, 2H, $^3J = 7.5$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 162.94 (d, $^1J_{\text{CF}} = 251.8$ Hz, $\text{C}_{\text{ipso-F}}$), 140.19, 137.87, 137.37, 131.31 (d, $J_{\text{CF}} = 8.0$ Hz), 129.89 (d, $J_{\text{CF}} = 7.0$ Hz), 128.70, 128.41, 127.60 (d, $J_{\text{CF}} = 3.2$ Hz), 126.82, 126.46, 119.01 (d, $^2J_{\text{CF}} = 23.1$ Hz), 115.85 (d, $^2J_{\text{CF}} = 21.1$ Hz), 51.52, 32.64, 31.22, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -109.20 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 1%), 287 (4), 230 (100), 202 (10), 175 (7), 117 (45), 109 (21), 91 (61), 65 (14), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0472.



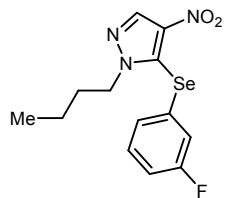
5-(4-fluorophenylselanyl)-4-nitro-1-(3-phenylpropyl)-1H-pyrazole (3c): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.21 (s, 1H, C(3)-pyrazole), 7.41 - 7.38 (m, 2H, CH_{Ar}), 7.30 (t, 2H, $^3J = 7.5$ Hz, CH_{Ar}), 7.22 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.13 (d, 2H, $^3J = 7.2$ Hz, CH_{Ar}), 6.97 (t, 2H, $^3J = 8.6$ Hz, CH_{Ar}), 4.22 (t, 2H, $^3J = 7.5$ Hz, CH_2), 2.59 (t, 2H, $^3J = 7.5$ Hz, CH_2), 2.10 (quint, 2H, $^3J = 7.5$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.02 (d, $^1J_{\text{CF}} = 250.0$ Hz, $\text{C}_{\text{ipso-F}}$), 140.18, 137.33, 137.08, 135.24 (d, $J_{\text{CF}} = 8.2$ Hz), 128.54, 128.31, 127.83, 126.29, 122.51 (d, $J_{\text{CF}} = 3.3$ Hz), 117.14 (d, $^2J_{\text{CF}} = 22.0$ Hz), 51.27, 32.50, 31.04, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -110.50 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 1%), 287 (4), 230 (100), 202 (10), 175 (6), 117 (42), 109 (42), 91 (57), 65 (13), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0473.



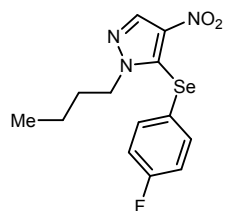
5-(2-methylphenylselanyl)-1-butyl-4-nitro-1H-pyrazole (4a): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.23 (s, 1H, C(3)-pyrazole), 7.24 - 7.20 (m, 2H, CH_{Ar}), 7.13 (d, 1H, $^3J = 7.5$ Hz, CH_{Ar}), 7.09 - 7.04 (m, 1H, CH_{Ar}), 4.09 (t, 2H, $^3J = 7.5$ Hz, CH_2), 2.40 (s, 3H, $\text{C}_{\text{Ar}}\text{-CH}_3$), 1.64 (quint, 2H, $^3J = 7.5$ Hz, CH_2), 1.19 (sext, 2H, $^3J = 7.5$ Hz, CH_2), 0.84 (t, 3H, $^3J = 7.3$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 139.34, 137.63, 137.19, 132.34, 131.05, 129.34, 128.87, 127.83, 127.45, 51.86, 31.75, 22.18, 19.72, 13.60, MS (GC, 70 eV): $m/z = 339$ (M^+ , 30%), 322 (9), 232 (100), 186 (15), 176 (25), 168 (58), 128 (10), 115 (17), 105 (63), 91 (96), 77 (18), 65 (31), 55 (26), 41 (45), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{14}\text{H}_{18}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 340.0564, found 340.0568.



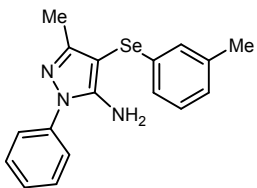
5-(2-fluorophenylselanyl)-1-butyl-4-nitro-1H-pyrazole (4b): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.24 (s, 1H, C(3)-pyrazole), 7.30 - 7.23 (m, 1H, CH_{Ar}), 7.15 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 7.11 - 7.05 (m, 1H, CH_{Ar}), 7.01 (td, 1H, $^3J = 8.4$ Hz, $^4J = 2.4$ Hz, CH_{Ar}), 4.24 (t, 2H, $^3J = 7.4$ Hz, CH_2), 1.73 (quint, 2H, $^3J = 7.5$ Hz, CH_2), 1.26 (sext, 2H, $^3J = 7.5$ Hz, CH_2), 0.89 (t, 3H, $^3J = 7.3$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 162.99 (d, $^1J_{\text{CF}} = 251.7$ Hz, $\text{C}_{\text{ipso-F}}$), 137.76, 137.33, 131.29 (d, $J_{\text{CF}} = 8.1$ Hz), 130.03 (d, $J_{\text{CF}} = 7.1$ Hz), 127.48 (d, $J_{\text{CF}} = 3.2$ Hz), 126.66, 118.88 (d, $^2J_{\text{CF}} = 23.1$ Hz), 115.78 (d, $^2J_{\text{CF}} = 21.1$ Hz), 51.97, 32.04, 19.74, 13.64, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -109.41 (CF), MS (GC, 70 eV): $m/z = 343$ (M^+ , 10%), 339 (21), 322 (5), 232 (97), 186 (11), 176 (29), 168 (100), 115 (10), 105 (39), 91 (44), 77 (9), 65 (17), 55 (27), 41 (38), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{13}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 344.0314, found 344.0326.



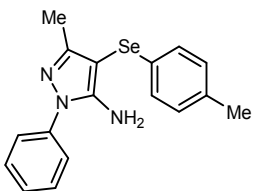
5-(3-fluorophenylselanyl)-1-butyl-4-nitro-1H-pyrazole (4c): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.21 (s, 1H, C(3)-pyrazole), 7.39 - 7.28 (m, 2H, CH_{Ar}), 7.08 (q, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 4.28 (t, 2H, $^3J = 7.4$ Hz, CH_2), 1.74 (quint, 2H, $^3J = 7.5$ Hz, CH_2), 1.27 (sext, 2H, $^3J = 7.5$ Hz, CH_2), 0.89 (t, 3H, $^3J = 7.4$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.21 (d, $^1J_{\text{CF}} = 245.5$ Hz, $\text{C}_{\text{ipso-F}}$), 137.81, 137.23, 134.29, 131.09 (d, $J_{\text{CF}} = 7.7$ Hz), 126.11, 125.55 (d, $J_{\text{CF}} = 3.4$ Hz), 116.22 (d, $^2J_{\text{CF}} = 22.7$ Hz), 115.12 (d, $^2J_{\text{CF}} = 21.4$ Hz), 51.92, 32.03, 19.73, 13.63, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -102.91 (CF), MS (GC, 70 eV): $m/z = 343$ (M^+ , 11%), 232 (42), 168 (100), 109 (53), 91 (12), 55 (17), 41 (25), HRMS (TOF MS ES+): calcd for $\text{C}_{13}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 344.0314, found 344.0316.



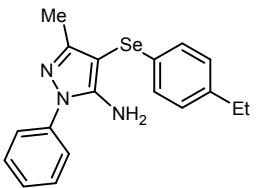
5-(4-fluorophenylselanyl)-1-butyl-4-nitro-1H-pyrazole (4d): yellow oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.16 (s, 1H, C(3)-pyrazole), 7.46 (d, 1H, $^3J = 8.4$ Hz, CH_{Ar}), 7.45 (d, 1H, $^3J = 8.4$ Hz, CH_{Ar}), 6.98 (t, 2H, $^3J = 8.6$ Hz, CH_{Ar}), 4.20 (t, 2H, $^3J = 7.4$ Hz, CH_2), 1.69 (quint, 2H, $^3J = 7.5$ Hz, CH_2), 1.23 (sext, 2H, $^3J = 7.5$ Hz, CH_2), 0.87 (t, 3H, $^3J = 7.3$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.08 (d, $^1J_{\text{CF}} = 250.0$ Hz, $\text{C}_{\text{ipso-F}}$), 137.28, 137.09, 135.15 (d, $J_{\text{CF}} = 8.2$ Hz), 127.72, 122.67 (d, $J_{\text{CF}} = 3.4$ Hz), 117.15 (d, $^2J_{\text{CF}} = 22.0$ Hz), 51.75, 31.89, 19.65, 13.55, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -110.75 (CF), MS (GC, 70 eV): $m/z = 343$ (M^+ , 23%), 232 (76), 190 (17), 175 (43), 168 (99), 109 (100), 95 (24), 83 (25), 55 (39), 41 (53), HRMS (TOF MS ES+): calcd for $\text{C}_{13}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 344.0314, found 344.0317.



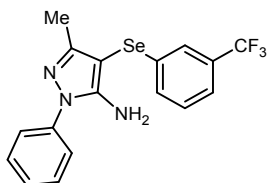
4-(m-tolylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5a): dark brown viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.61 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.49 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.35 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.11 (t, 1H, $^3J = 7.6$ Hz, CH_{Ar}), 7.06 (br.s, 1H, CH_{Ar}), 7.01 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 6.97 (d, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 4.23 (br. s, 2H, NH_2), 2.293 (s, 3H, CH_3), 2.290 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.31, 148.69, 139.21, 138.75, 132.74, 129.74, 129.19, 128.64, 127.56, 126.95, 125.10, 123.54, 84.76, 21.54, 13.25, MS (GC, 70 eV): $m/z = 343$ (M^+ , 26%), 263 (100), 222 (13), 131 (15), 119 (24), 91 (15), 77 (45), 66 (12), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{17}\text{H}_{18}\text{N}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 344.0666, found 344.0676.



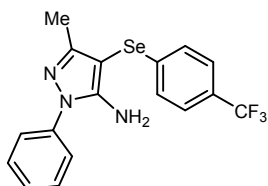
4-(p-tolylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5b): pale yellow crystals, mp. 98-99 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.47 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.33 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.14 (d, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 7.04 (d, 2H, $^3J = 8.00$ Hz, CH_{Ar}), 4.23 (br. s, 2H, NH_2), 2.287 (s, 3H, CH_3), 2.282 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.10, 148.51, 138.81, 135.75, 130.06, 129.58, 129.06, 128.26, 127.32, 123.36, 84.94, 20.99, 13.19, MS (GC, 70 eV): $m/z = 343$ (M^+ , 27%), 263 (100), 222 (12), 131 (11), 119 (17), 91 (14), 77 (35), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{17}\text{H}_{18}\text{N}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 344.0666, found 344.0674.



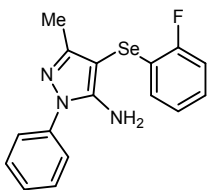
4-(4-ethylphenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5c): dark brown viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.47 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.33 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.16 (d, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 7.06 (d, 2H, $^3J = 8.2$ Hz, CH_{Ar}), 4.23 (br. s, 2H, NH_2), 2.58 (q, 2H, $^3J = 7.6$ Hz, CH_2), 2.28 (s, 3H, CH_3), 1.20 (t, 3H, $^3J = 7.6$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.19, 148.58, 142.21, 138.79, 129.61, 129.36, 128.92, 128.27, 127.38, 123.43, 84.91, 28.41, 15.65, 13.19, MS (GC, 70 eV): $m/z = 357$ (M^+ , 25%), 277 (100), 262 (32), 131 (9), 119 (16), 77 (34), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{20}\text{N}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 358.0822, found 358.0831.



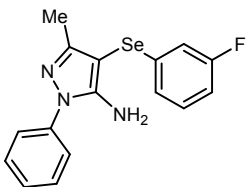
4-(3-(trifluoromethyl)phenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5d): dark green powder, mp. 104-105 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.60 - 7.47 (m, 3H, CH_{Ar}), 7.40 (d, 1H, $^3J = 7.3$ Hz, CH_{Ar}), 7.37 - 7.30 (m, 3H, CH_{Ar}), 4.25 (br. s, 2H, NH_2), 2.26 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.12, 148.78, 138.65, 134.59, 131.54 (q, $^2J_{\text{CF}} = 32.2$ Hz, $\text{C}_{\text{ipso}}\text{-CF}_3$), 123.88 (q, $^1J_{\text{CF}} = 272.8$ Hz, CF_3), 131.02, 129.74, 129.59, 127.68, 124.52 (dd, $J_{\text{CF}} = 7.6$ Hz, $J_{\text{CF}} = 3.7$ Hz), 123.61, 122.75 (dd, $J_{\text{CF}} = 7.1$ Hz, $J_{\text{CF}} = 3.4$ Hz), 83.50, 13.14, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -62.09 (CF_3), MS (GC, 70 eV): $m/z = 397$ (M^+ , 40%), 317 (100), 276 (13), 131 (19), 119 (36), 77 (53), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 398.0383, found 398.0392.



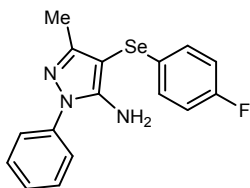
4-(4-(trifluoromethyl)phenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5e): dark brown viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.51 - 7.42 (m, 4H, CH_{Ar}), 7.35 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.30 (m, 2H, CH_{Ar}), 4.25 (br. s, 2H, NH_2), 2.25 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.13, 148.78, 138.69, 138.62, 129.70, 128.07 (q, $^2J_{\text{CF}} = 32.5$ Hz, $\text{C}_{\text{ipso}}\text{-CF}_3$), 127.62, 125.94 (dd, $J_{\text{CF}} = 7.1$ Hz, $J_{\text{CF}} = 3.4$ Hz), 124.28 (q, $^1J_{\text{CF}} = 271.9$ Hz, CF_3), 123.49, 83.23, 77.16, 13.10, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -61.77 (CF_3), MS (GC, 70 eV): $m/z = 397$ (M^+ , 43%), 317 (100), 276 (13), 131 (16), 119 (33), 77 (48), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{N}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 398.0383, found 398.0393.



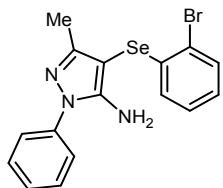
4-(2-fluorophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5f): light brown powder, mp. 97-99 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.55 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.44 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.31 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.16 - 7.09 (m, 1H, CH_{Ar}), 7.02 - 6.94 (m, 3H, CH_{Ar}), 4.28 (br. s, 2H, NH_2), 2.24 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 160.15 (d, $^1J_{\text{CF}} = 241.1$ Hz, $\text{C}_{\text{ipso-F}}$), 153.30, 148.93, 138.57, 129.52, 129.49 (d, $J_{\text{CF}} = 7.3$ Hz), 127.59 (d, $J_{\text{CF}} = 7.3$ Hz), 127.36, 124.88 (d, $J_{\text{CF}} = 3.0$ Hz), 123.30, 119.52 (d, $^2J_{\text{CF}} = 22.2$ Hz), 115.20 (d, $^2J_{\text{CF}} = 22.1$ Hz), 81.63, 12.99, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -107.38 (CF), MS (GC, 70 eV): $m/z = 347$ (M^+ , 39%), 267 (100), 250 (9), 226 (10), 131 (16), 119 (30), 77 (51), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{FN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 348.0415, found 348.0424.



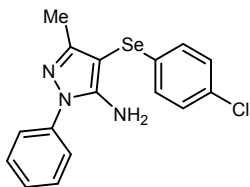
4-(3-fluorophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5g): black viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.59 (d, 2H, $^3J = 7.6$ Hz, CH_{Ar}), 7.48 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.35 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.17 (td, 1H, $^3J = 8.0$ Hz, $^3J = 5.9$ Hz, CH_{Ar}), 7.01 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 6.92 - 6.87 (m, 1H, CH_{Ar}), 6.84 (td, 1H, $^3J = 8.4$ Hz, $^3J = 2.4$ Hz), 4.23 (br. s, 2H, NH_2), 2.26 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.33 (d, $^1J_{\text{CF}} = 249.2$ Hz, $\text{C}_{\text{ipso-F}}$), 153.11, 148.69, 138.65, 135.37 (d, $J_{\text{CF}} = 6.2$ Hz), 130.42 (d, $J_{\text{CF}} = 8.0$ Hz), 129.66, 127.55, 123.51, 123.35 (d, $J_{\text{CF}} = 2.8$ Hz), 114.68 (d, $^2J_{\text{CF}} = 23.3$ Hz), 112.84 (d, $^2J_{\text{CF}} = 21.4$ Hz), 83.80, 13.11, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -111.27 (CF), MS (GC, 70 eV): $m/z = 347$ (M^+ , 35%), 267 (100), 226 (13), 131 (15), 119 (30), 77 (49), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{FN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 348.0415, found 348.0422.



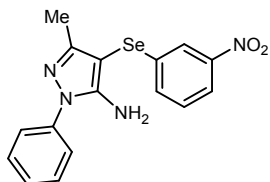
4-(4-fluorophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5h): light brown viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.2$ Hz, CH_{Ar}), 7.50 - 7.45 (m, 2H, CH_{Ar}), 7.34 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.22 - 7.17 (m, 2H, CH_{Ar}), 6.93 (t, 2H, $^3J = 8.8$ Hz, CH_{Ar}), 4.24 (br. s, 2H, NH_2), 2.27 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.76 (d, $^1J_{\text{CF}} = 244.8$ Hz, $\text{C}_{\text{ipso-F}}$), 153.04, 148.57, 138.73, 129.97 (d, $J_{\text{CF}} = 7.6$ Hz), 129.70, 127.55, 127.32 (d, $J_{\text{CF}} = 2.9$ Hz), 123.49, 116.42 (d, $^2J_{\text{CF}} = 21.7$ Hz), 84.99, 13.20, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -116.26 (CF), MS (GC, 70 eV): $m/z = 347$ (M^+ , 31%), 267 (100), 226 (14), 131 (12), 119 (25), 77 (45), 66 (14), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{FN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 348.0415, found 348.0426.



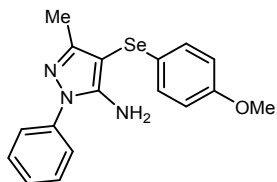
4-(2-bromophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5i): green crystals, mp. 109-110 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.60 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.53 - 7.44 (m, 3H, CH_{Ar}), 7.36 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.13 (td, 1H, $^3J = 7.8$ Hz, $^4J = 1.3$ Hz, CH_{Ar}), 7.03 (td, 1H, $^3J = 7.6$ Hz, $^4J = 1.6$ Hz, CH_{Ar}), 6.85 (dd, 1H, $^3J = 7.9$ Hz, $^4J = 1.6$ Hz, CH_{Ar}), 4.25 (br. s, 2H, NH_2), 2.26 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.55, 149.01, 138.61, 135.48, 132.90, 129.77, 128.03, 127.95, 127.70, 127.08, 123.59, 122.16, 84.35, 13.14, MS (GC, 70 eV): $m/z = 407$ (M^+ , 40), 329 (46), 327 (46), 247 (30), 233 (11), 156 (12), 131 (35), 119 (56), 104 (14), 77 (100), 66 (28), 51 (24), 39 (17), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{BrN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 407.9615, found 407.9617.



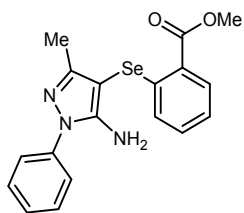
4-(4-chlorophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5j): dark brown viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.59 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.50 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.37 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.21 - 7.13 (m, 4H, CH_{Ar}), 4.24 (br. s, 2H, NH_2), 2.27 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.04, 148.63, 138.64, 131.91, 131.30, 129.67, 129.33, 129.27, 127.54, 123.45, 84.22, 13.14, MS (GC, 70 eV): $m/z = 363$ (M^+ , 29%), 283 (100), 247 (12), 131 (14), 119 (32), 77 (61), 66 (18), 51 (15), 39 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{ClN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 364.0120, found 364.0122.



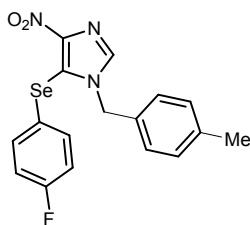
4-(3-nitrophenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5k): green powder, mp. 150-151 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.08 (t, 1H, $^4J = 1.9$ Hz, CH_{Ar}), 8.00 (ddd, 1H, $^3J = 8.0$ Hz, $^4J = 2.2$ Hz, $^4J = 0.9$ Hz, CH_{Ar}), 7.60 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.54 - 7.47 (m, 3H, CH_{Ar}), 7.38 (t, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 4.28 (br. s, 2H, NH_2), 2.27 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 153.05, 148.94, 148.89, 138.46, 135.88, 133.64, 129.93, 129.86, 127.95, 123.79, 122.68, 120.99, 83.21, 13.17, MS (GC, 70 eV): $m/z = 374$ (M^+ , 40%), 294 (100), 247 (17), 131 (30), 119 (52), 77 (70), 66 (16), 51 (16), 39 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{N}_4\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 375.0360, found 375.0365.



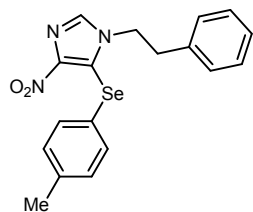
4-(4-methoxyphenylselanyl)-3-methyl-1-phenyl-1H-pyrazol-5-amine (5l): dark yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.58 (dd, 2H, $^3J = 8.5$ Hz, $^4J = 1.1$ Hz, CH_{Ar}), 7.48 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.34 (t, 1H, $^3J = 7.4$ Hz, CH_{Ar}), 7.21 (d, 2H, $^3J = 8.9$ Hz, CH_{Ar}), 6.79 (d, 2H, $^3J = 8.8$ Hz, CH_{Ar}), 4.23 (br. s, 2H, NH_2), 3.76 (s, 3H, OCH_3), 2.29 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 158.63, 153.03, 148.45, 138.77, 130.45, 129.72, 127.52, 123.53, 122.79, 115.14, 85.95, 55.46, 13.26, MS (GC, 70 eV): $m/z = 359$ (M^+ , 19%), 279 (100), 264 (35), 119 (20), 77 (42), 66 (10), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{18}\text{N}_3\text{OSe}$ ($\text{M} + \text{H}$) $^+$ 360.0615, found 360.0631.



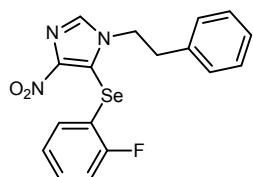
methyl 2-[(5-amino-3-methyl-1-phenyl-1H-pyrazol-4-yl)selenanyl]benzoate (5m): dark green crystals, mp. 160-163 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.07 (dd, 1H, $^3J = 7.8$ Hz, $^4J = 1.4$ Hz, CH_{Ar}), 7.61 (dd, 2H, $^3J = 8.4$ Hz, $^4J = 1.0$ Hz, CH_{Ar}), 7.48 (t, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 7.36 - 7.28 (m, 2H, CH_{Ar}), 7.22 - 7.17 (m, 1H, CH_{Ar}), 7.13 (dd, 1H, $^3J = 8.9$ Hz, $^4J = 0.8$ Hz, CH_{Ar}), 4.21 (br. s, 2H, NH_2), 3.97 (s, 3H, COOCH_3), 2.22 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 167.64, 153.82, 149.09, 139.31, 138.82, 133.00, 131.82, 129.66, 127.70, 127.42, 125.09, 123.46, 85.23, 52.43, 13.19, MS (GC, 70 eV): $m/z = 387$ (M^+ , 100%), 307 (64), 275 (75), 252 (22), 215 (20), 184 (14), 172 (43), 157 (12), 131 (44), 119 (61), 104 (17), 91 (16), 77 (95), 66 (21), 51 (17), 39 (11), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 388.0564, found 388.0578.



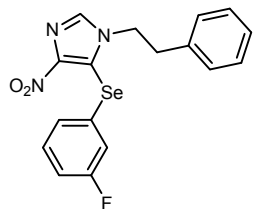
5-(4-fluorophenylselenanyl)-1-[(4-methylphenyl)methyl]-4-nitro-1H-imidazole (6): light yellow crystals, mp. 114-115 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.55 (s, 1H, C(2)-imidazole), 7.36 - 7.28 (m, 2H, CH_{Ar}), 7.12 (d, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 6.95 - 6.88 (m, 4H, CH_{Ar}), 5.17 (s, 2H, CH_2), 2.34 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.06 (d, $^1J_{\text{CF}} = 249.6$ Hz, $\text{C}_{\text{ipso-F}}$), 150.69, 138.99, 137.88, 134.90 (d, $J_{\text{CF}} = 8.1$ Hz), 131.05, 130.02, 127.55, 123.03 (d, $J_{\text{CF}} = 3.5$ Hz), 117.80, 117.07 (d, $^2J_{\text{CF}} = 22.0$ Hz), 51.06, 21.23, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -111.27 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 8%), 280 (3), 105 (100), 79 (14), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0313.



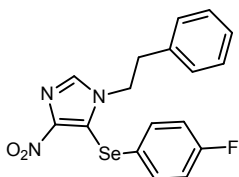
5-(p-tolylselanyl)-4-nitro-1-phenethyl-1H-imidazole (7a): yellow powder, mp. 94-95 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.32 (d, 2H, $^3J = 8.1$ Hz, CH_{Ar}), 7.30 - 7.22 (m, 4H, CH_{Ar}), 7.09 (d, 2H, $^3J = 8.0$ Hz CH_{Ar}), 6.95 (d, 2H, $^3J = 6.4$ Hz, CH_{Ar}), 4.22 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.90 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.31 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 150.46, 139.01, 137.73, 136.32, 132.39, 130.85, 129.16, 128.74, 127.55, 125.02, 48.99, 36.86, 21.27, MS (GC, 70 eV): $m/z = 387$ (M^+ , 8%), 280 (27), 105 (100), 91 (33), 79 (23), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{18}\text{H}_{18}\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 388.0564, found 388.0566.



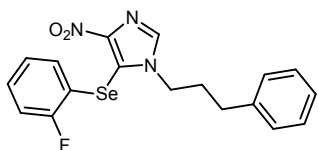
5-(2-fluorophenylselanyl)-4-nitro-1-phenethyl-1H-imidazole (7b): yellow powder, mp. 100-101 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.33 (s, 1H, C(2)-imidazole), 7.33 - 7.22 (m, 5H, CH_{Ar}), 7.10 - 7.03 (m, 2H, CH_{Ar}), 7.02 - 6.97 (m, 2H, CH_{Ar}), 4.37 (t, 2H, $^3J = 7.0$ Hz, CH_2), 2.97 (t, 2H, $^3J = 7.0$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 161.05 (d, $^1J_{\text{CF}} = 244.6$ Hz, $\text{C}_{\text{ipso-F}}$), 150.96, 137.79, 136.21, 133.89, 130.84 (d, $J_{\text{CF}} = 7.7$ Hz), 129.18, 128.77, 127.60, 125.56 (d, $J_{\text{CF}} = 3.3$ Hz), 116.17 (d, $^2J_{\text{CF}} = 22.7$ Hz), 115.96, 115.64 (d, $^2J_{\text{CF}} = 21.5$ Hz), 48.98, 37.28, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -103.60 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 11%), 280 (18), 105 (100), 91 (48), 79 (29), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0316.



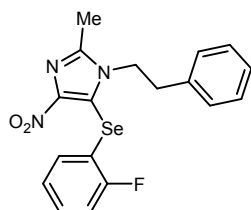
5-(3-fluorophenylselanyl)-4-nitro-1-phenethyl-1H-imidazole (7c): yellow powder, mp. 71-72 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.35 (s, 1H, C(2)-imidazole), 7.30 - 7.21 (m, 4H, CH_{Ar}), 7.10 (d, 1H, $^3J = 7.8$ Hz, CH_{Ar}), 7.02 (d, 1H, $^3J = 8.3$ Hz, CH_{Ar}), 6.99 - 6.94 (m, 3H, CH_{Ar}), 4.29 (t, 2H, $^3J = 7.0$ Hz, CH_2), 2.94 (t, 2H, $^3J = 7.0$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.00 (d, $^1J_{\text{CF}} = 251.6$ Hz, $\text{C}_{\text{ipso-F}}$), 150.96, 138.04, 136.05, 131.26 (d, $J_{\text{CF}} = 8.1$ Hz), 130.69 (d, $J_{\text{CF}} = 6.9$ Hz), 129.15, 128.67, 127.58, 126.66 (d, $J_{\text{CF}} = 3.1$ Hz), 118.06 (d, $^2J_{\text{CF}} = 23.1$ Hz), 116.30, 115.46 (d, $^2J_{\text{CF}} = 21.1$ Hz), 48.99, 37.02, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -109.35 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 12%), 280 (14), 105 (100), 91 (49), 79 (31), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0321.



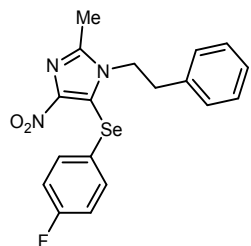
5-(4-fluorophenylselanyl)-4-nitro-1-phenethyl-1H-imidazole (7d): yellow powder, mp. 105-106 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.45 - 7.37 (m, 2H, CH_{Ar}), 7.29 (s, 1H, C(2)-imidazole), 7.28 - 7.22 (m, 3H, CH_{Ar}), 7.01 - 6.93 (m, 4H, CH_{Ar}), 4.29 (t, 2H, $^3J = 7.0$ Hz, CH_2), 2.94 (t, 2H, $^3J = 7.0$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.01 (d, $^1J_{\text{CF}} = 249.7$ Hz, $\text{C}_{\text{ipso-F}}$), 150.50, 137.75, 136.12, 134.45 (d, $J_{\text{CF}} = 8.1$ Hz), 129.17, 128.68, 127.59, 123.31 (d, $J_{\text{CF}} = 3.3$ Hz), 117.63, 117.25 (d, $^2J_{\text{CF}} = 22.0$ Hz), 48.90, 36.99, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -111.13 (CF), MS (GC, 70 eV): $m/z = 391$ (M^+ , 7%), 280 (13), 105 (100), 91 (42), 79 (25), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 392.0314, found 392.0318.



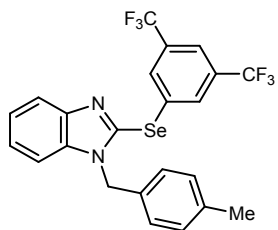
5-(2-fluorophenylselanyl)-4-nitro-1-phenylpropyl-1H-imidazole (8): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.78 (br. s. 1H, C(2)-imidazole), 7.30 - 7.19 (m, 5H, CH_{Ar}), 7.10 - 7.02 (m, 4H, CH_{Ar}), 4.08 (t, 2H, $^3J = 7.4$ Hz, CH_2), 2.60 (t, 2H, $^3J = 7.4$ Hz, CH_2), 2.06 (quint, 2H, $^3J = 7.4$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 160.94 (d, $^1J_{\text{CF}} = 244.9$ Hz, $\text{C}_{\text{ipso-F}}$), 139.54, 133.66, 130.74 (d, $J_{\text{CF}} = 7.7$ Hz), 128.74, 128.24, 126.58, 125.50 (d, $J_{\text{CF}} = 3.2$ Hz), 116.11 (d, $^2J_{\text{CF}} = 22.5$ Hz), 115.47 (d, $^2J_{\text{CF}} = 21.4$ Hz), 47.36, 32.50, 31.87, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -103.55 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 17%), 294 (13), 230 (26), 184 (38), 117 (68), 91 (100), HRMS (TOF MS ES+): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0469.



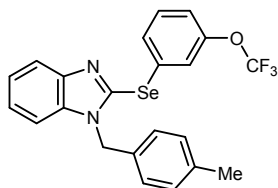
5-(2-fluorophenylselanyl)-2-methyl-4-nitro-1-phenethyl-1H-imidazole (9a): dark yellow powder, mp. 85-86 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.33 - 7.23 (m, 5H, CH_{Ar}), 7.05 (q, 2H, $^3J = 7.8$ Hz, CH_{Ar}), 7.01 - 6.98 (m, 2H, CH_{Ar}), 4.31 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.93 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.21 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 160.92 (d, $^1J_{\text{CF}} = 244.1$ Hz, $\text{C}_{\text{ipso-F}}$), 150.07, 147.01, 136.40, 133.55, 133.54 (d, $J = 1.9$ Hz), 130.57 (d, $J_{\text{CF}} = 7.7$ Hz), 129.19, 128.94, 127.62, 125.52 (d, $J_{\text{CF}} = 3.3$ Hz), 116.10 (d, $^2J_{\text{CF}} = 22.3$ Hz), 115.31, 47.96, 36.93, 13.96, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -103.97 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 14%), 294 (12), 230 (12), 213 (12), 184 (8), 105 (100), 91 (43), 79 (30), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0475.



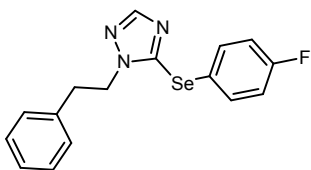
5-(4-fluorophenylselanyl)-2-methyl-4-nitro-1-phenethyl-1H-imidazole (9b): yellow powder, mp. 108-109 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.43 (dd, 2H, $^3J = 8.7$ Hz, $^3J = 5.2$ Hz, CH_{Ar}), 7.32 - 7.26 (m, 3H, CH_{Ar}), 6.98 (m, 4H, CH_{Ar}), 4.24 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.90 (t, 2H, $^3J = 7.1$ Hz, CH_2), 2.16 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 162.98 (d, $^1J_{\text{CF}} = 249.1$ Hz, $\text{C}_{\text{ipso-F}}$), 149.67, 146.94, 136.36, 134.11 (d, $J_{\text{CF}} = 8.1$ Hz), 129.23, 128.85, 127.66, 123.86 (d, $J_{\text{CF}} = 2.8$ Hz), 117.24 (d, $^2J_{\text{CF}} = 22.0$ Hz), 116.96, 47.87, 36.74, 13.93, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -111.54 (CF), MS (GC, 70 eV): $m/z = 405$ (M^+ , 11%), 294 (18), 230 (10), 213 (10), 105 (100), 91 (36), 79 (26), HRMS (TOF MS ES $^+$): calcd for $\text{C}_{18}\text{H}_{17}\text{FN}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 406.0470, found 406.0466.



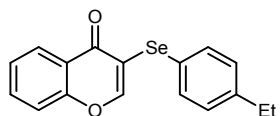
2-(3,5-bis(trifluoromethyl)phenylselanyl)-1-[(4-methylphenyl)methyl]-1H-benzo[d]imidazole (10a): yellow powder, mp. 94-95 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.86 - 7.83 (m, 3H, CH_{Ar}), 7.67 (s, 1H, CH_{Ar}), 7.36 - 7.29 (m, 3H, CH_{Ar}), 6.96 (d, H, $^3J = 7.9$ Hz, CH_{Ar}), 6.83 (d, H, $^3J = 7.9$ Hz, CH_{Ar}), 5.48 (s, 2H, CH_2), 2.24 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 141.91, 137.82, 136.11, 132.41, 132.25 - 132.13 (m, $\text{C}_{\text{ipso}}\text{-CF}_3$), 131.00, 129.53, 126.26, 124.16, 122.98, 122.64 (q, $^1J_{\text{CF}} = 272.9$ Hz, CF_3), 121.72 (m), 120.18, 110.27, 48.90, 20.92. $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -62.37 (CF_3), MS (GC, 70 eV): $m/z = 514$ (M^+ , 8%), 433 (3), 317 (11), 105 (100), 79 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{23}\text{H}_{17}\text{F}_6\text{N}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 515.0461, found 515.0462.



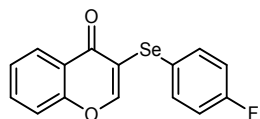
2-(3-(trifluoromethoxy)phenylselanyl)-1-[(4-methylphenyl)methyl]-1H-benzo[d]imidazole (10b): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.85 - 7.83 (m, 1H, CH_{Ar}), 7.40 (d, 1H, $^3J = 7.9$ Hz, CH_{Ar}), 7.34 (s, 1H, CH_{Ar}), 7.30 - 7.25 (m, 3H, CH_{Ar}), 7.22 (t, 1H, $^3J = 8.0$ Hz, CH_{Ar}), 7.08 (d, 1H, $^3J = 8.3$ Hz, CH_{Ar}), 7.02 (d, 2H, $^3J = 7.9$ Hz, CH_{Ar}), 6.89 (d, 2H, $^3J = 8.0$ Hz, CH_{Ar}), 5.44 (s, 2H, CH_2), 2.28 (s, 3H, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 149.53, 144.01, 143.15, 137.82, 136.04, 132.62, 130.67, 130.64, 130.11, 129.58, 126.58, 124.71, 123.86, 122.81, 120.40 (q, $J_{\text{CF}} = 257.9$ Hz, OCF_3), 120.35, 120.14, 110.48, 49.08, 21.12, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -57.15 (CF_3), MS (GC, 70 eV): $m/z = 462$ (M^+ , 9%), 382 (8), 265 (13), 105 (100), 79 (13), HRMS (TOF MS ES+): calcd for $\text{C}_{22}\text{H}_{18}\text{F}_3\text{N}_2\text{OSe}$ ($\text{M} + \text{H}$) $^+$ 463.0536, found 463.0557.



5-(4-fluorophenylselanyl)-1-phenethyl-1H-1,2,4-triazole (11): yellow powder, mp. 87-88 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 7.97 (s, 1H, C(3)-triazole), 7.45 - 7.41 (m, 2H, CH_{Ar}), 7.28 - 7.22 (m, 3H, CH_{Ar}), 7.04 - 7.02 (m, 2H, CH_{Ar}), 7.00 - 6.95 (m, 2H, CH_{Ar}), 4.44 (t, 2H, $^3J = 7.2$ Hz, CH_2), 3.10 (t, 2H, $^3J = 7.2$ Hz, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 163.16 (d, $^1J_{\text{CF}} = 249.4$ Hz, $\text{C}_{\text{ipso-F}}$), 152.78, 137.16, 135.80 (d, $J_{\text{CF}} = 8.2$ Hz), 128.91, 128.89, 127.14, 121.67 (d, $J_{\text{CF}} = 3.3$ Hz), 117.02 (d, $^2J_{\text{CF}} = 21.9$ Hz), 51.24, 36.32, $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -111.33 (CF), MS (GC, 70 eV): $m/z = 347$ (M^+ , 37%), 243 (100), 216 (14), 175 (23), 163 (26), 136 (19), 122 (18), 104 (70), 91 (82), 77 (32), 65 (30), 55 (54), HRMS (TOF MS ES+): calcd for $\text{C}_{16}\text{H}_{15}\text{FN}_3\text{Se}$ ($\text{M} + \text{H}$) $^+$ 348.0415, found 348.0420.

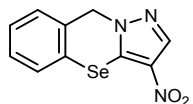


3-(4-ethylphenylselanyl)-4H-chromen-4-one (12a): yellow viscous oil, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.24 (dd, 1H, $^3J = 8.3$ Hz, $^4J = 1.6$ Hz, CH_{Ar}), 7.79 (s, 1H, CH_{Ar}), 7.70 - 7.62 (m, 1H, CH_{Ar}), 7.55 (d, 2H, $^3J = 8.1$ Hz, CH_{Ar}), 7.44 - 7.38 (m, 2H, CH_{Ar}), 7.15 (d, 2H, $^3J = 8.1$ Hz, CH_{Ar}), 2.63 (q, 2H, $^3J = 7.6$ Hz, CH_2), 1.22 (t, 3H, $^3J = 7.6$ Hz, CH_3), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 175.43, 156.47, 155.03, 144.92, 134.78, 133.88, 129.39, 126.45, 125.60, 124.25, 123.17, 118.68, 118.16, 28.68, 15.55, MS (GC, 70 eV): $m/z = 330$ (M^+ , 46%), 279 (15), 249 (48), 235 (38), 210 (23), 195 (17), 167 (45), 149 (100), 115 (48), 105 (16), 89 (16), 71 (25), 57 (33), 43 (23), HRMS (TOF MS ES+): calcd for $\text{C}_{17}\text{H}_{15}\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 331.0237, found 331.0245.

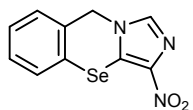


3-(4-fluorophenylselanyl)-4H-chromen-4-one (12b): brown powder, mp. 84-85 °C, ^1H NMR (500 MHz, CDCl_3): δ (ppm): 8.23 (dd, 1H, $^3J = 8.1$ Hz, $^4J = 1.4$ Hz, CH_{Ar}), 7.89 (s, 1H, CH_{Ar}), 7.67 (ddd, 1H, $^3J = 8.7$ Hz, $^3J = 7.2$ Hz, $^4J = 1.6$ Hz, CH_{Ar}), 7.62 (dd, 2H, $^3J = 8.8$ Hz, $^3J = 5.4$ Hz, CH_{Ar}), 7.47 - 7.37 (m, 2H, CH_{Ar}), 7.00 (t, 2H, $^3J = 8.7$ Hz, CH_{Ar}), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 175.31, 163.09 (d, $^1J_{\text{CF}} = 248.5$ Hz, $\text{C}_{\text{ipso-F}}$), 156.47, 155.68, 136.55 (d, $J_{\text{CF}} = 8.1$ Hz), 134.04, 126.46, 125.76, 123.26, 122.64 (d, $J_{\text{CF}} = 3.4$ Hz), 118.21, 118.17,

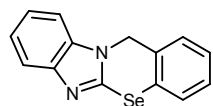
116.90 (d, $^2J_{CF} = 21.7$ Hz), $^{19}\text{F}\{^1\text{H}\}$ NMR (188.34 MHz, CDCl_3): δ (ppm): -112.24 (CF), MS (GC, 70 eV): $m/z = 320$ (M^+ , 79%), 239 (56), 200 (51), 183 (16), 120 (100), 92 (47), 75 (16), 63 (25), HRMS (TOF MS ES+): calcd for $\text{C}_{15}\text{H}_{10}\text{FO}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 320.9830, found 320.9837.



3-nitro-9H-pyrazolo[5,1-b][1,3]benzoselenazine (13a): green powder, mp. 195-196 °C, ^1H NMR (500 MHz, CDCl_3): 8.18 (s, 1H, C(2)), 7.55 - 7.53 (m, 1H, CH_{Ar}), 7.37 - 7.34 (m, 3H, CH_{Ar}), 5.27 (s, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 136.55, 131.06, 130.33, 129.43, 129.05, 128.94, 128.37, 125.09, 53.97, MS (GC, 70 eV): $m/z = 281$ (M^+ , 100%), 235 (10), 206 (10), 169 (22), 155 (44), 126 (20), 115 (33), 105 (17), 89 (32), 77 (14), 63 (17), HRMS (TOF MS ES+): calcd for $\text{C}_{10}\text{H}_8\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 281.9782, found 281.9785.



3-nitro-9H-imidazo[5,1-b][1,3]benzoselenazine (13b): yellow powder, mp. 228-229 °C, ^1H NMR (500 MHz, DMSO-d_6): 8.16 (s, 1H, C(2)), 7.78 - 7.75 (m, 1H, CH_{Ar}), 7.52 - 7.50 (m, 1H, CH_{Ar}), 7.42 - 7.37 (m, 2H, CH_{Ar}), 5.31 (s, 2H, CH_2), ^{13}C NMR (126 MHz, DMSO-d_6): δ (ppm): 144.87, 138.03, 131.33, 129.55, 129.13, 129.01, 128.06, 125.78, 123.28, 48.85, MS (GC, 70 eV): $m/z = 281$ (M^+ , 100%), 235 (20), 208 (58), 196 (10), 181 (23), 169 (54), 155 (17), 128 (18), 116 (17), 89 (50), 77 (11), 63 (21), HRMS (TOF MS ES+): calcd for $\text{C}_{10}\text{H}_8\text{N}_3\text{O}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 281.9782, found 281.9785.



12H-benzimidazo[2,1-b][1,3]benzoselenazine (13c): colorless crystals, mp. 174-175 °C, ^1H NMR (500 MHz, CDCl_3): 7.70 (s, 1H, CH_{Ar}), 7.46 - 7.21 (m, 7H, CH_{Ar}), 5.09 (s, 2H, CH_2), ^{13}C NMR (126 MHz, CDCl_3): δ (ppm): 144.45, 143.24, 135.03, 131.96, 129.81, 128.82, 128.42, 127.47, 126.94, 122.32, 122.10, 118.81, 108.48, 47.92, MS (GC, 70 eV): $m/z = 286$ (M^+ , 41%), 206 (100), 103 (10), 77 (12), HRMS (TOF MS ES+): calcd for $\text{C}_{14}\text{H}_{11}\text{N}_2\text{Se}$ ($\text{M} + \text{H}$) $^+$ 287.0087, found 287.0092.

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(C) Copies ^1H and ^{13}C NMR spectra.

Compound **sm3**

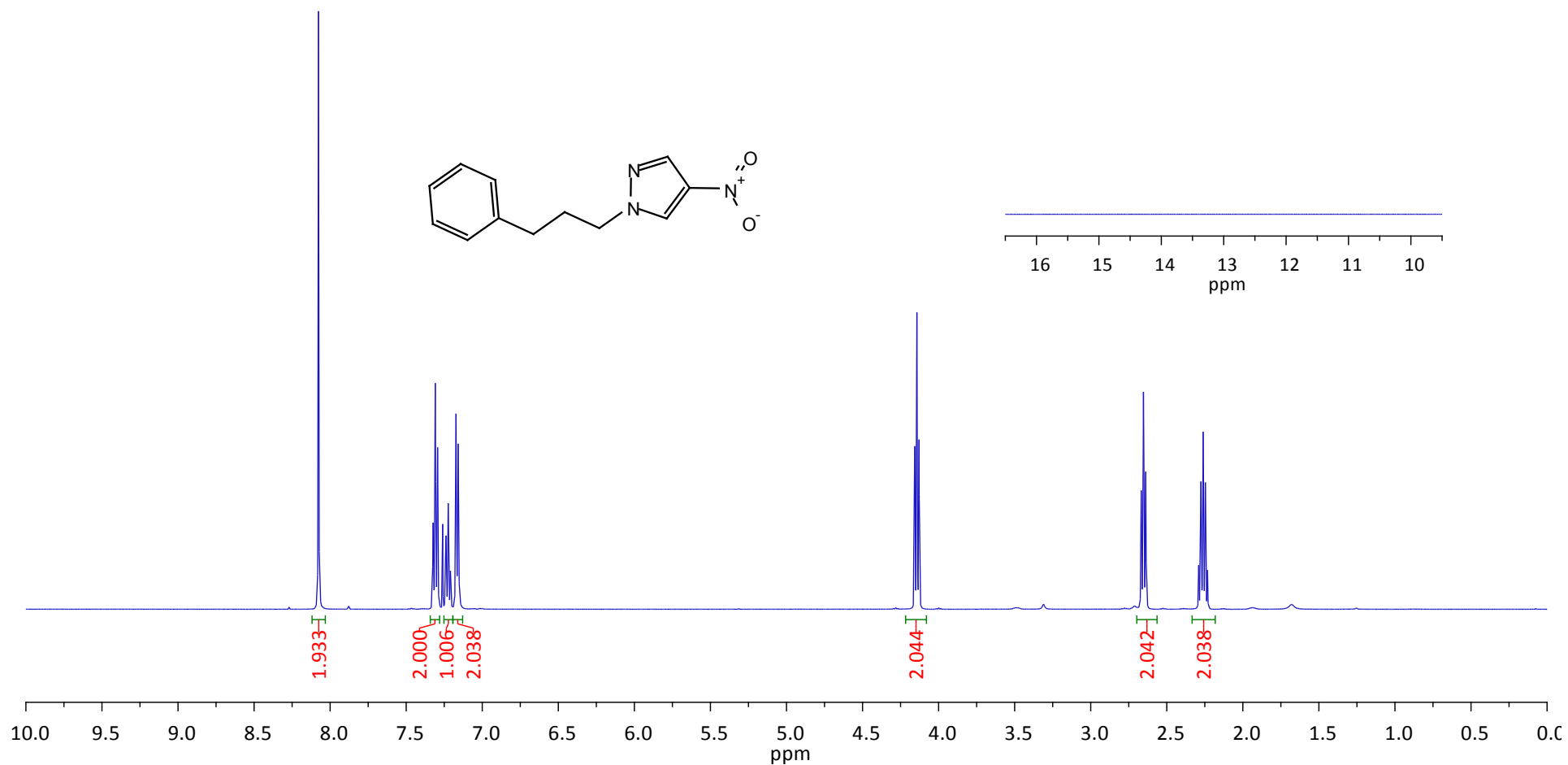
8.077
7.323
7.309
7.294
7.260
7.224
7.172
7.158

4.143

2.653

2.261

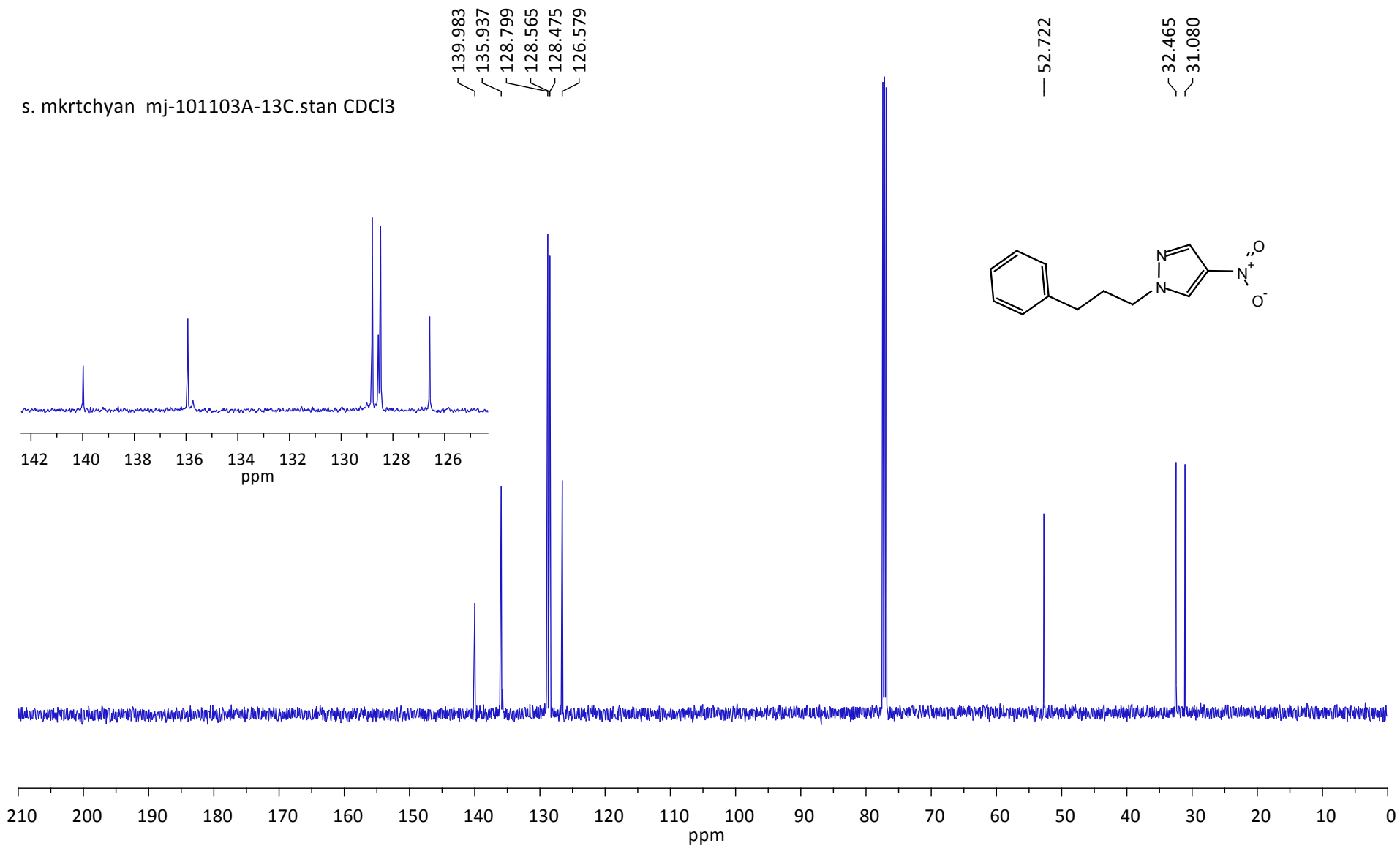
s. mkrtyan mj-1011031H.stan CDCl3



Comment s. mkrtyan mj-1011031H.stan CDCl3
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 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **sm3**

s. mkrtyan mj-101103A-13C.stan CDCl3



Comment s. mkrtyan mj-101103A-13C.stan CDCl3
Number of Scans 512
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

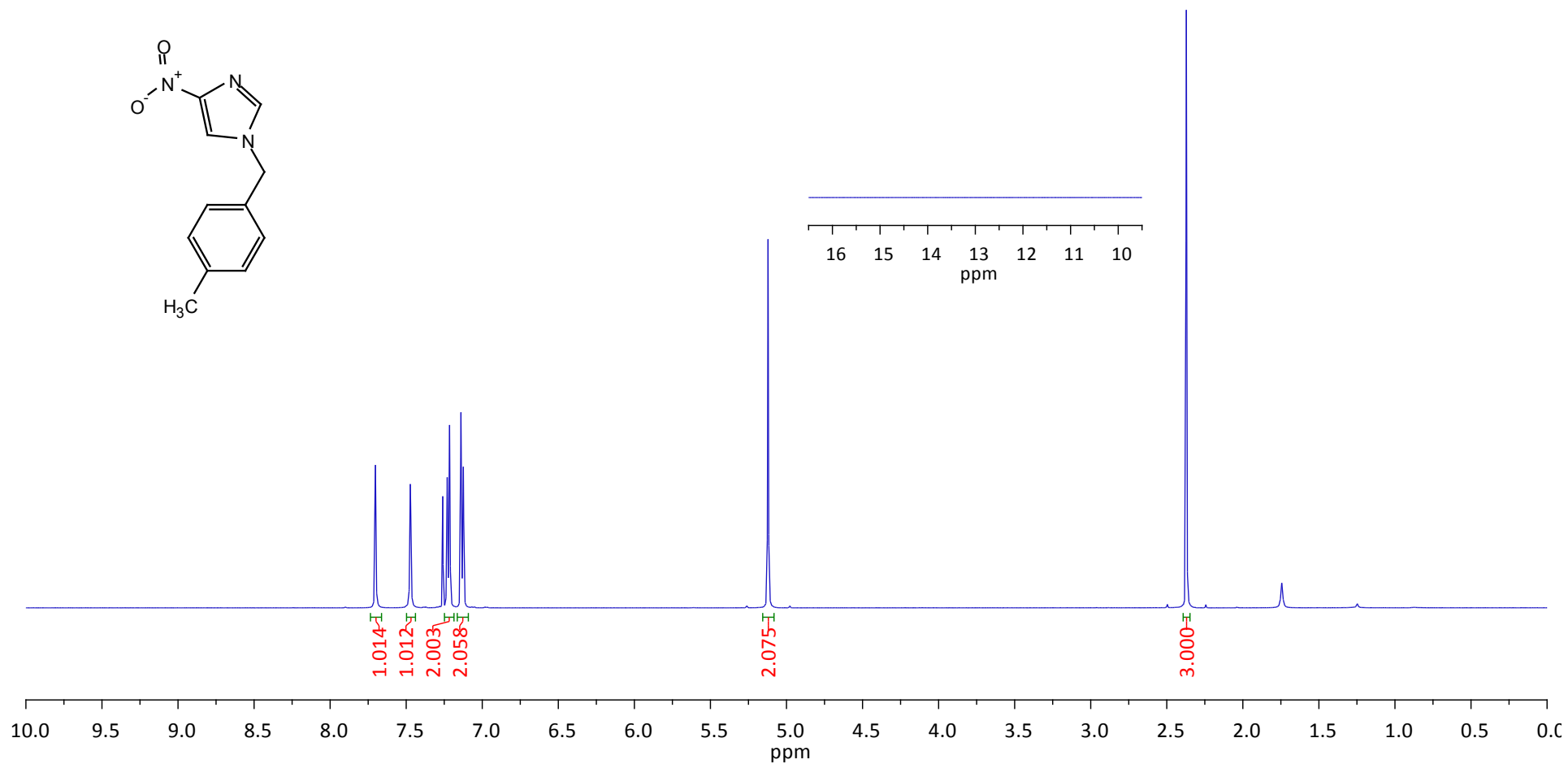
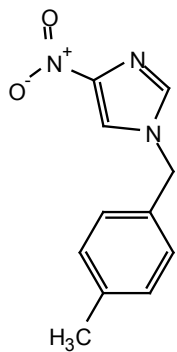
Compound **sm6**

7.702
7.473
7.230
7.215
7.140
7.124

5.121

2.371

s. mkrtyan =mj-137=1H.stan CDCl3



Comment s. mkrtyan =mj-137=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **sm6**

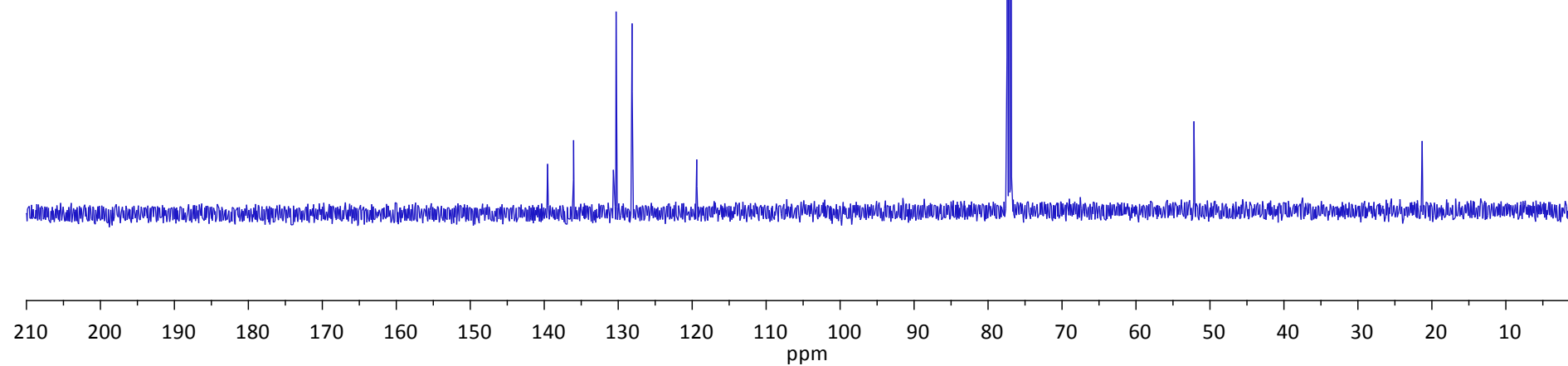
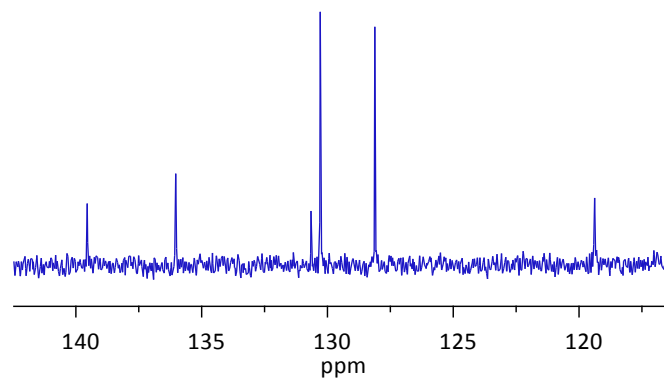
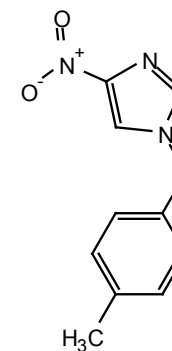
s. mkrtyan =mj-137=A-13C.stan CDCl3

139.551
136.034
130.653
130.287
128.116

119.378

52.169

21.314



Comment	s. mkrtyan =mj-137=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **sm8**

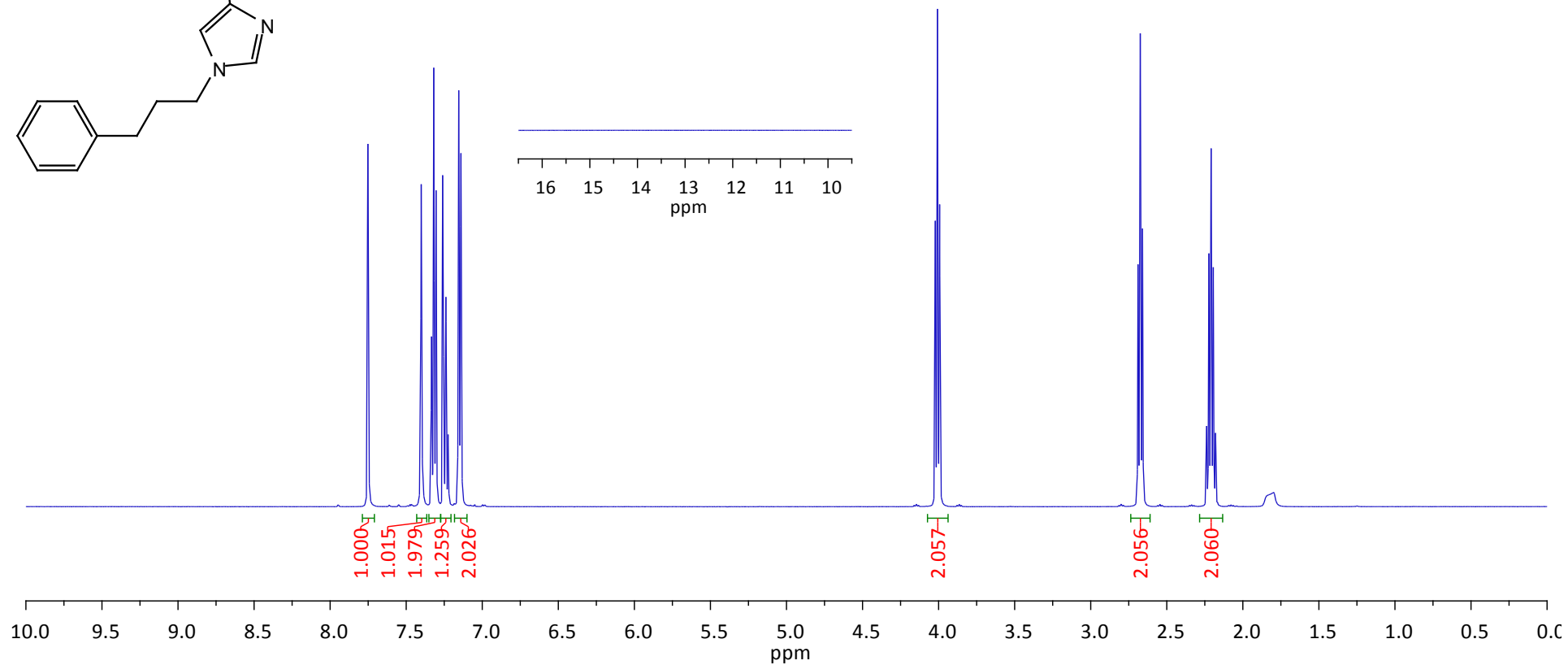
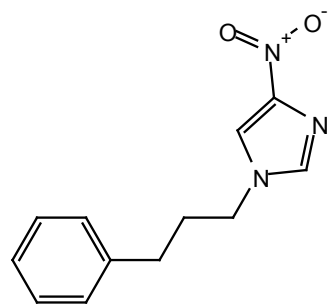
7.752
7.401
7.399
7.260
7.239
7.154
7.140

4.008
3.993

2.674

2.209

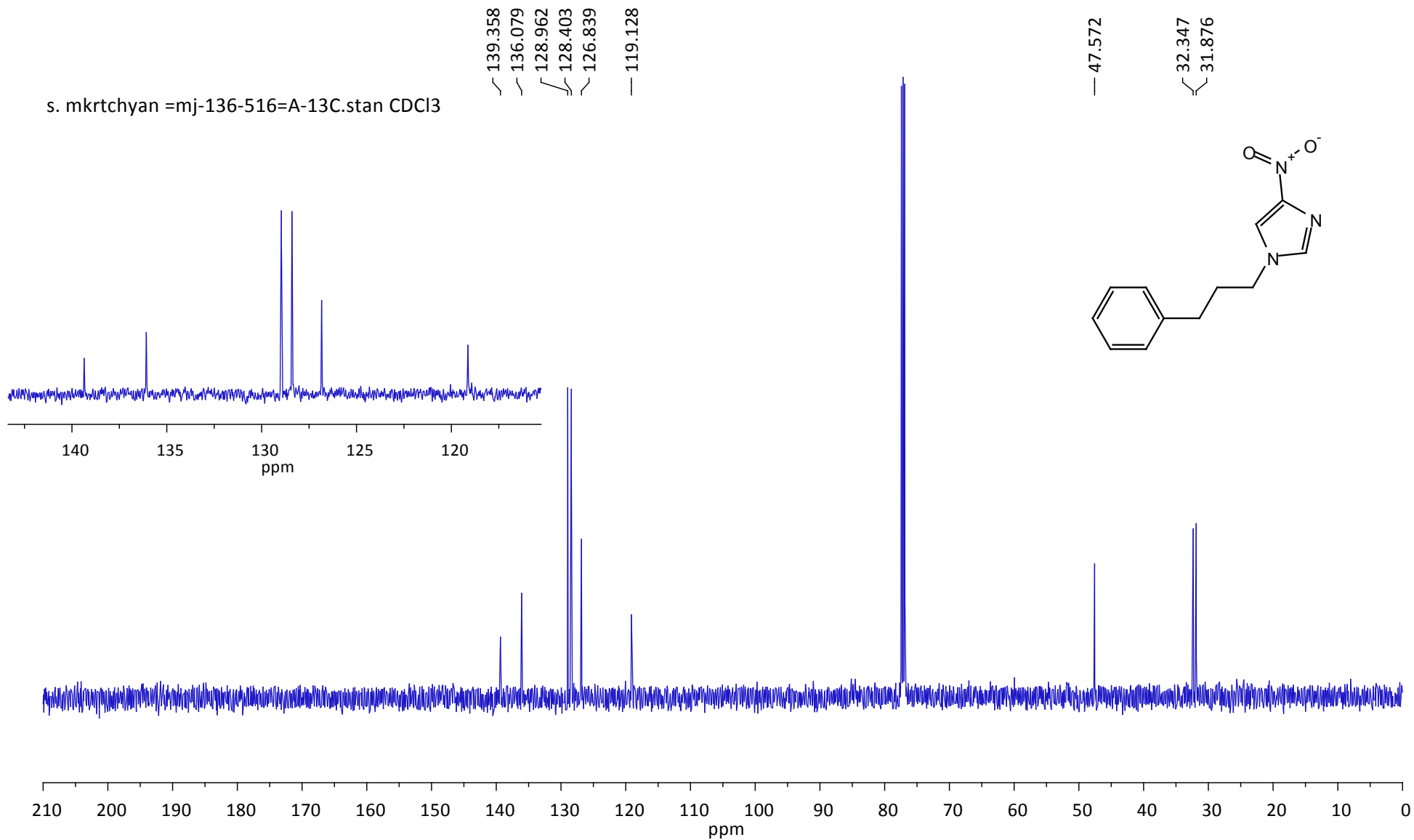
s. mkrtyan =mj-136-516=1H.stan CDCl3



Comment s. mkrtyan =mj-136-516=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

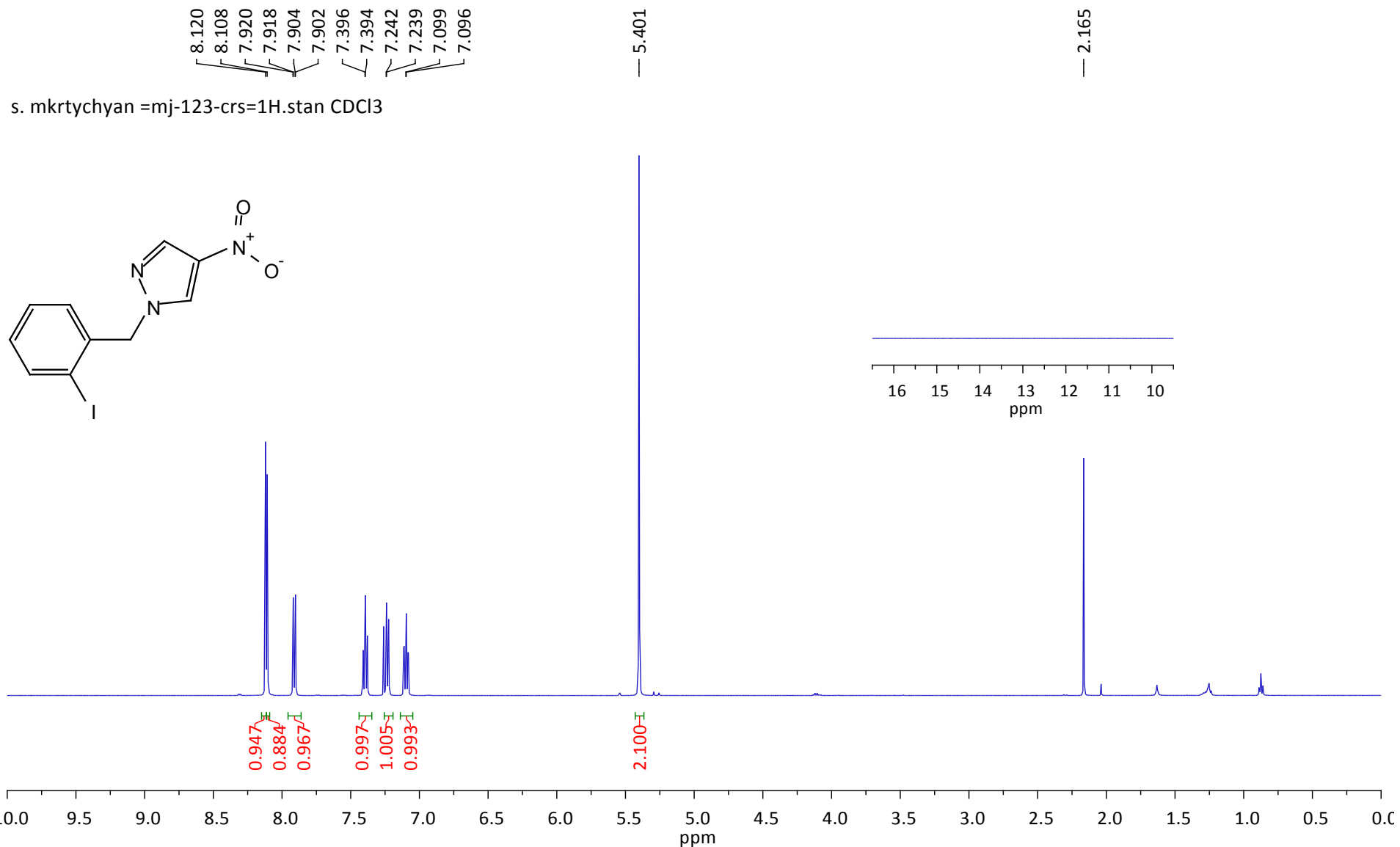
Compound **sm8**

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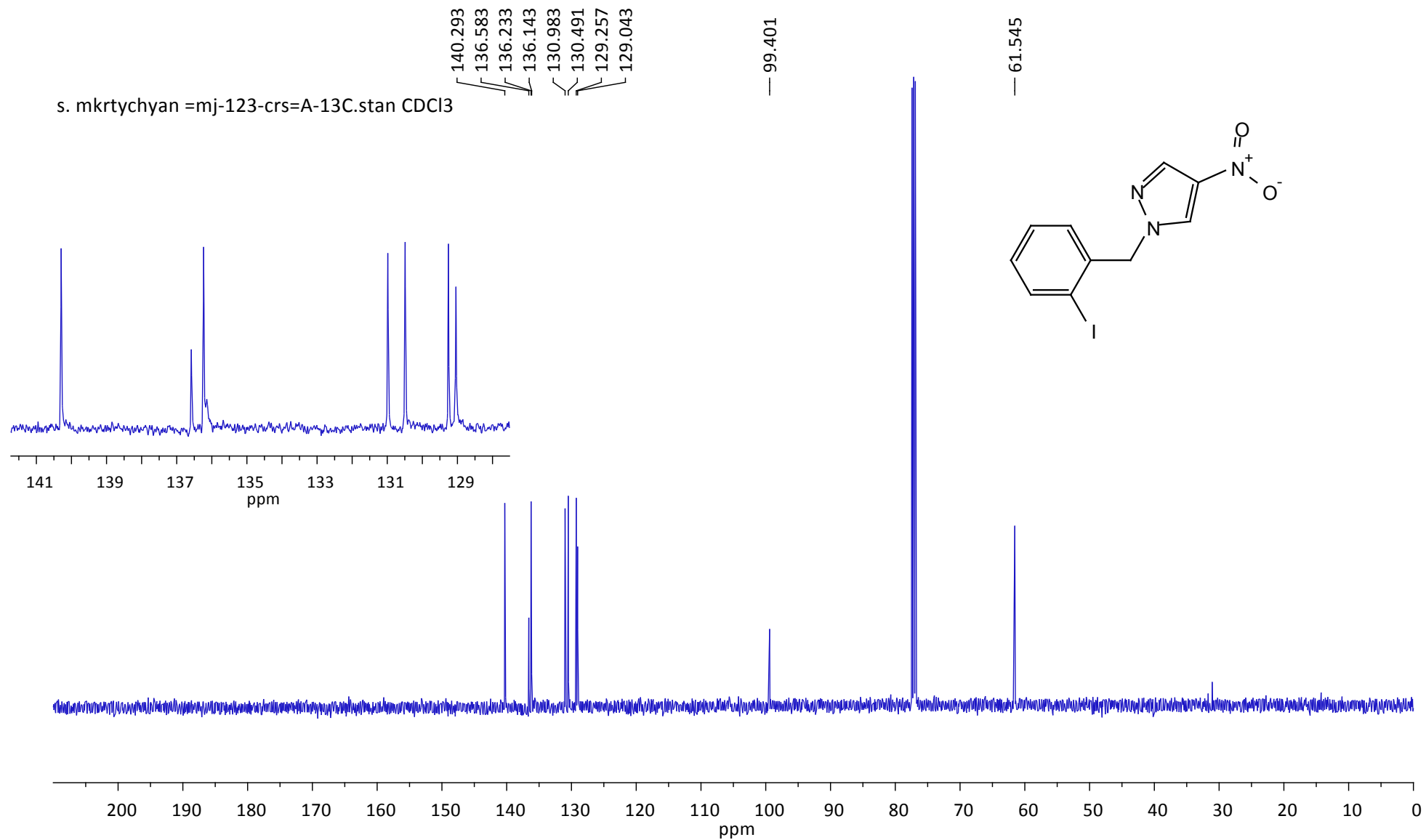
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Number of Scans	128
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **sm13**



Comment s. mkrtychyan =mj-123-crs=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **sm13**



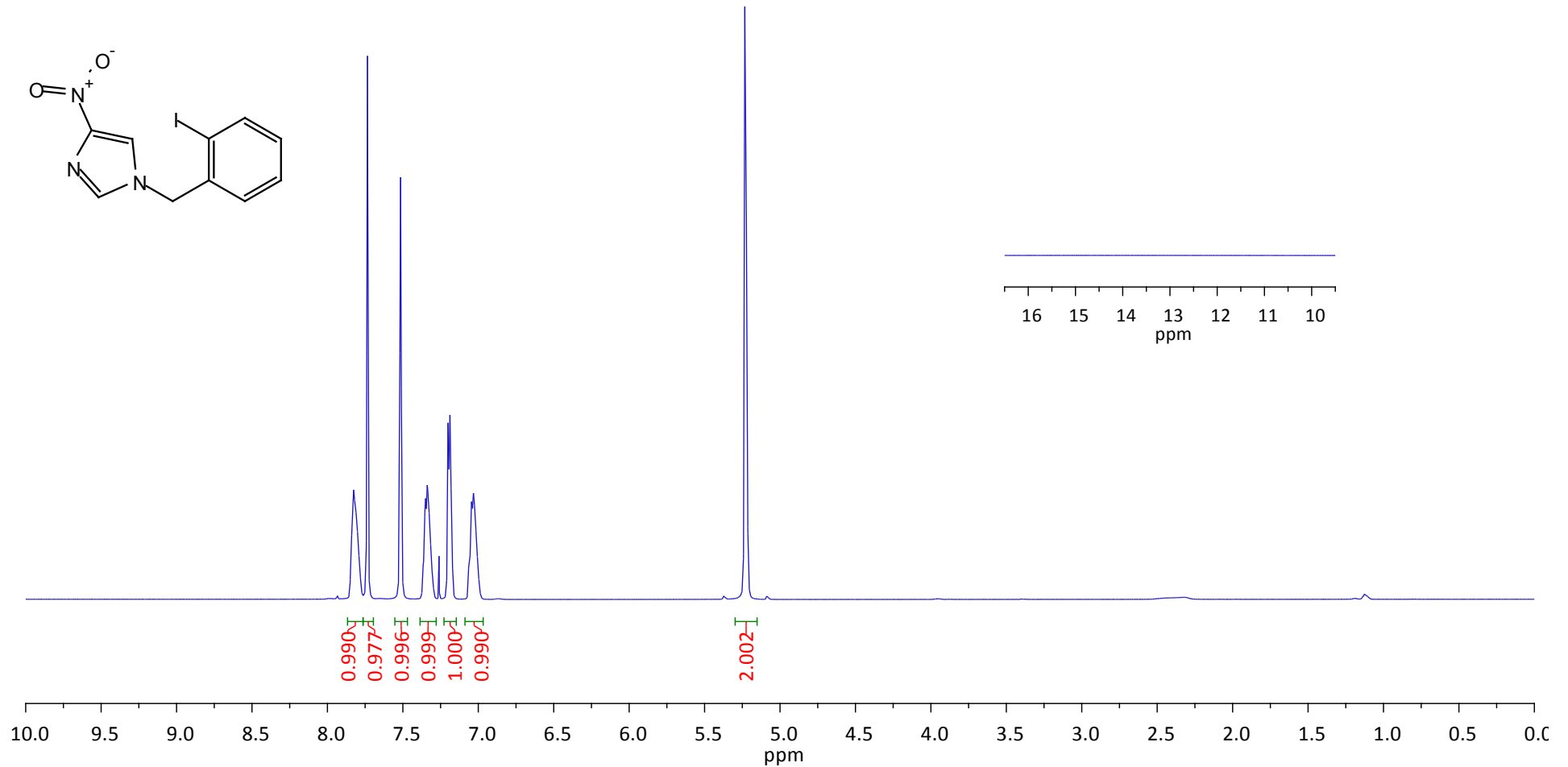
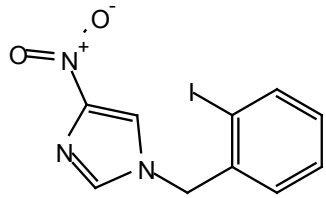
Comment	s. mkrtychyan =mj-123-crs=A-13C.stan CDCl ₃
Number of Scans	224
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **sm14**

7.826
7.735
7.515
7.349
7.338
7.260
7.201
7.188
7.044
7.032

5.233

s. mkrtyan =mja-140-crs1=1H.stan CDCl3



Comment s. mkrtyan =mja-140-crs1=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **sm14**

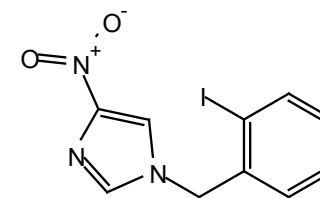
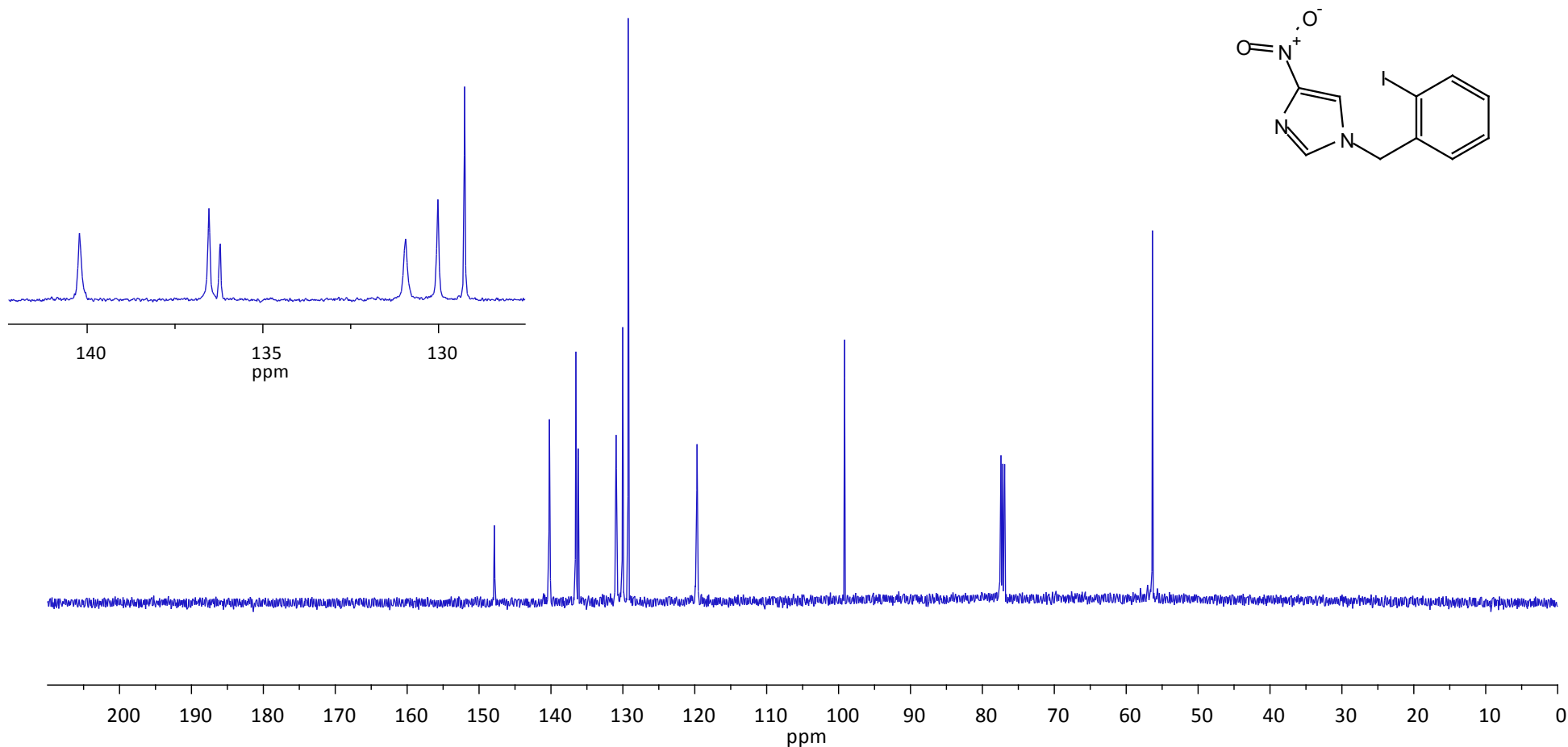
s. mkrtyan =mja-140-crs1=A-13C.stan CDCl3

147.870
140.219
136.533
136.210
130.940
130.019
129.258

119.685

99.164

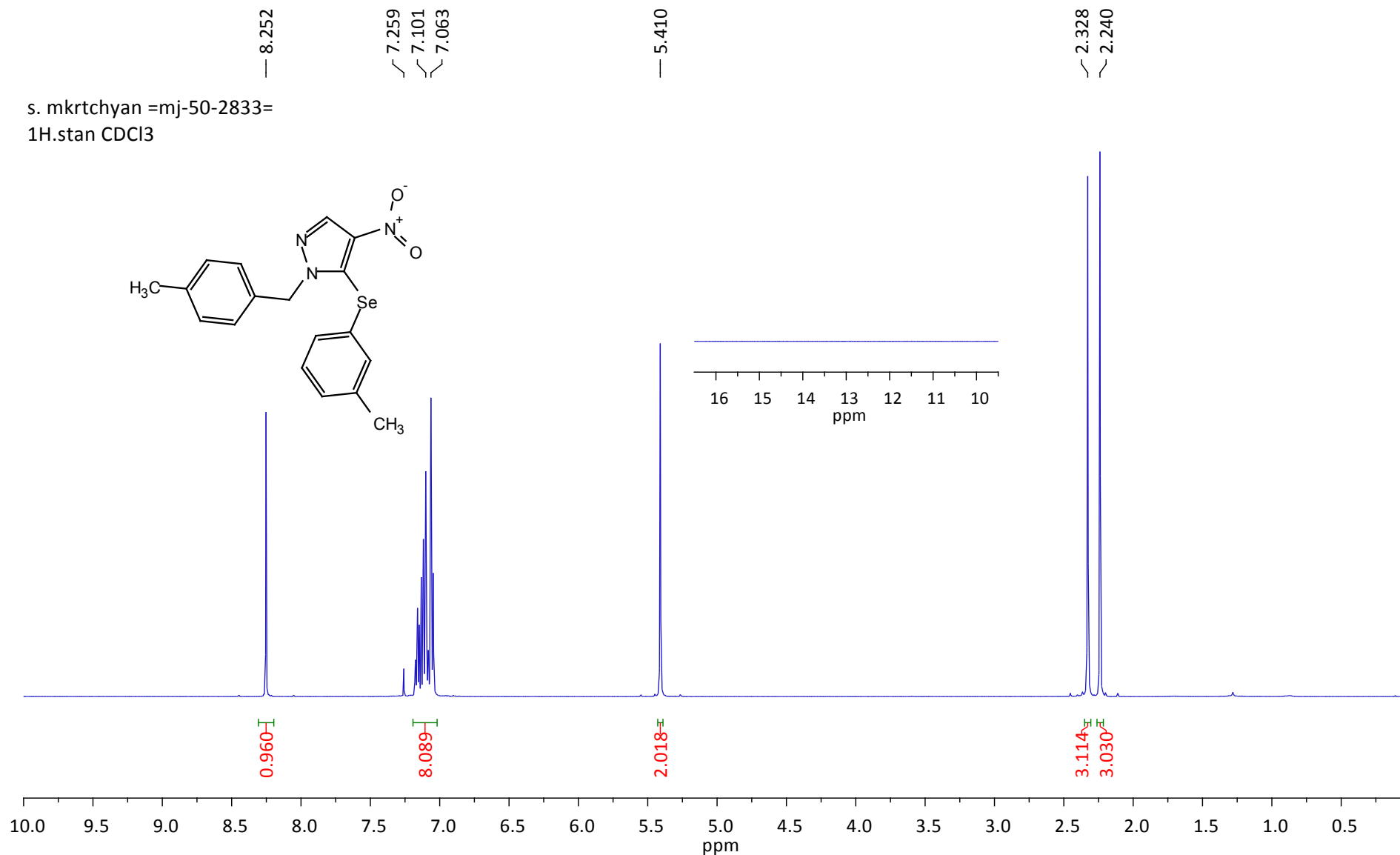
56.344



Comment	s. mkrtyan =mja-140-crs1=A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **1a**

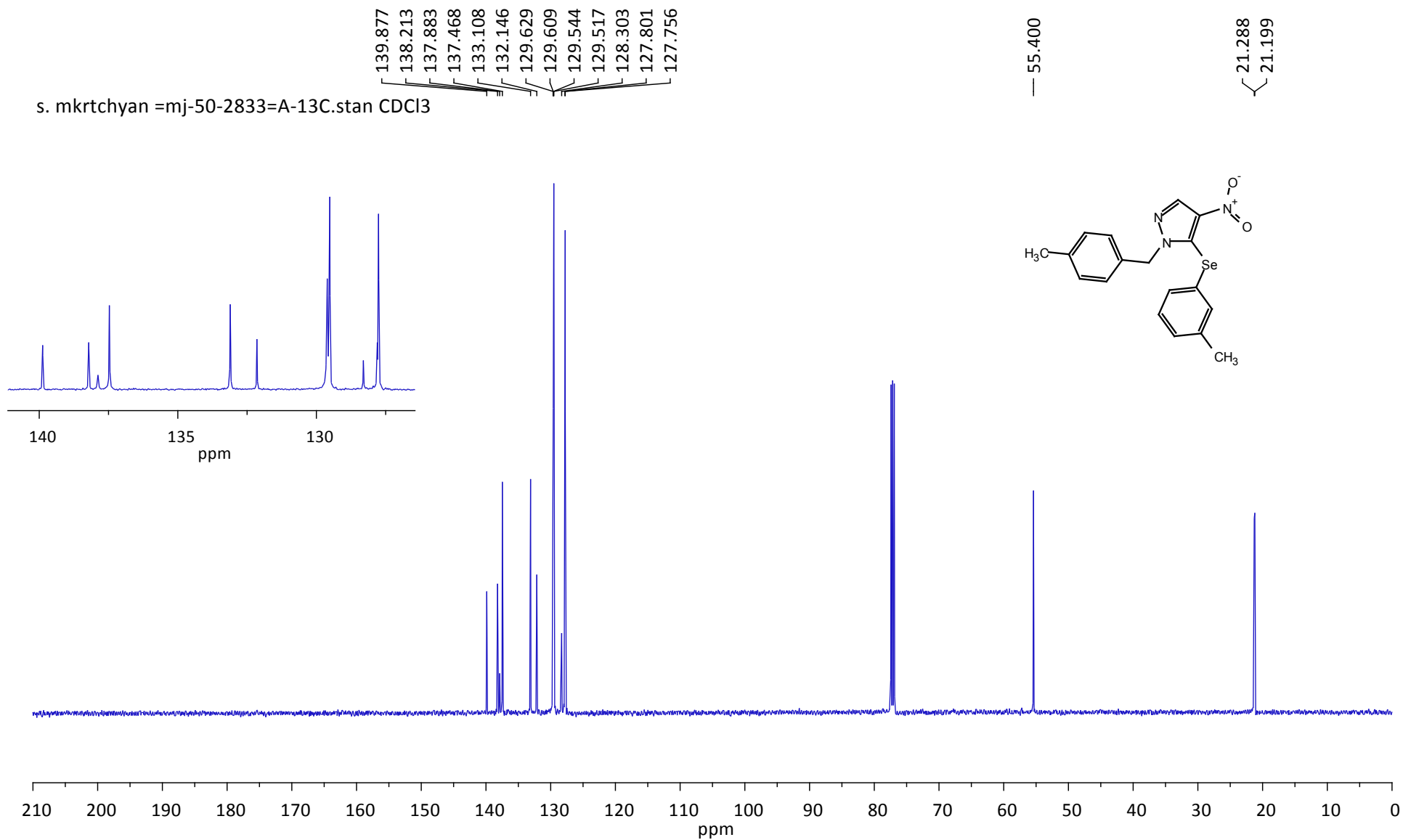
s. mkrtyan =mj-50-2833=
1H.stan CDCl3



Comment	s. mkrtyan =mj-50-2833=1H.stan CDCl3
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound 1a

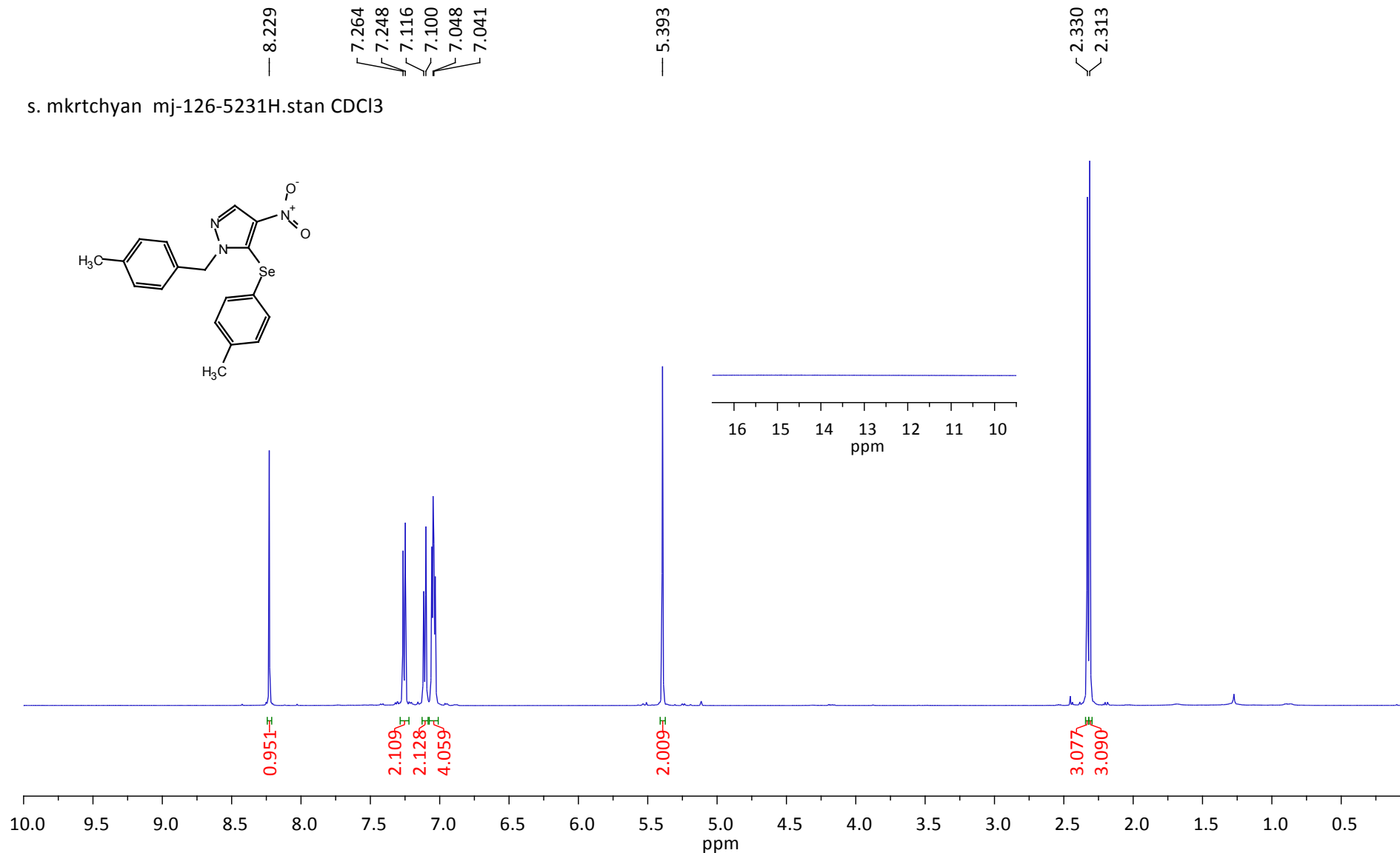
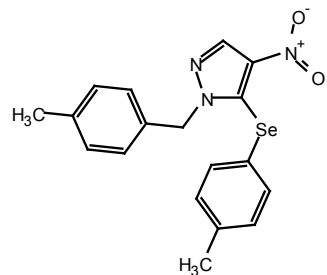
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Comment	s. mkrtyan =mj-50-2833=A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

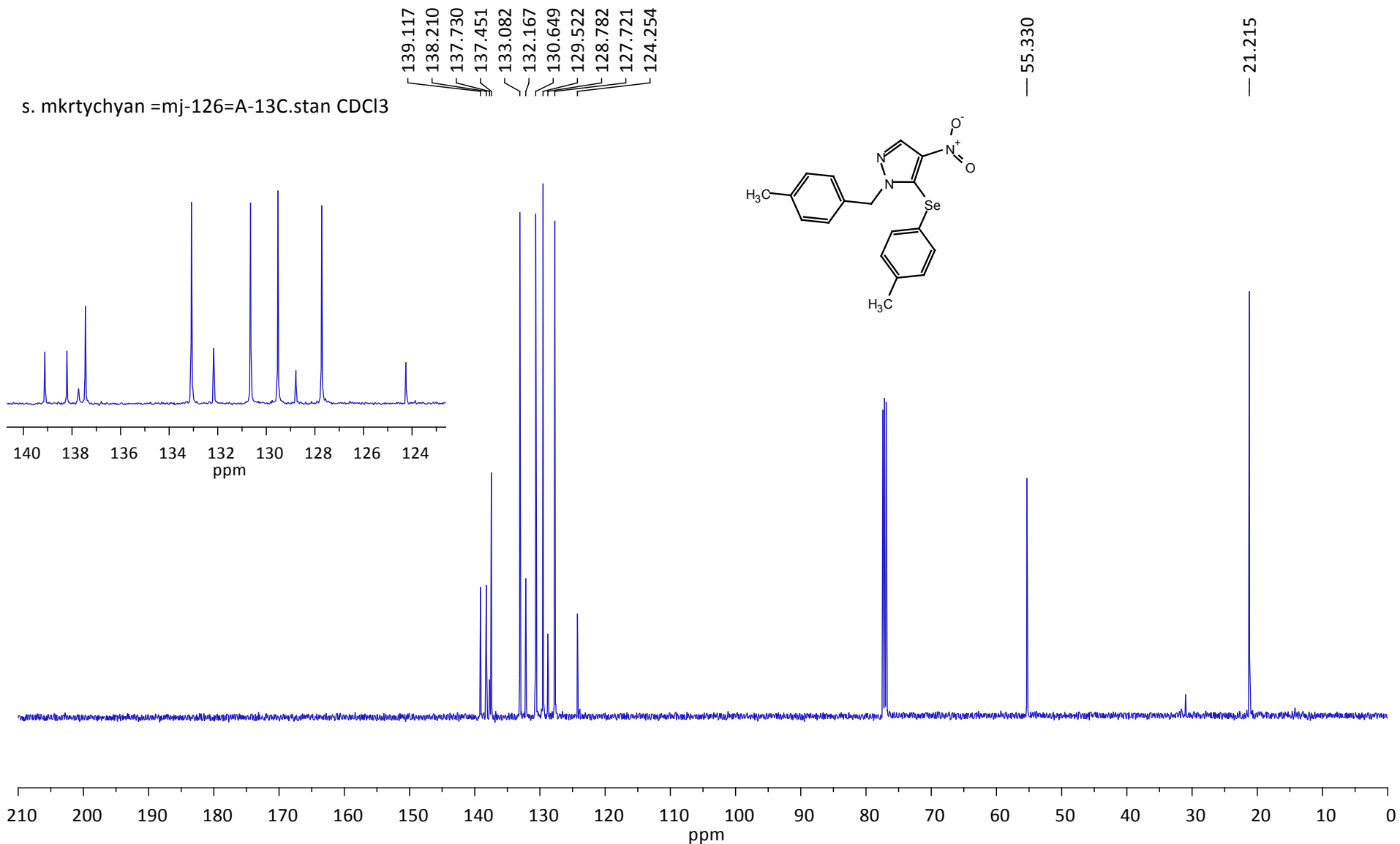
Compound **1b**

s. mkrтчyаn mj-126-5231H.stаn CDCl3



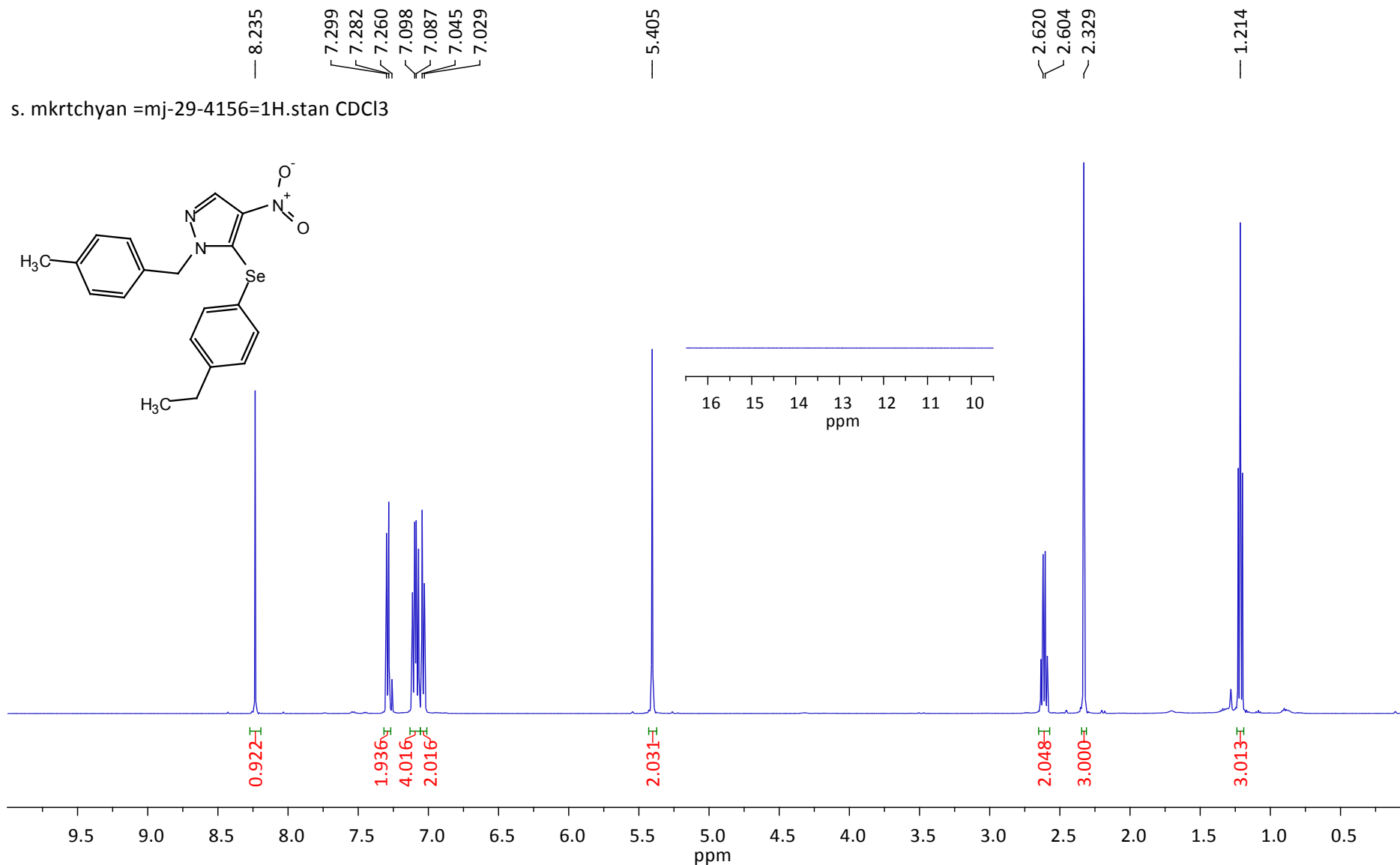
Comment s. mkrтчyаn mj-126-5231H.stаn CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **1b**



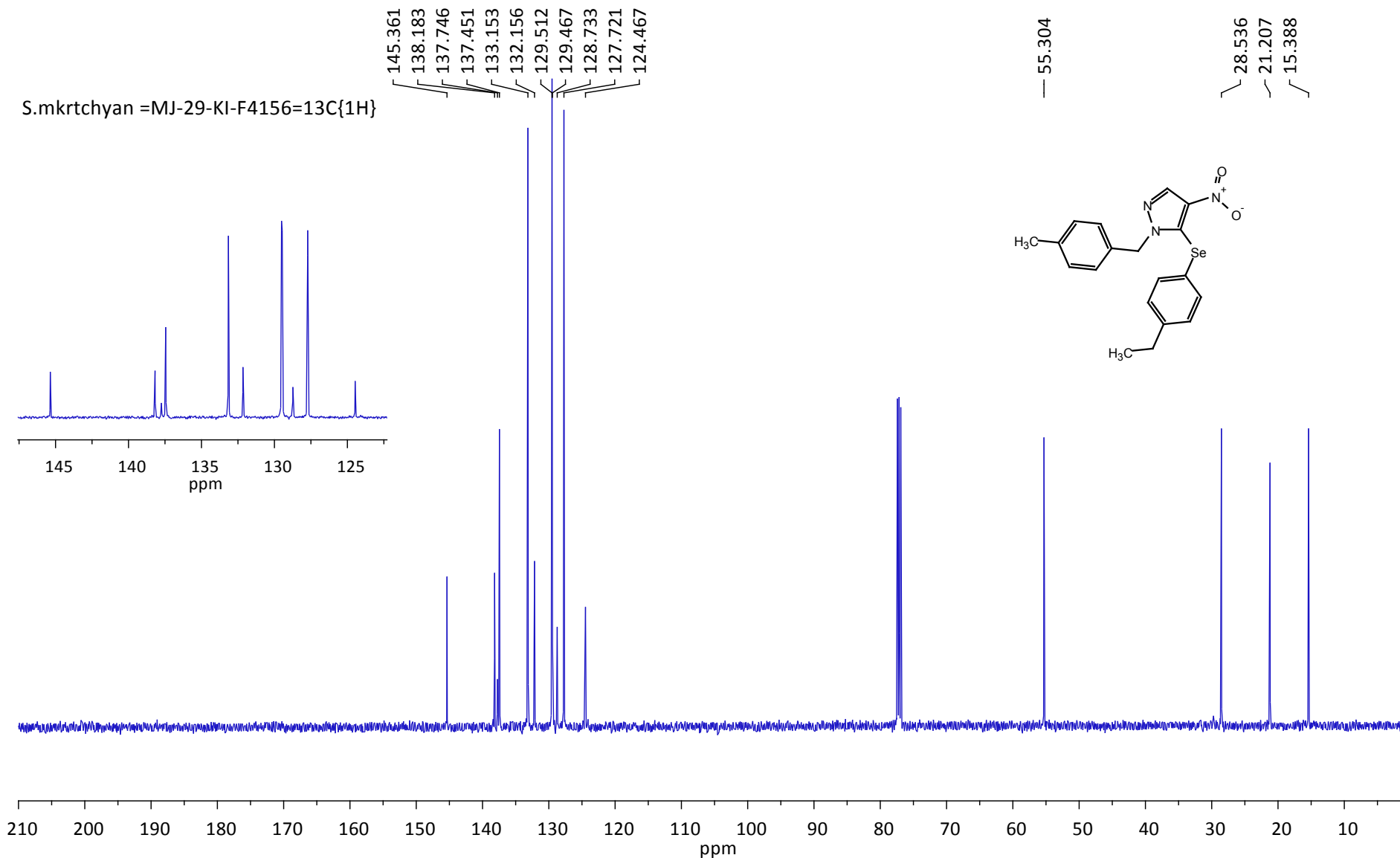
Comment	s. mkrtychyan =mj-126=A-13C.stan CDCl ₃
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **1c**



Comment	S.mkrtyan =MJ-29-KI-F4156=1H.stan CDCl3
Number of Scans	16
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound 1c



Comment S.mkrtyan =MJ-29-KI-F4156=13C{1H}

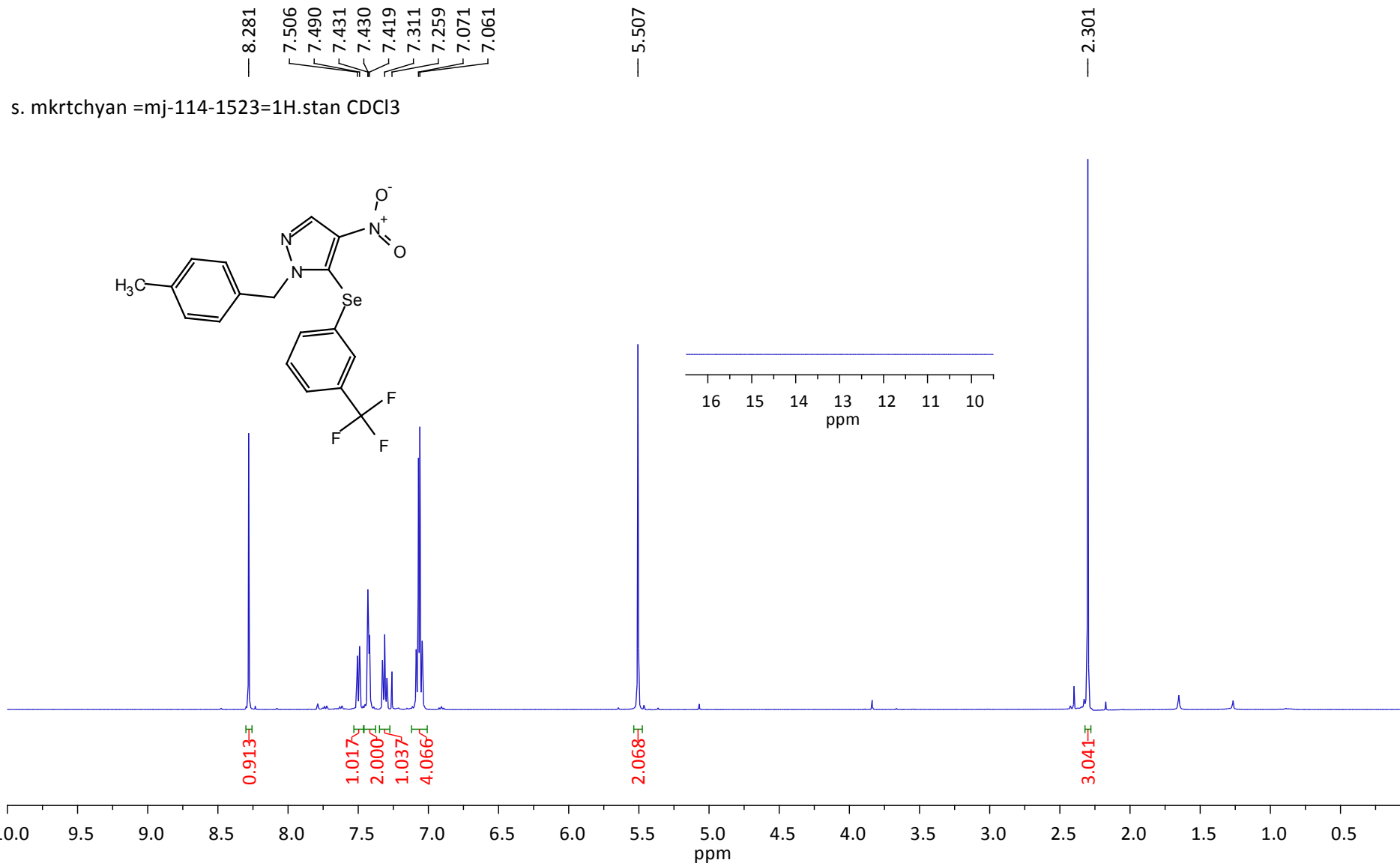
Number of Scans 256

Spectrometer Frequency 125.76

Spectral Width 36057.7

Spectral Size 65536

Compound **1d**

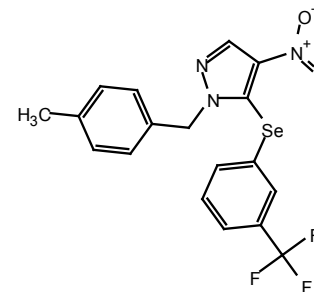


Comment s. mkrtyan =mj-114-1523=1H.stan CDCl₃
 Number of Scans 32
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **1d**

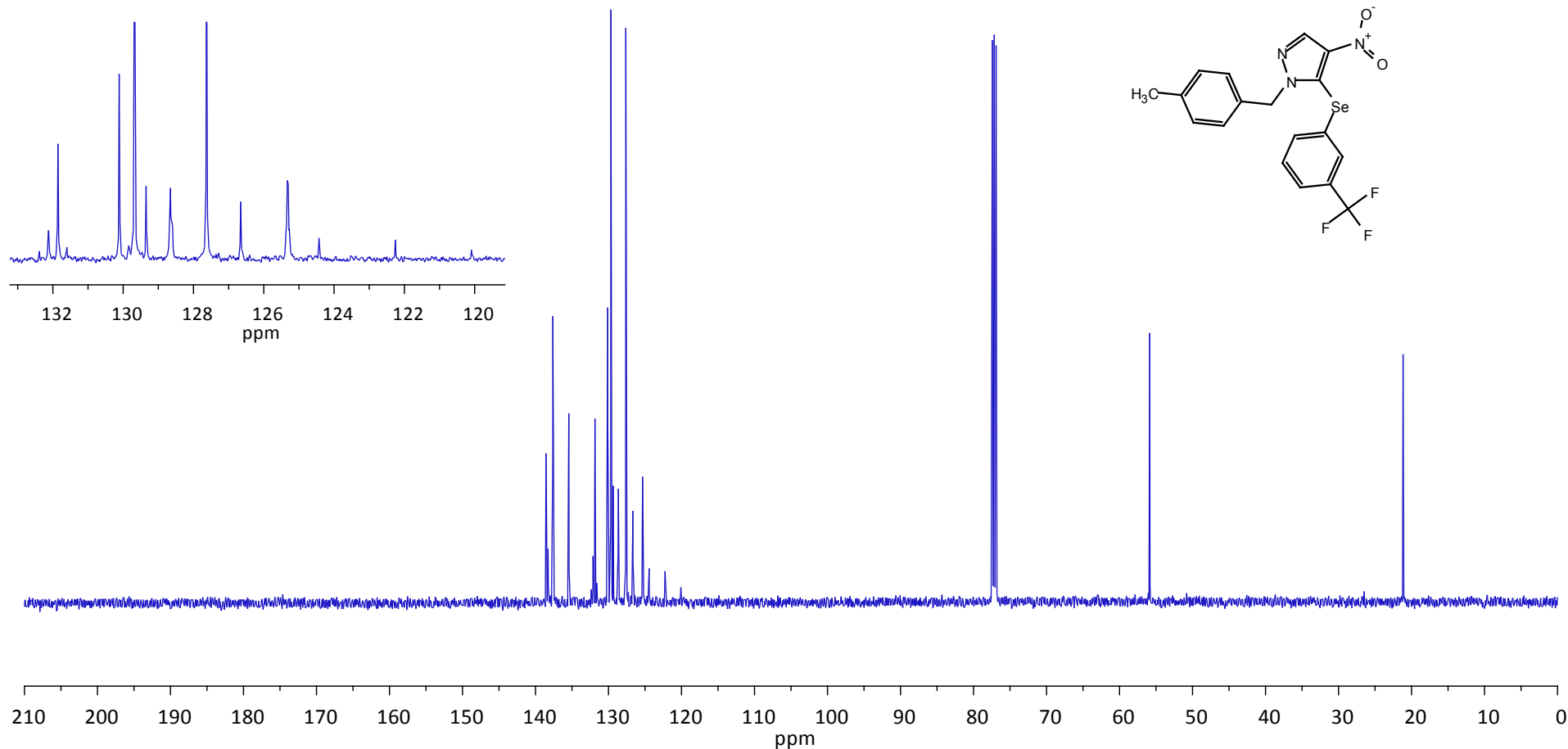
138.557
138.277
137.629
135.435
132.384
132.124
131.854
131.602
130.113
129.676
129.347
128.657
128.627
127.627
126.655
125.332
125.304
124.428
122.258
120.089

s. mkrtyan =mj-114-1523=A-13C.stan CDCl3



— 55.868

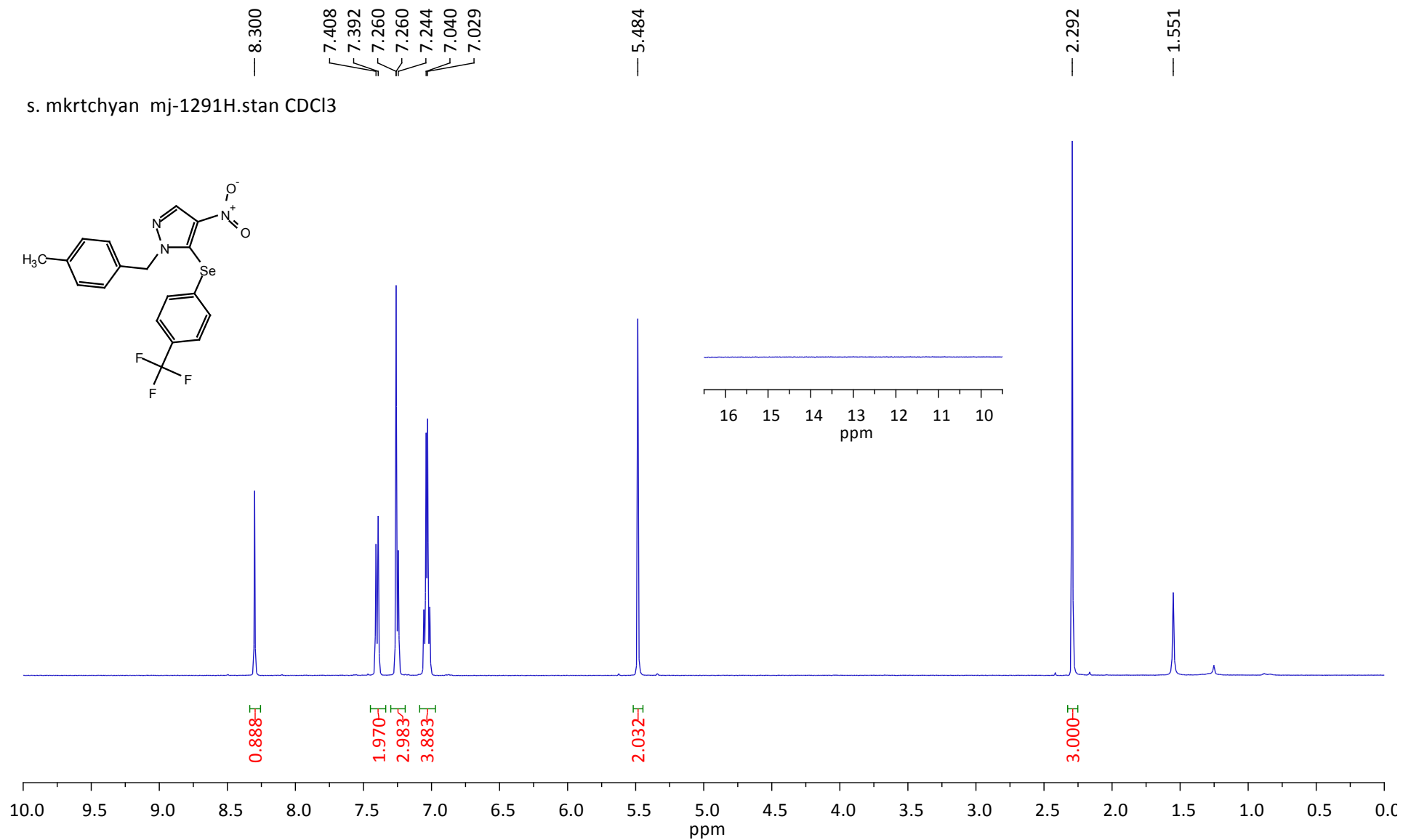
— 21.159



Comment s. mkrtyan =mj-114-1523=A-13C.stan CDCl3
 Number of Scans 336
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

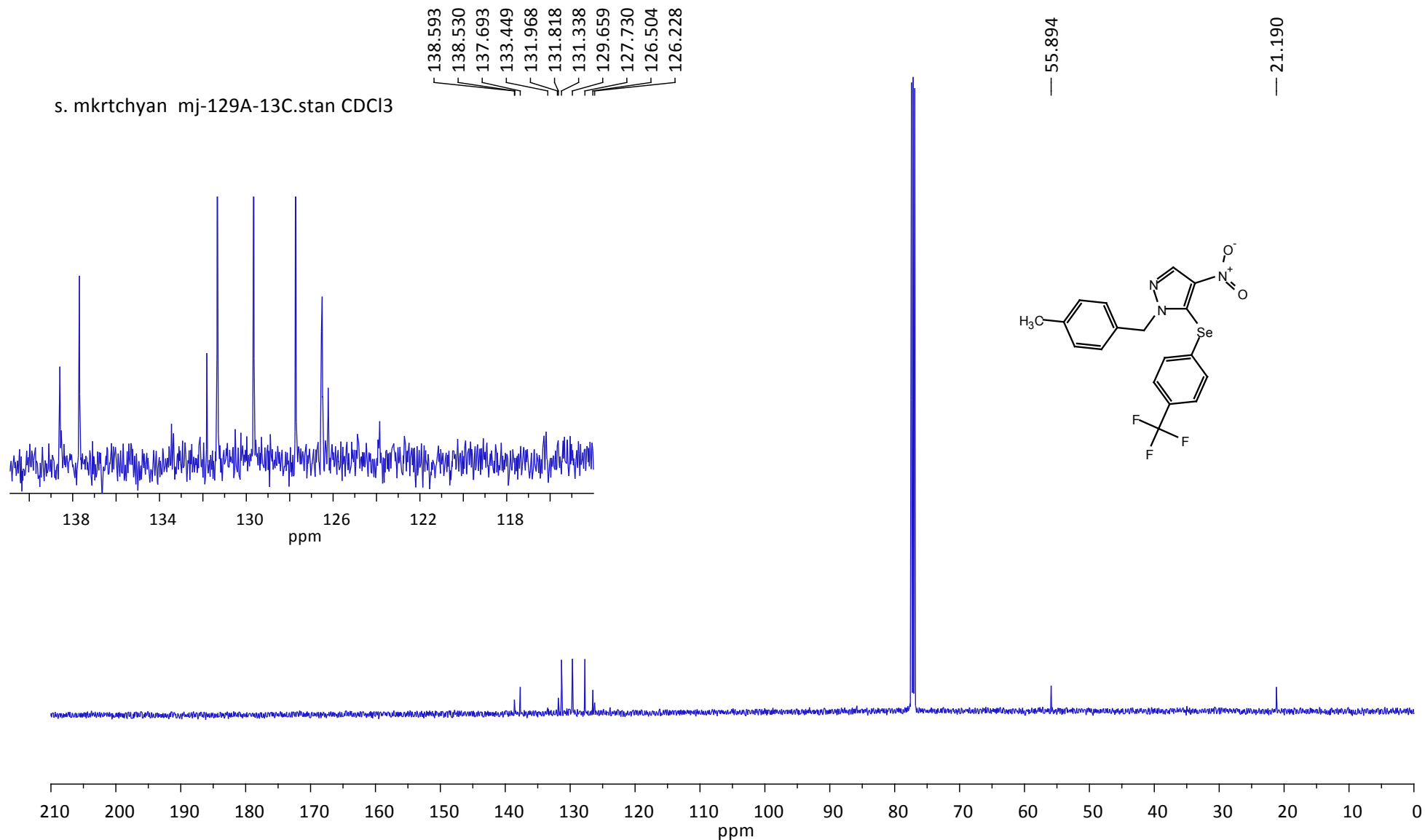
Compound **1e**

s. mkrtyan mj-1291H.stan CDCl₃



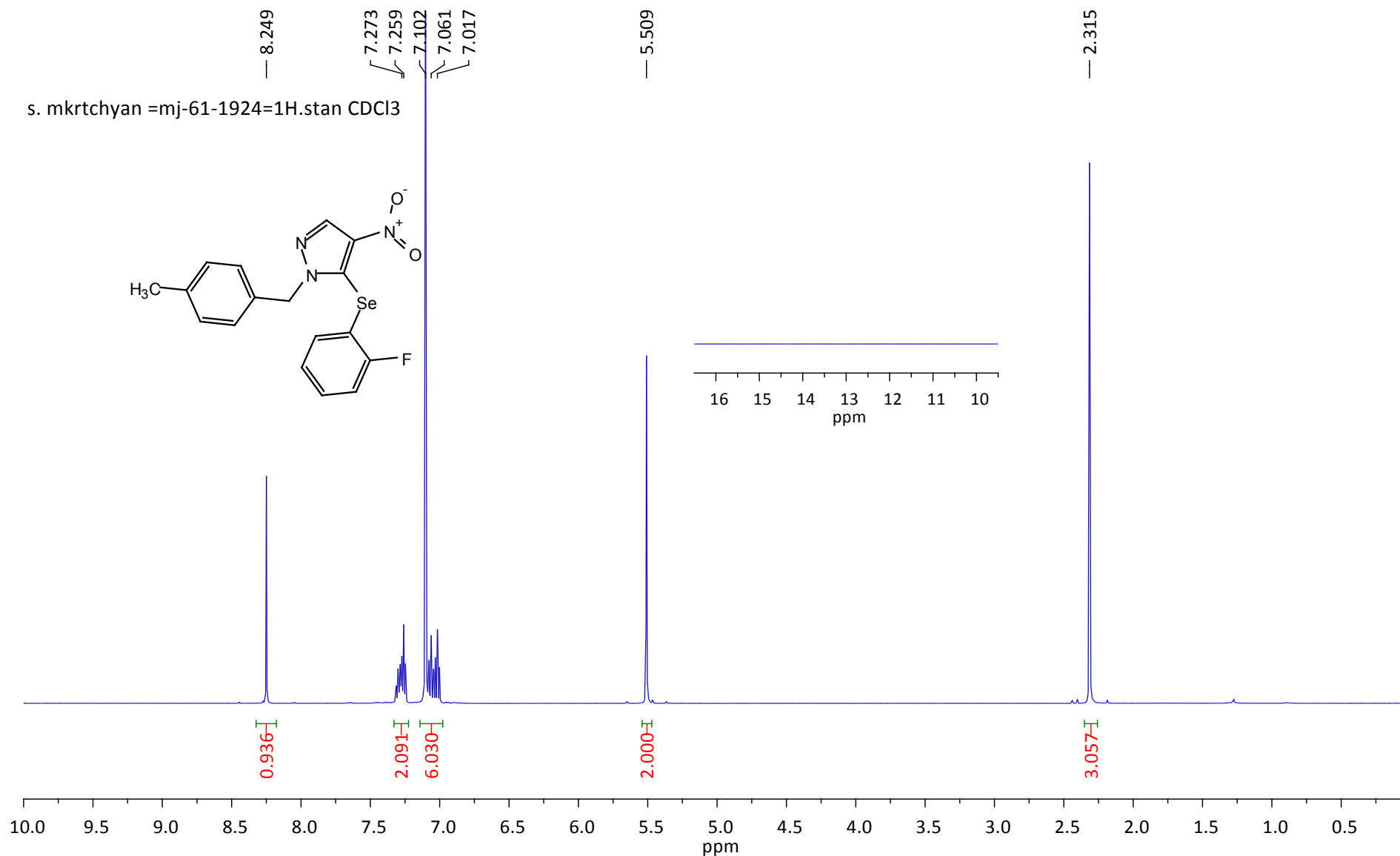
Comment	s. mkrtyan mj-1291H.stan CDCl ₃
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound **1e**



Comment s. mkrтчyan mj-129A-13C.stan CDCl3
Number of Scans 2048
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

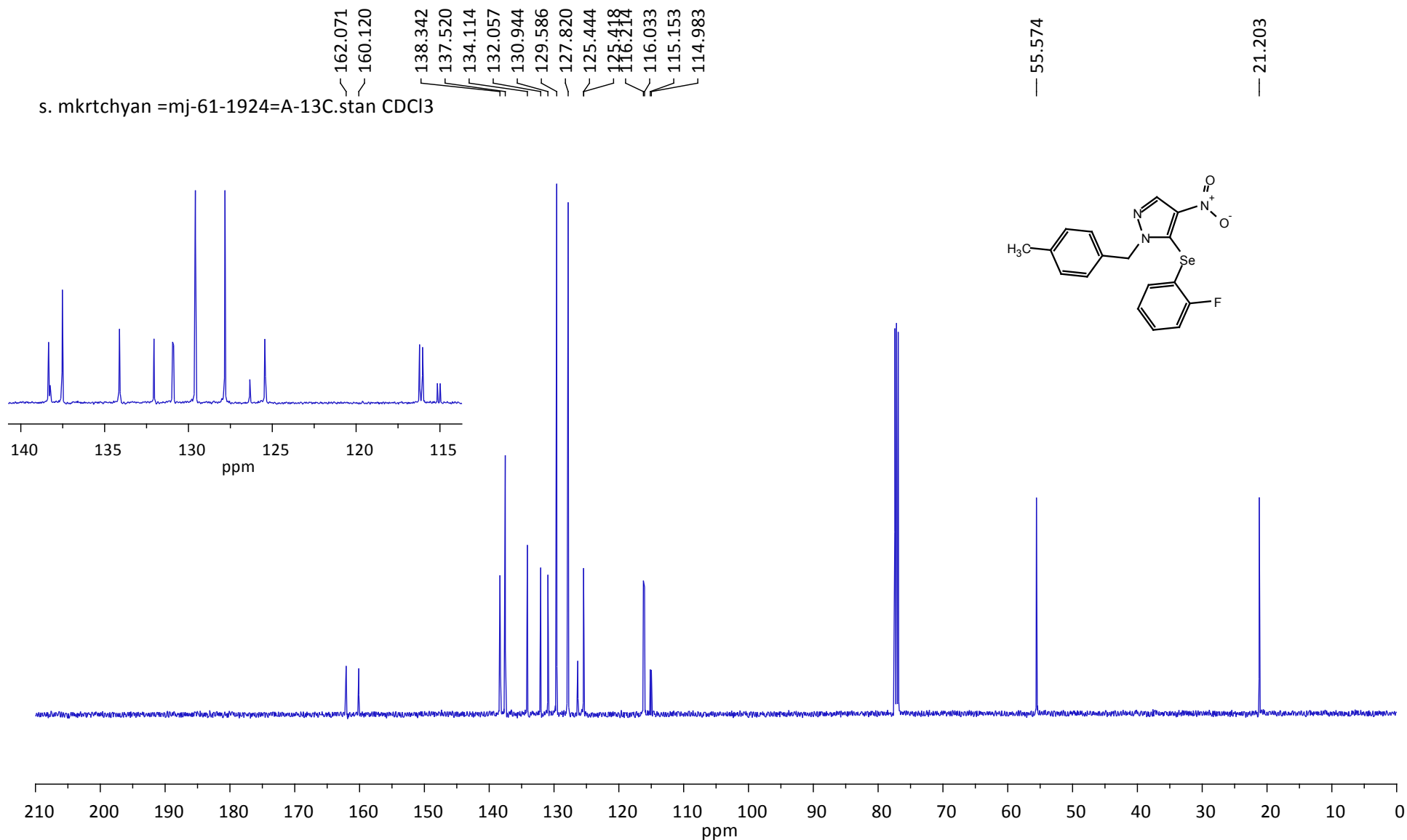
Compound **1f**



Comment s. mkrtyan =mj-61-1924=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **1f**

s. mkrtchyan =mj-61-1924=A-13C.stan CDCl₃



Comment s. mkrtchyan =mj-61-1924=A-13C.stan CDCl₃

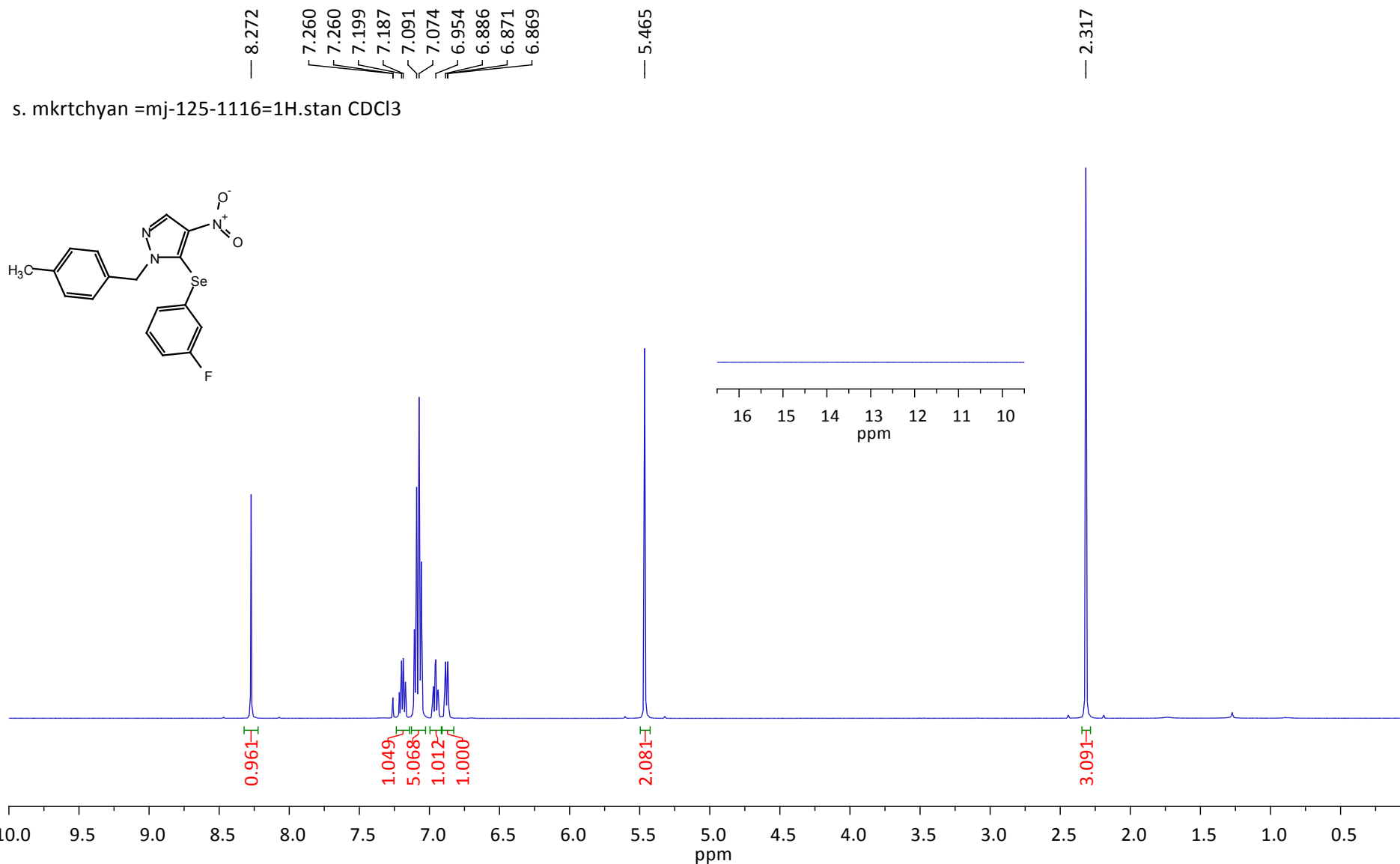
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Spectral Width 36057.7

Spectral Size 65536

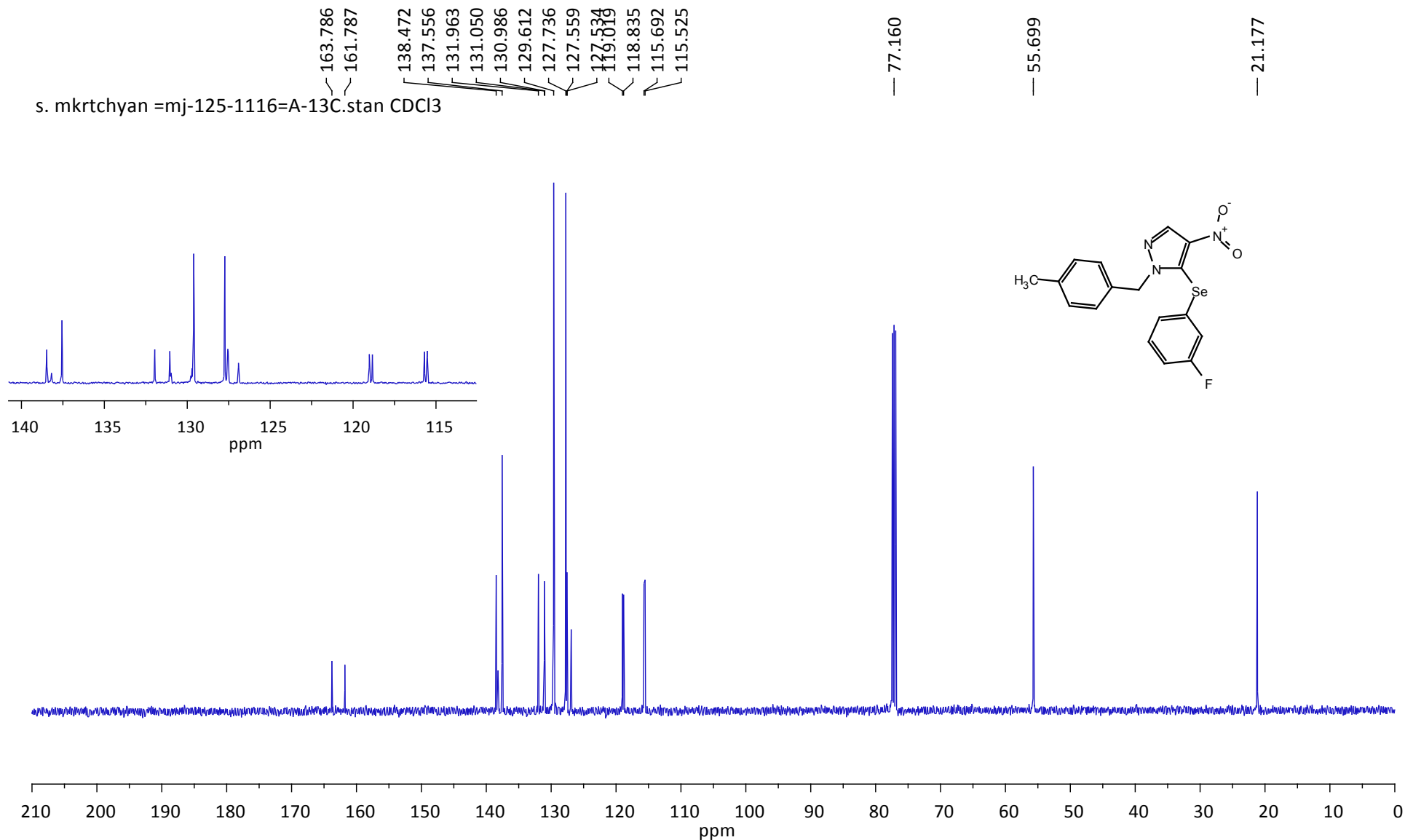
Compound **1g**



Comment s. mkrтчyan =mj-125-1116=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **1g**

s. mkrtyan =mj-125-1116=A-13C.stan CDCl₃



Comment s. mkrtyan =mj-125-1116=A-13C.stan CDCl₃

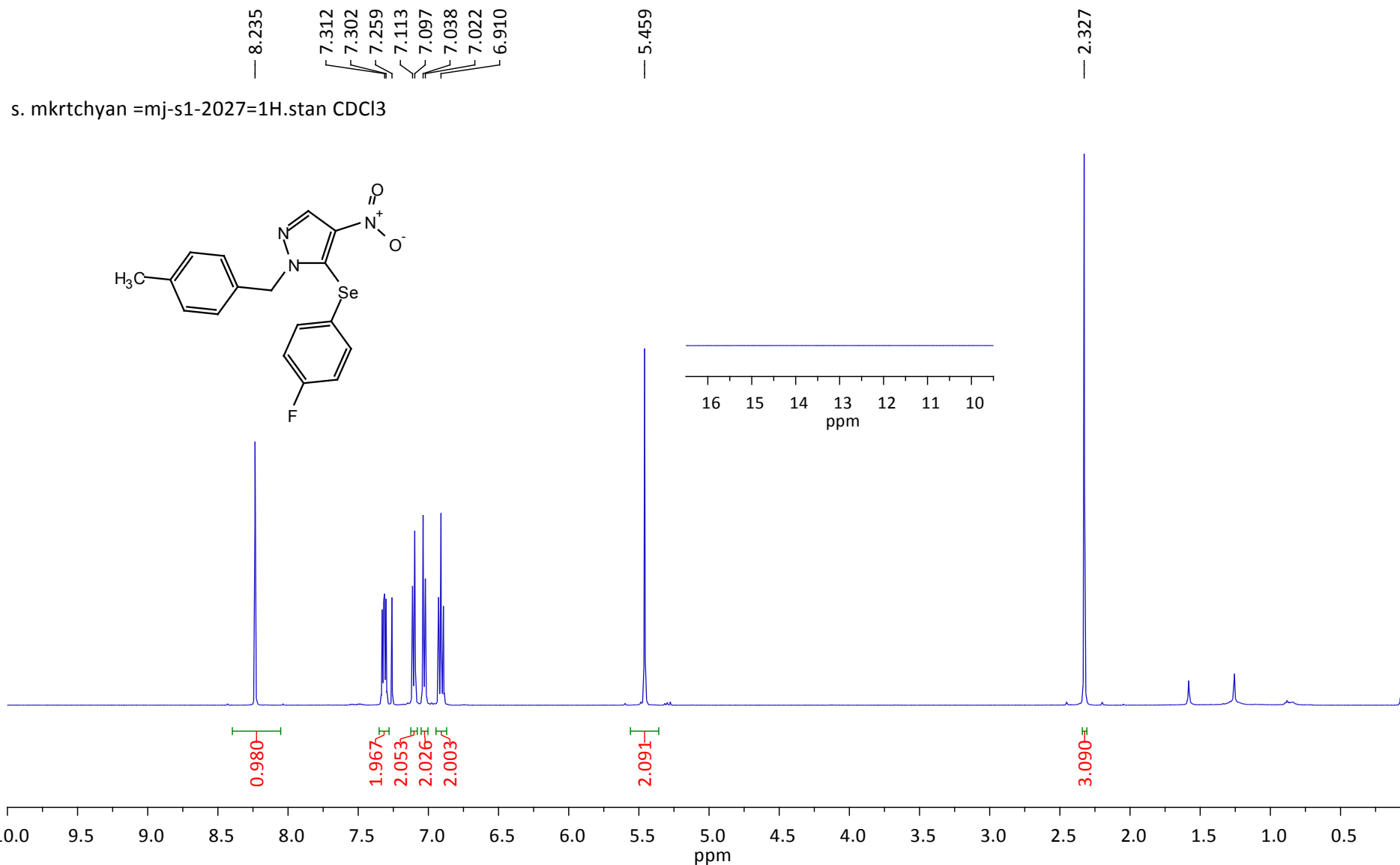
Number of Scans 256

Spectrometer Frequency 125.76

Spectral Width 36057.7

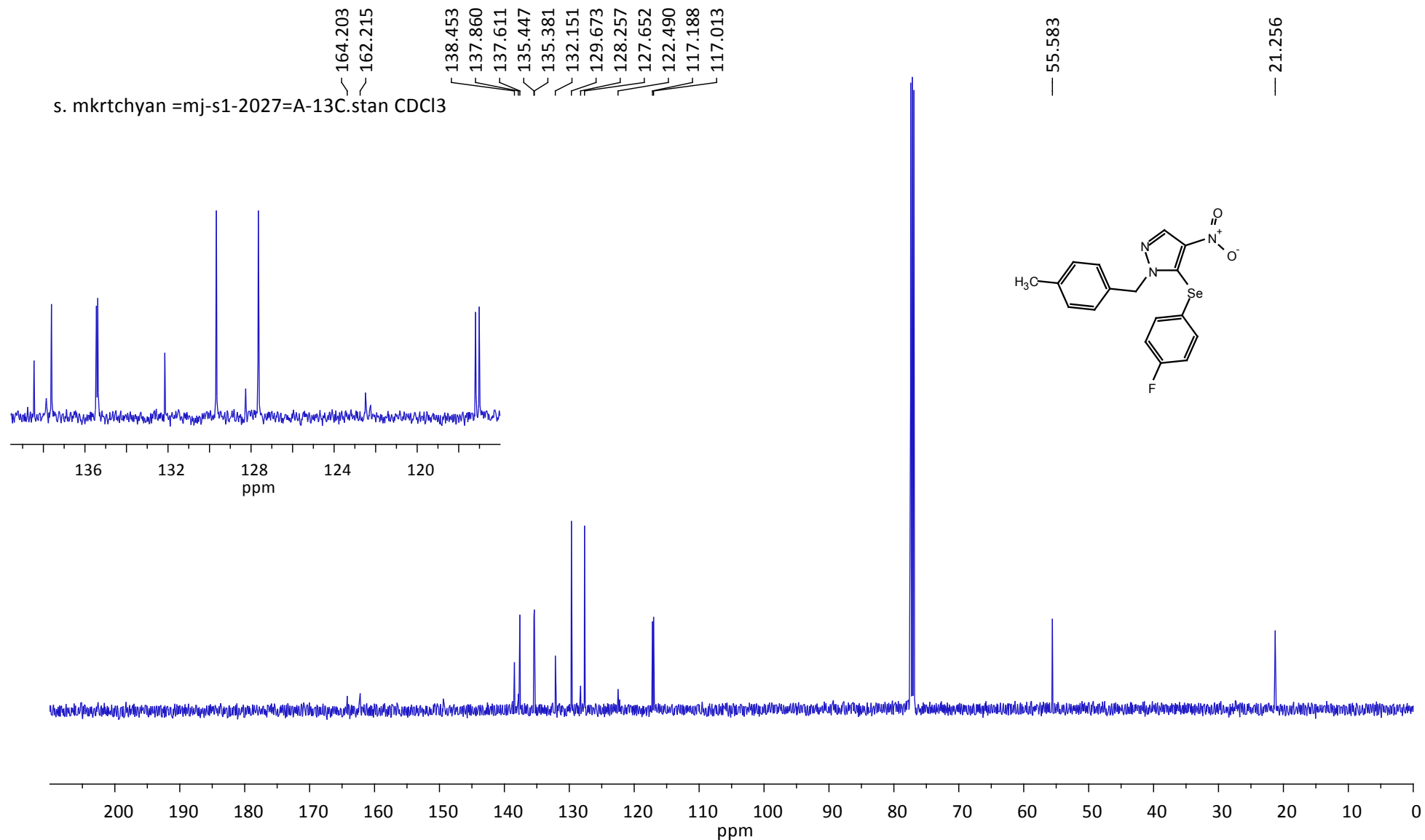
Spectral Size 65536

Compound **1h**



Comment	s. mkrtyan =mj-s1-2027=1H.stan CDCl ₃
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

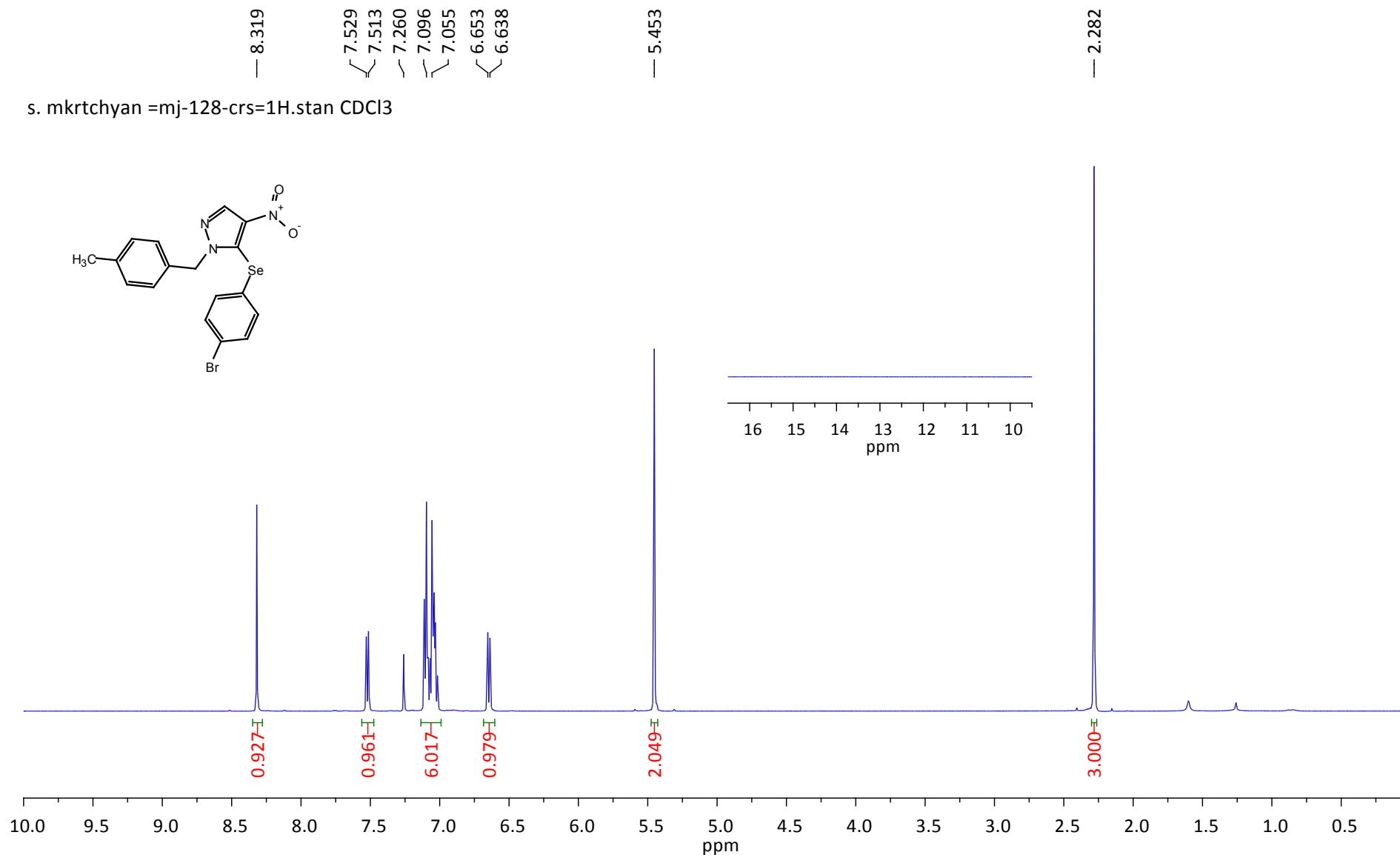
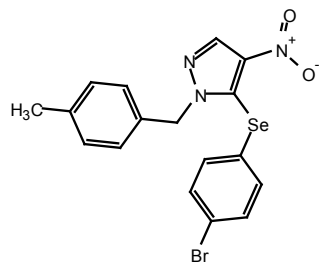
Compound **1h**



Comment	s. mkrtyan =mj-s1-2027=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

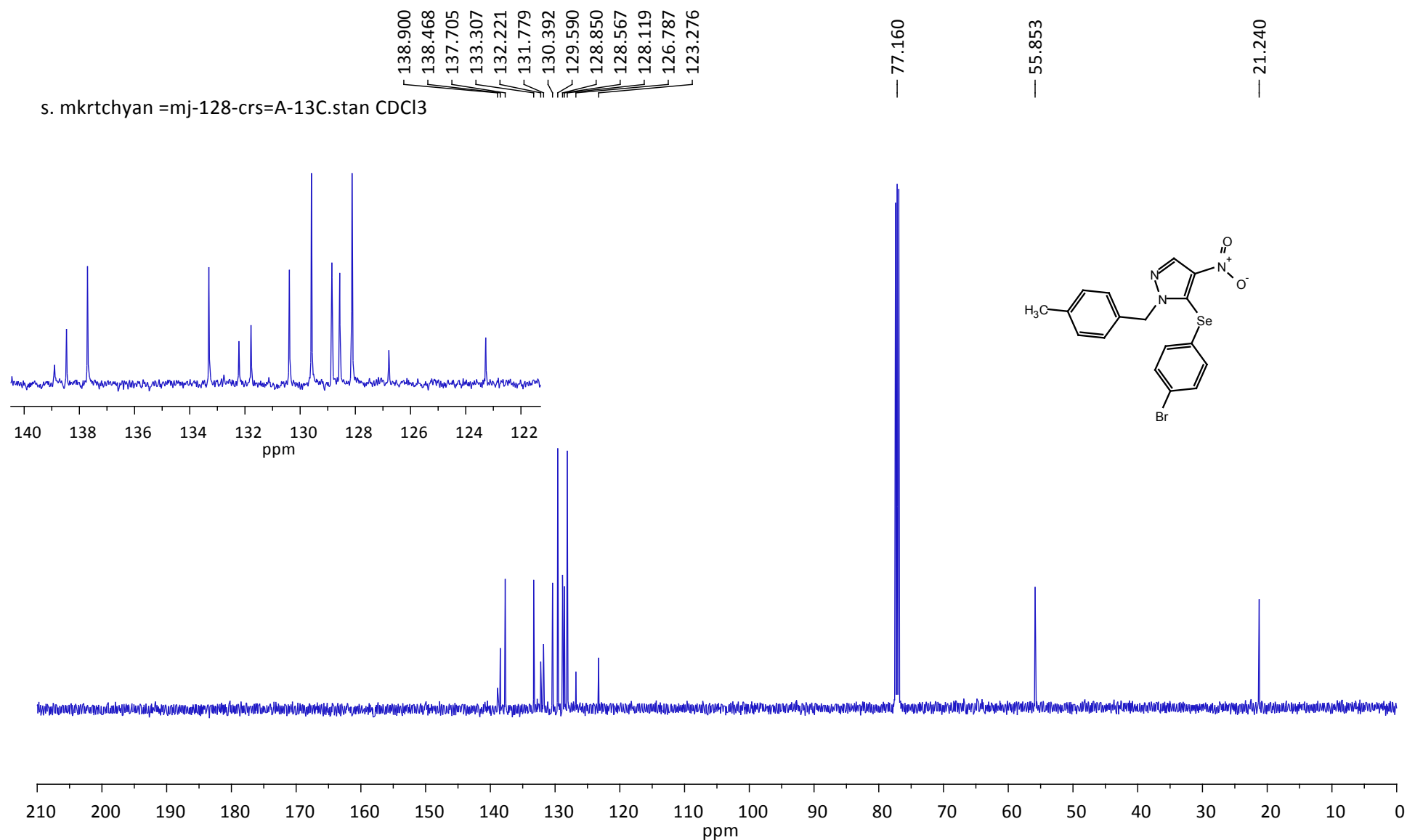
Compound **1i**

s. mkrтчyan =mj-128-crs=1H.stan CDCl3



Comment s. mkrтчyan =mj-128-crs=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **1i**



s. mkrtchyan =mj-128-crs=A-13C.stan CDCl3

Comment s. mkrtchyan =mj-128-crs=A-13C.stan CDCl3

Number of Scans 256

Spectrometer Frequency 125.76

Spectral Width 36057.7

Spectral Size 65536

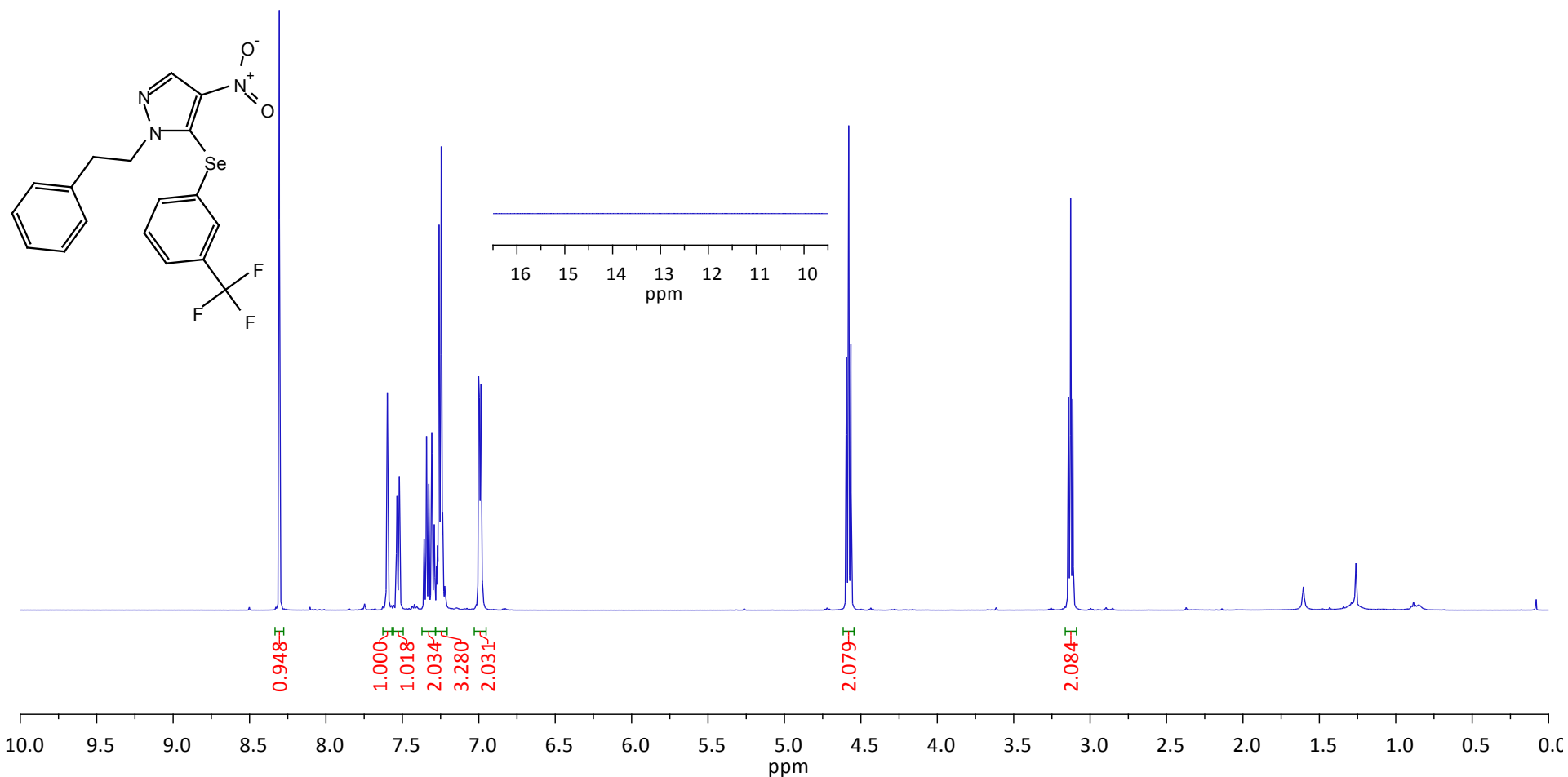
Compound 2a

8.305
7.599
7.535
7.520
7.342
7.308
7.260
7.260
7.246
7.001
6.997
6.986
6.982

4.580

3.128

s. mkrtychyan =mj-...-f3445=1H.stan CDCl3

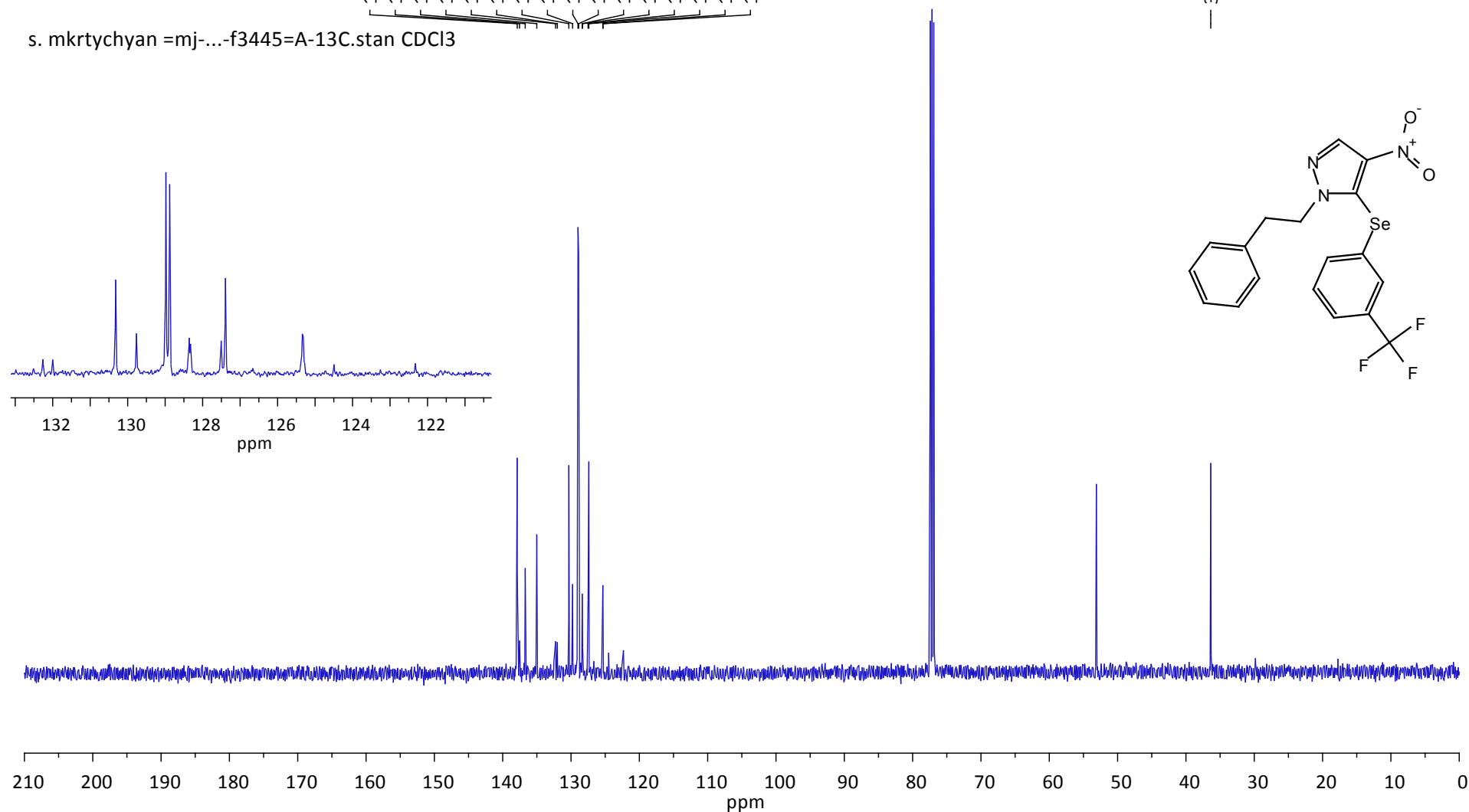


Comment s. mkrtychyan =mj-...-f3445=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 2a

137.876
137.540
136.704
135.011
132.261
131.999
130.321
129.767
128.980
128.878
128.357
128.328
127.505
127.391
125.341
125.313

s. mkrtychyan =mj-...-f3445=A-13C.stan CDCl3



Comment	s. mkrtychyan =mj-...-f3445=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

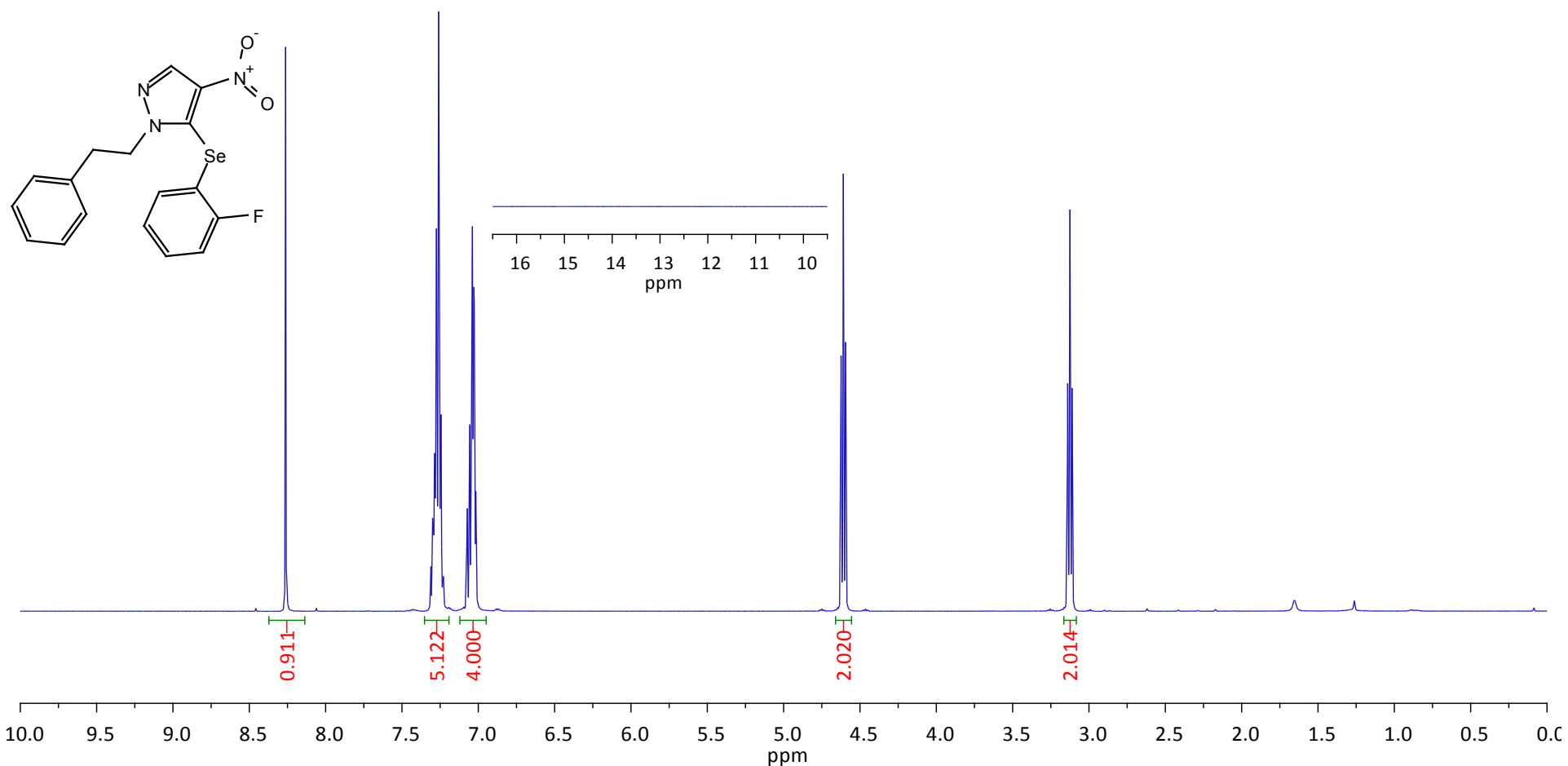
Compound **2b**

8.262
7.287
7.283
7.275
7.260
7.247
7.244
7.055
7.046
7.039
7.029
7.027

4.609

3.125

s. mkrtyan =mj...-f4749=1H.stan CDCl3



Comment s. mkrtyan =mj...-f4749=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

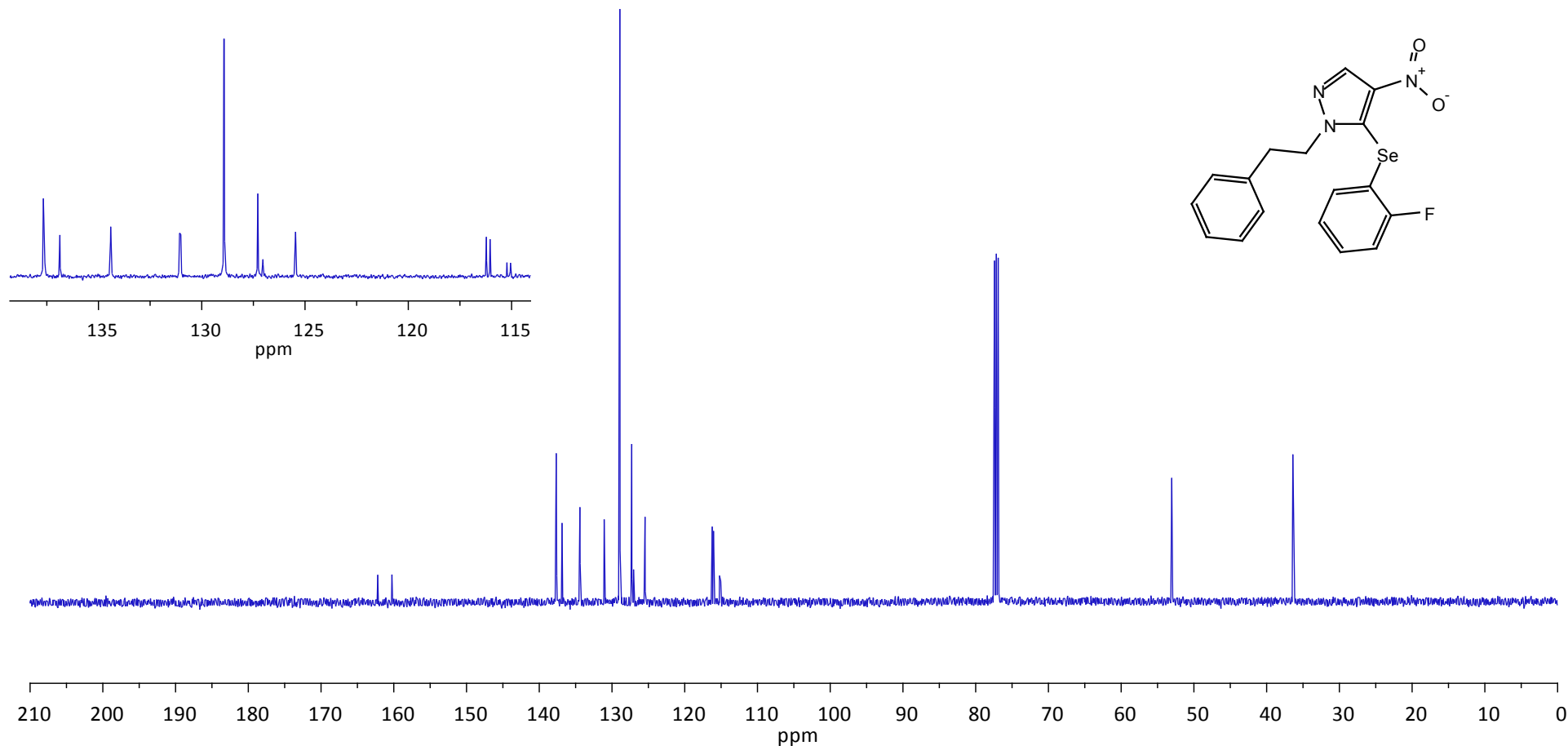
Compound **2b**

s. mkrtyan =mj...-f4749=A-13C.stan CDCl₃

162.202
160.252
137.666
136.868
134.407
131.074
131.012
128.920
127.286
125.483
125.456
116.226
116.039
115.223
115.053

— 53.043

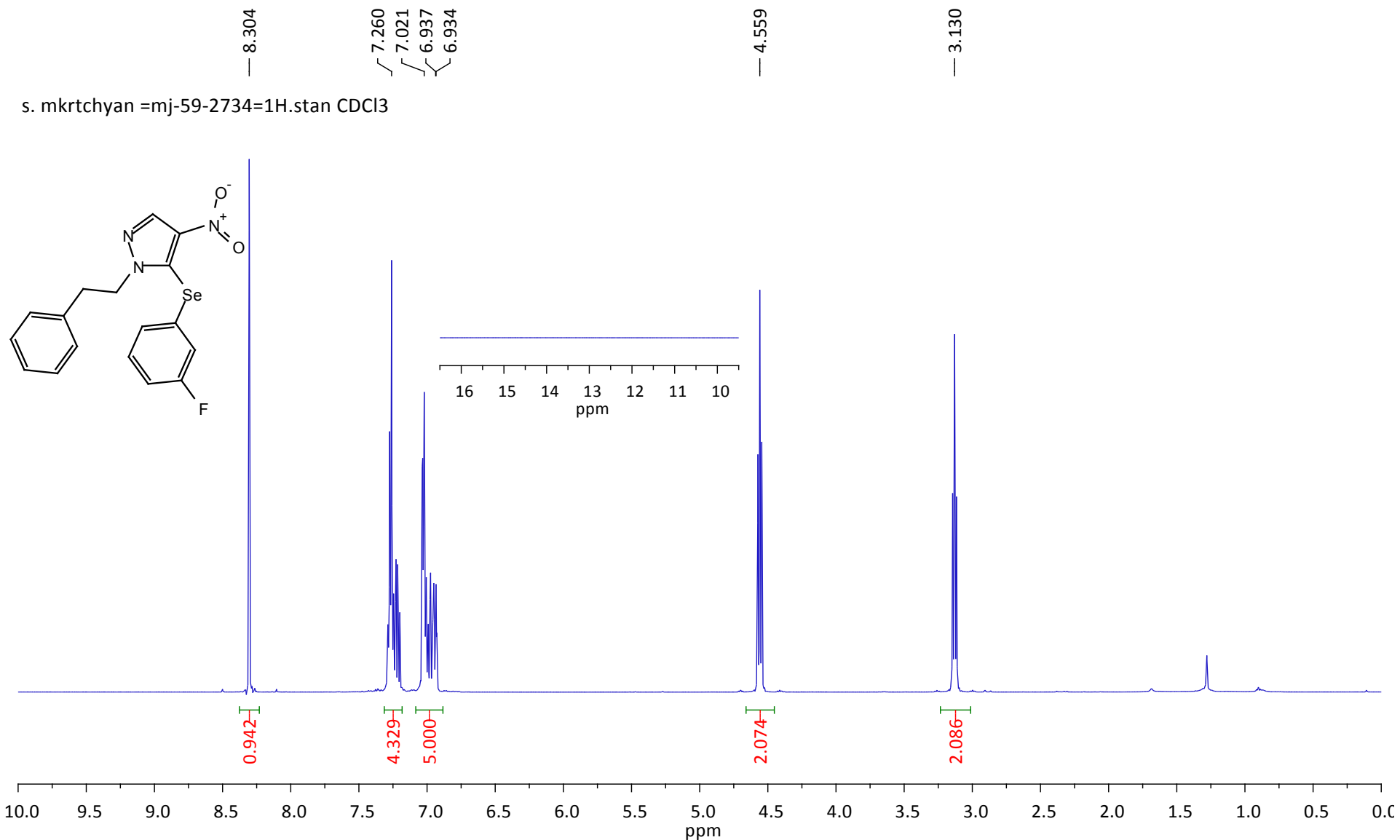
— 36.395



Comment	s. mkrtyan =mj...-f4749=A-13C.stan CDCl ₃
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **2c**

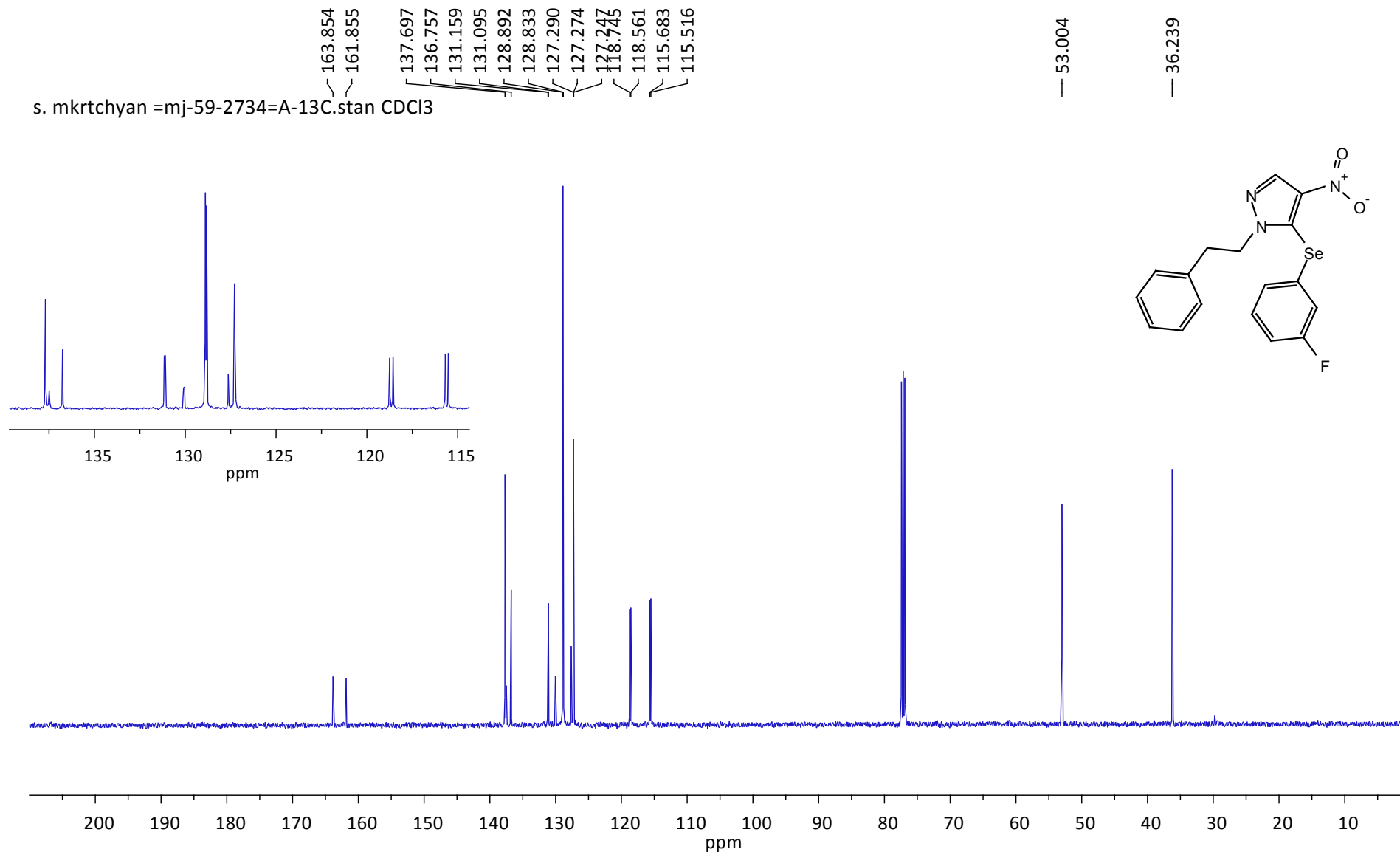
s. mkrtyan =mj-59-2734=1H.stan CDCl3



Comment	s. mkrtyan =mj-59-2734=1H.stan CDCl3
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

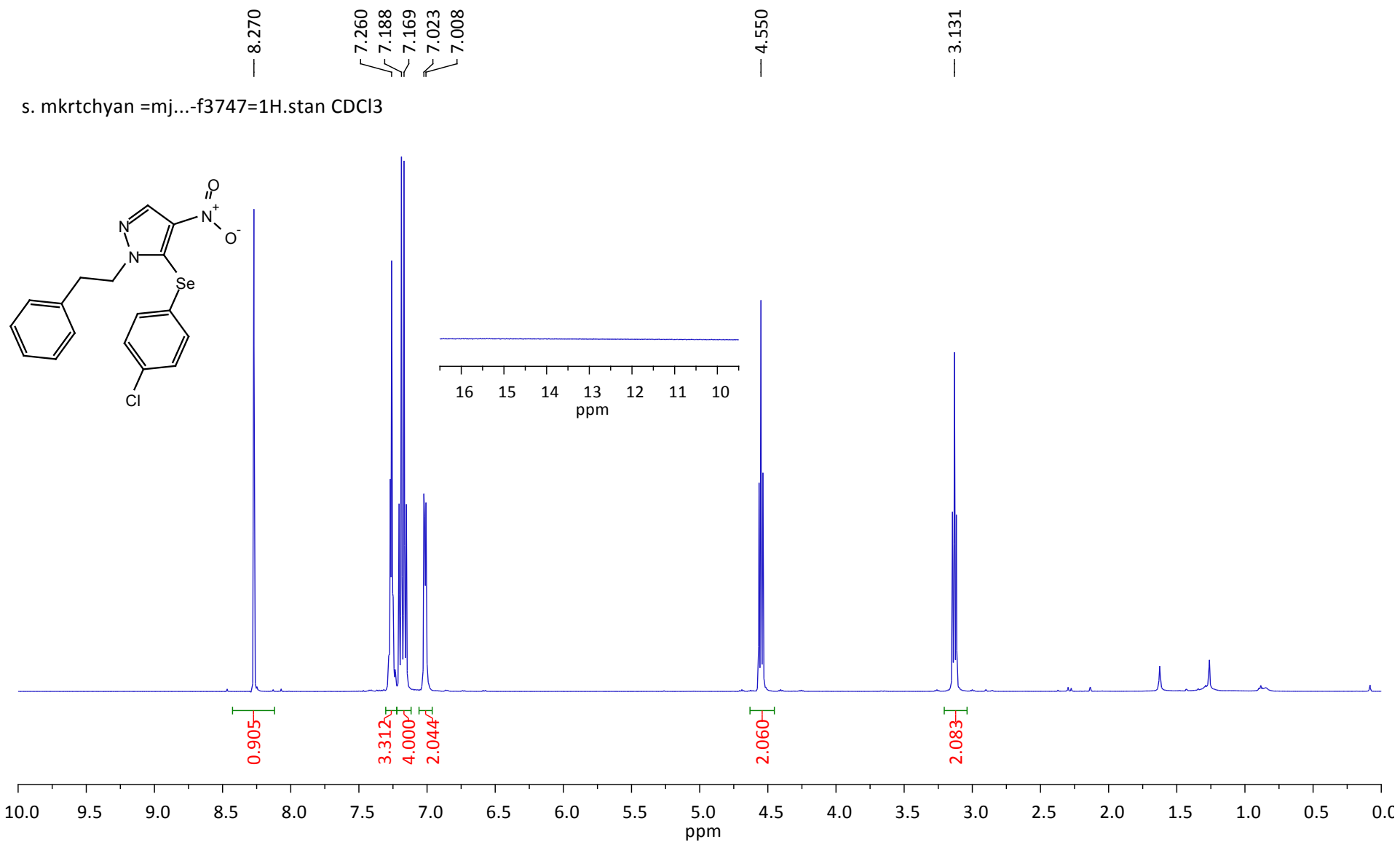
Compound 2c

s. mkrtyan =mj-59-2734=A-13C.stan CDCl3



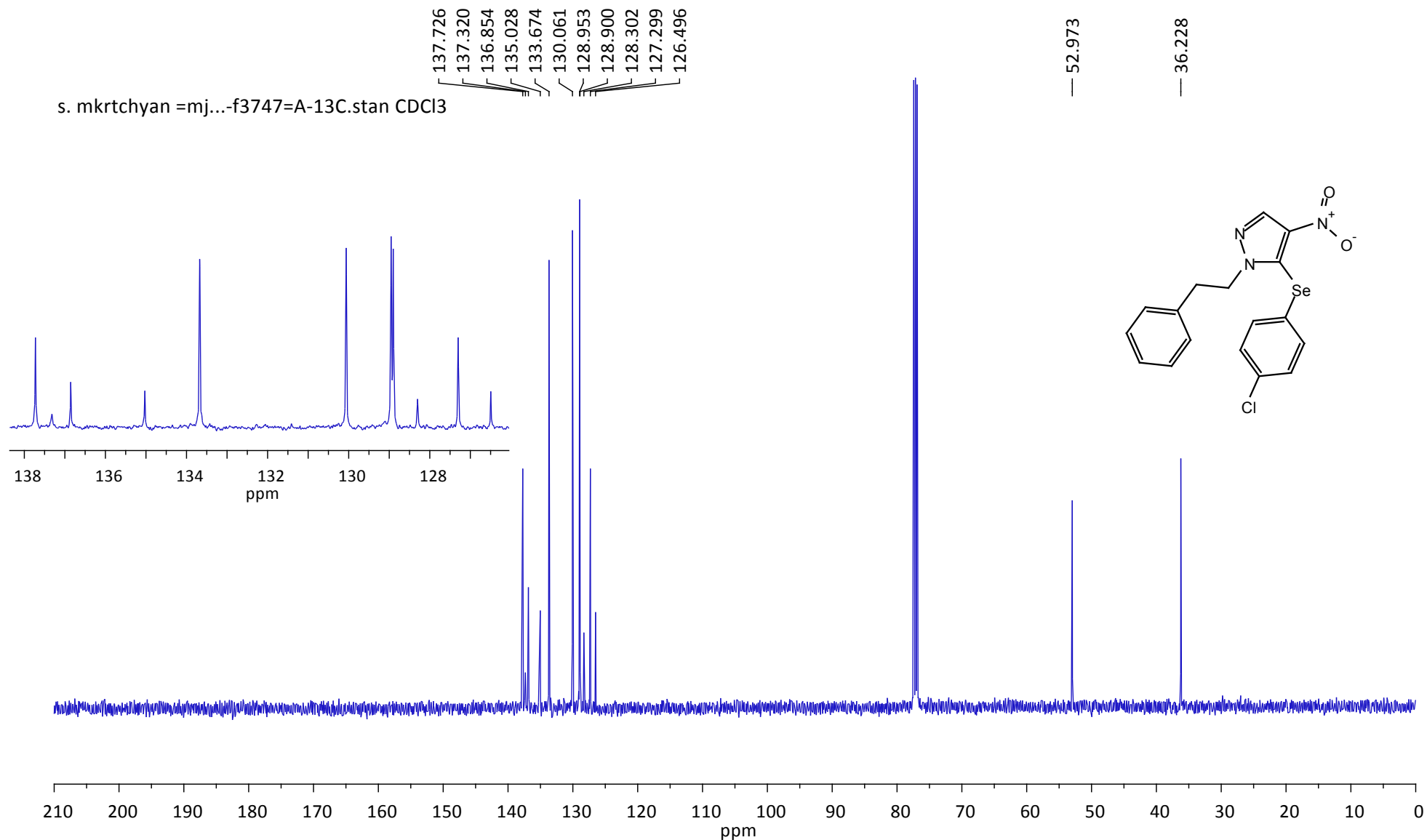
Comment	s. mkrtyan =mj-59-2734=A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **2d**



Comment s. mkrtyan =mj...-f3747=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

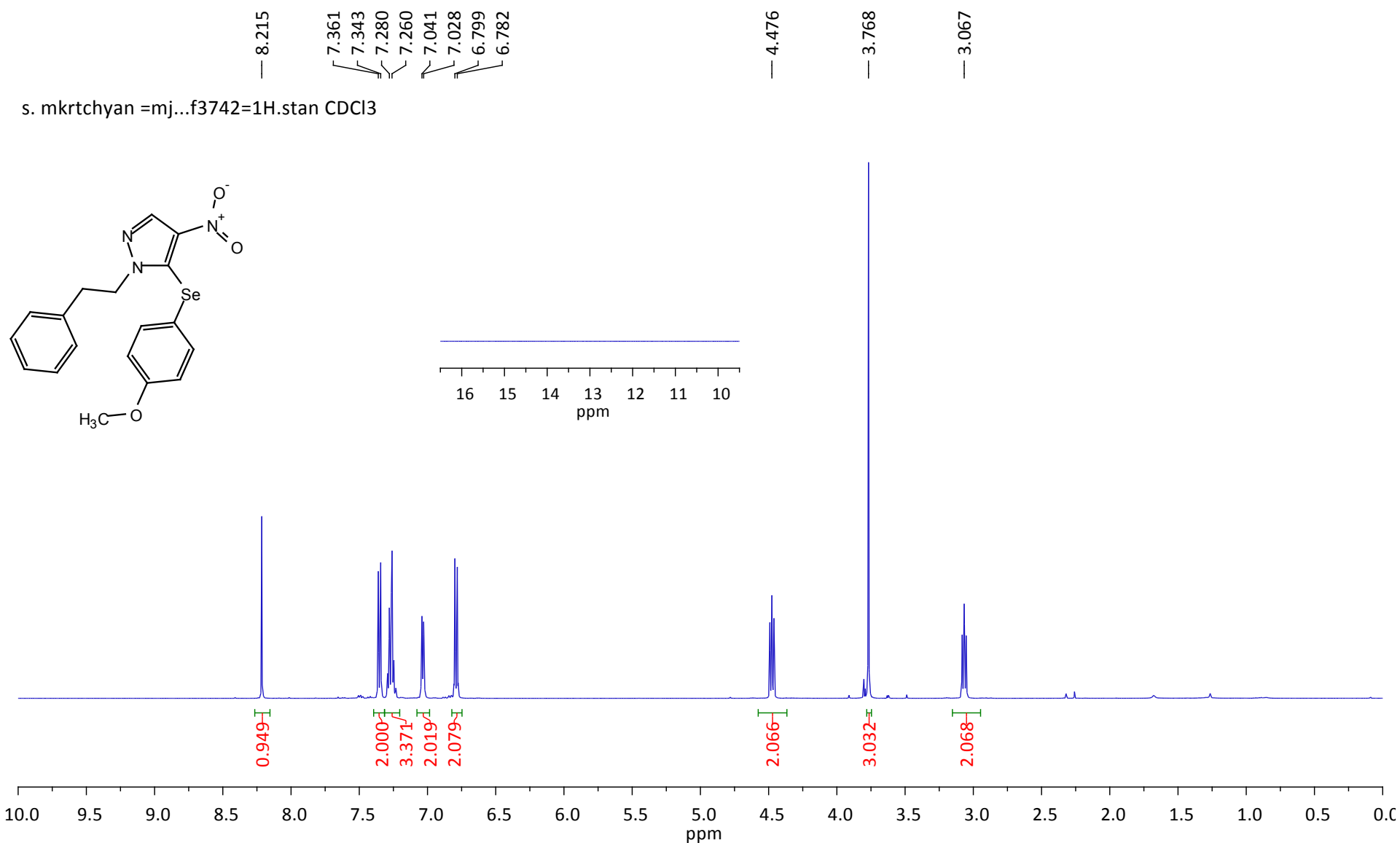
Compound 2d



Comment	s. mkrtyan =mj...-f3747=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

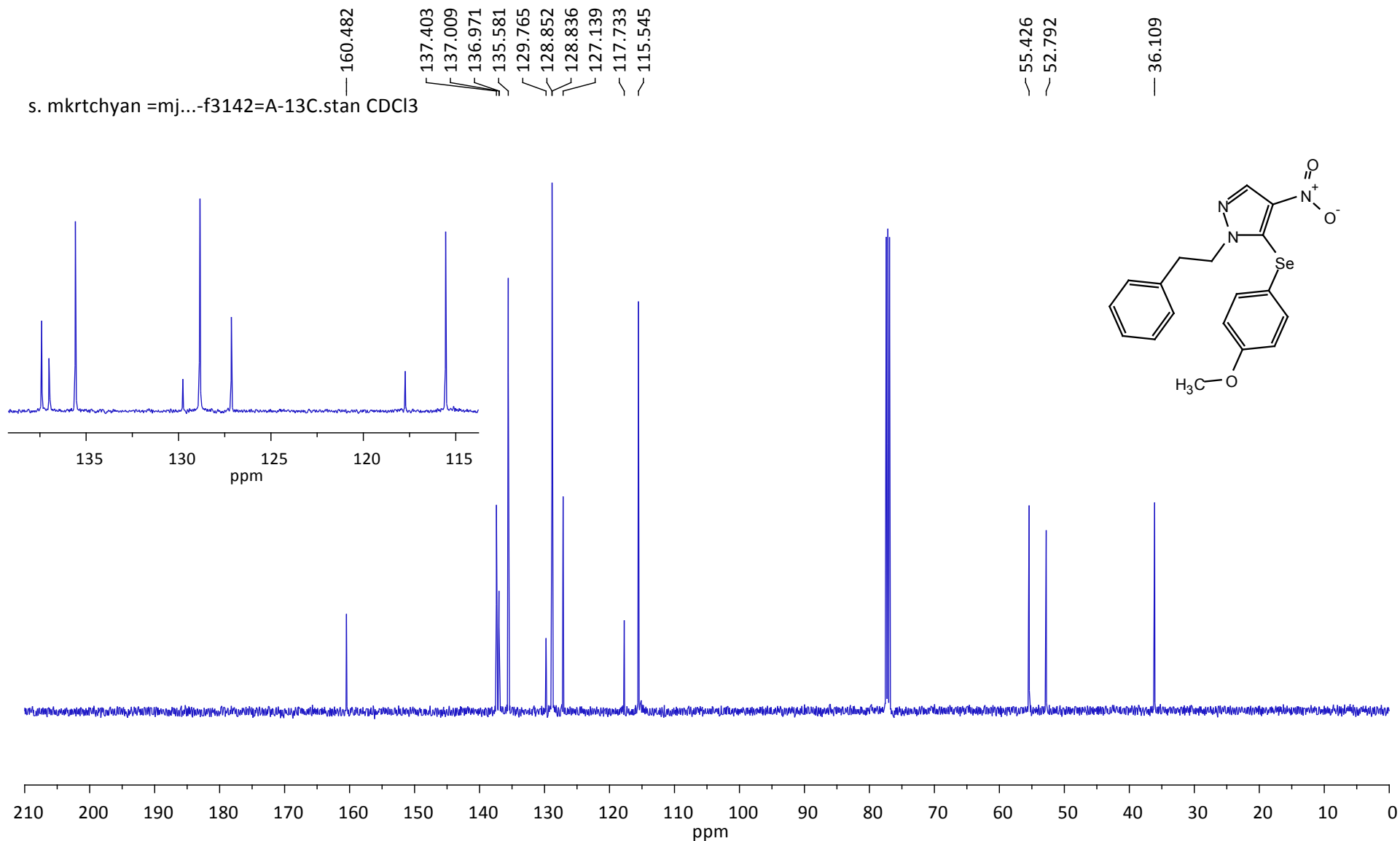
Compound **2e**

s. mkrtyan =mj...f3742=1H.stan CDCl3



Comment s. mkrtyan =mj...f3742=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 2e



Comment s. mkrtyan =mj...-f3142=
A-13C.stan CDCl3 {C:\NMR_Data\Service\CBMM} nmrsu 9

Number of Scans 256

Spectrometer Frequency 125.76

Spectral Width 36057.7

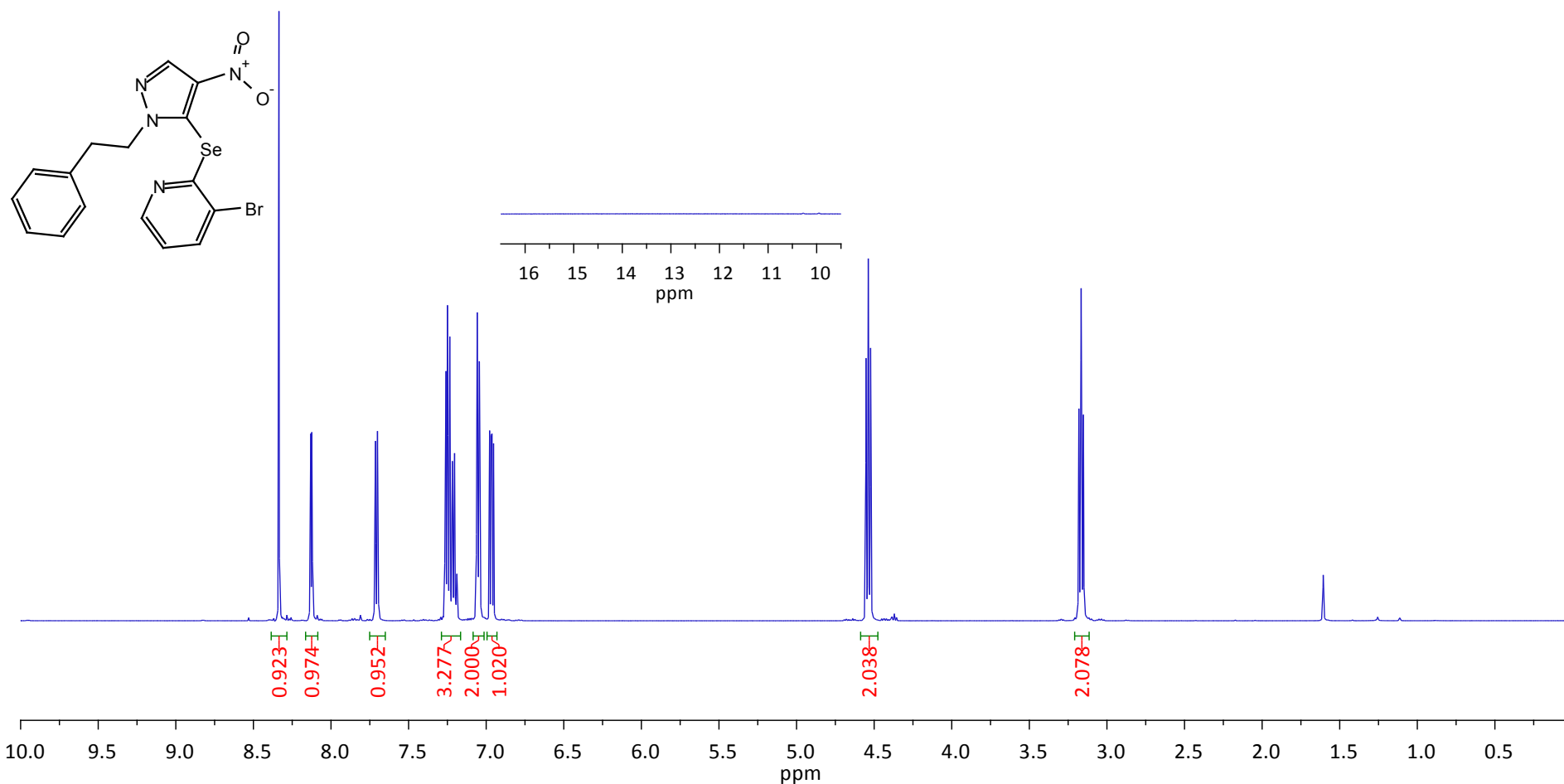
Compound **2f**

8.335
8.133
8.130
8.124
8.121
7.700
7.697
7.249
7.235
7.058
7.044
6.978
6.969
6.962
6.953

4.538

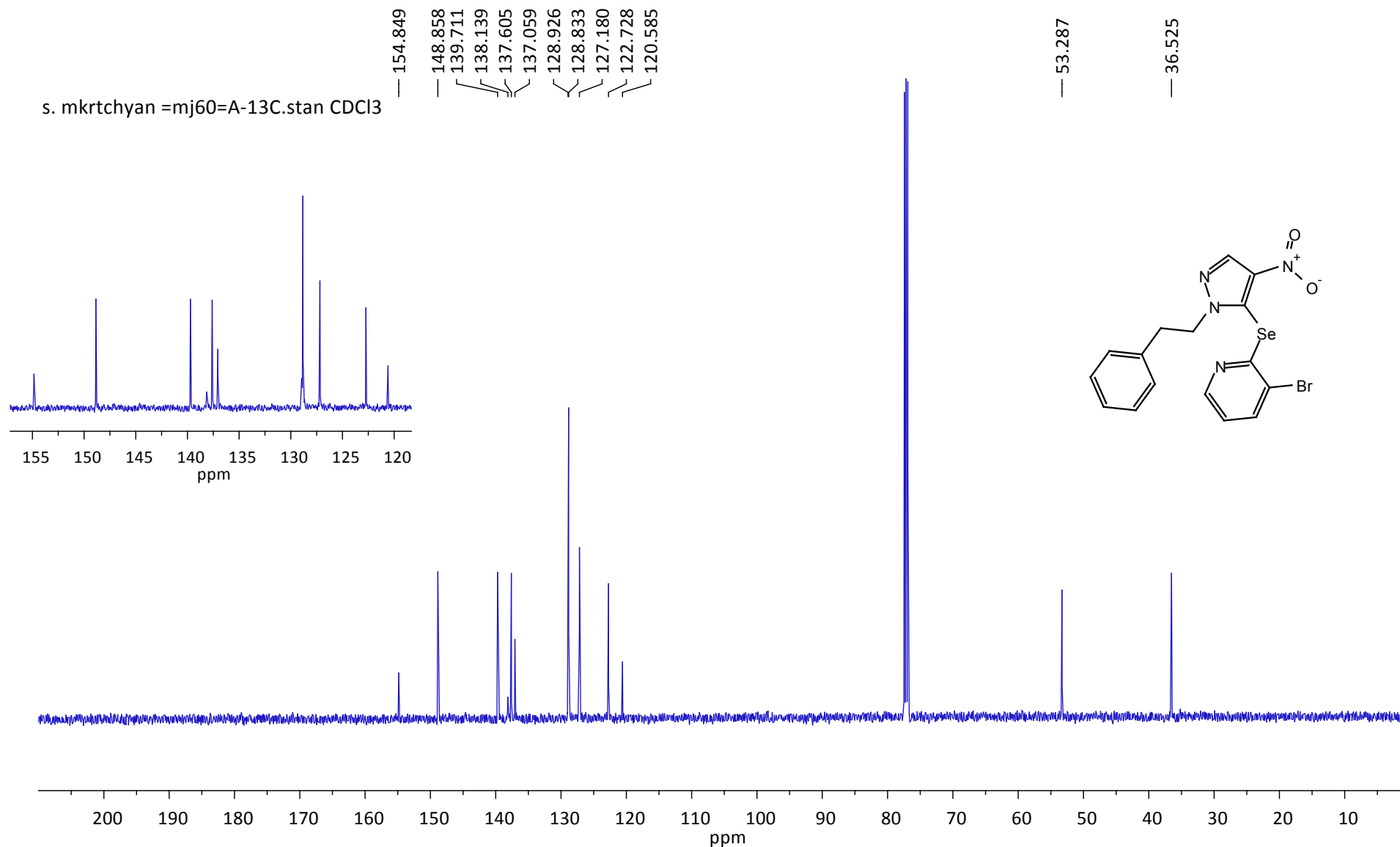
3.166

s. mkrtyan =mj60=1H.stan CDCl3



Comment s. mkrtyan =mj60=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **2f**



Comment s. mkrtchyan =mj60=
A-13C.stan CDCl₃ {C:\NMR_Data\Service\CBMM} nmrsu 6

Number of Scans 512
Spectrometer Frequency 125.76
Spectral Width 36057.7

Compound 3a

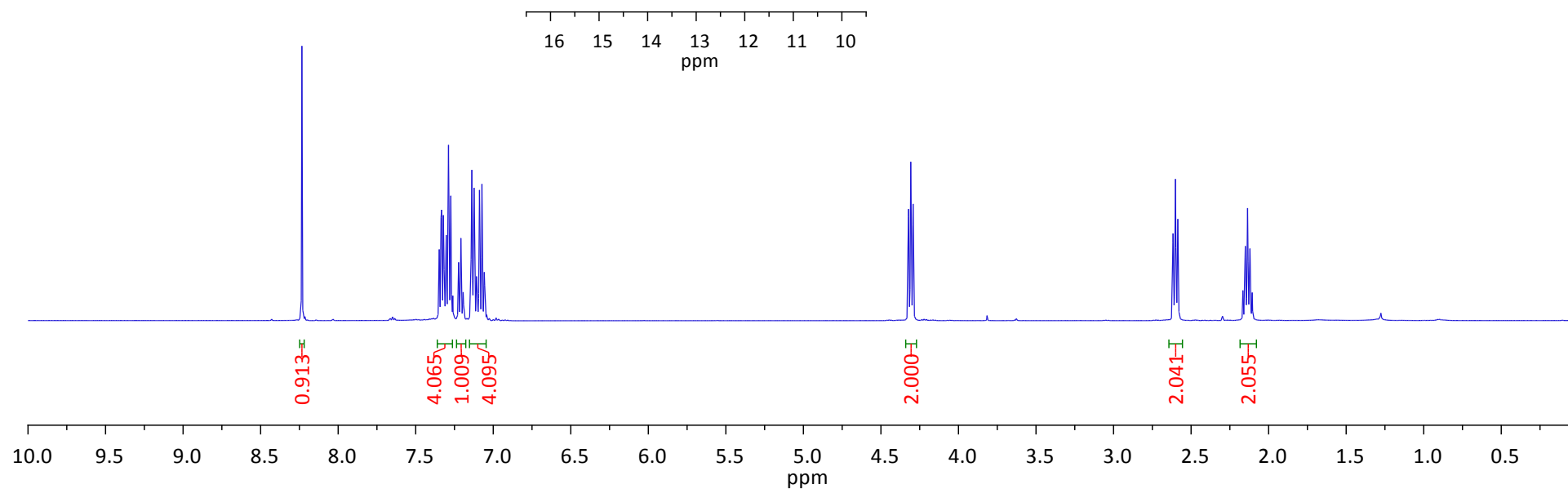
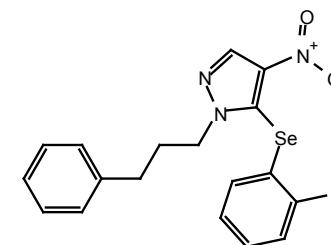
8.234
7.348
7.336
7.333
7.322
7.303
7.289
7.273
7.223
7.209
7.138
7.124
7.108
7.089
7.073
7.058

4.308

2.601

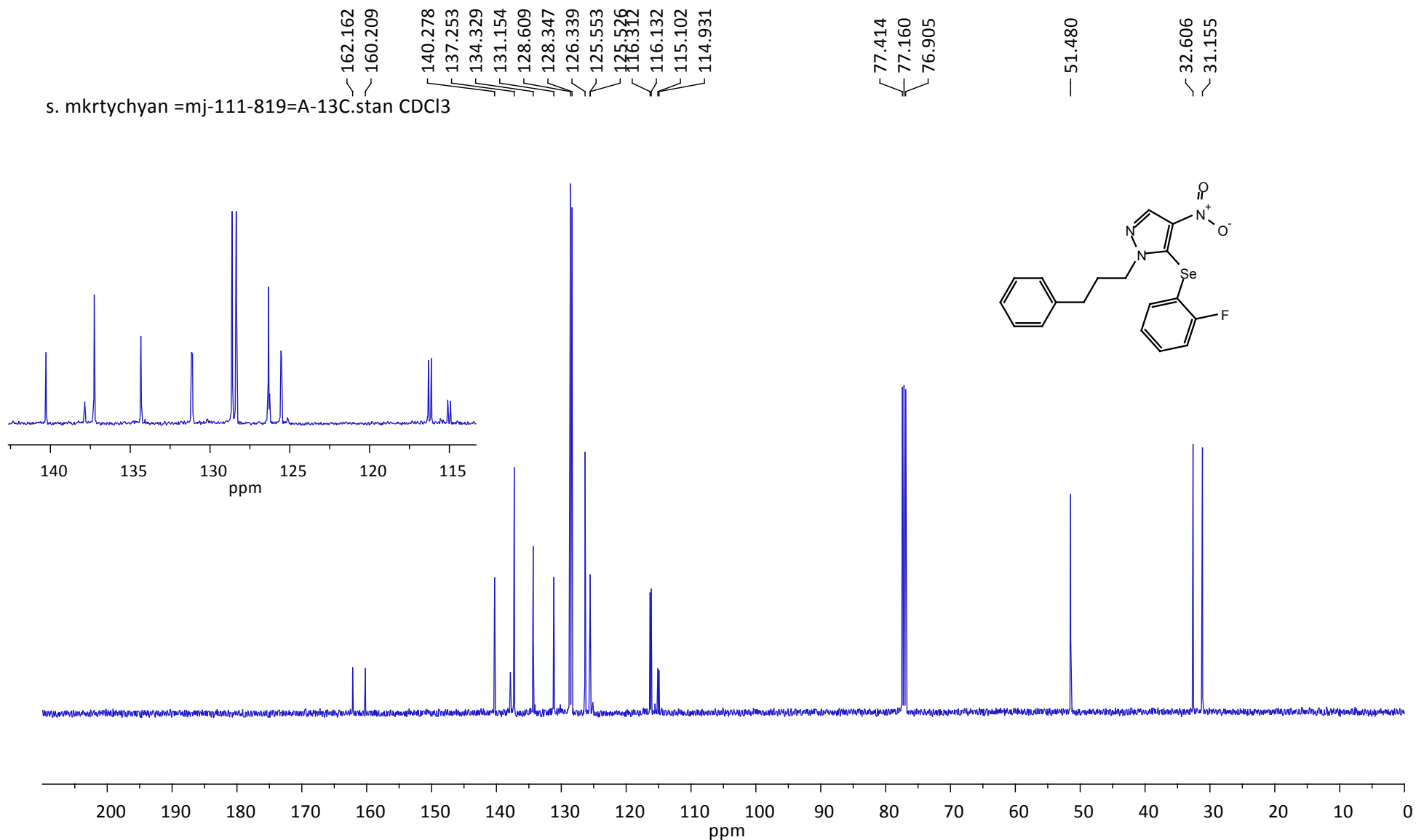
2.136

mkrtychyan =mj-111-819=1H.stan CDCl3



Comment	s. mkrtychyan =mj-111-819=1H.stan CDCl3
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound 3a



Comment s. mkrtychyan =mj-111-819=A-13C.stan CDCl3
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound **3b**

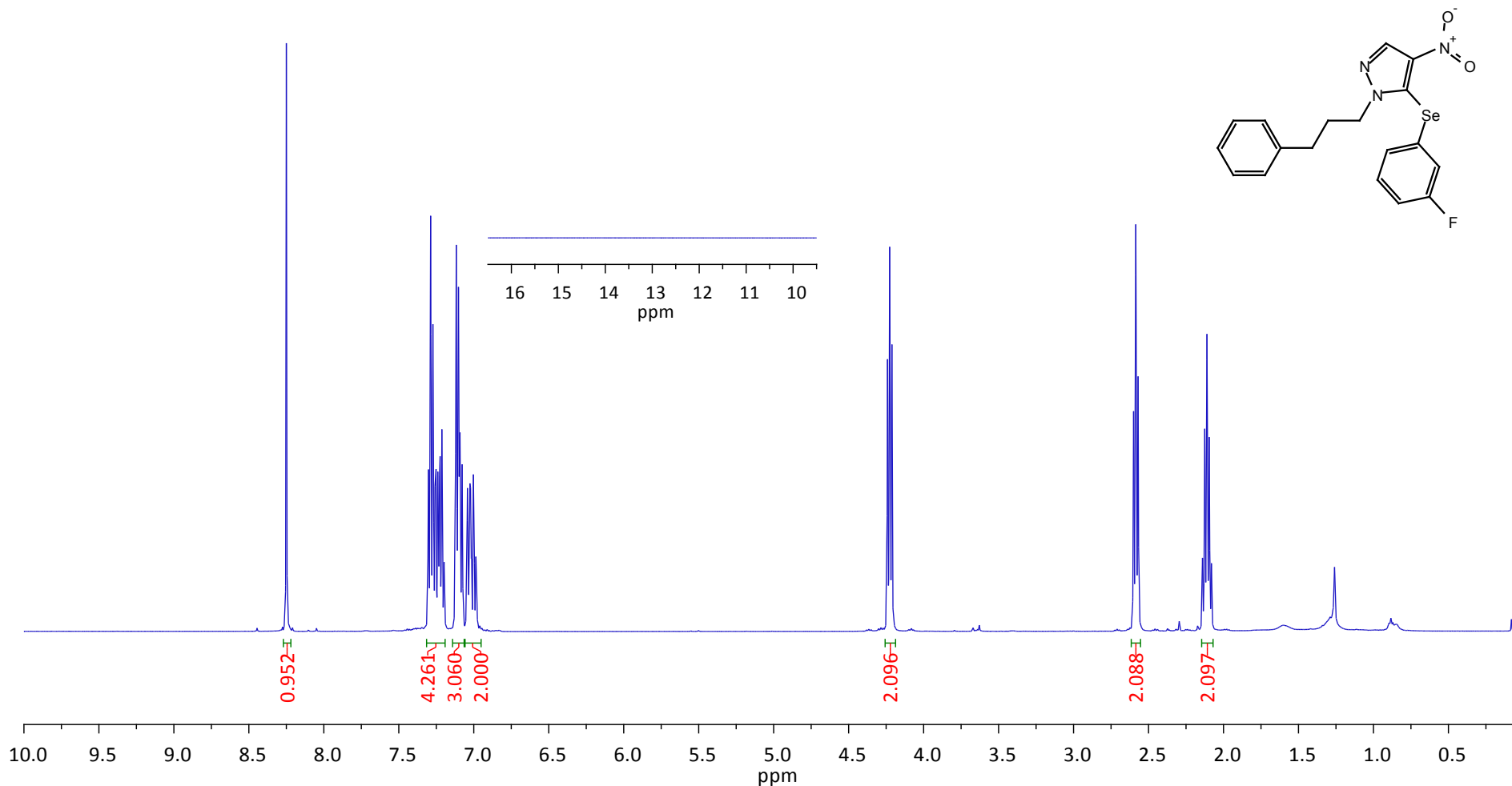
8.250
7.302
7.288
7.273
7.252
7.240
7.227
7.225
7.213
7.117
7.102
7.094
7.042
7.026
7.022
7.003
6.986
6.981

4.226

2.585

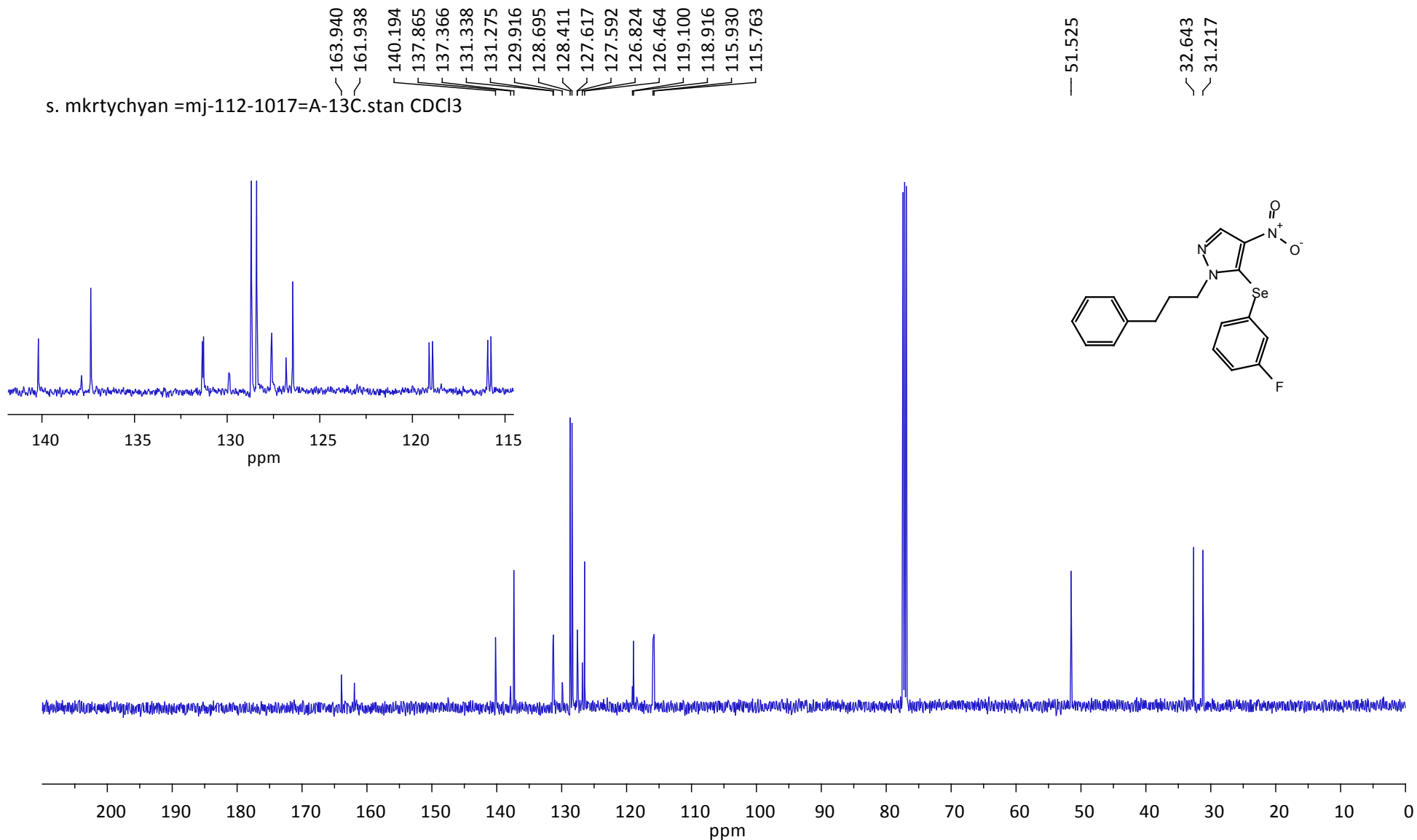
2.110

s. mkrtychyan =mj-112-1017=1H.stan CDCl3



Comment s. mkrtychyan =mj-112-1017=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

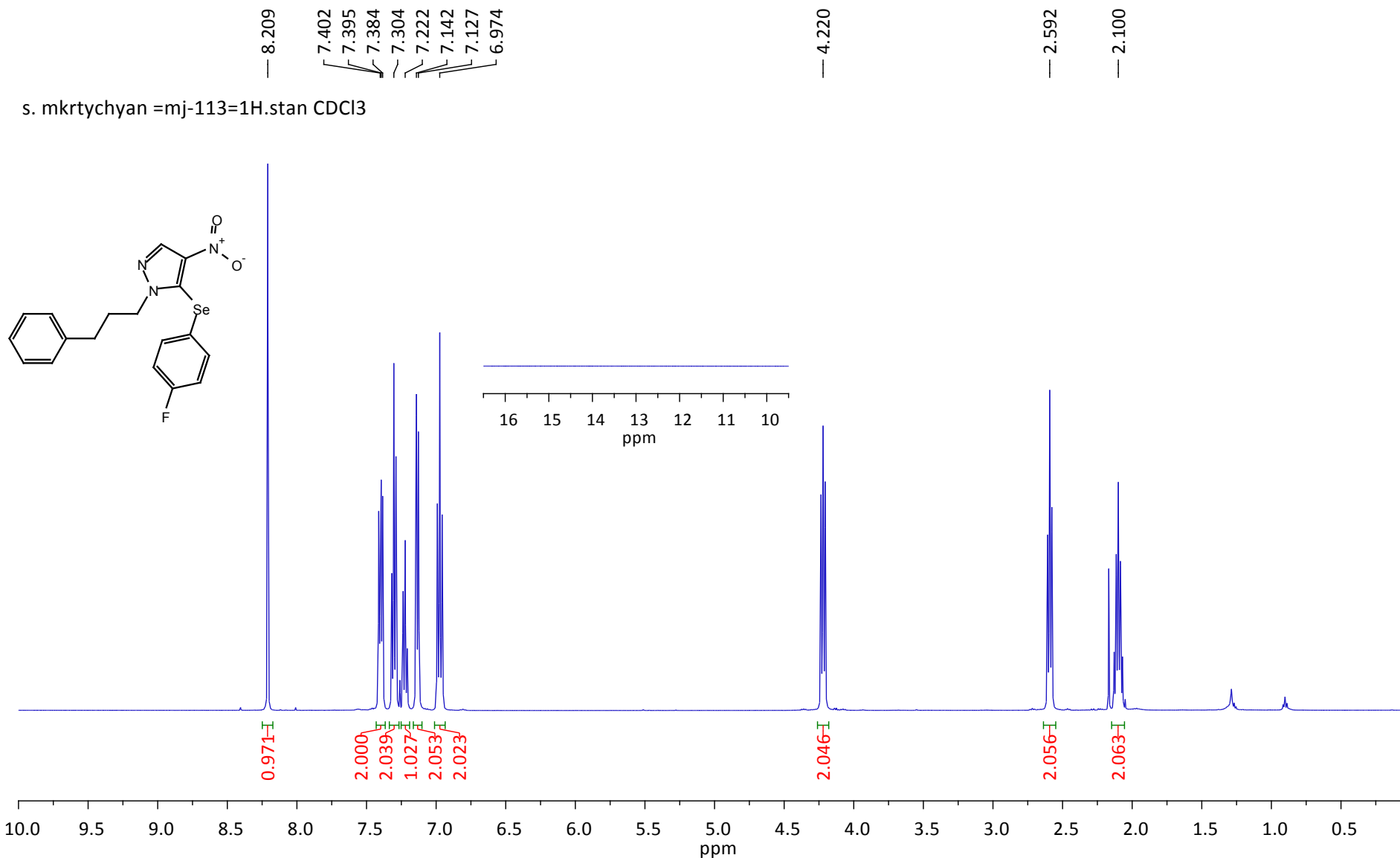
Compound **3b**



Comment s. mkrtychyan =mj-112-1017=A-13C.stan CDCl3
 Number of Scans 256
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound **3c**

s. mkrtychyan =mj-113=1H.stan CDCl3



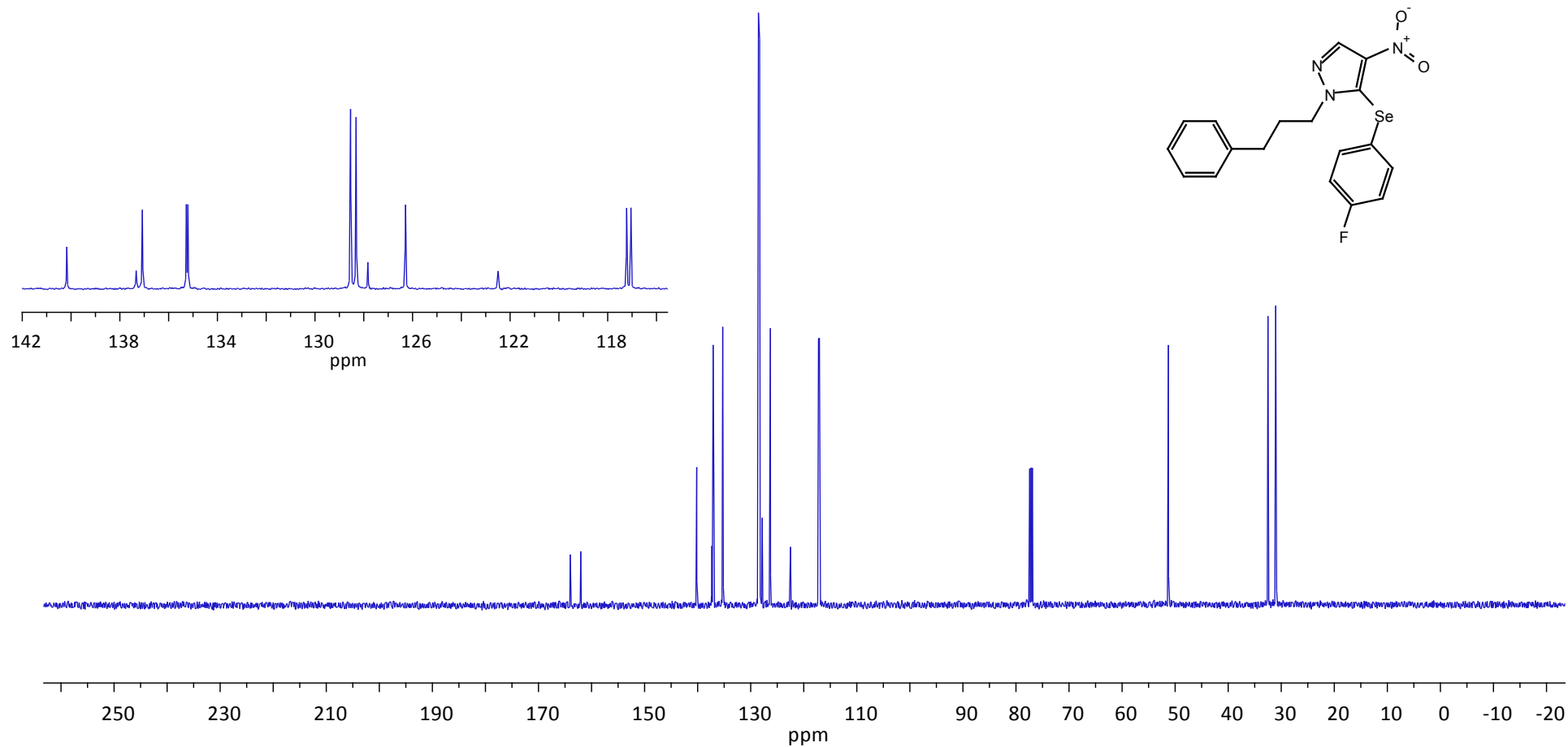
Comment s. mkrtychyan =mj-113=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **3c**

164.012
162.024
140.176
137.329
137.075
135.273
135.208
128.541
128.312
127.831
126.290
122.519
122.493
117.223
117.048

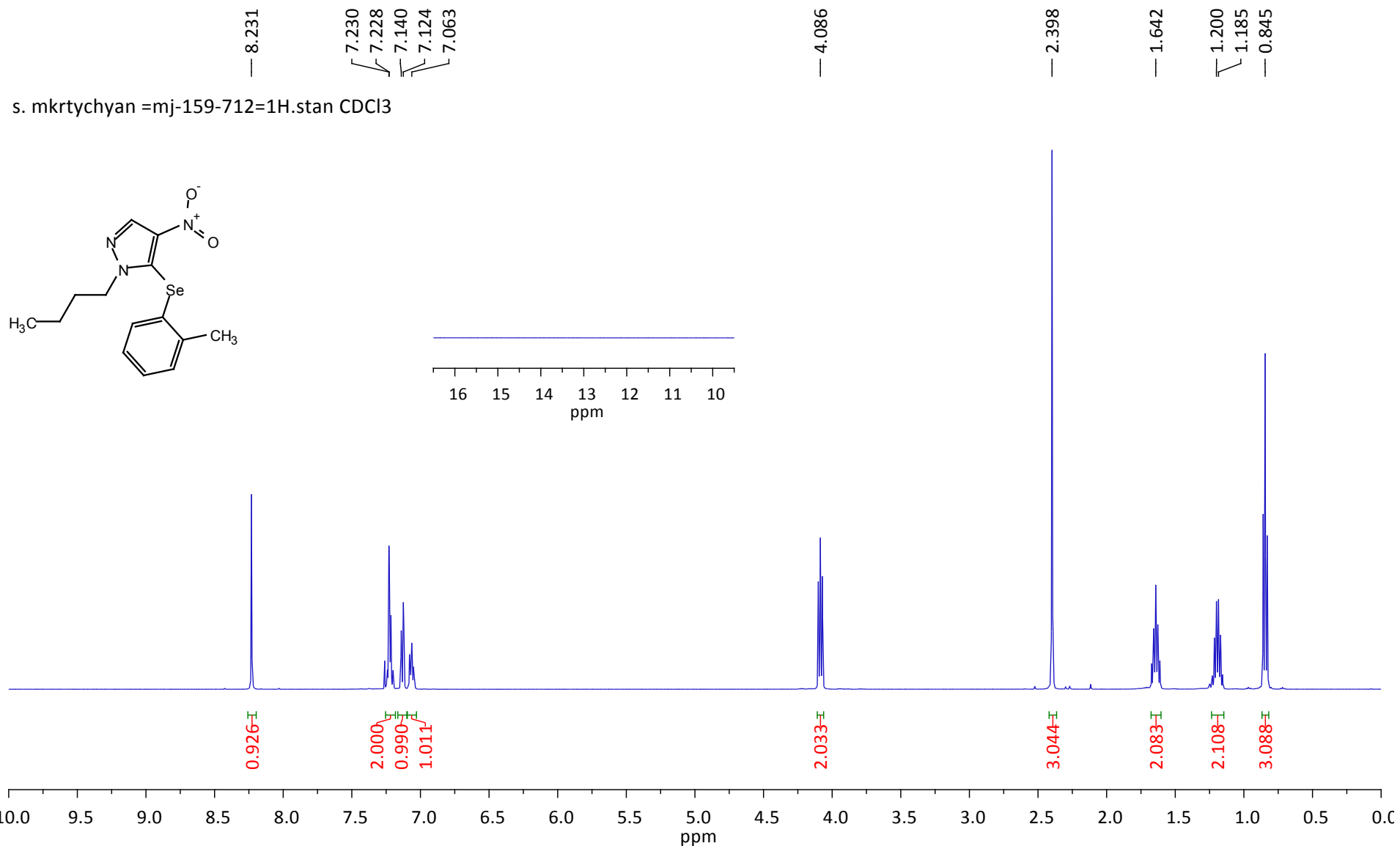
51.271
32.501
31.041

s. mkrtychyan =mj-113=A-13C.stan CDCl3



Comment s. mkrtychyan =mj-113=A-13C.stan CDCl3
 Number of Scans 128
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound **4a**



Comment s. mkrtychyan =mj-159-712=1H.stan CDCl₃

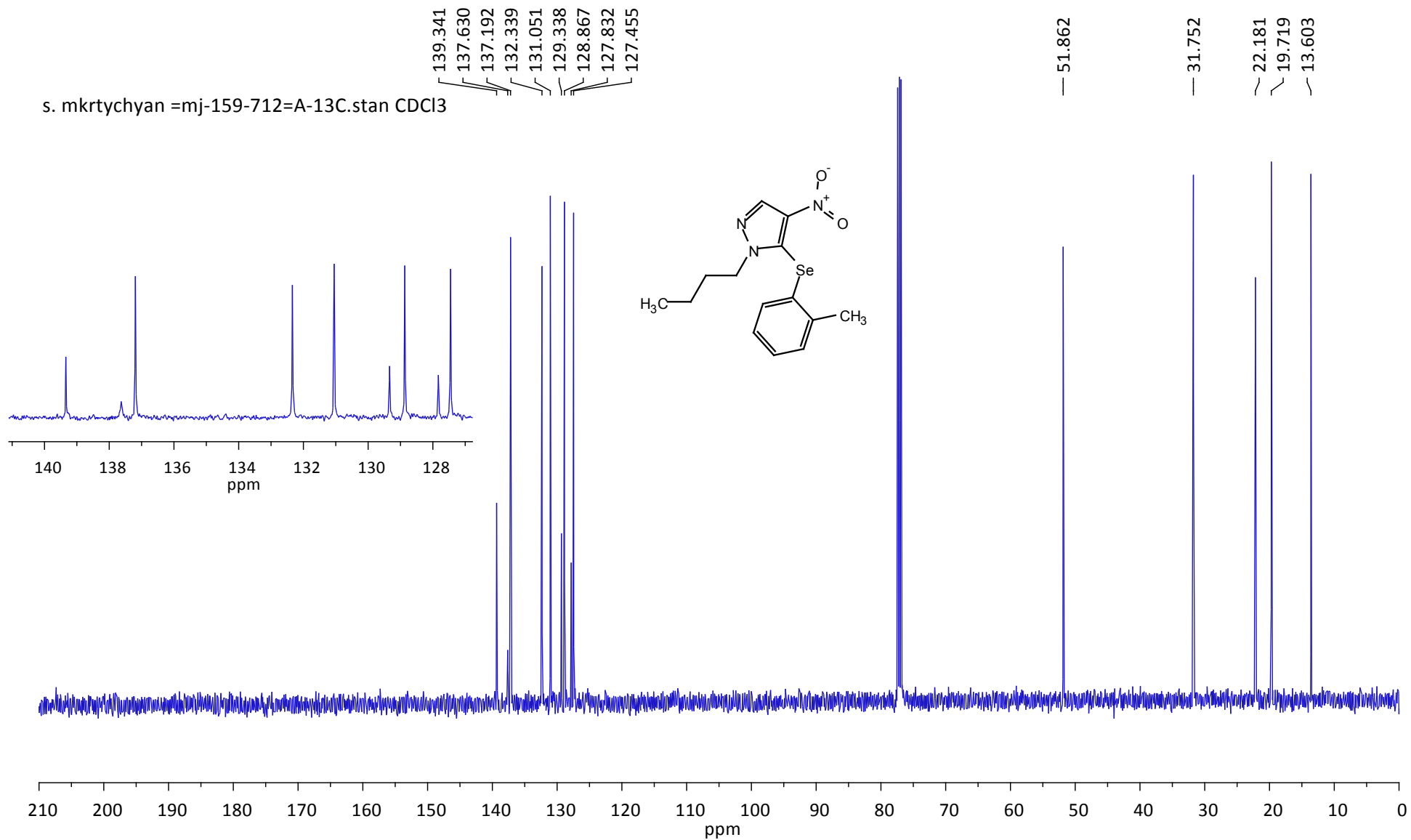
Number of Scans 24

Spectrometer Frequency 500.13

Spectral Width 12335.5

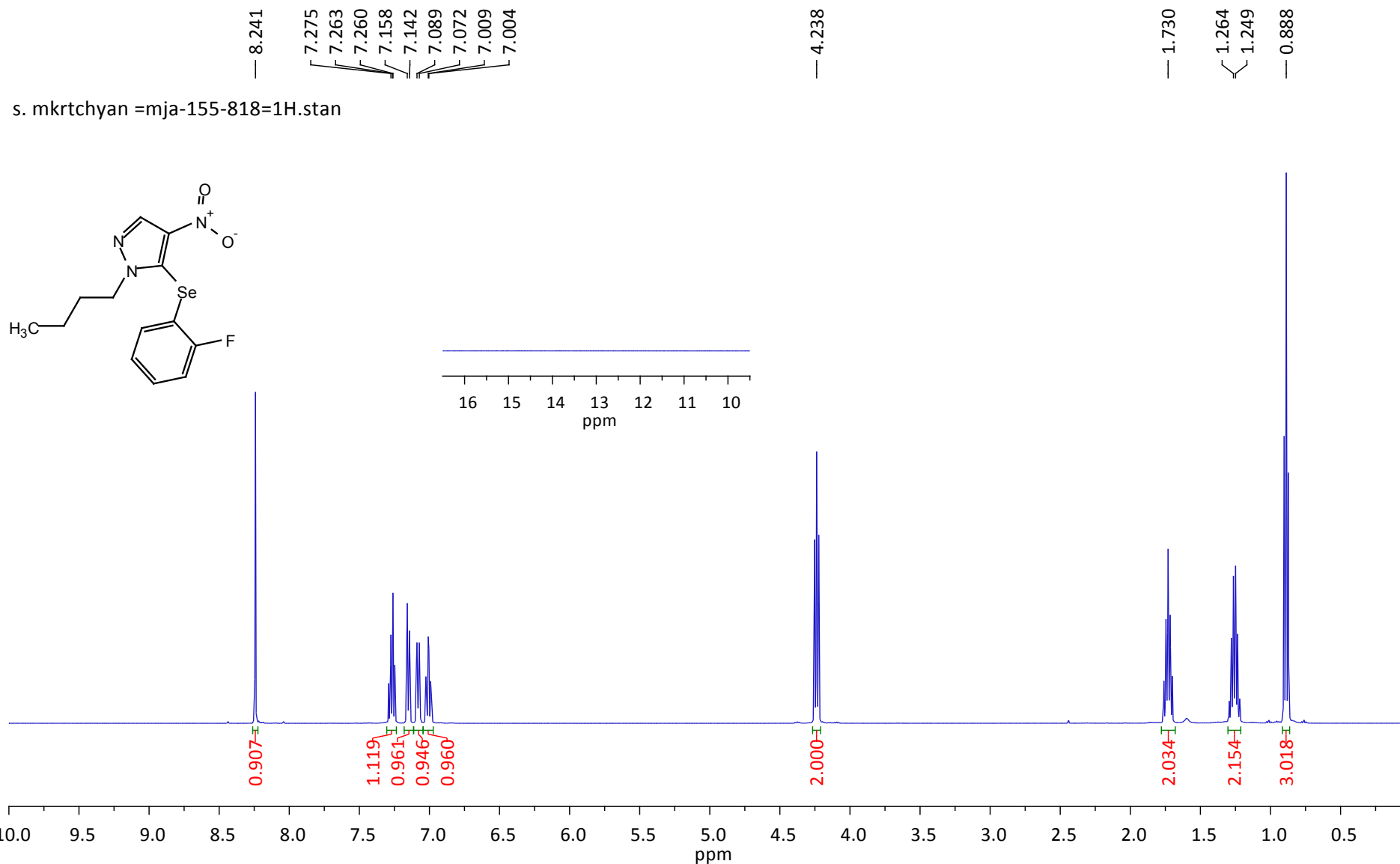
Spectral Size 65536

Compound 4a



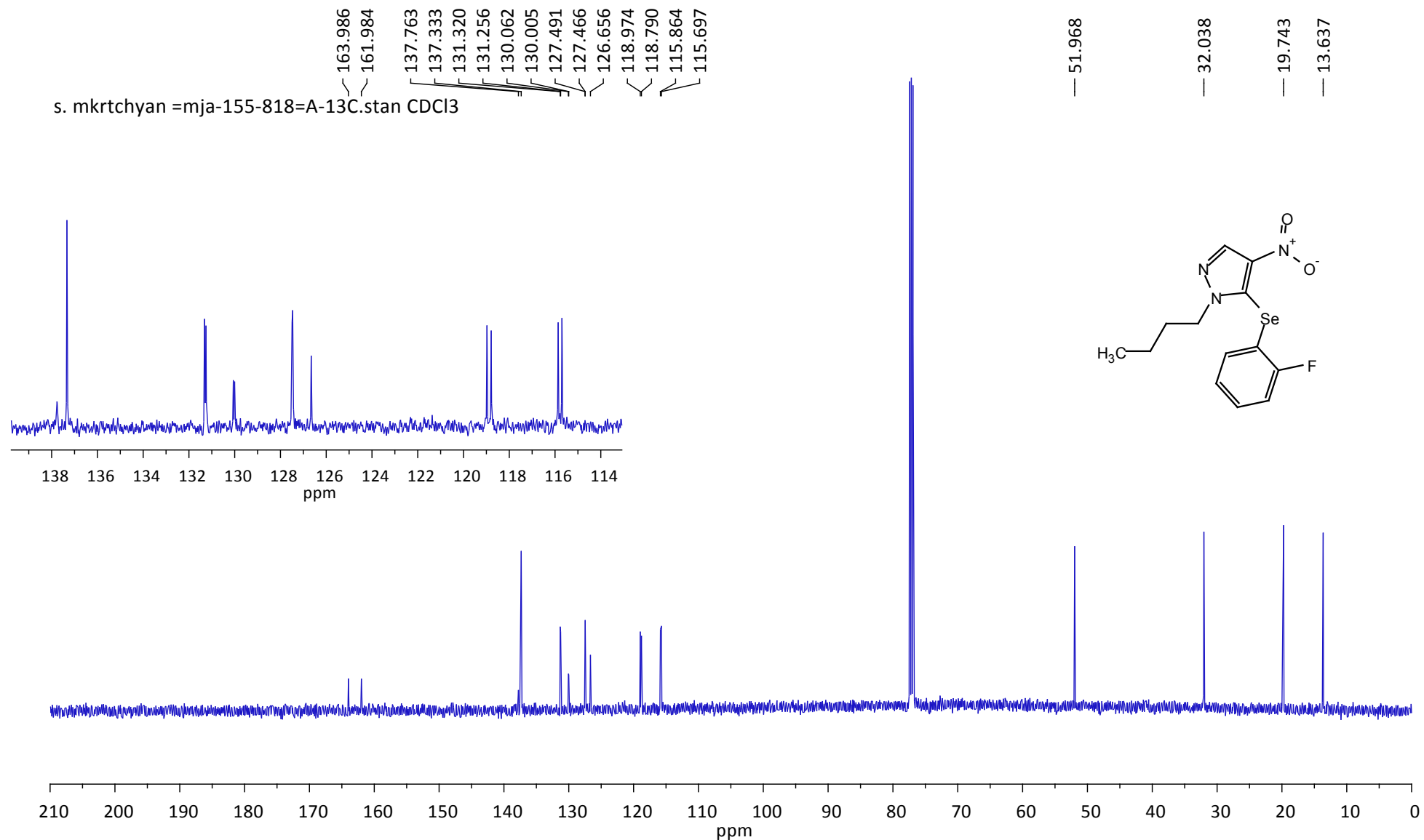
Comment s. mkrtychyan =mj-159-712=A-13C.stan CDCl3
Number of Scans 296
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

Compound **4b**



Comment s. mkrtyan =mja-155-818=1H.stan
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

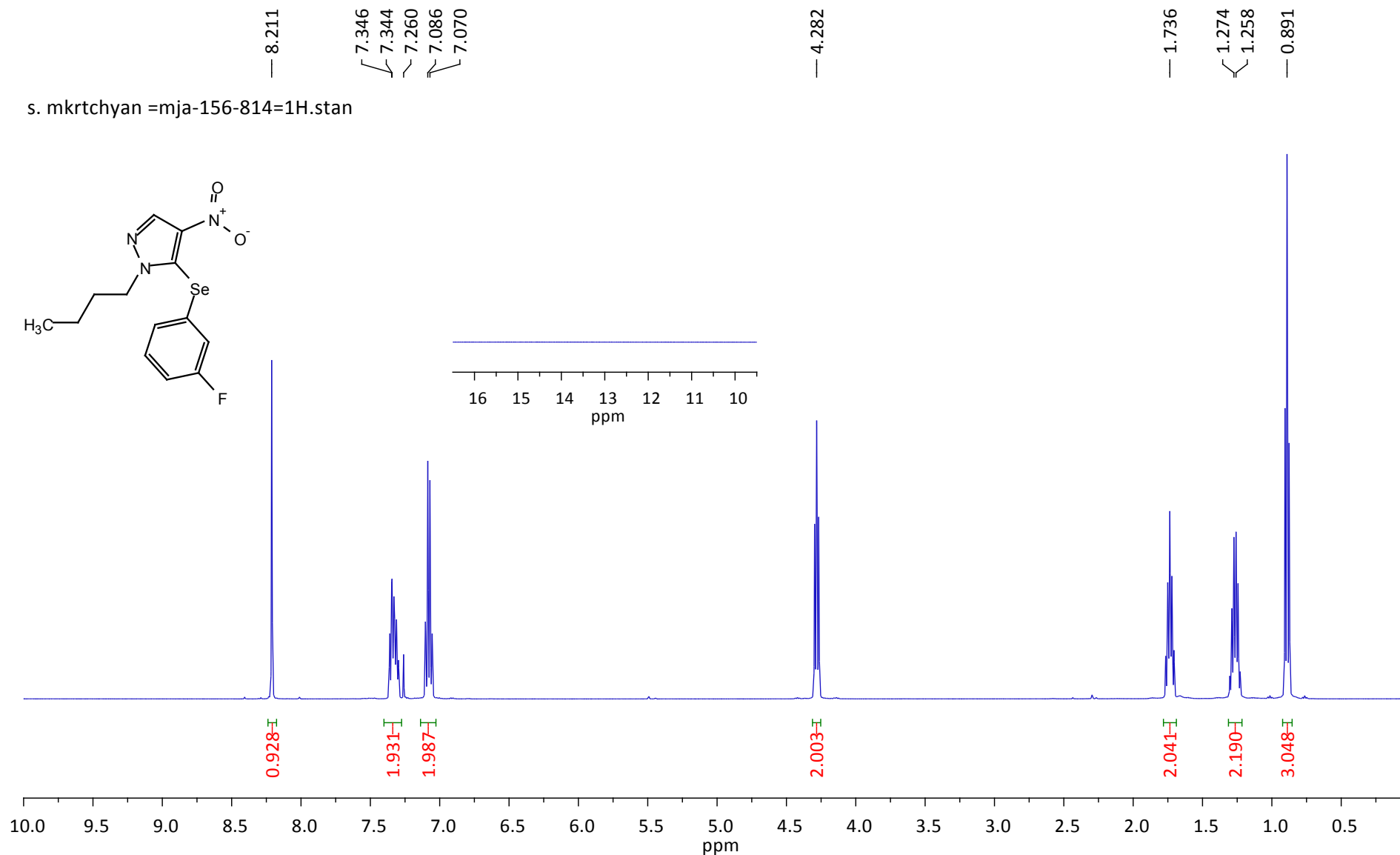
Compound **4b**



Comment	s. mkrtyan =mja-155-818=A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

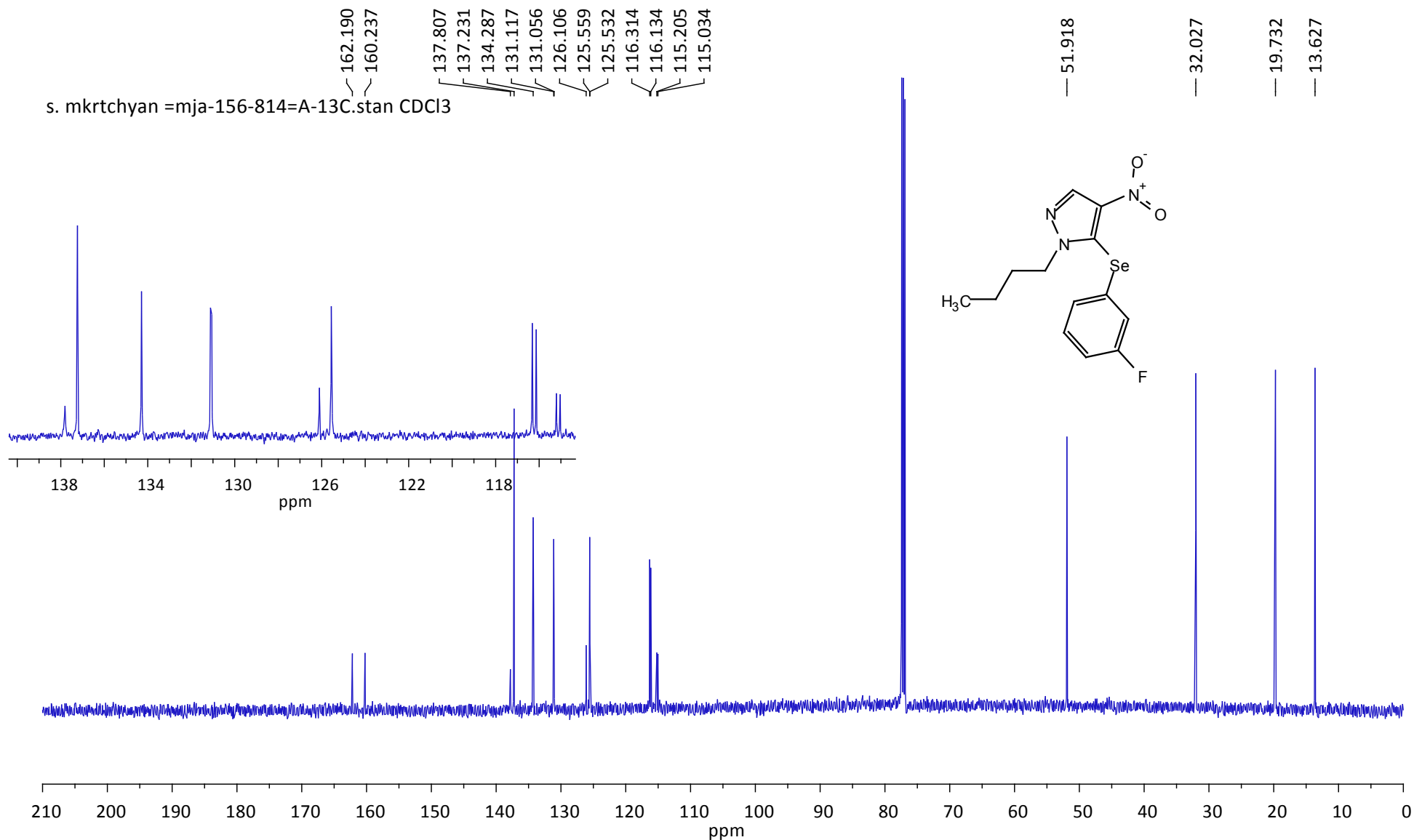
Compound **4c**

s. mkrтчhyan =mja-156-814=1H.stan



Comment s. mkrтчhyan =mja-156-814=1H.stan
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **4c**



Comment s. mkrtyan =mja-156-814=A-13C.stan CDCl3

Number of Scans 512

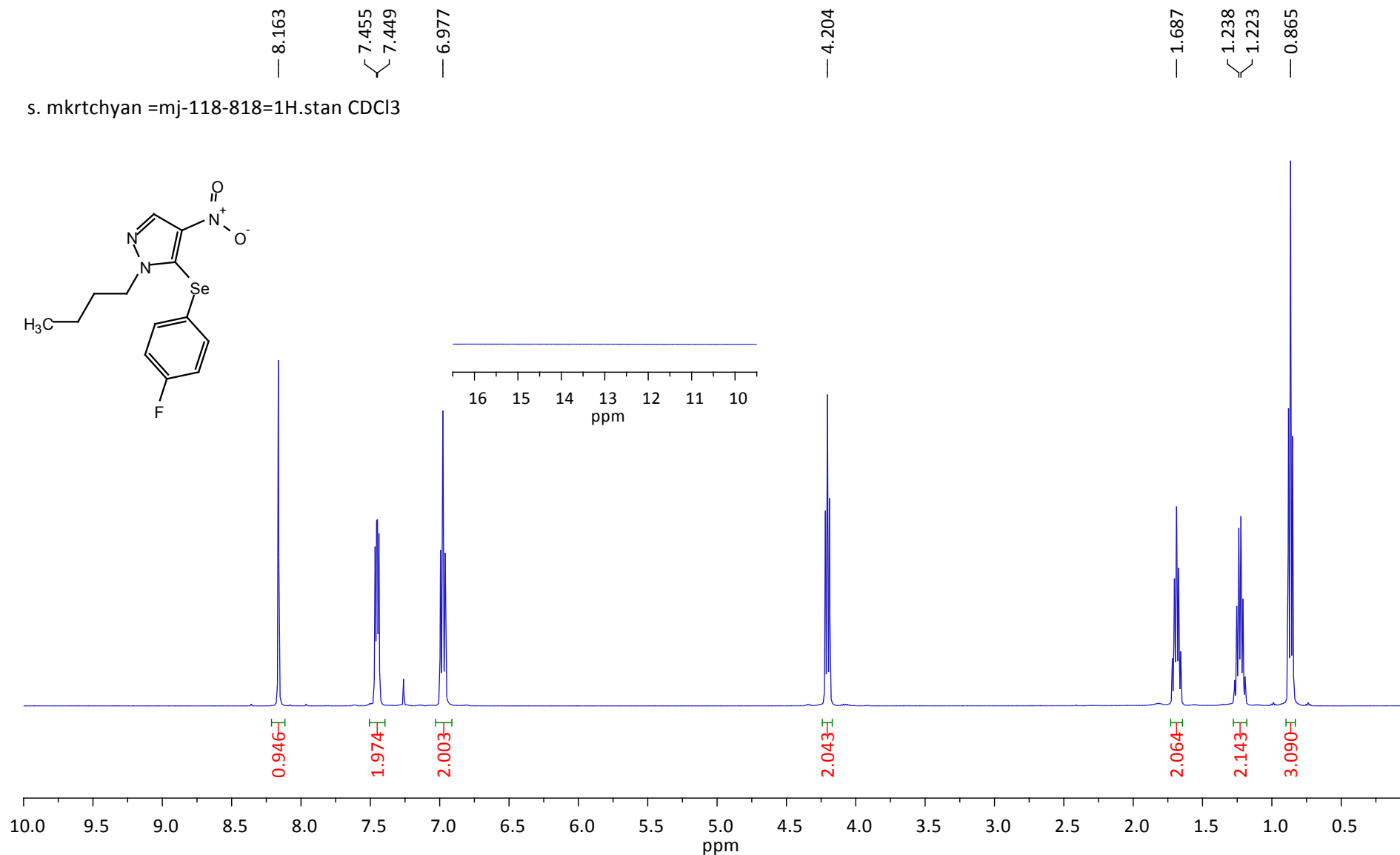
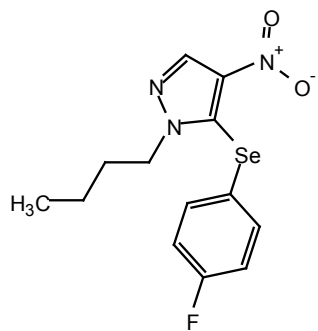
Spectrometer Frequency 125.76

Spectral Width 36057.7

Spectral Size 65536

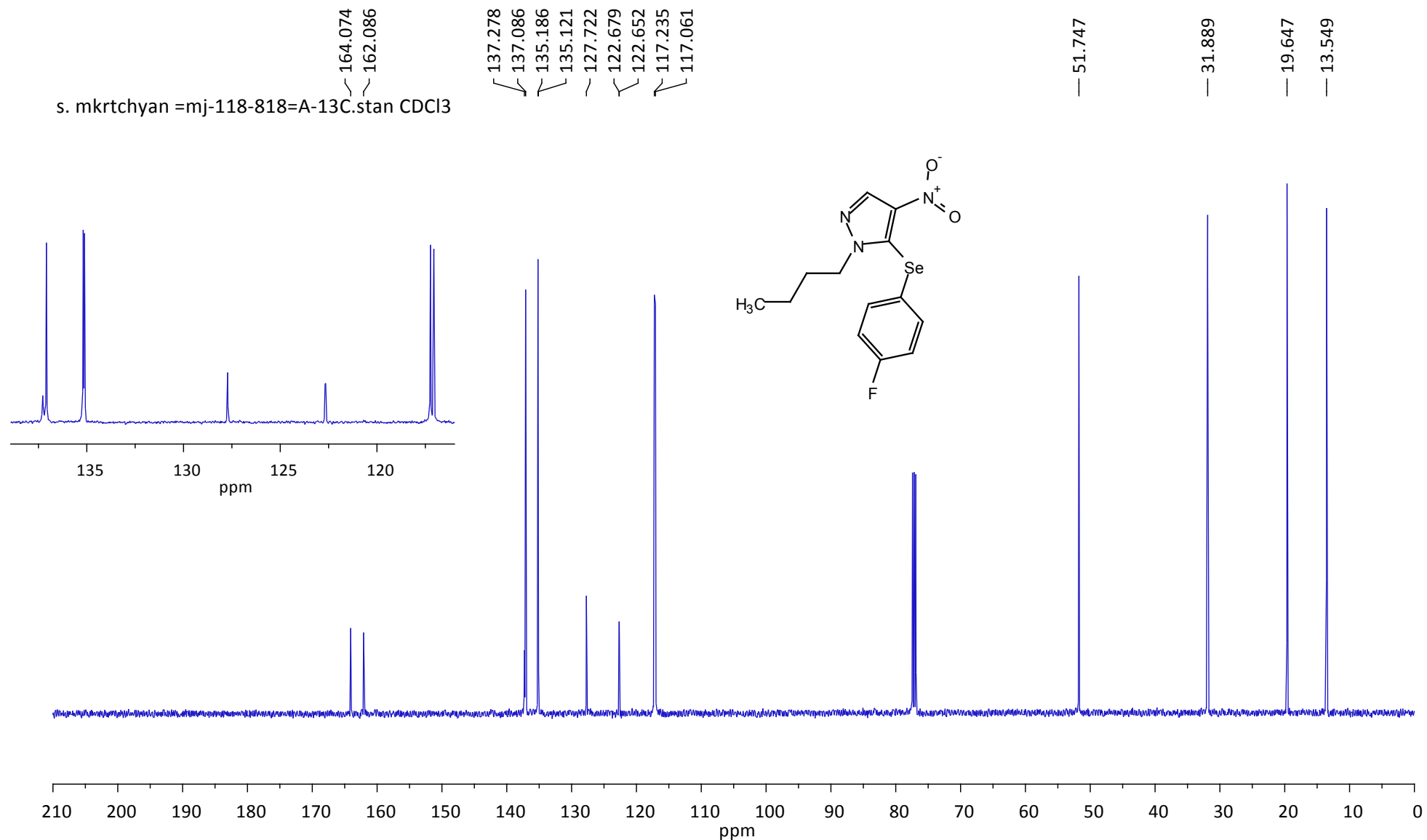
Compound **4d**

s. mkrtyan =mj-118-818=1H.stan CDCl3



Comment s. mkrtyan =mj-118-818=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **4d**



Comment s. mkrtyan =mj-118-818=A-13C.stan CDCl3
 Number of Scans 256
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

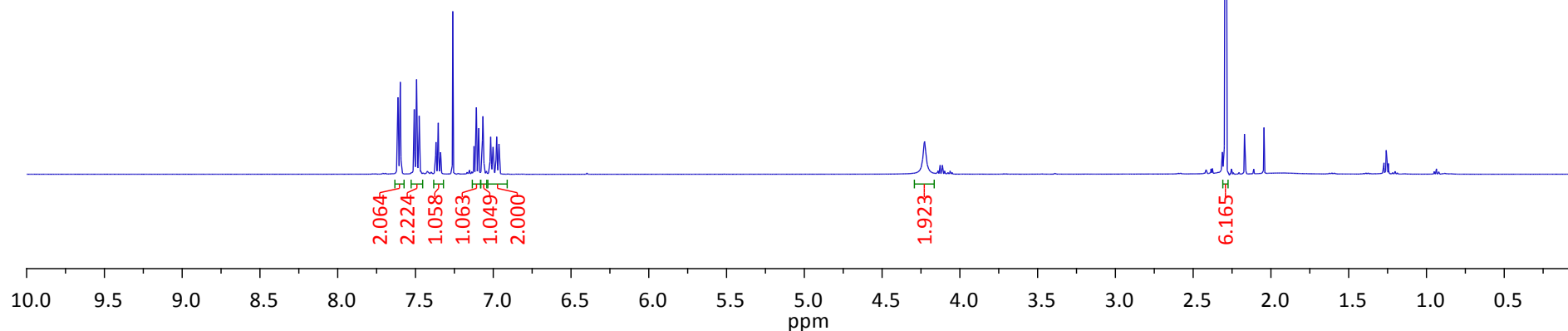
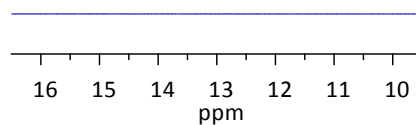
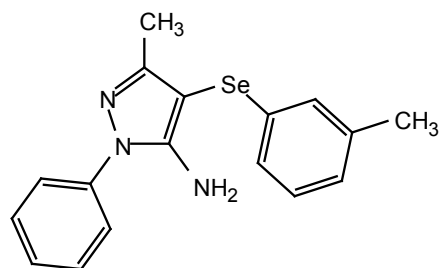
Compound 5a

7.612
7.598
7.596
7.493
7.353
7.260
7.108
7.066
7.017
6.978

— 4.227

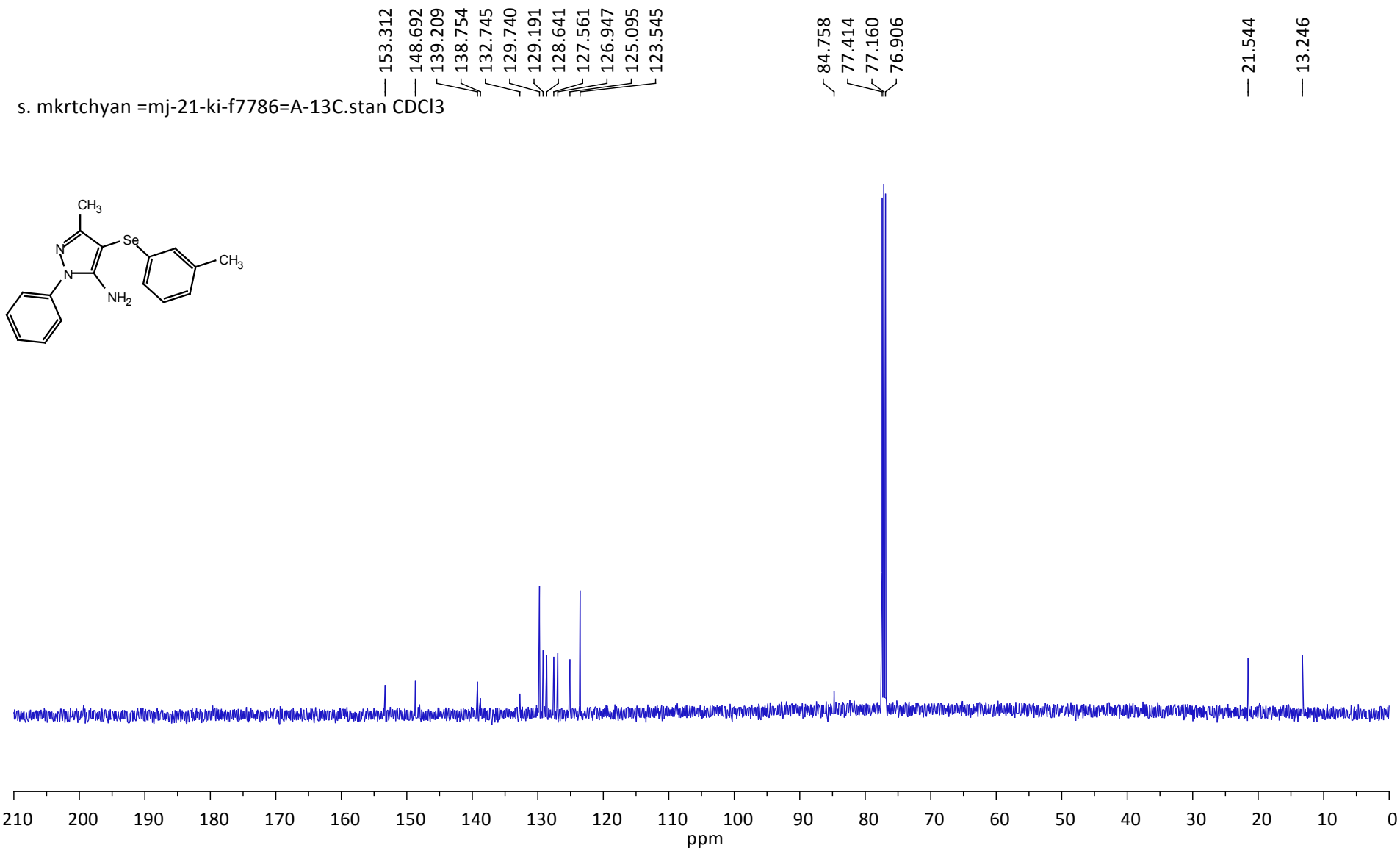
— 2.290

s. mkrtyan =mj-21-ki-f7786=1H.stan CDCl3



Comment s. mkrtyan =mj-21-ki-f7786=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 5a



Comment s. mkrtyan =mj-21-ki-f7786=A-13C.stan CDCl3
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

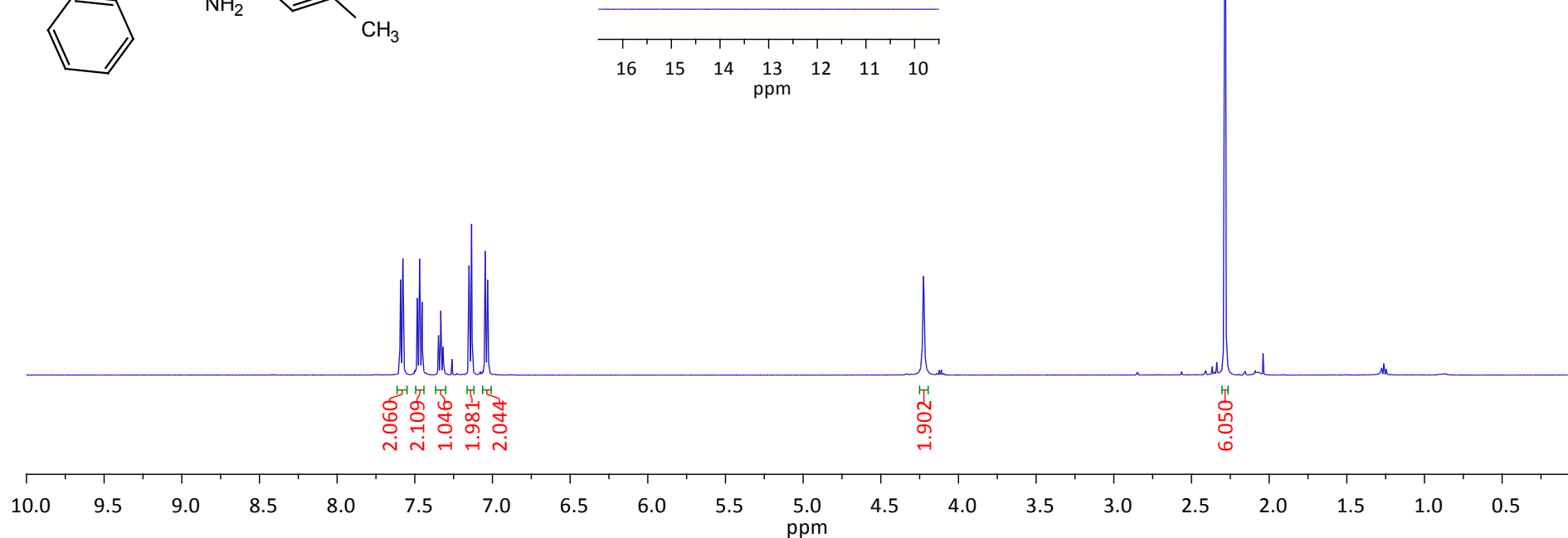
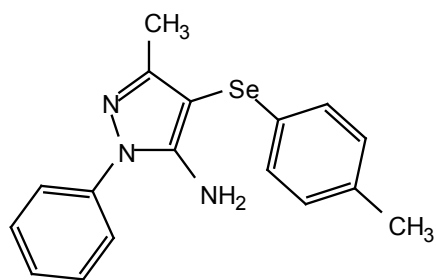
Compound **5b**

7.577
7.575
7.469
7.333
7.260
7.151
7.134
7.047
7.031

— 4.225

— 2.287
— 2.282

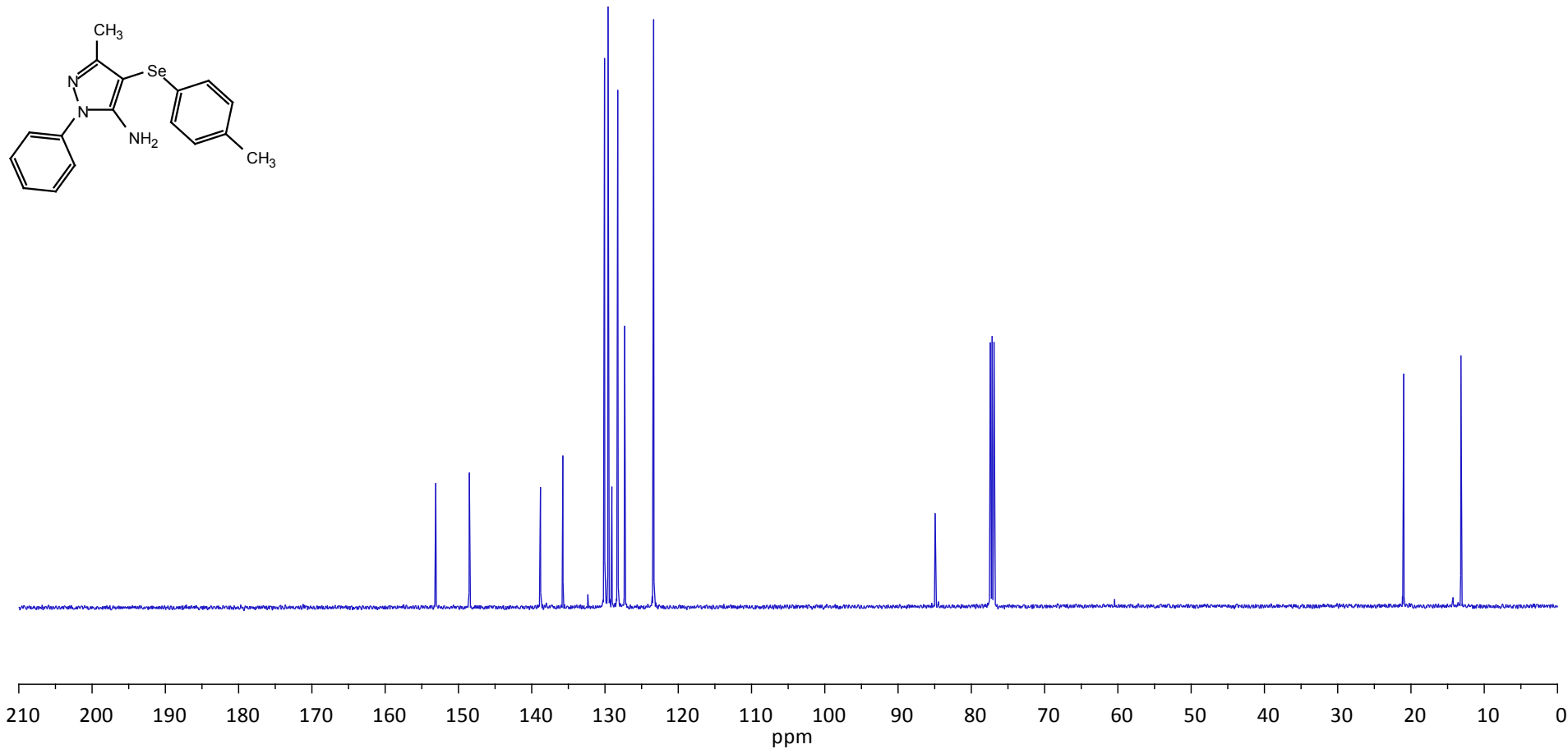
s. mkrtyan =mj-1-k1f2028=1H.stan CDCl3



Comment s. mkrtyan =mj-1-k1f2028=1H.stan CDCl3
Number of Scans 32
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **5b**

s. mkrtyan =mj-1-k1f2028=A-13C.stan CDCl₃



Comment	s. mkrtyan =mj-1-k1f2028=A-13C.stan CDCl ₃
Number of Scans	1024
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound 5c

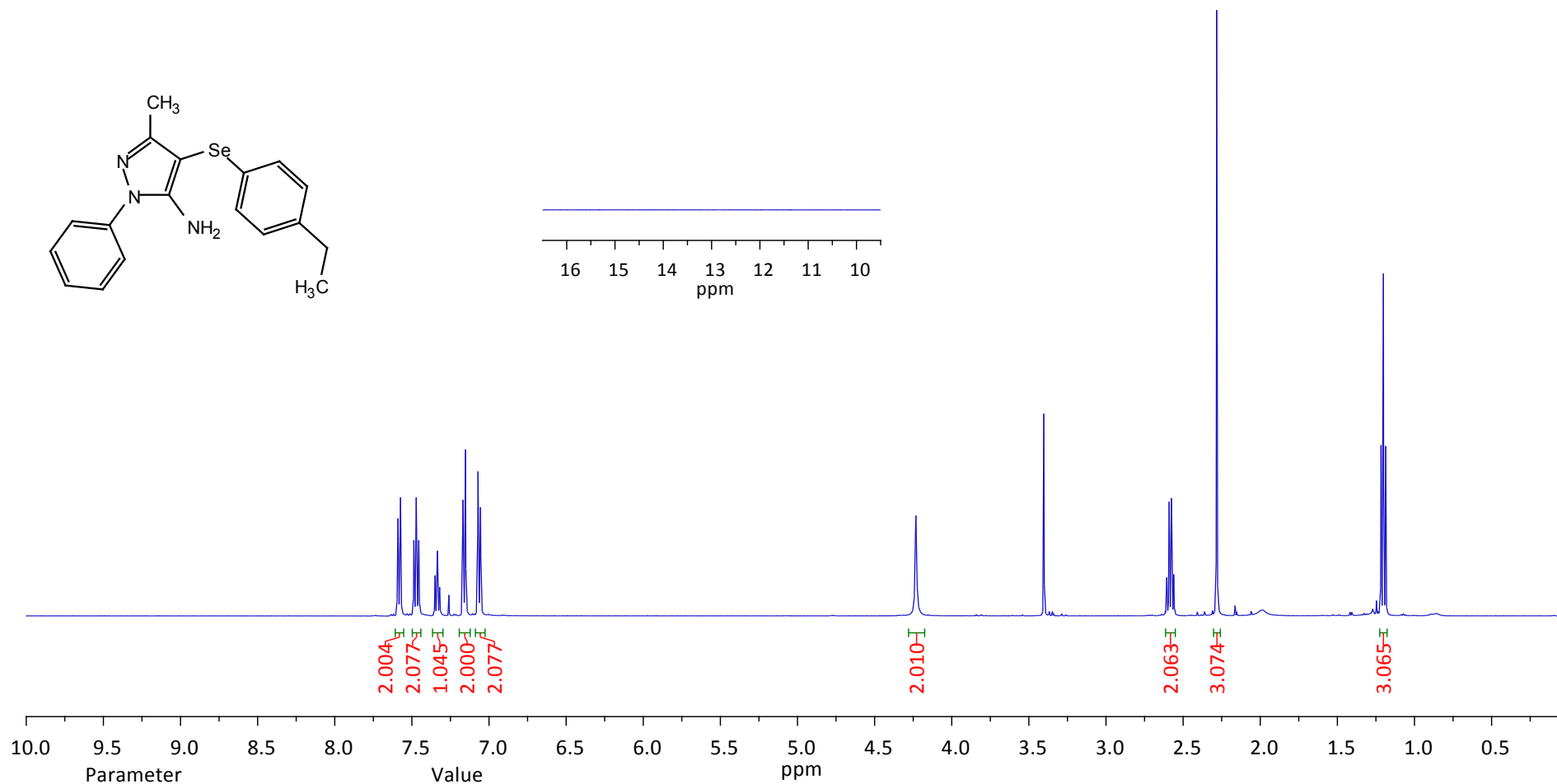
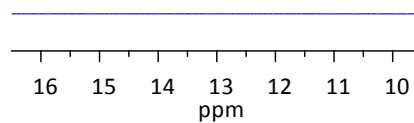
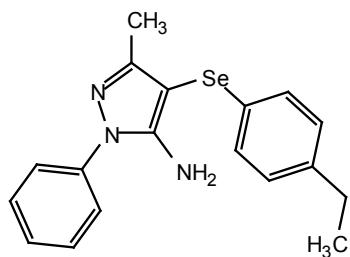
7.575
7.574
7.472
7.335
7.260
7.169
7.153
7.071
7.055

— 4.232

2.591
2.576
~ 2.282

— 1.202

s. mkrtyan =mj-1-k1f67112=1H.stan CDCl3



Comment s. mkrtyan =mj-1-k1f67112=1H.stan CDCl3
 Number of Scans 32
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 5c

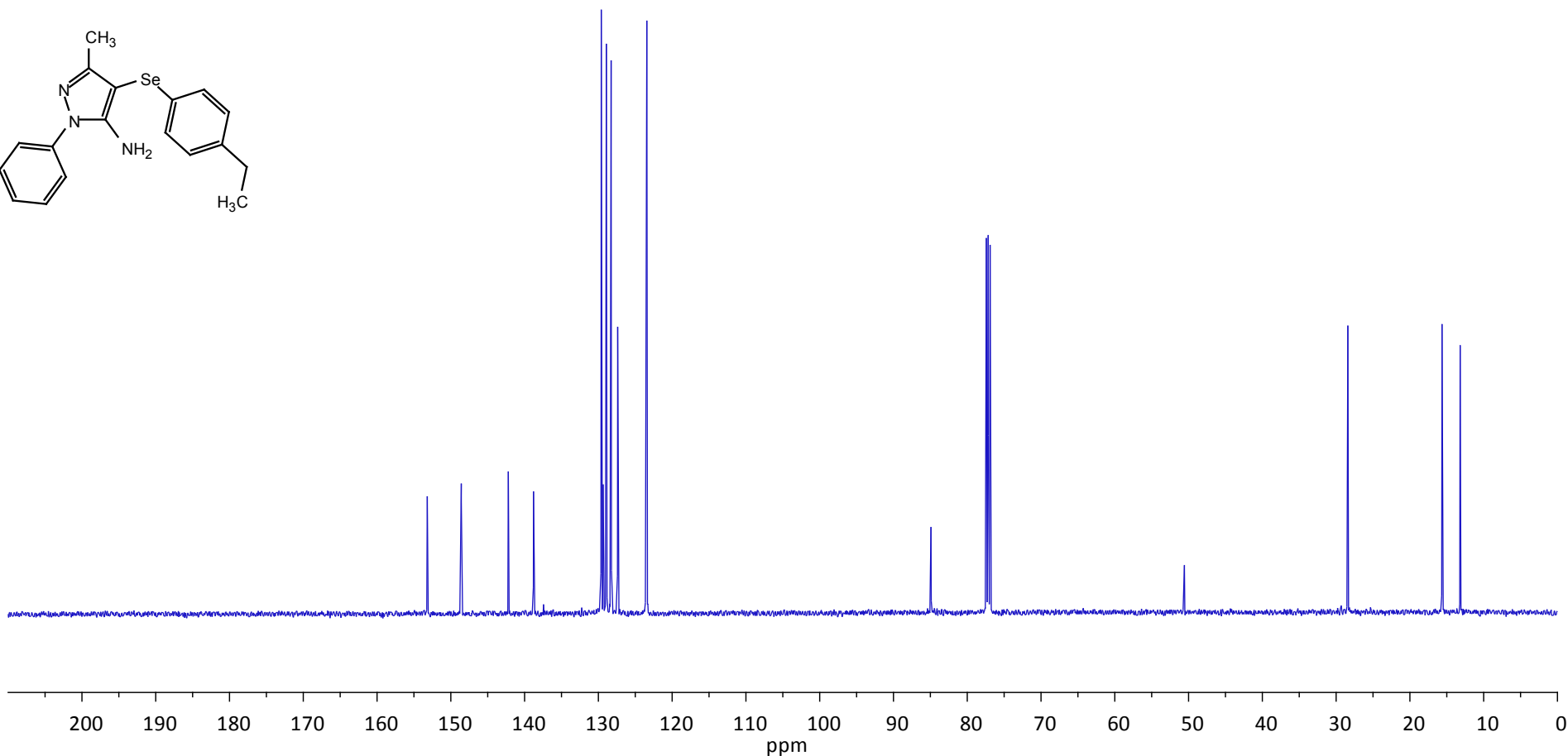
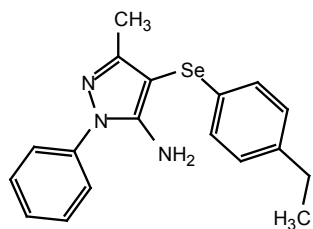
s. mkrtyan =mj-2-k1f67112=A-13C.stan CDCl3

153.193
148.581
142.208
138.792
129.612
129.360
128.918
128.271
127.385
123.432

84.914
77.414
77.160
76.905

28.410

15.648
13.190



Comment s. mkrtyan =mj-2-k1f67112=A-13C.stan CDCl3
 Number of Scans 1024
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

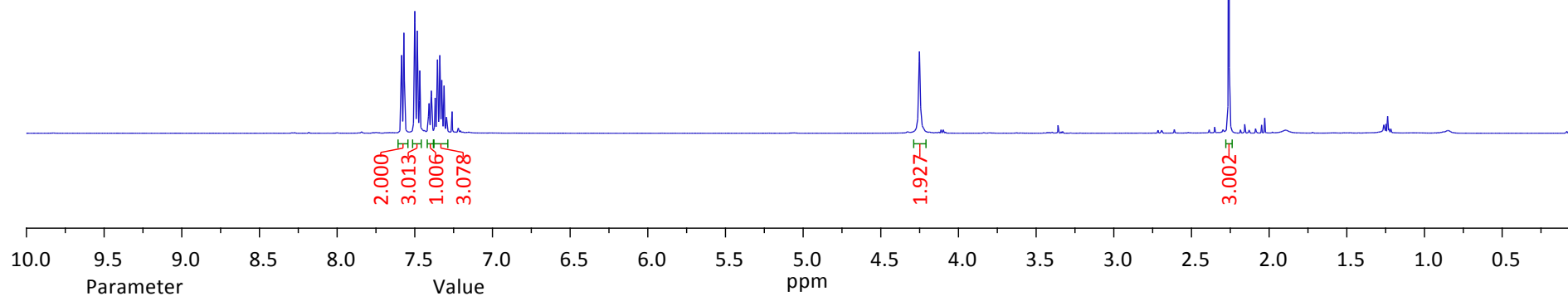
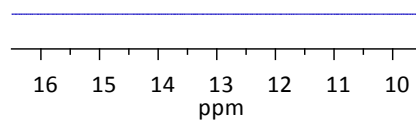
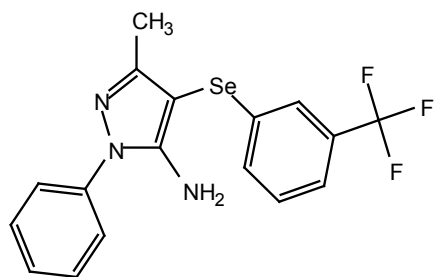
Compound 5d

7.570
7.568
7.500
7.485
7.354
7.339
7.260

— 4.251

— 2.259

s. mkrtyan =mj-4-k1-f6078=1H.stan CDCl3



Comment	s. mkrtyan =mj-4-k1-f6078=1H.stan CDCl3
Number of Scans	32
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

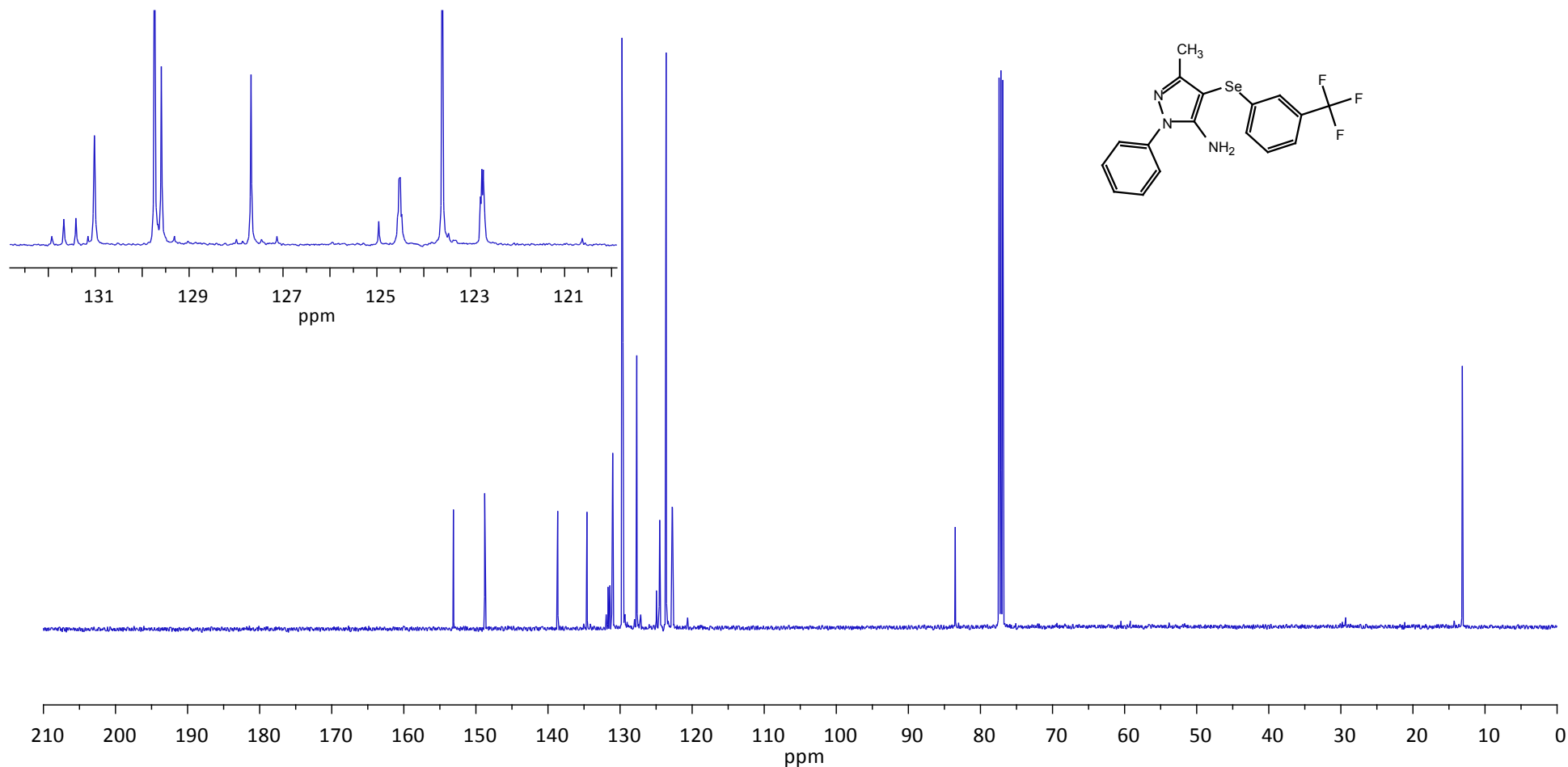
Compound 5d

s. mkrtyan =mj-4-k1-f6078=A-13C.stan CDCl3

153.124
148.781
138.650
134.590
131.670
131.413
131.020
129.737
129.591
127.682
124.960
124.531
124.500
123.607
122.763
122.733

— 83.495

— 13.145



Comment s. mkrtyan =mj-4-k1-f6078=A-13C.stan CDCl3
Number of Scans 2560
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

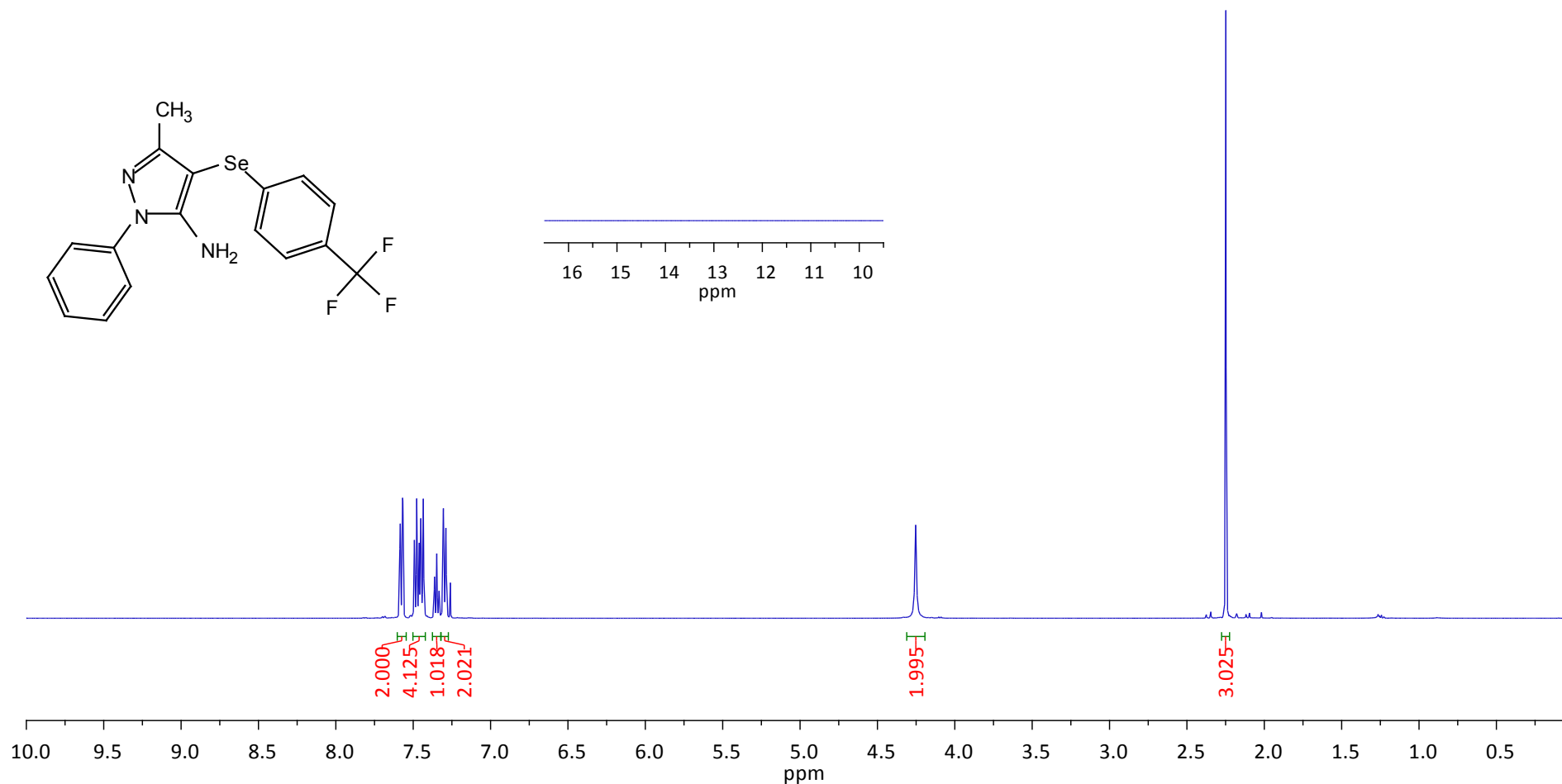
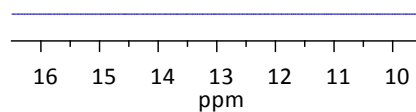
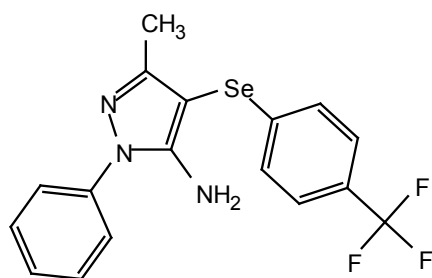
Compound 5e

7.584
7.569
7.567
7.477
7.435
7.348
7.305
7.289
7.260

— 4.253

— 2.248

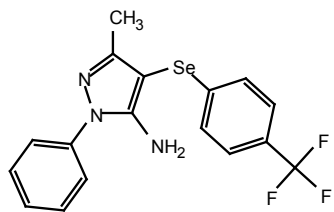
m. jakubczyk =mj-25-ki-f32=1H.stan CDCl3



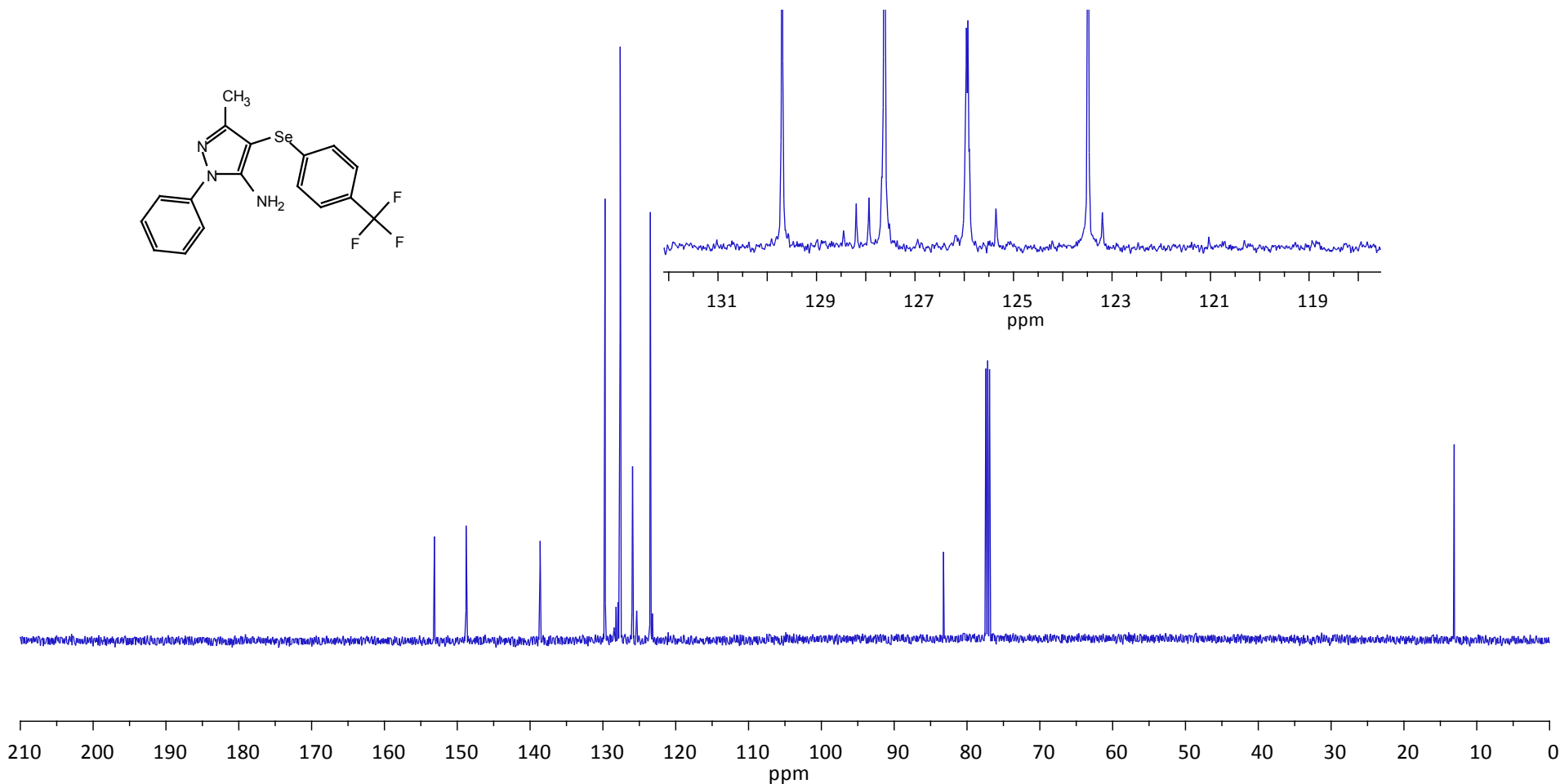
Comment m. jakubczyk =mj-25-ki-f32=1H.stan CDCl3
 Number of Scans 32
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 5e

m. jakubczyk =mj-25-ki-f32=A-13C.stan CDCl₃



153.132
148.780
138.695
138.617
129.699
128.194
127.936
127.623
125.955
125.926
125.356
123.486
123.194
83.233
77.160
13.101



Comment m. jakubczyk =mj-25-ki-f32=A-13C.stan CDCl₃
 Number of Scans 256
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

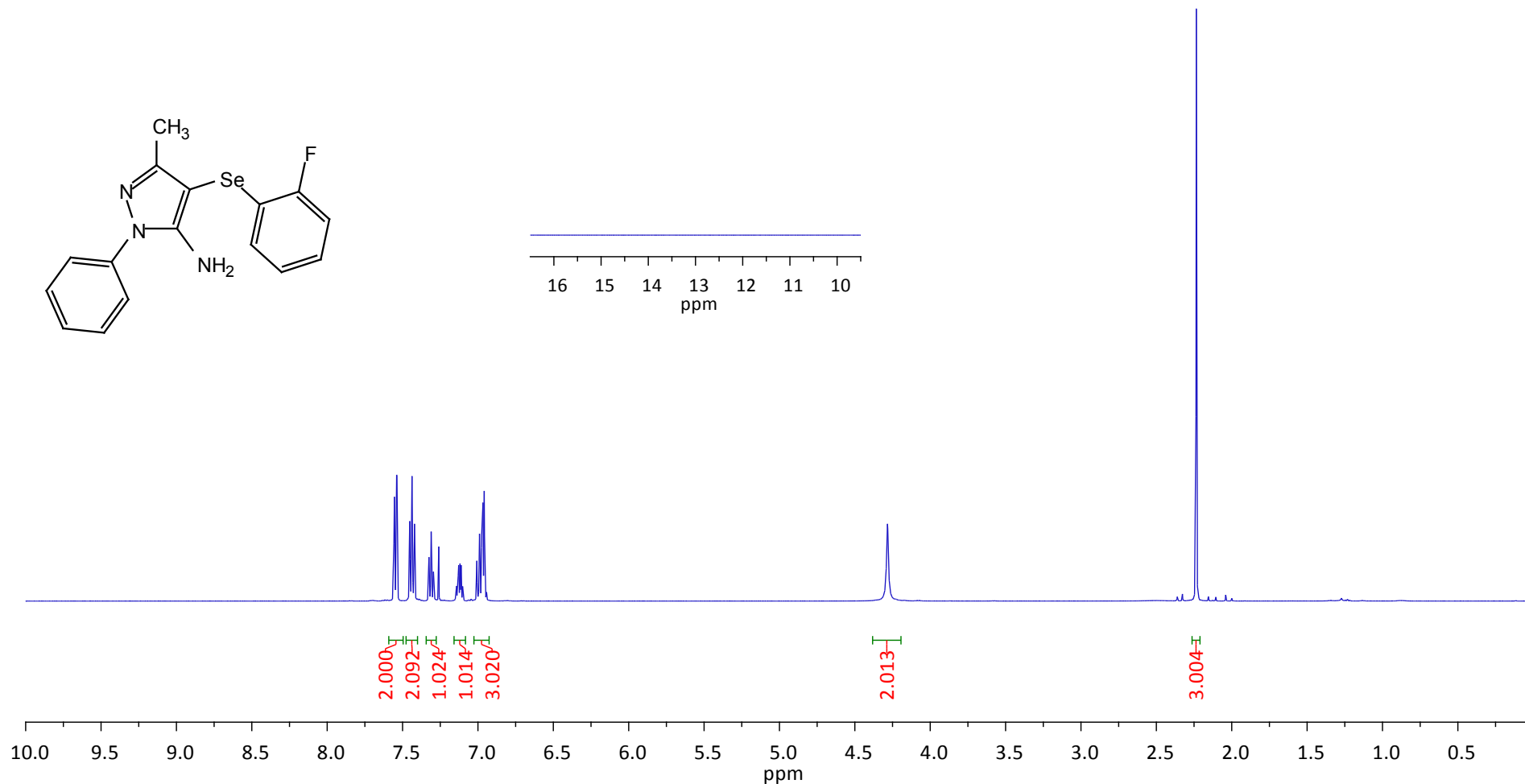
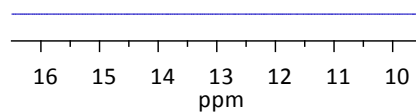
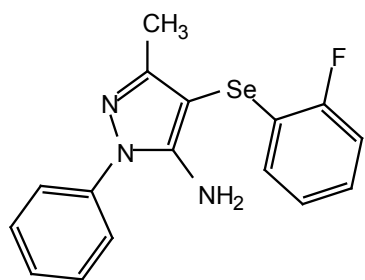
Compound 5f

7.554
7.539
7.537
7.437
7.310
7.260
6.990
6.973
6.972
6.967
6.958

4.284

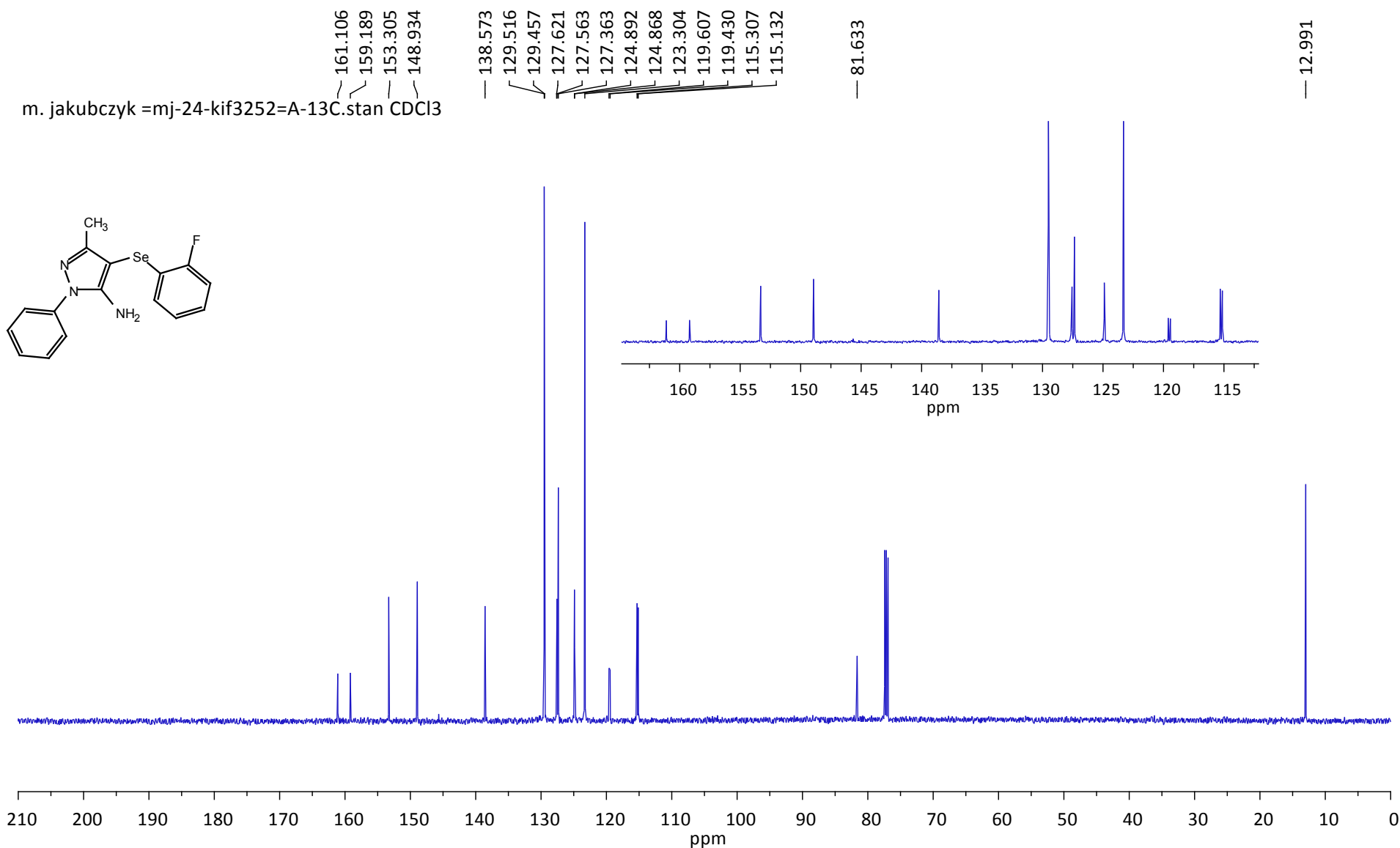
2.235

m. jakubczyk =mj-24-ki-f3252=1H.stan CDCl3



Comment m. jakubczyk =mj-24-ki-f3252=1H.stan CDCl3
Number of Scans 32
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 5f



Comment m. jakubczyk =mj-24-kif3252=A-13C.stan CDCl3

Number of Scans 256

Spectrometer Frequency 125.76

Spectral Width 36057.7

Spectral Size 65536

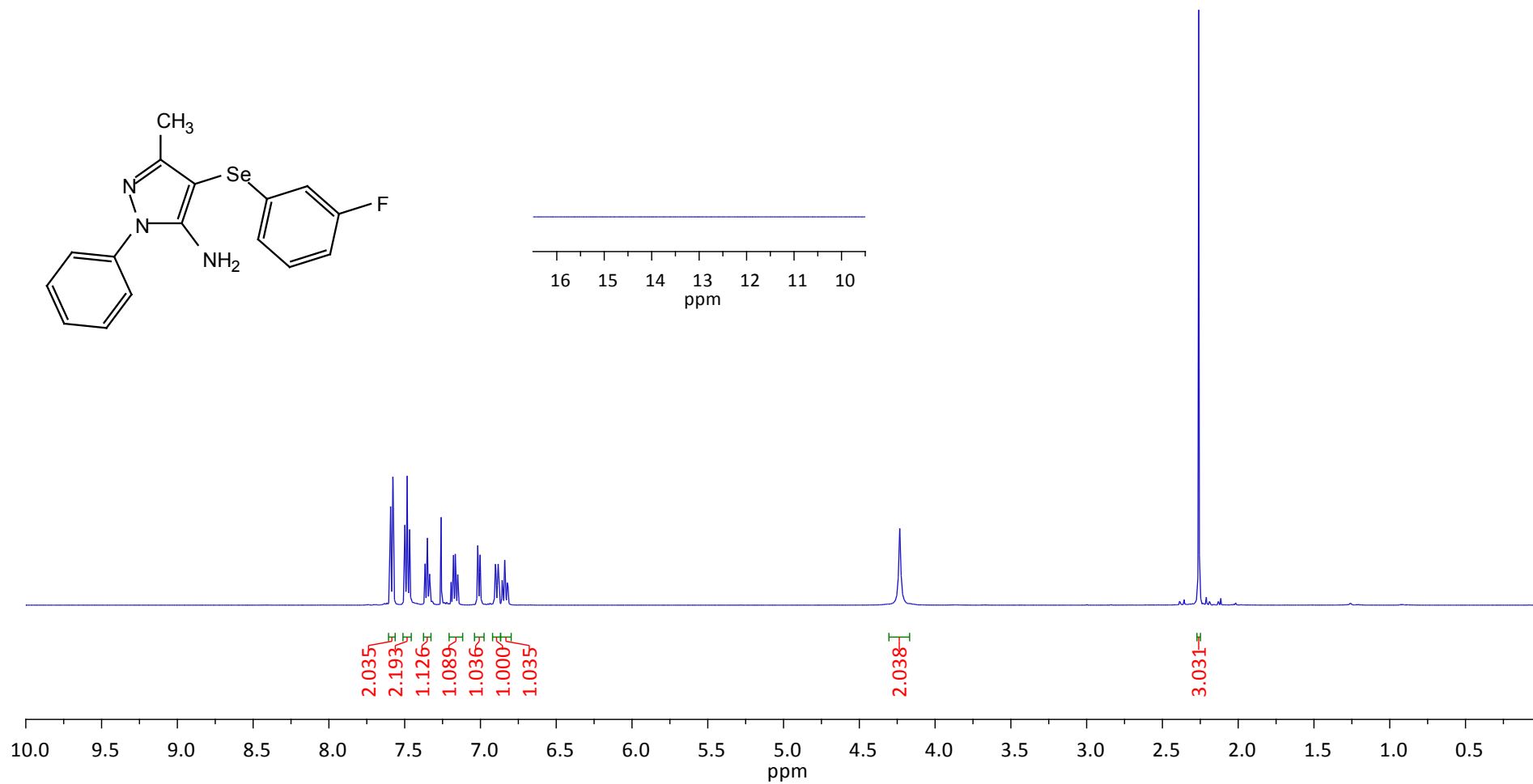
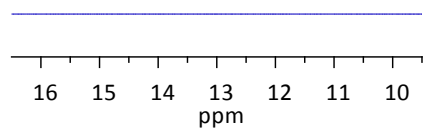
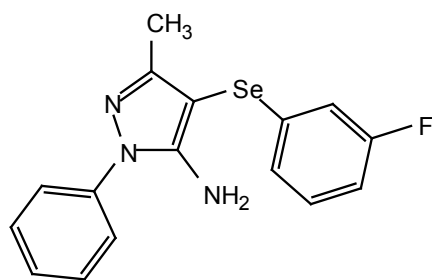
Compound 5g

7.593
7.578
7.484
7.350
7.178
7.166
7.018
7.002
6.901
6.883
6.840

4.233

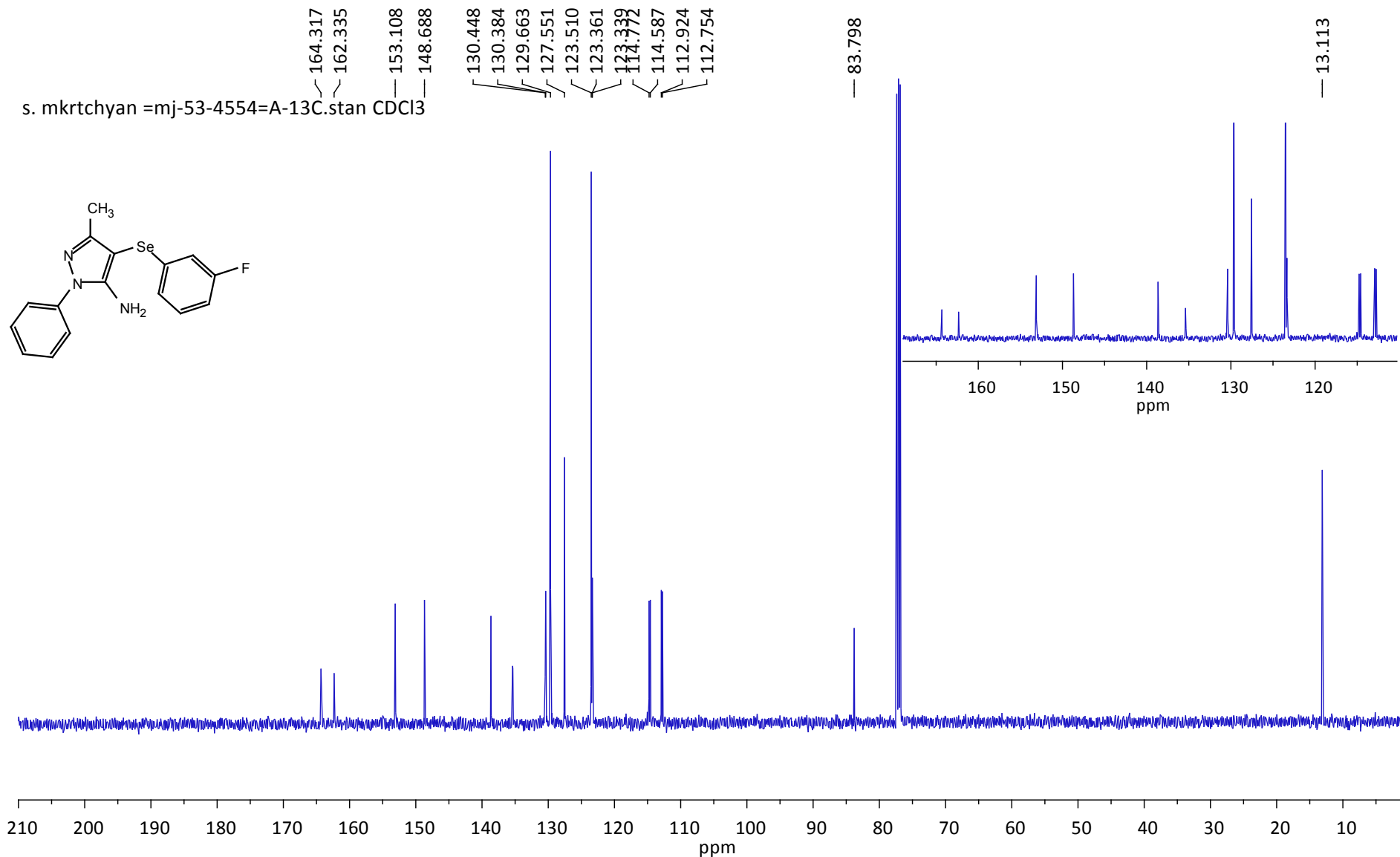
2.260

s. mkrtyan =mj-53-4554=1H.stan CDCl3



Comment s. mkrtyan =mj-53-4554=1H.stan CDCl3
Number of Scans 32
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 5g



Comment s. mkrтчyan =mj-53-4554=A-13C.stan CDCl3
 Number of Scans 256
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

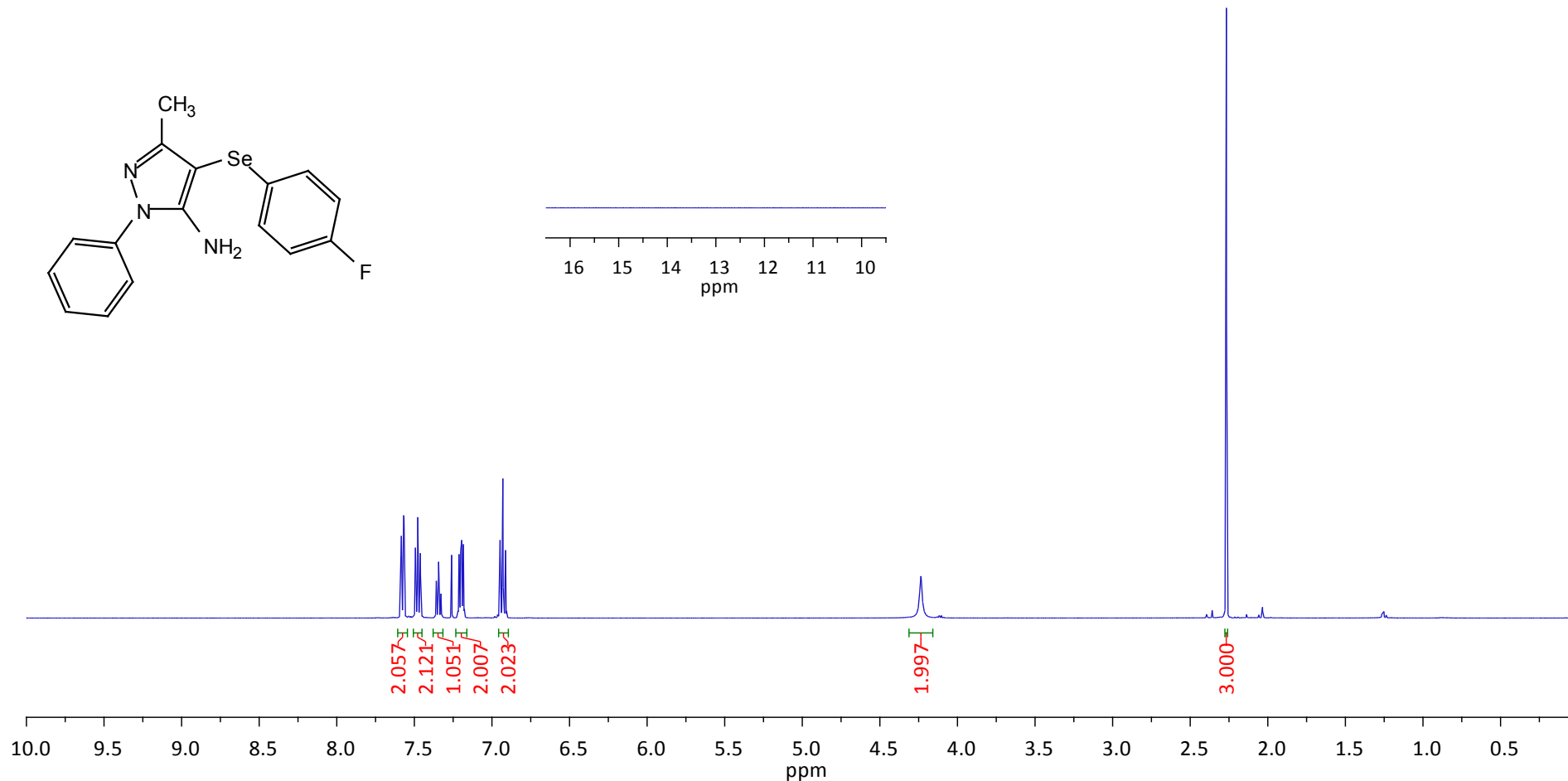
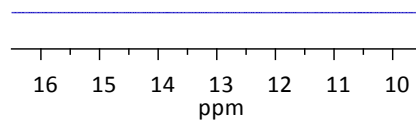
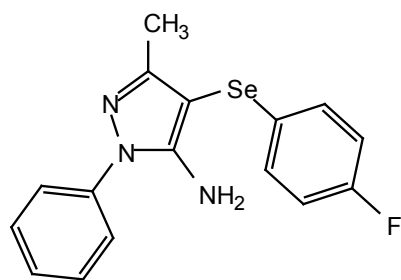
Compound 5h

7.584
7.569
7.567
7.478
7.344
7.260
7.212
7.202
7.195
7.184
6.930

4.236

2.267

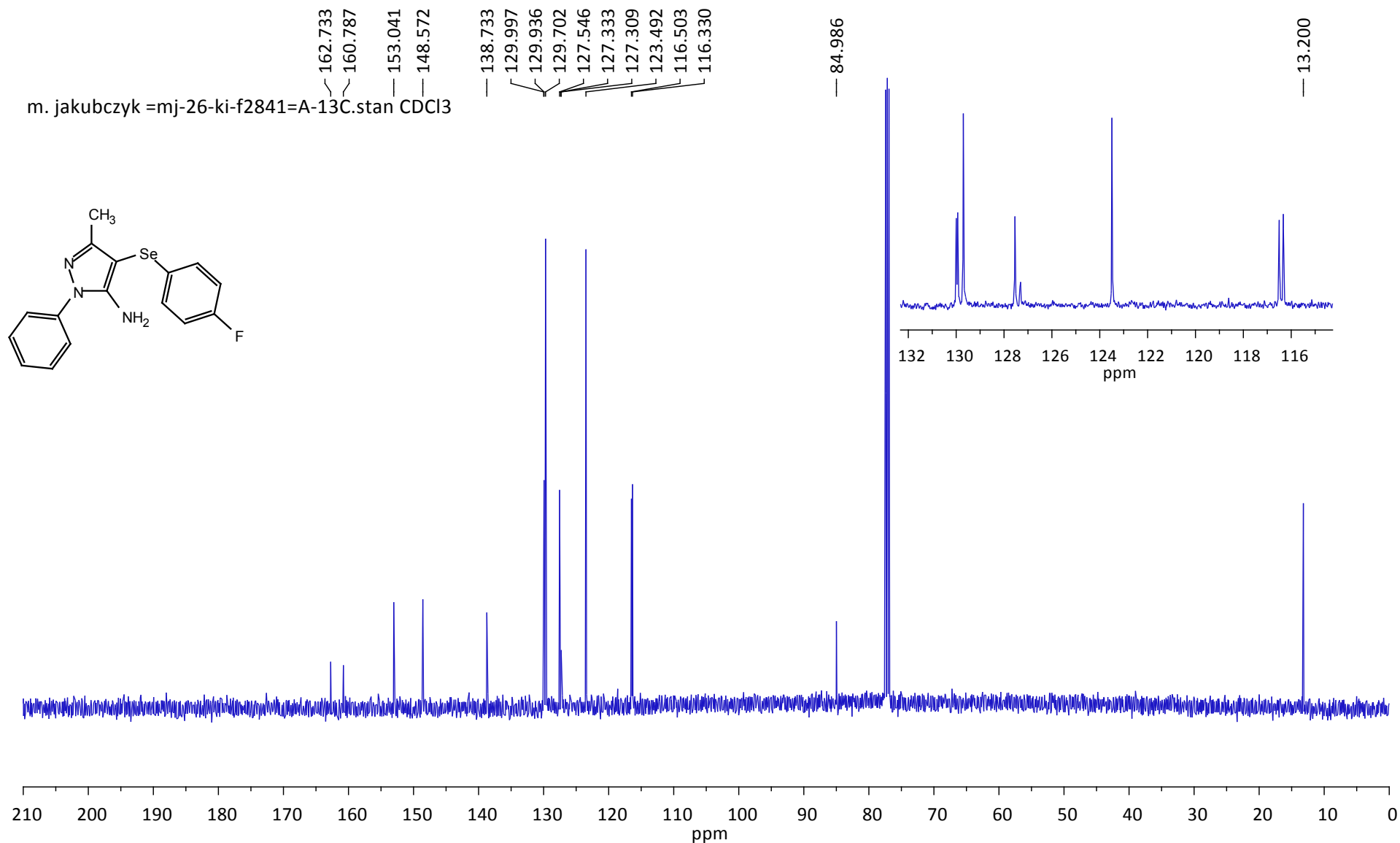
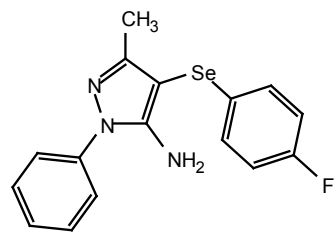
m. jakubczyk =mj-26-ki-f2841=1H.stan CDCl3



Comment m. jakubczyk =mj-26-ki-f2841=1H.stan CDCl3
 Number of Scans 32
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 5h

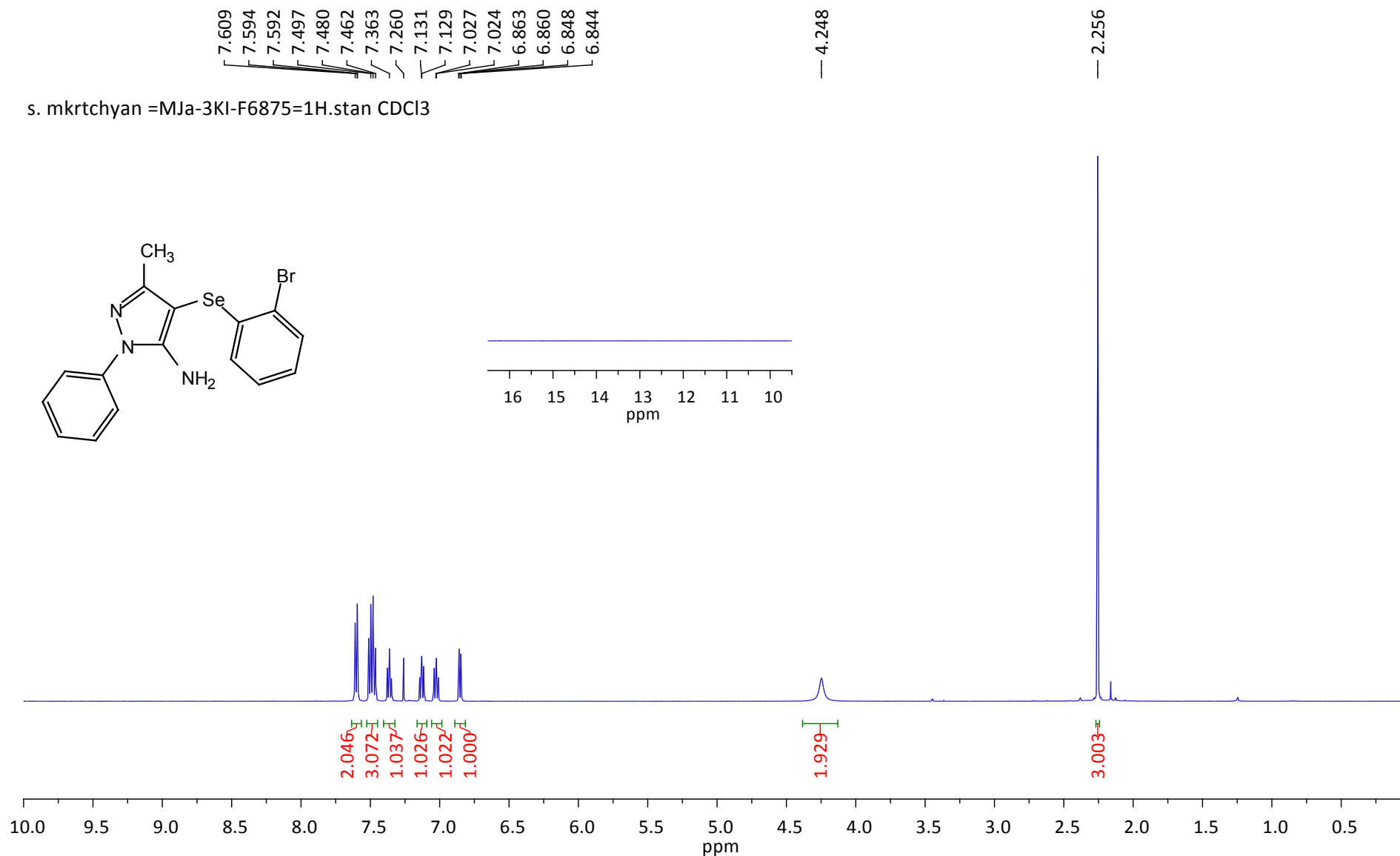
m. jakubczyk =mj-26-ki-f2841=A-13C.stan CDCl3



Comment	m. jakubczyk =mj-26-ki-f2841=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound 5i

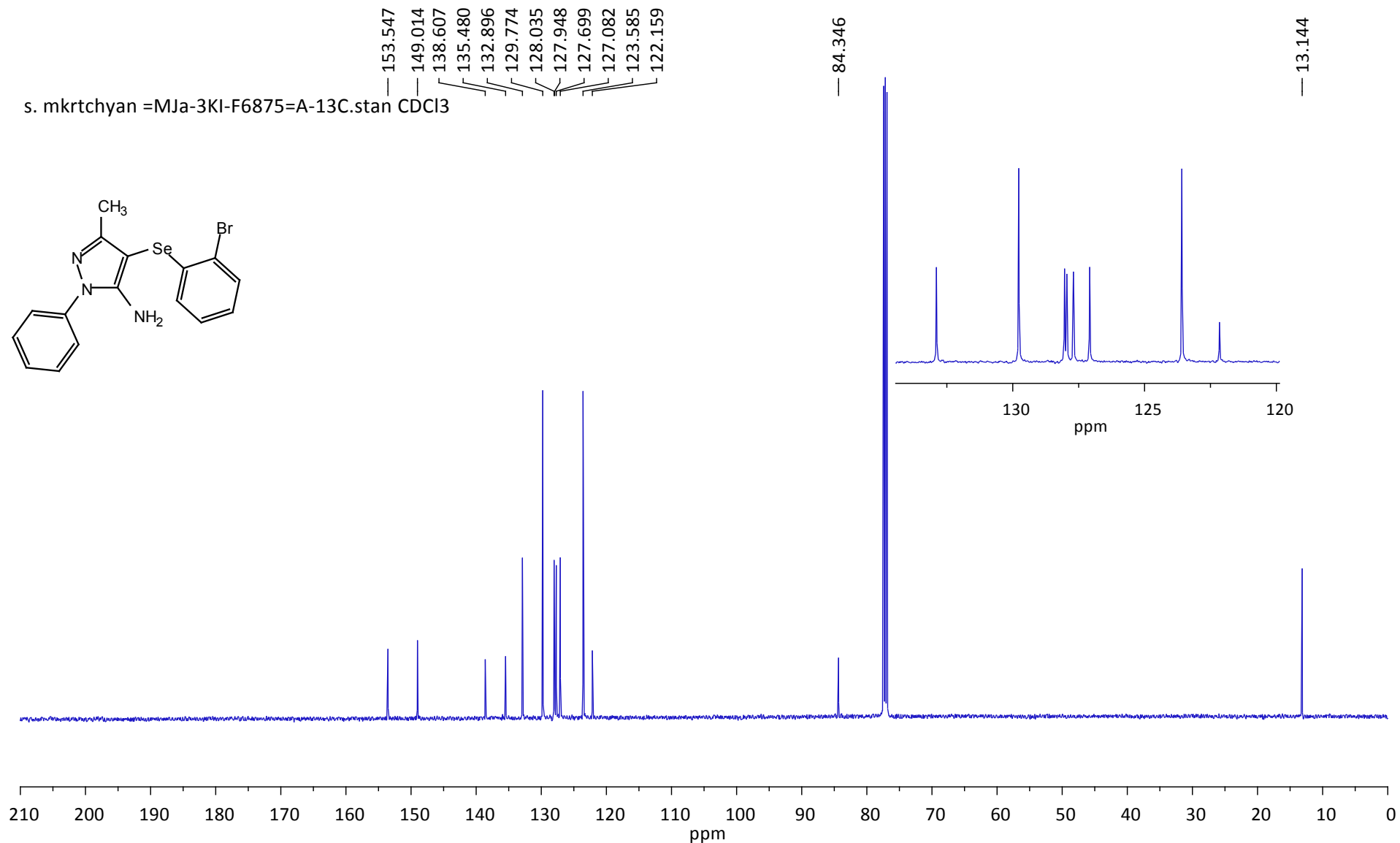
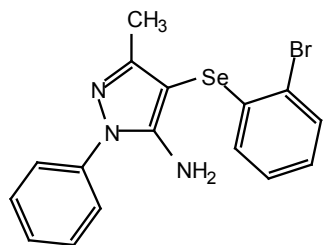
s. mkrtyan =MJa-3KI-F6875=1H.stan CDCl3



Comment	s. mkrtyan =MJa-3KI-F6875=1H.stan CDCl3
Number of Scans	32
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound 5i

s. mkrtyan =MJa-3KI-F6875=A-13C.stan CDCl3

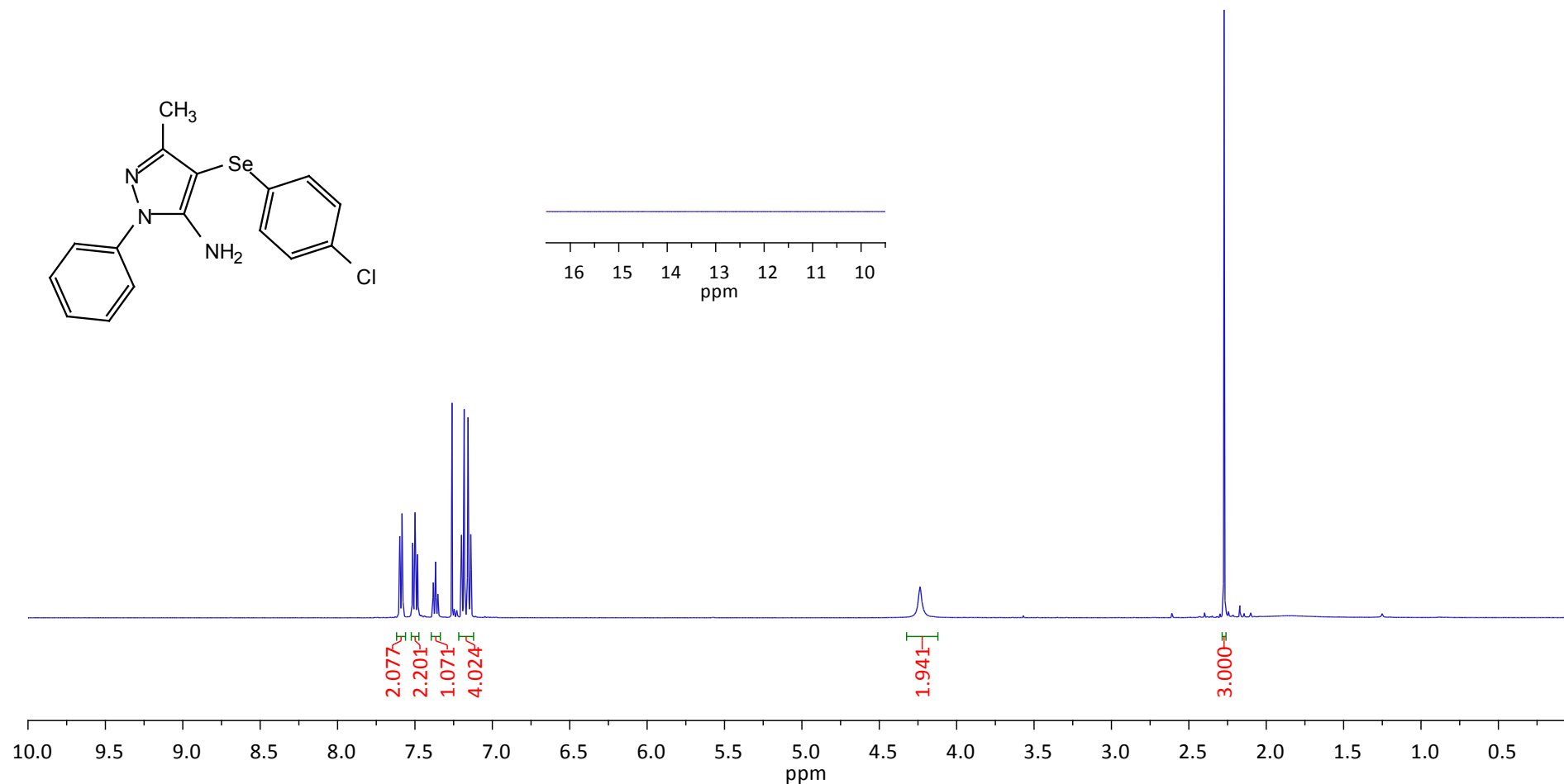
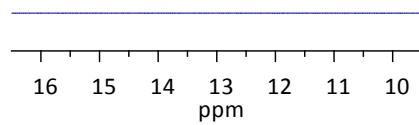
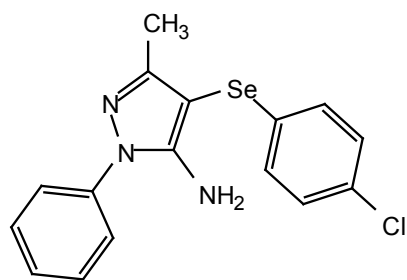


Comment	s. mkrtyan =MJa-3KI-F6875=A-13C.stan CDCl3
Number of Scans	3072
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound 5j

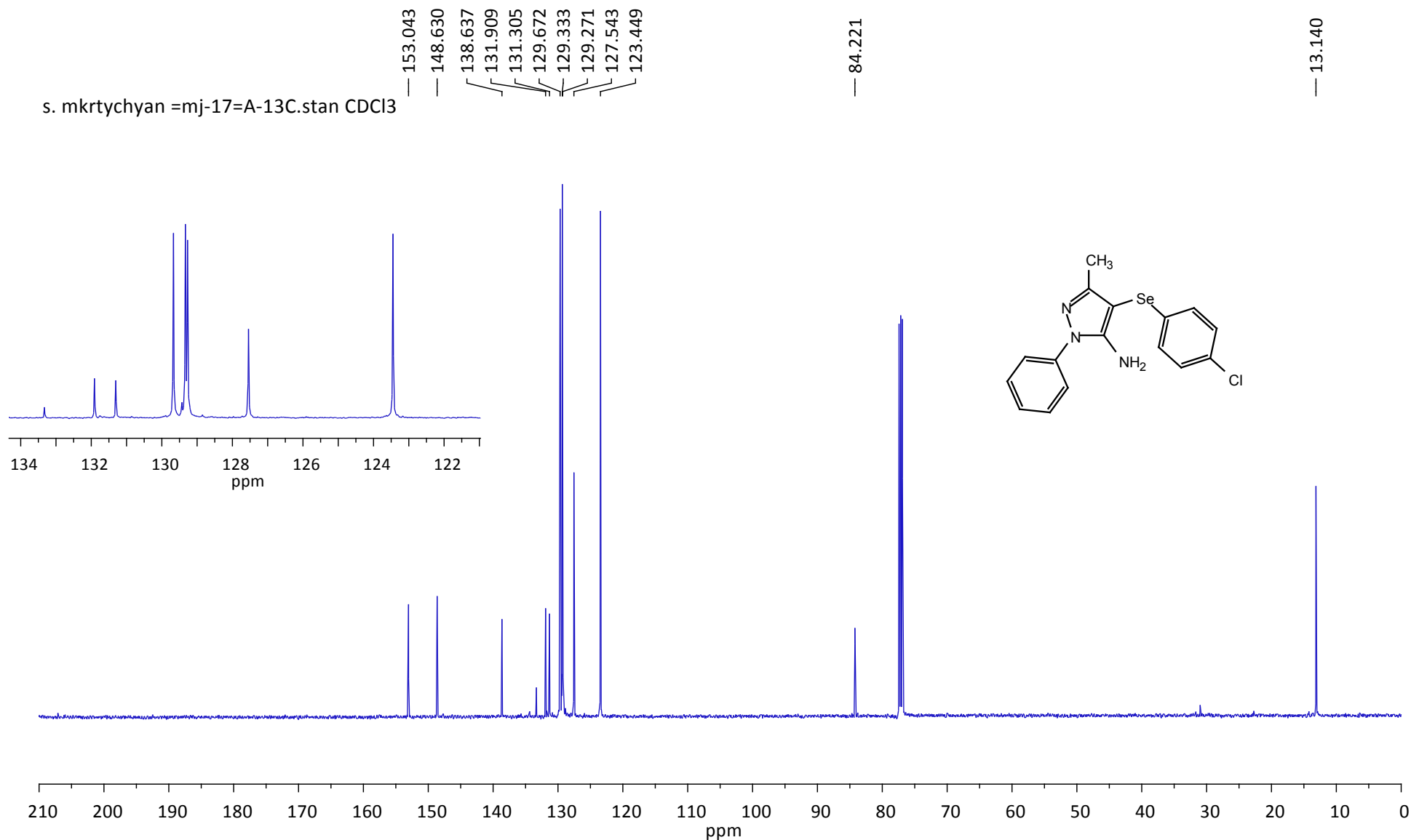
7.600
7.598
7.583
7.581
7.500
7.367
7.260
7.182
7.157

s. mkrtyan =mj-17-ki-f53593=1H.stan CDCl3



Comment s. mkrtyan =mj-17-ki-f53593=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 5j



Comment s. mkrtychyan =mj-17=A-13C.stan CDCl3
 Number of Scans 1744
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

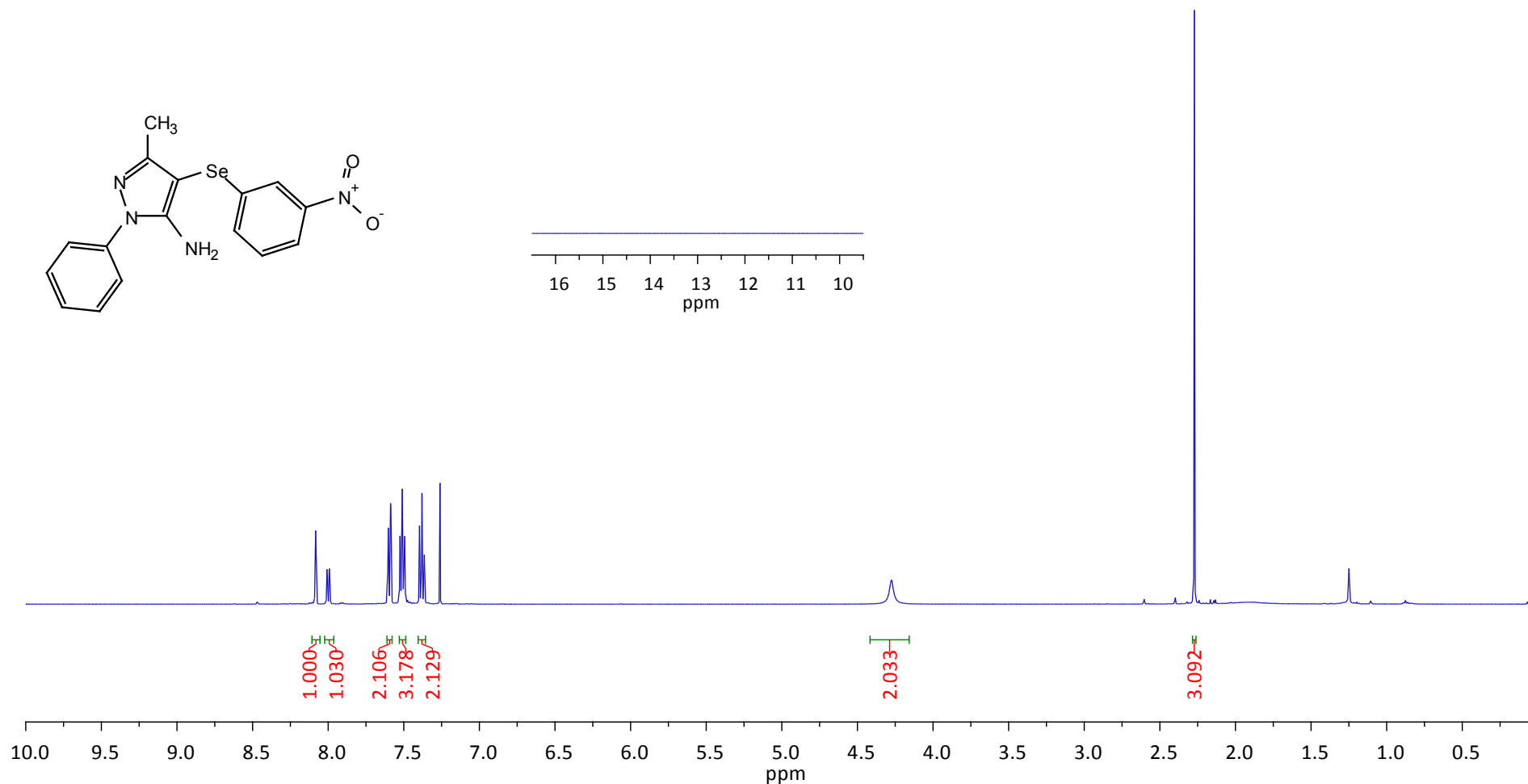
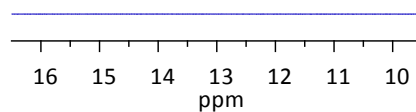
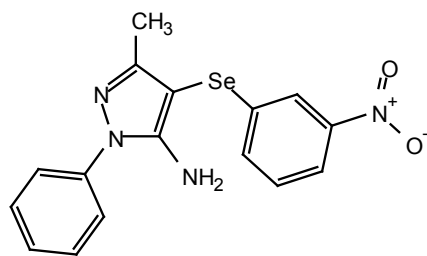
Compound 5k

8.083
8.010
8.008
8.005
8.004
7.994
7.992
7.989
7.987
7.605
7.602
7.588
7.586
7.510
7.380
7.260

— 4.275

— 2.272

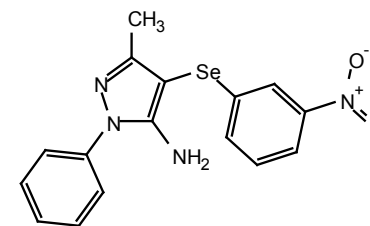
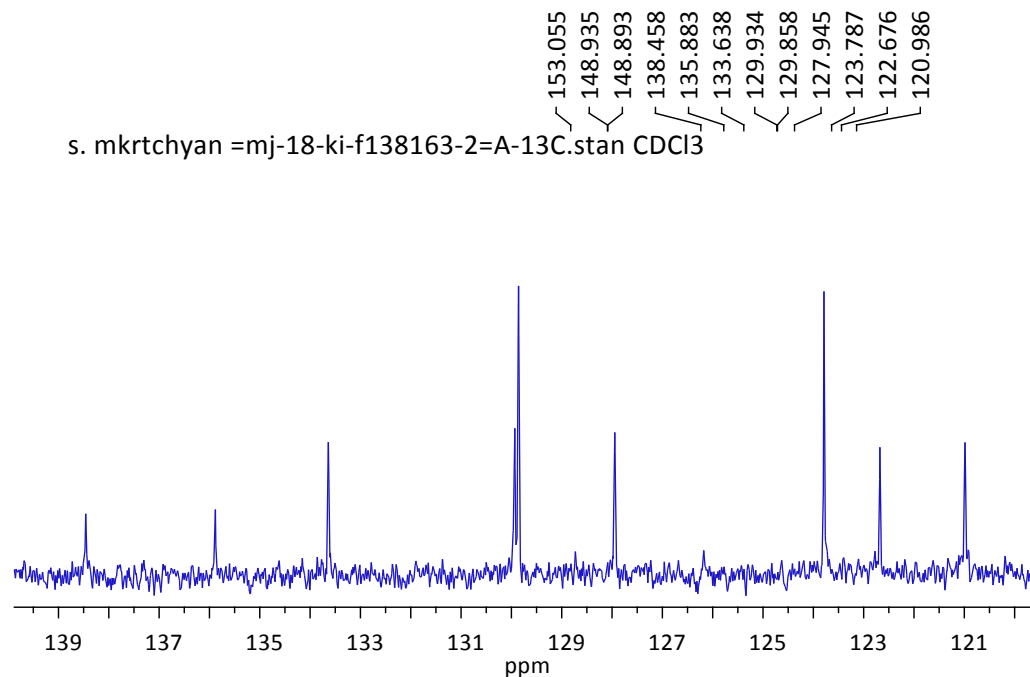
s. mkrtyan =mj-18-ki-f138163-2=1H.stan CDCl3



Comment s. mkrtyan =mj-18-ki-f138163-2=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

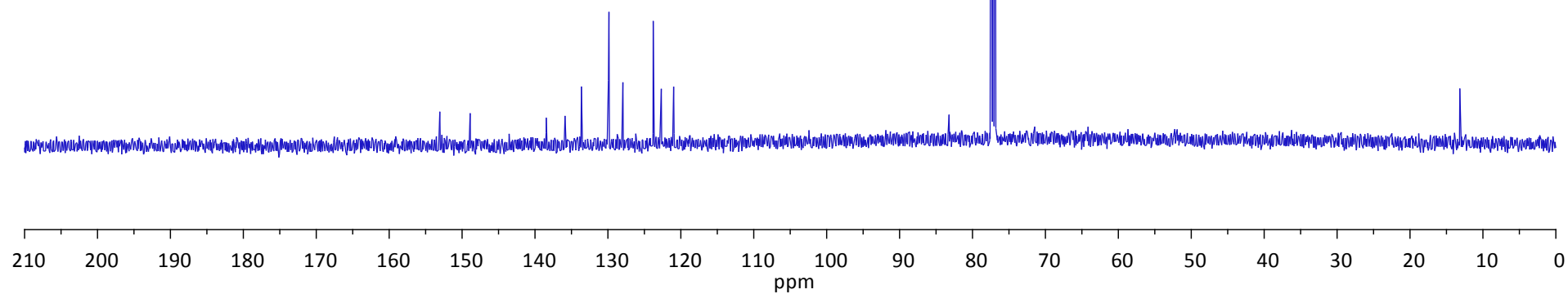
Compound 5k

s. mkrtyan =mj-18-ki-f138163-2=A-13C.stan CDCl₃



— 83.214

— 13.167



Comment s. mkrtyan =mj-18-ki-f138163-2=A-13C.stan CDCl₃
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

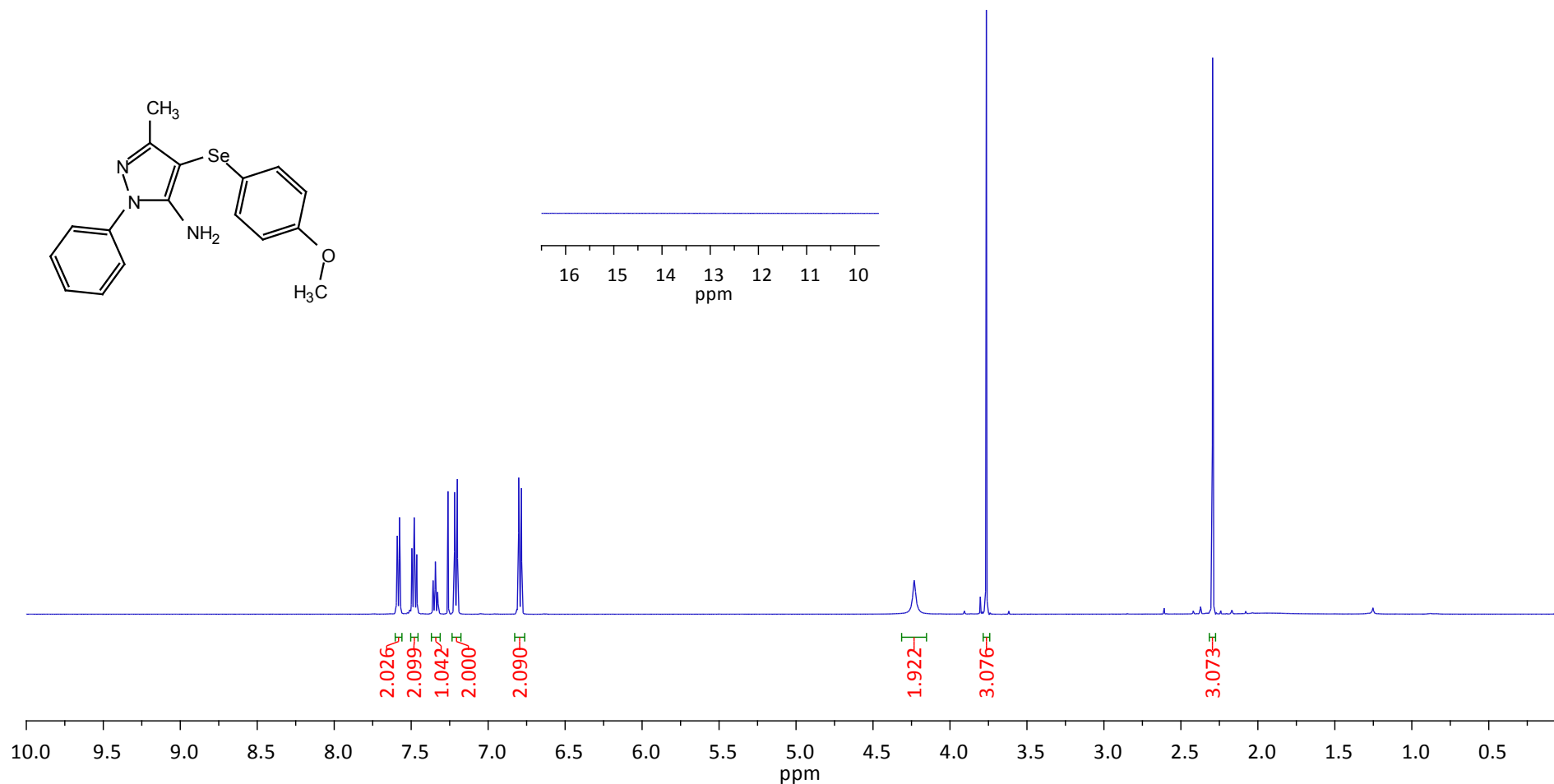
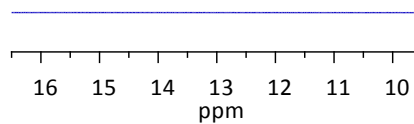
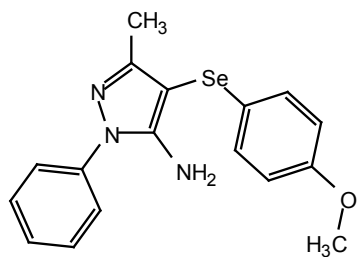
Compound 5I

7.593
7.590
7.576
7.574
7.480
7.343
7.261
7.218
7.200
6.801
6.784

4.232

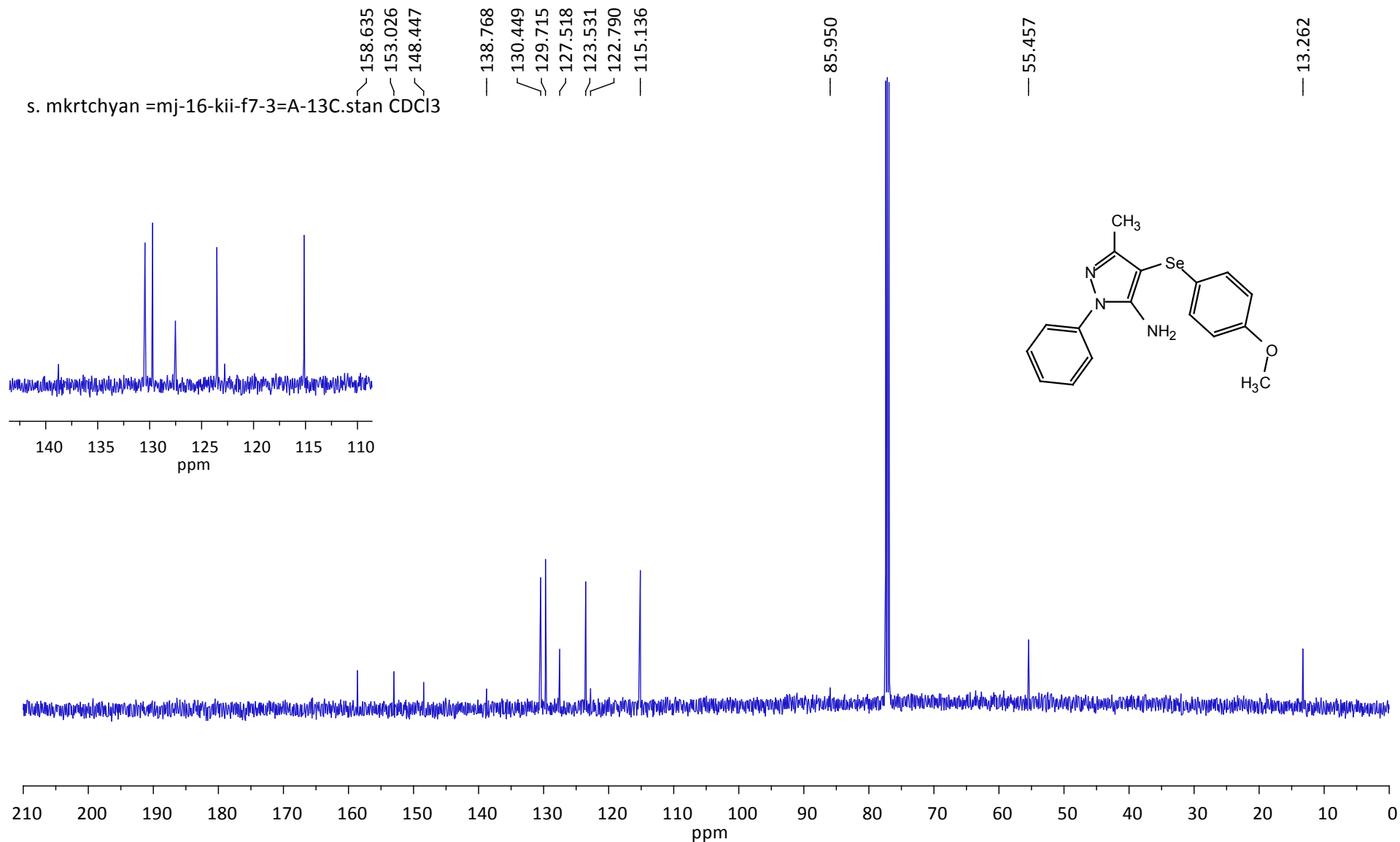
3.764

s. mkrtyan =mj-16-kii-f7-3=1H.stan CDCl3



Comment	s. mkrtyan =mj-16-kii-f7-3=1H.stan CDCl3
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12336.0
Spectral Size	65536

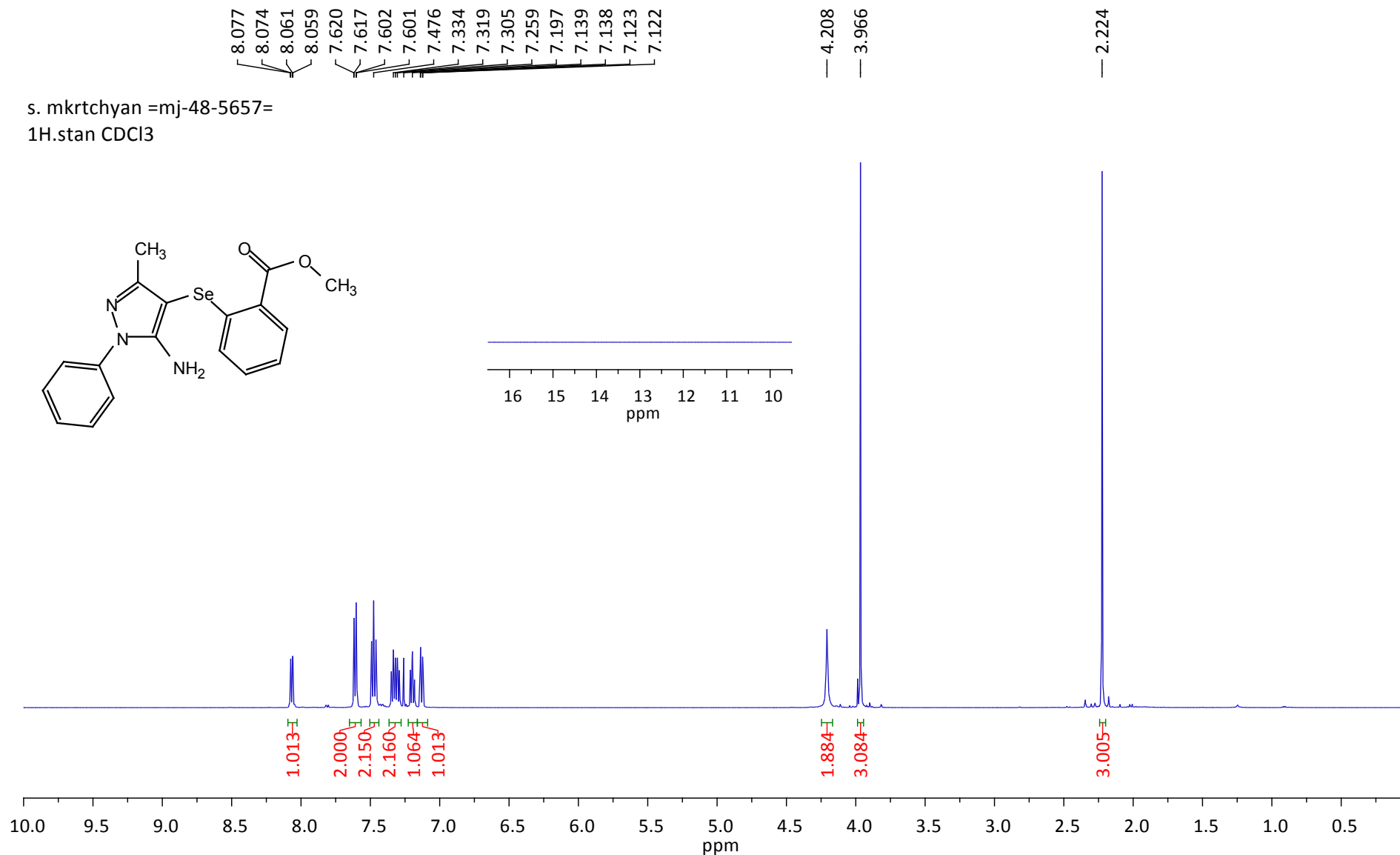
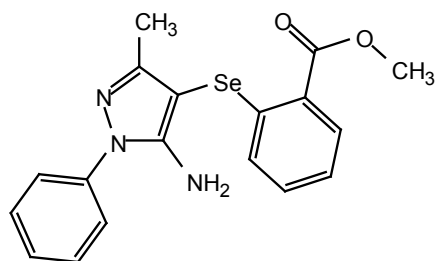
Compound 5I



Comment s. mkrtyan =mj-16-kii-f7-3=A-13C.stan CDCl3
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound 5m

s. mkrtyan =mj-48-5657=
1H.stan CDCl3



Comment s. mkrtyan =mj-48-5657=
1H.stan CDCl3

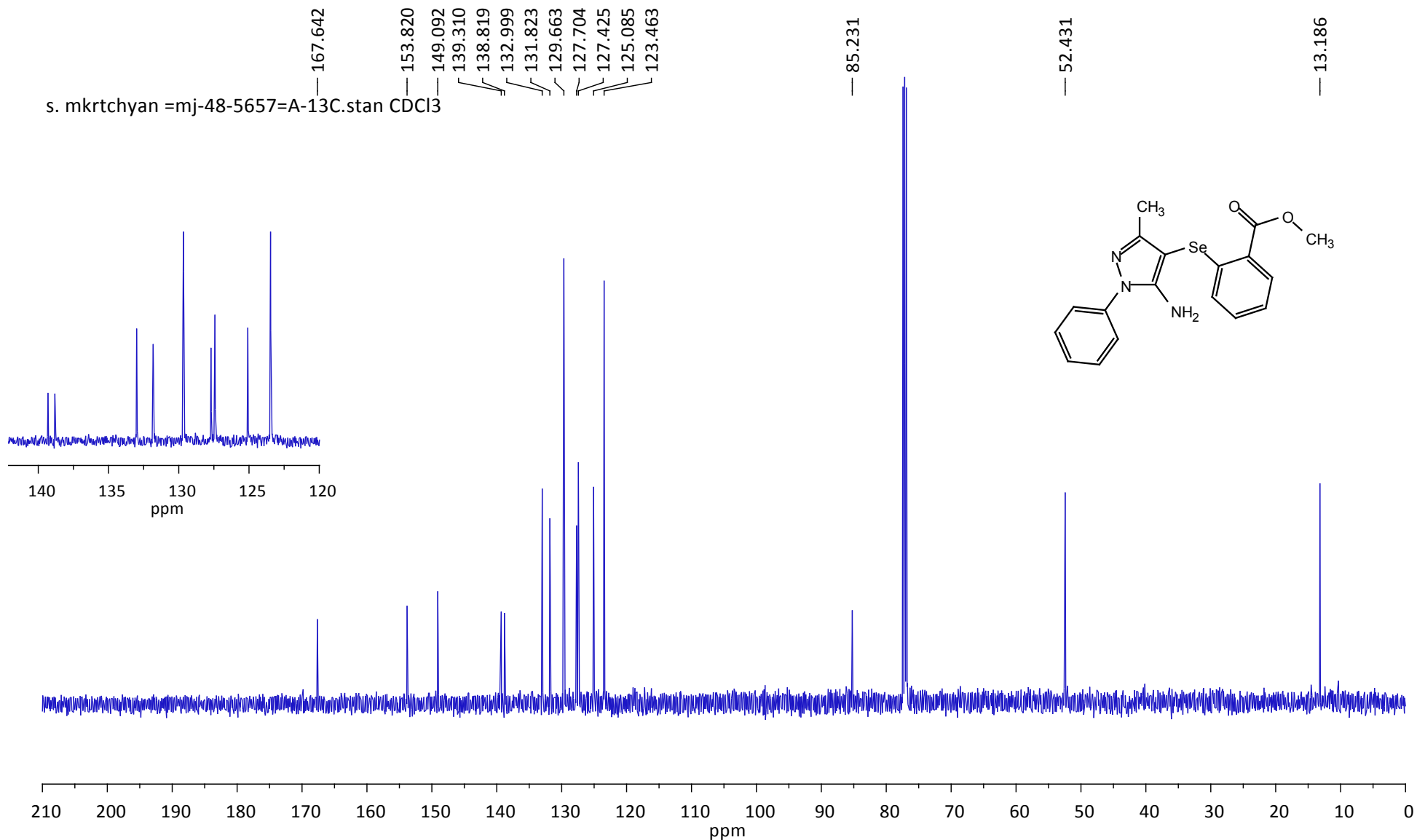
Number of Scans 24

Spectrometer Frequency 500.13

Spectral Width 12335.5

Chemical Shift Range 10.000 - 0.000

Compound 5m



Comment s. mkrtyan =mj-48-5657=A-13C.stan CDCl3
 Number of Scans 128
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

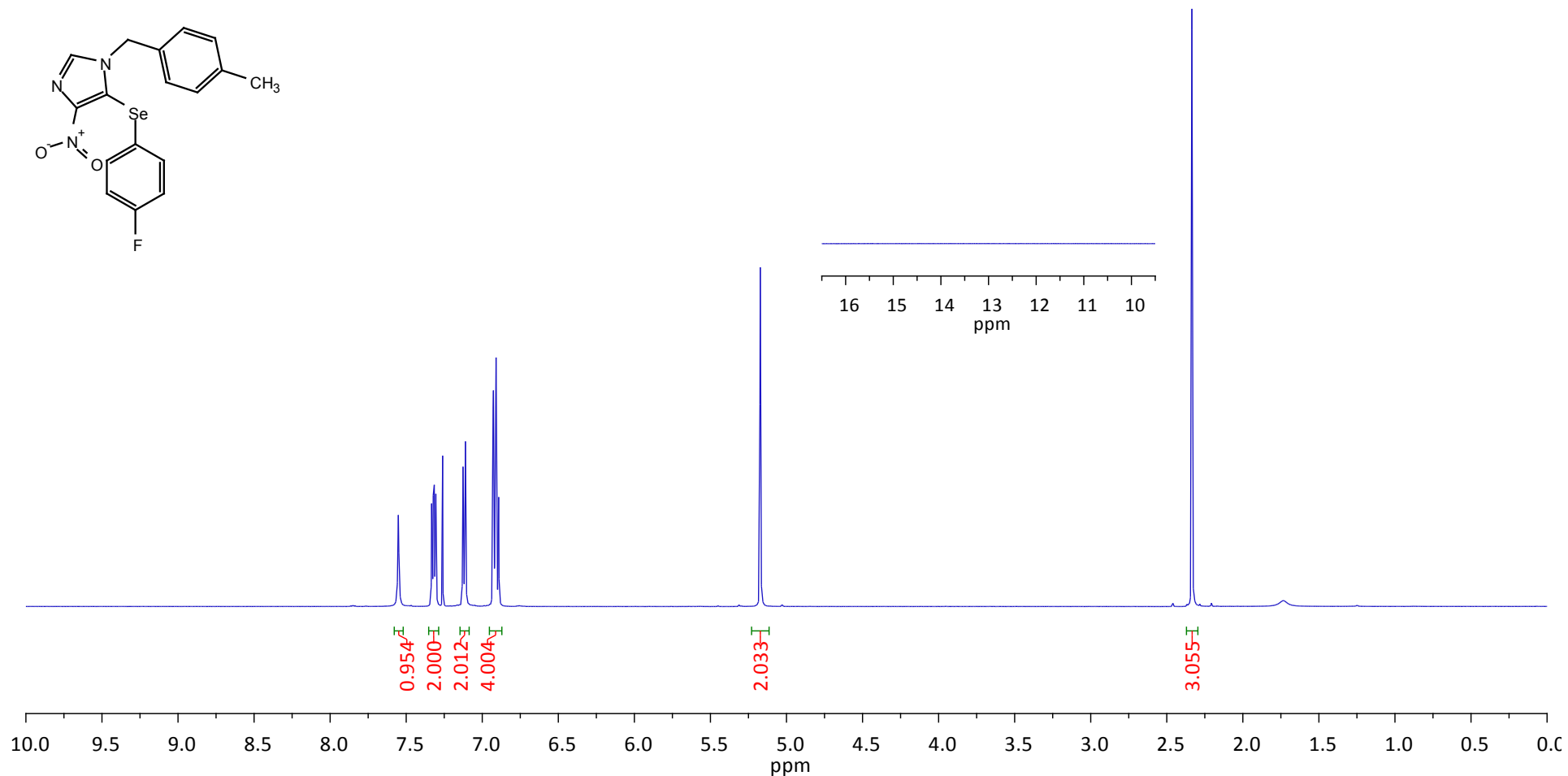
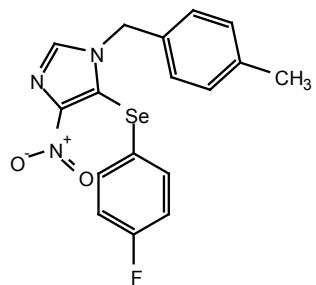
Compound 6

7.552
7.333
7.323
7.315
7.305
7.260
7.126
7.111
6.909

5.172

2.335

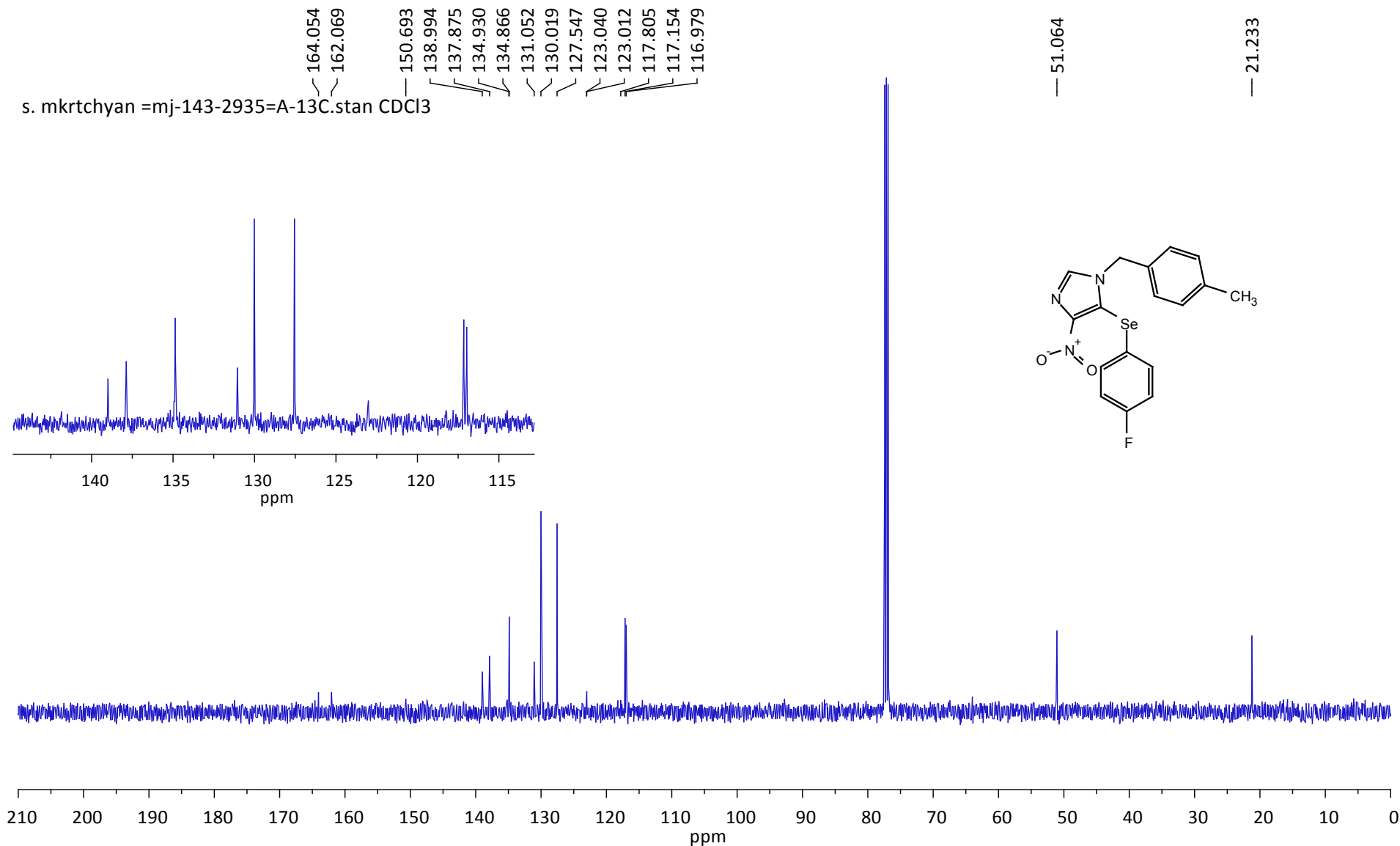
s. mkrtyan =mj-143-2935=1H.stan CDCl3



Comment s. mkrtyan =mj-143-2935=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 6

s. mkrtyan =mj-143-2935=A-13C.stan CDCl3



Comment s. mkrtyan =mj-143-2935=A-13C.stan CDCl3
 Number of Scans 128
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound 7a

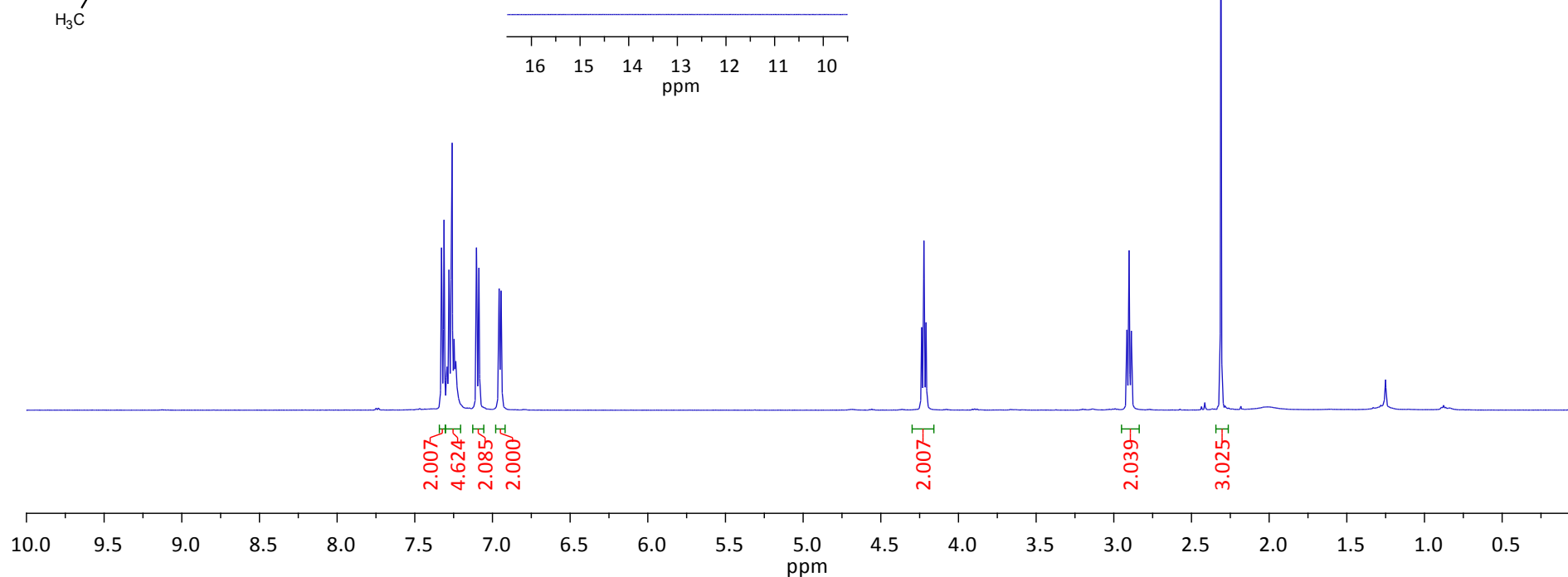
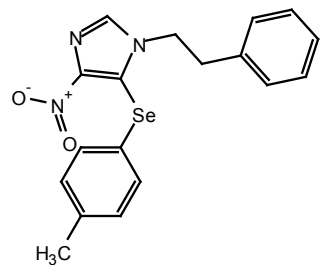
7.328
7.312
7.259
7.103
7.087
6.960
6.957
6.945

4.223

2.901

2.311

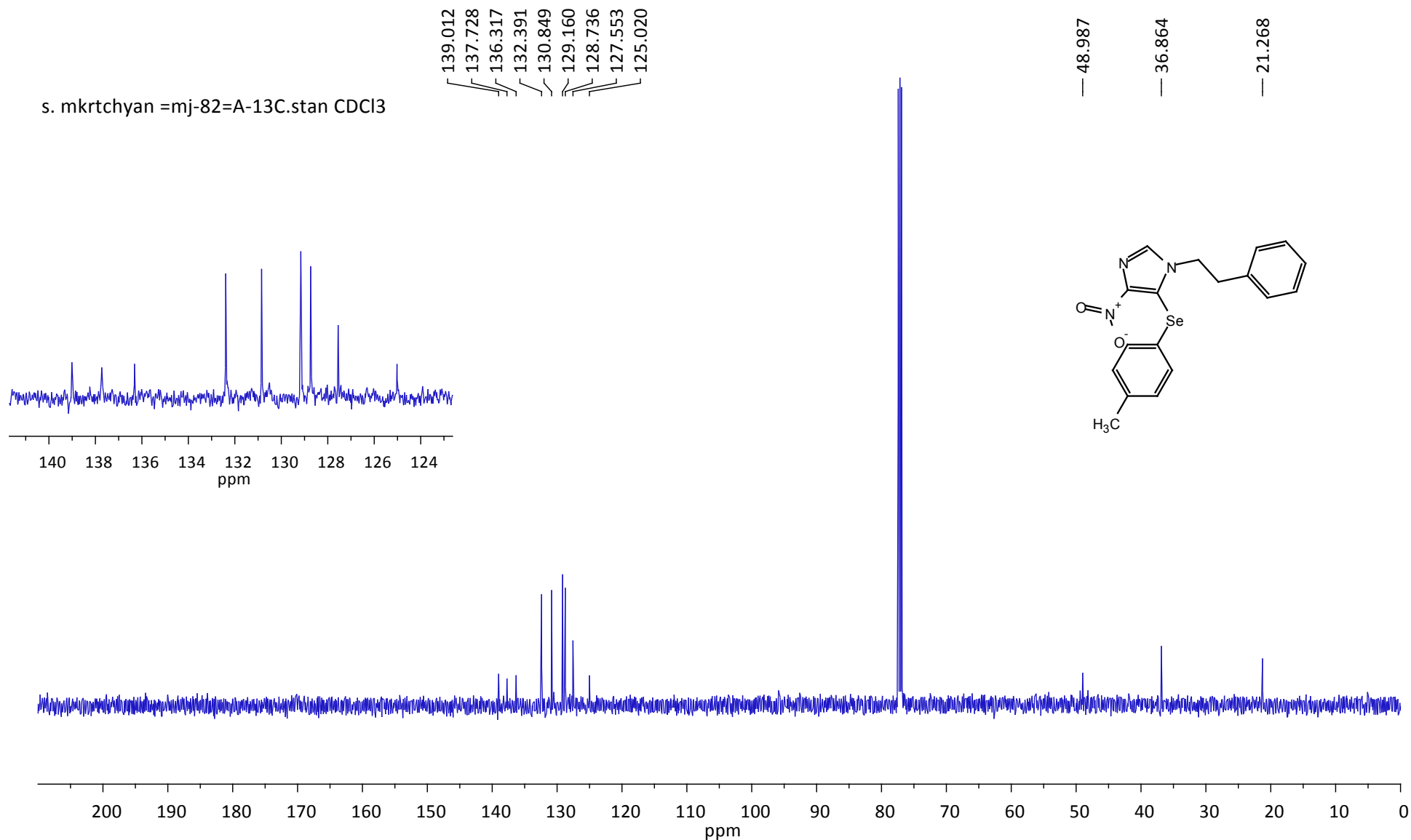
s. mkrtyan =mj-82=1H.stan CDCl3



Comment s. mkrtyan =mj-82=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 7a

s. mkrtchyan =mj-82=A-13C.stan CDCl3



Comment	s. mkrtchyan =mj-82=A-13C.stan CDCl3
Number of Scans	128
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

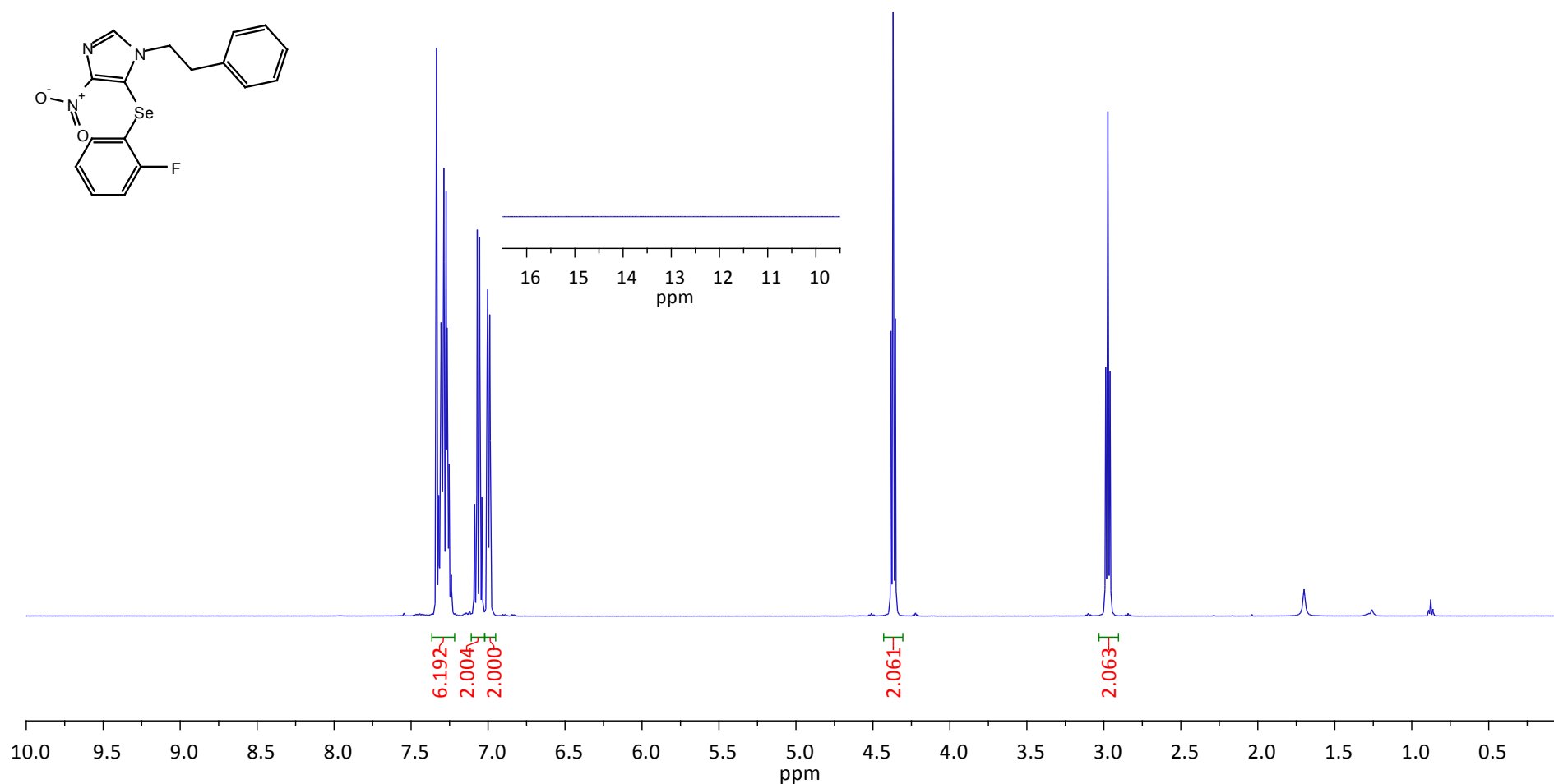
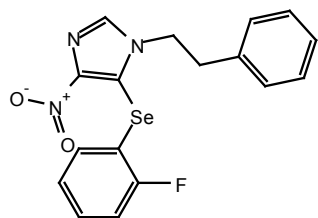
Compound **7b**

7.334
7.287
7.272
7.070
7.054
7.002
6.989

4.369

2.974

s. mkrtyan =mj-62-3041=1H.stan CDCl3



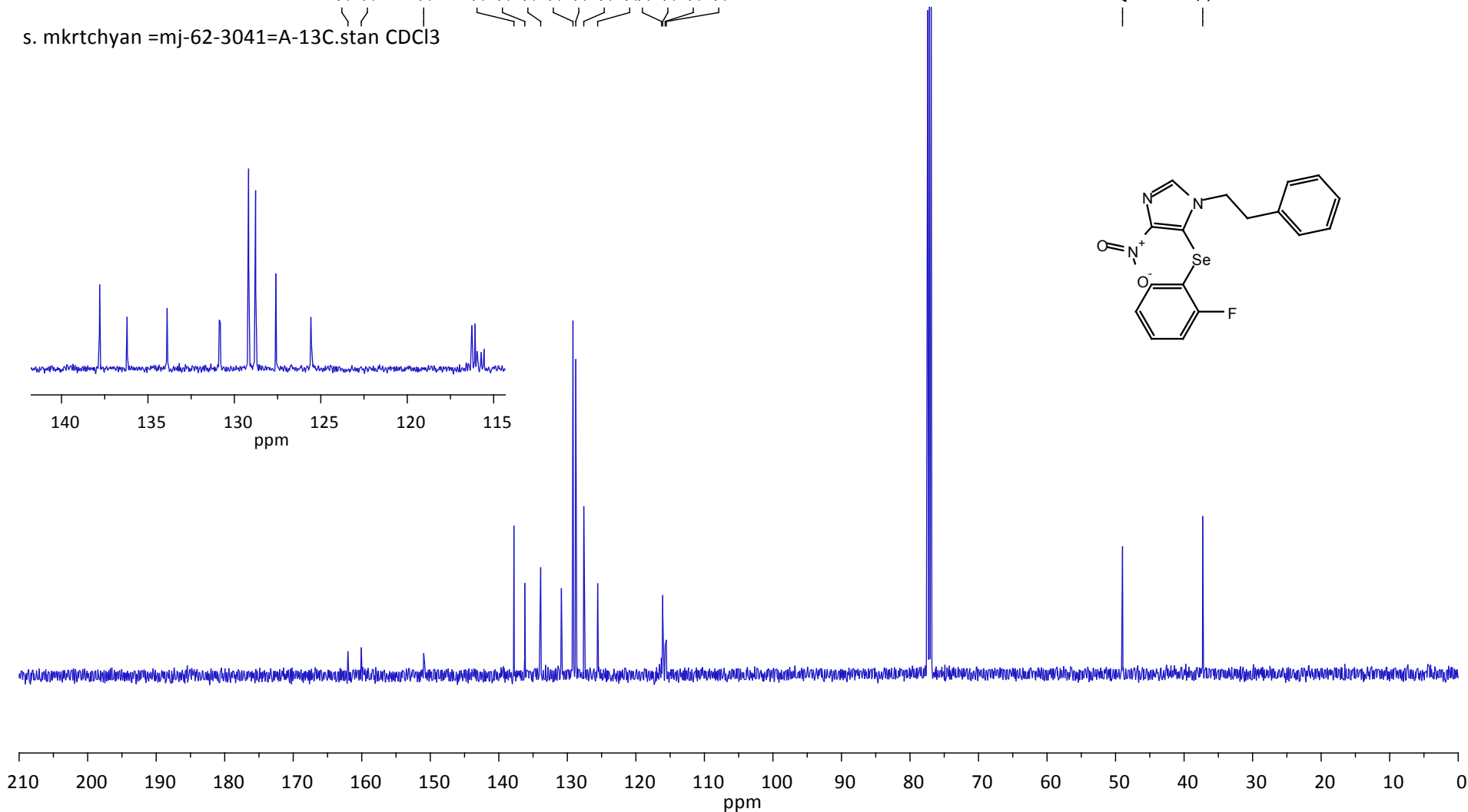
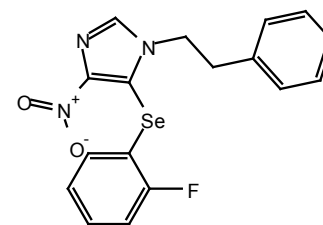
Comment s. mkrtyan =mj-62-3041=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **7b**

s. mkrtyan =mj-62-3041=A-13C.stan CDCl₃

162.019
160.074
150.964
137.793
136.205
133.891
129.179
128.774
127.599
125.575
116.261
116.080
115.721
115.551

48.985
37.279



Comment s. mkrtyan =mj-62-3041=A-13C.stan CDCl₃
 Number of Scans 256
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

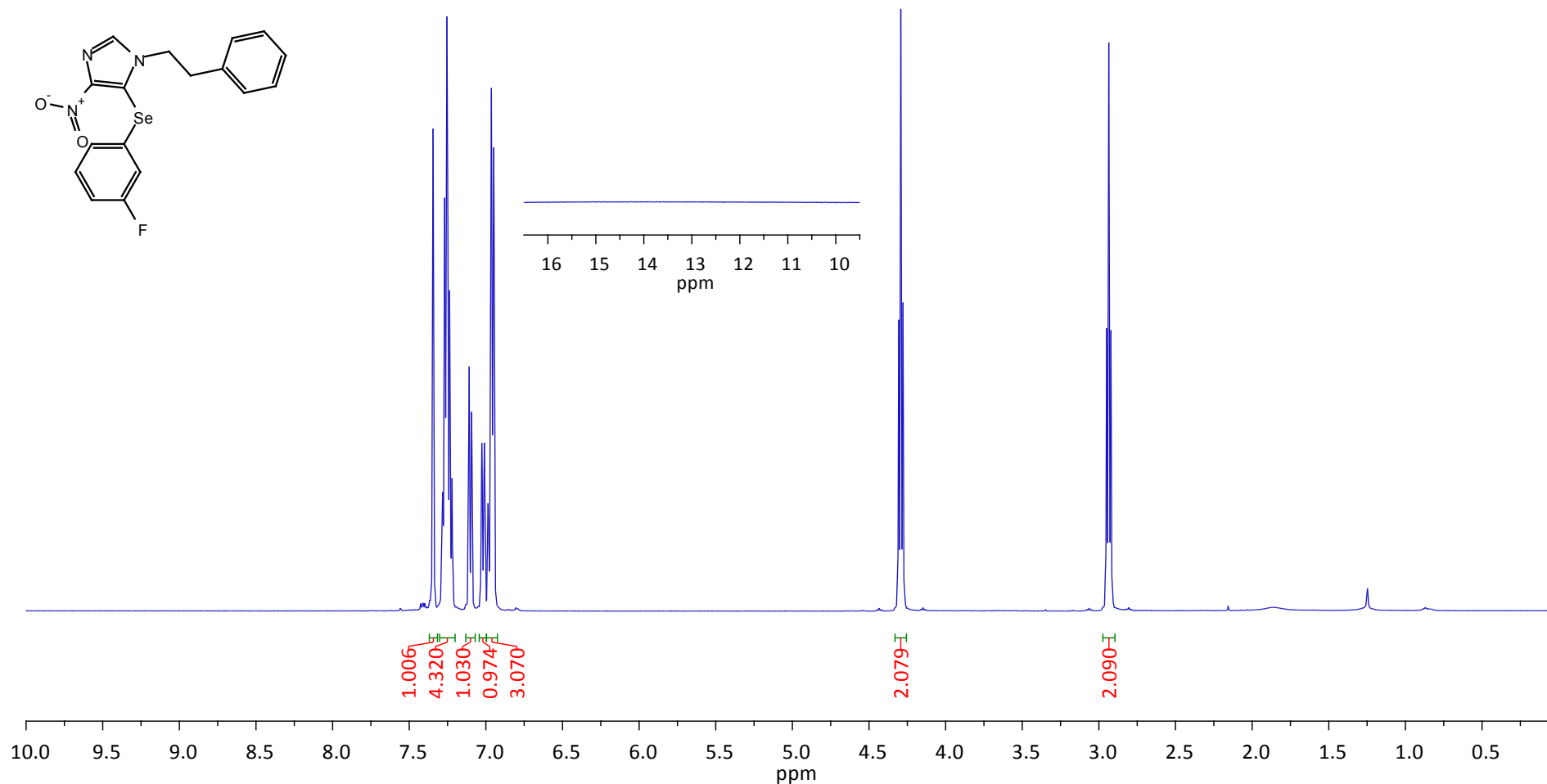
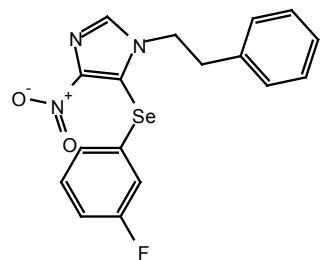
Compound 7c

7.345
7.254
7.109
7.093
7.026
7.010
6.964

4.292

2.936

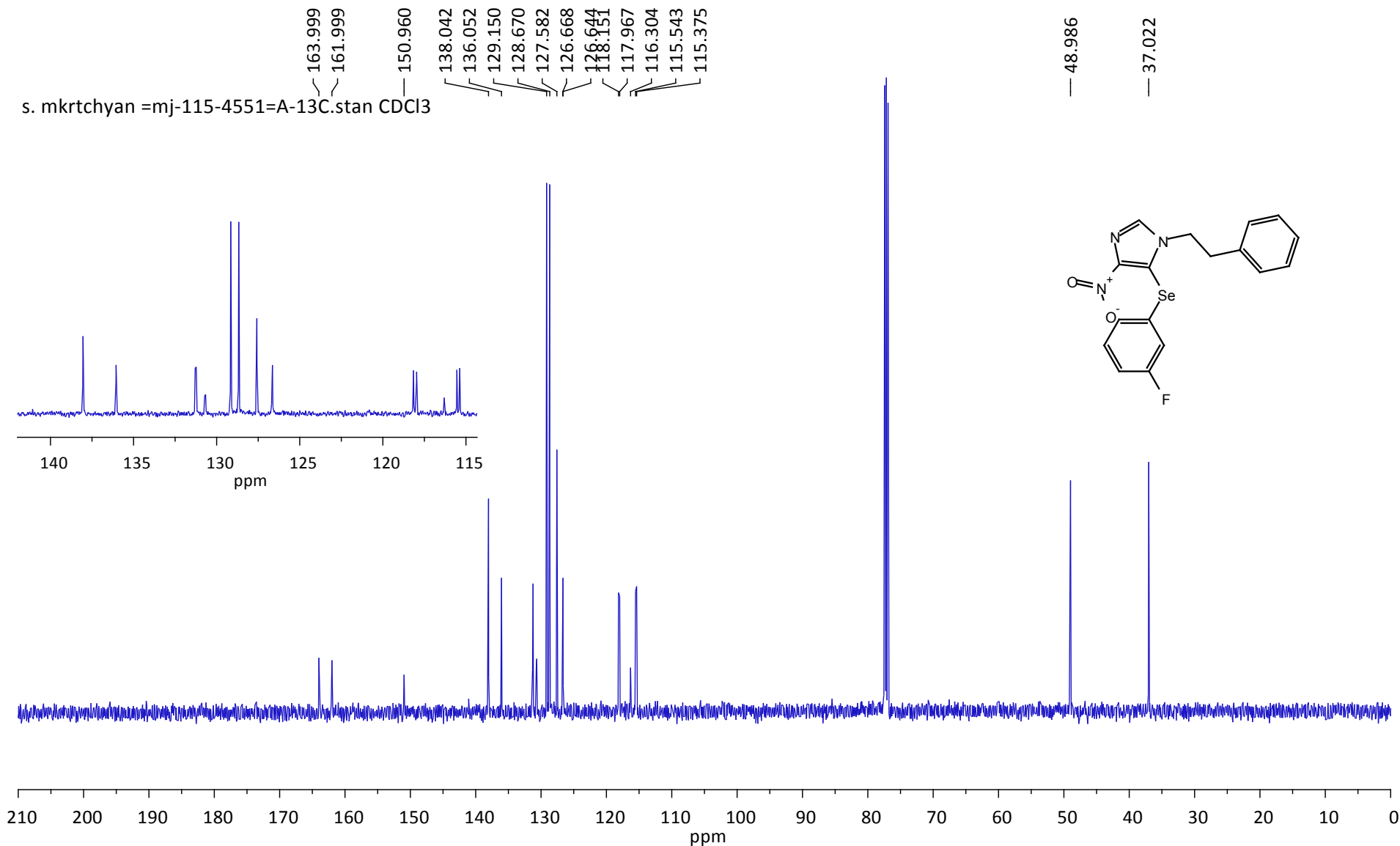
s. mkrtyan =mj-115-4551=1H.stan CDCl3



Comment s. mkrtyan =mj-115-4551=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 7c

s. mkrtyan =mj-115-4551=A-13C.stan CDCl3



Comment s. mkrtyan =mj-115-4551=A-13C.stan CDCl3
 Number of Scans 164
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

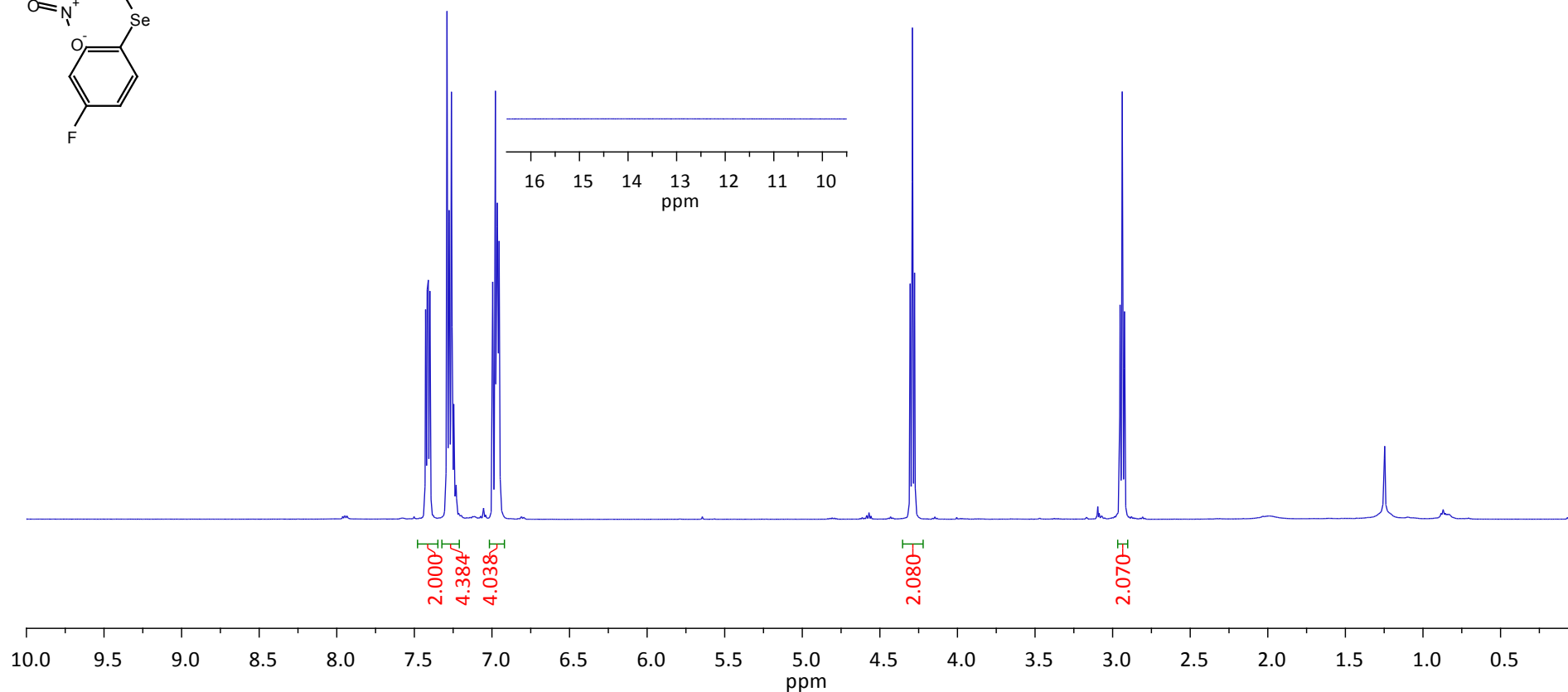
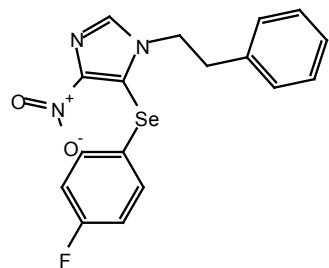
Compound 7d

7.428
7.417
7.410
7.400
7.290
7.261
7.259
6.978
6.966

4.291

2.938

s. mkrtyan =mj63-512=1H.stan CDCl3

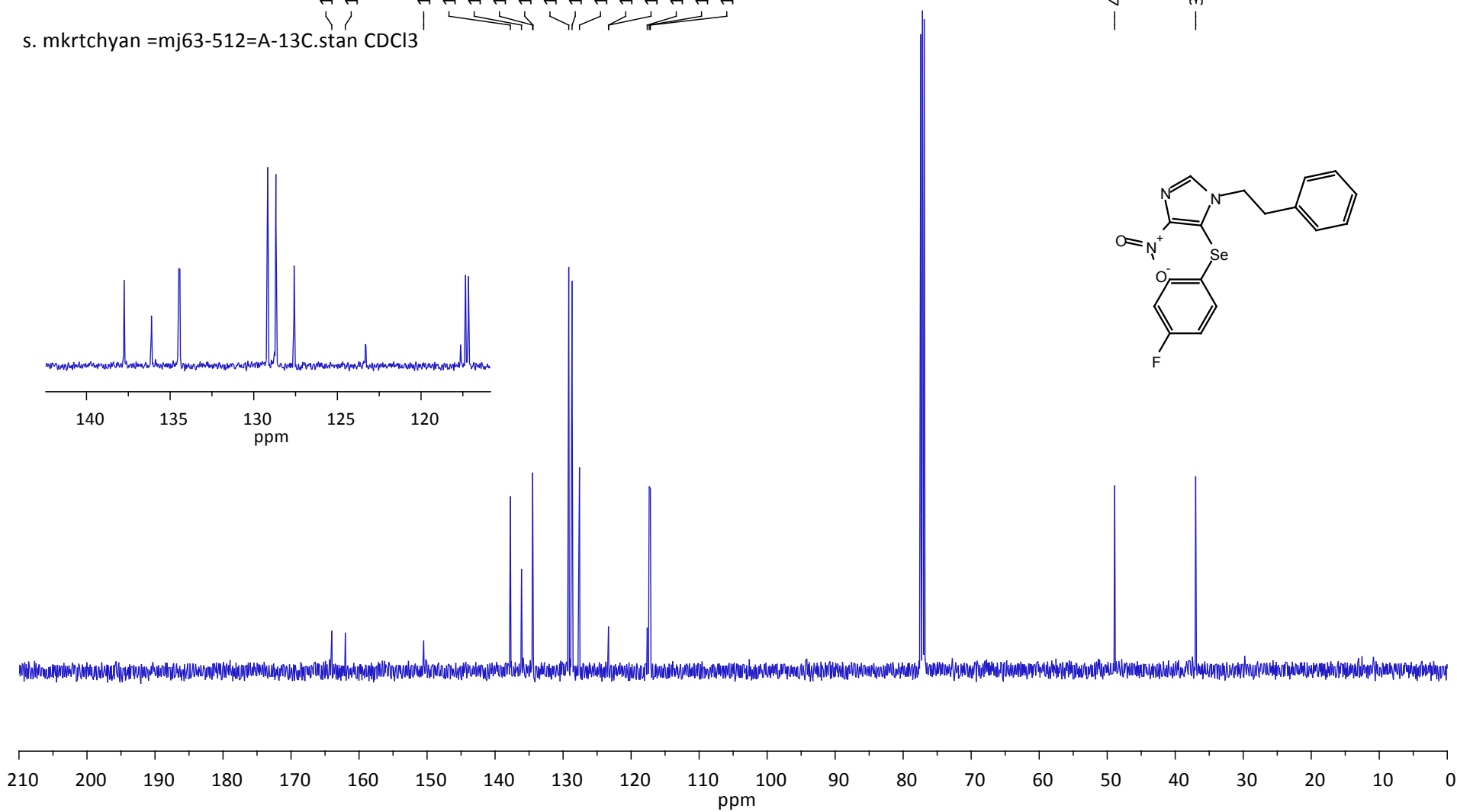
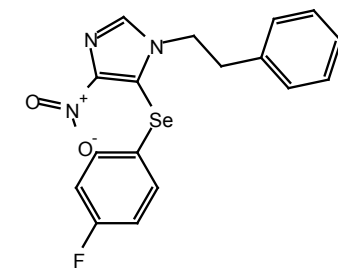


Comment s. mkrtyan =mj63-512=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 7d

s. mkrtyan =mj63-512=A-13C.stan CDCl3

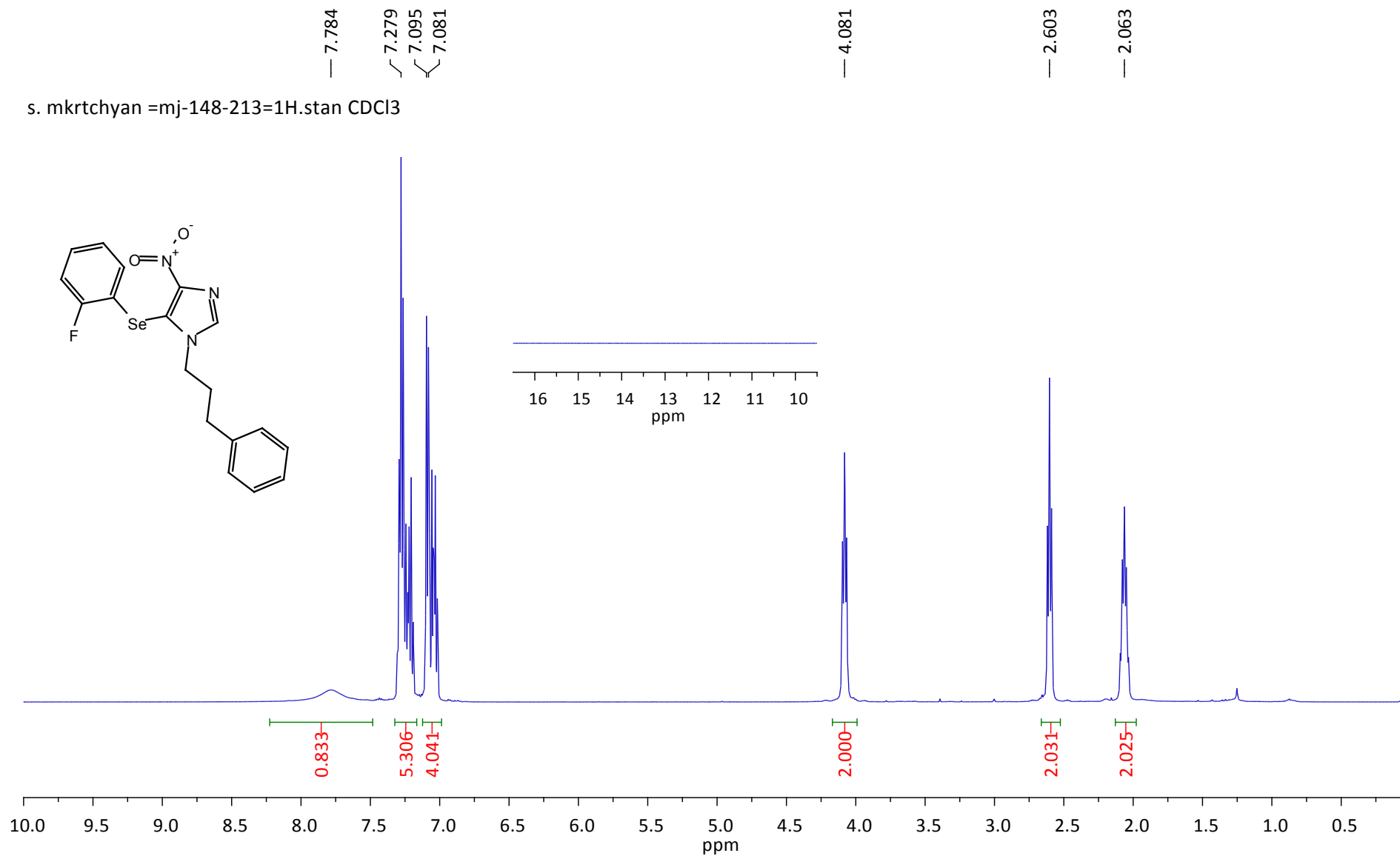
— 48.899
— 36.989



Comment s. mkrtyan =mj63-512=A-13C.stan CDCl3
 Number of Scans 128
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

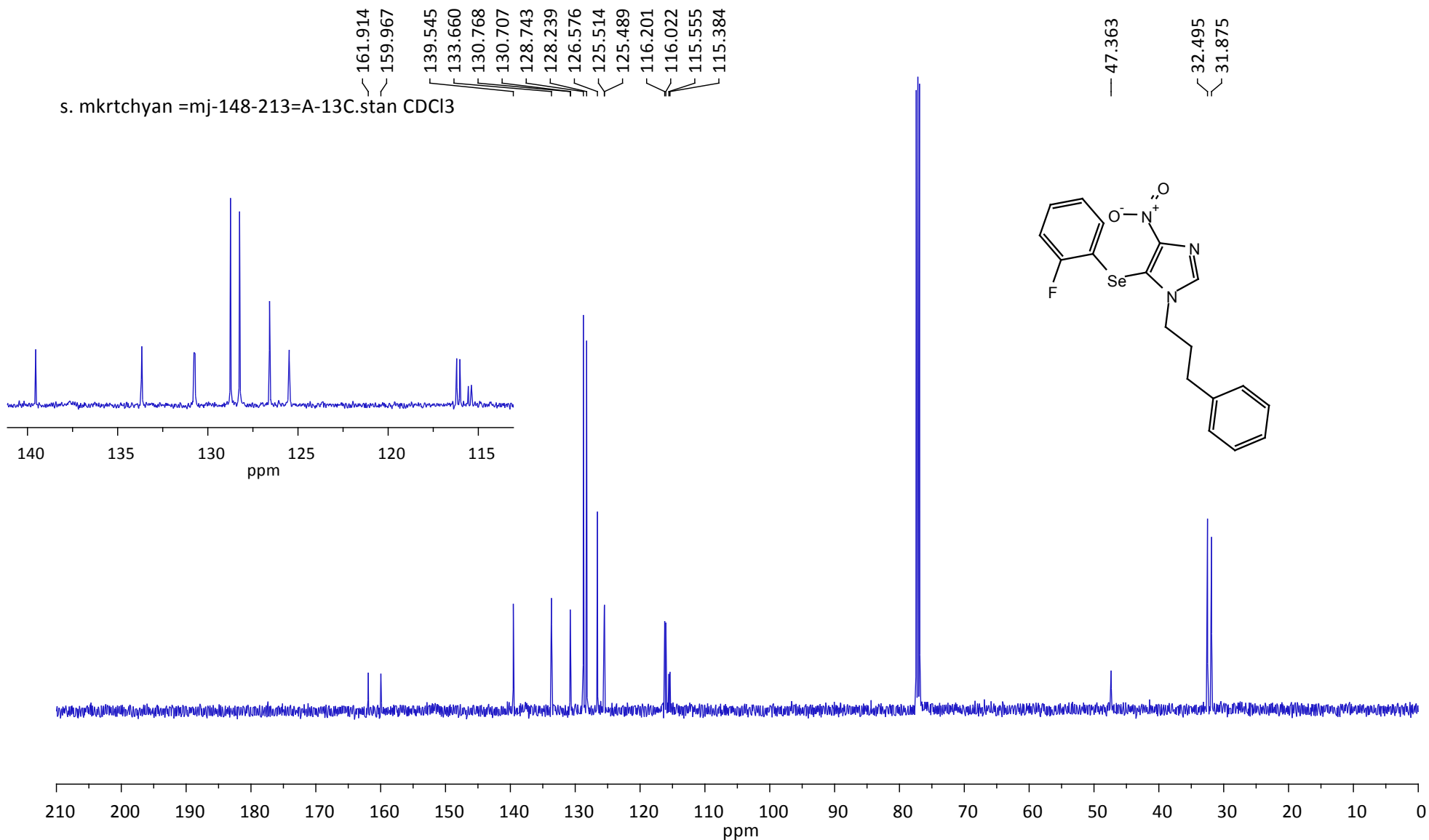
Compound 8

s. mkrtyan =mj-148-213=1H.stan CDCl3



Comment s. mkrtyan =mj-148-213=1H.stan CDCl3
Number of Scans 16
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 8



Comment s. mkrtyan =mj-148-213=A-13C.stan CDCl3
 Number of Scans 148
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound 9a

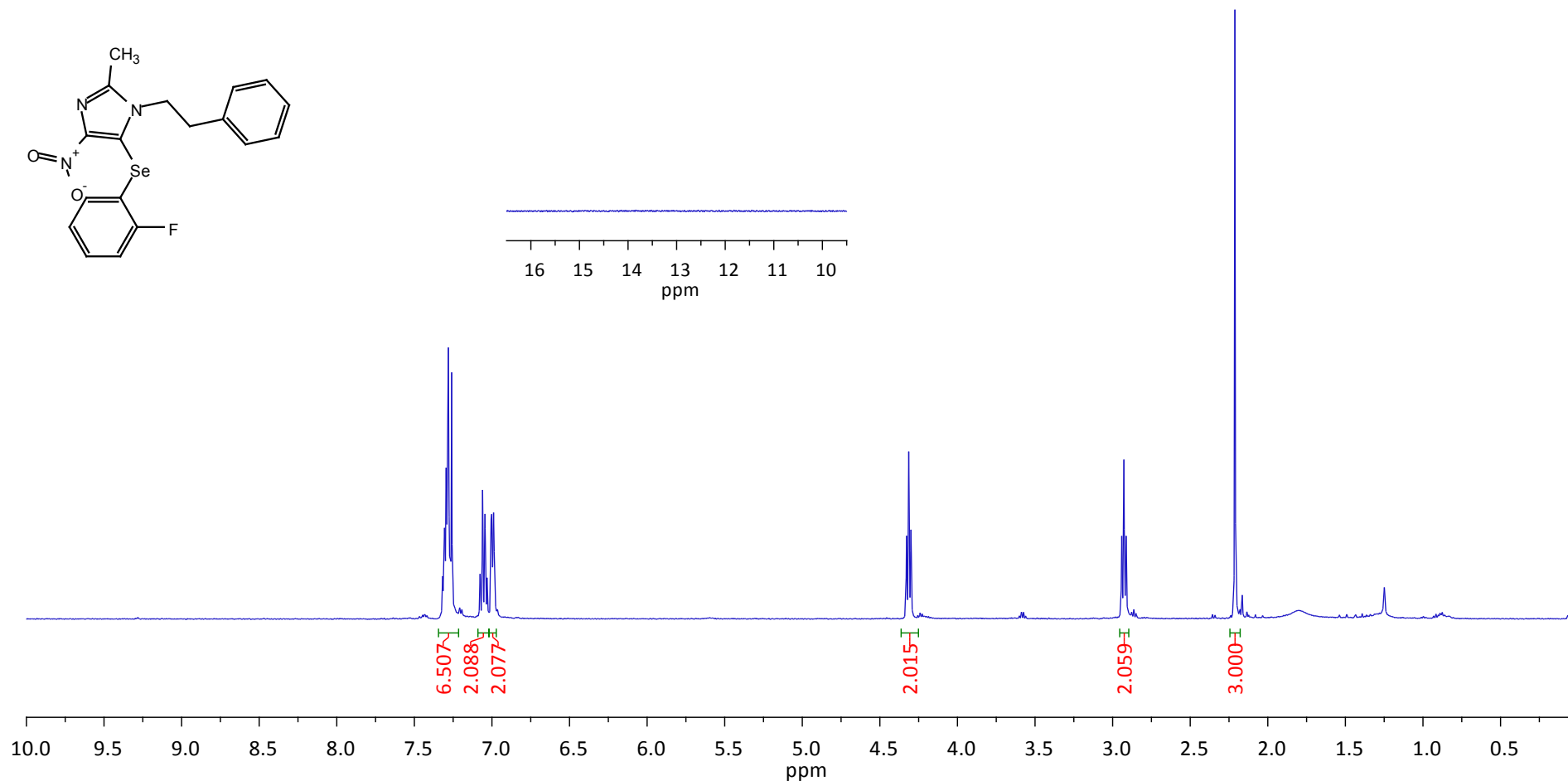
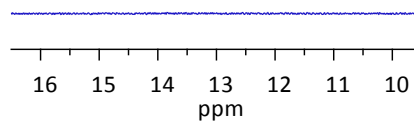
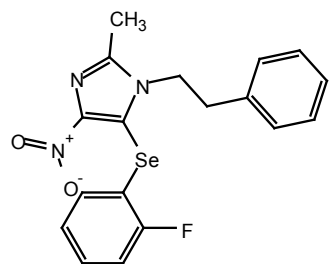
7.295
7.281
7.260
7.060
7.045
7.005
7.001
6.990

— 4.314

— 2.927

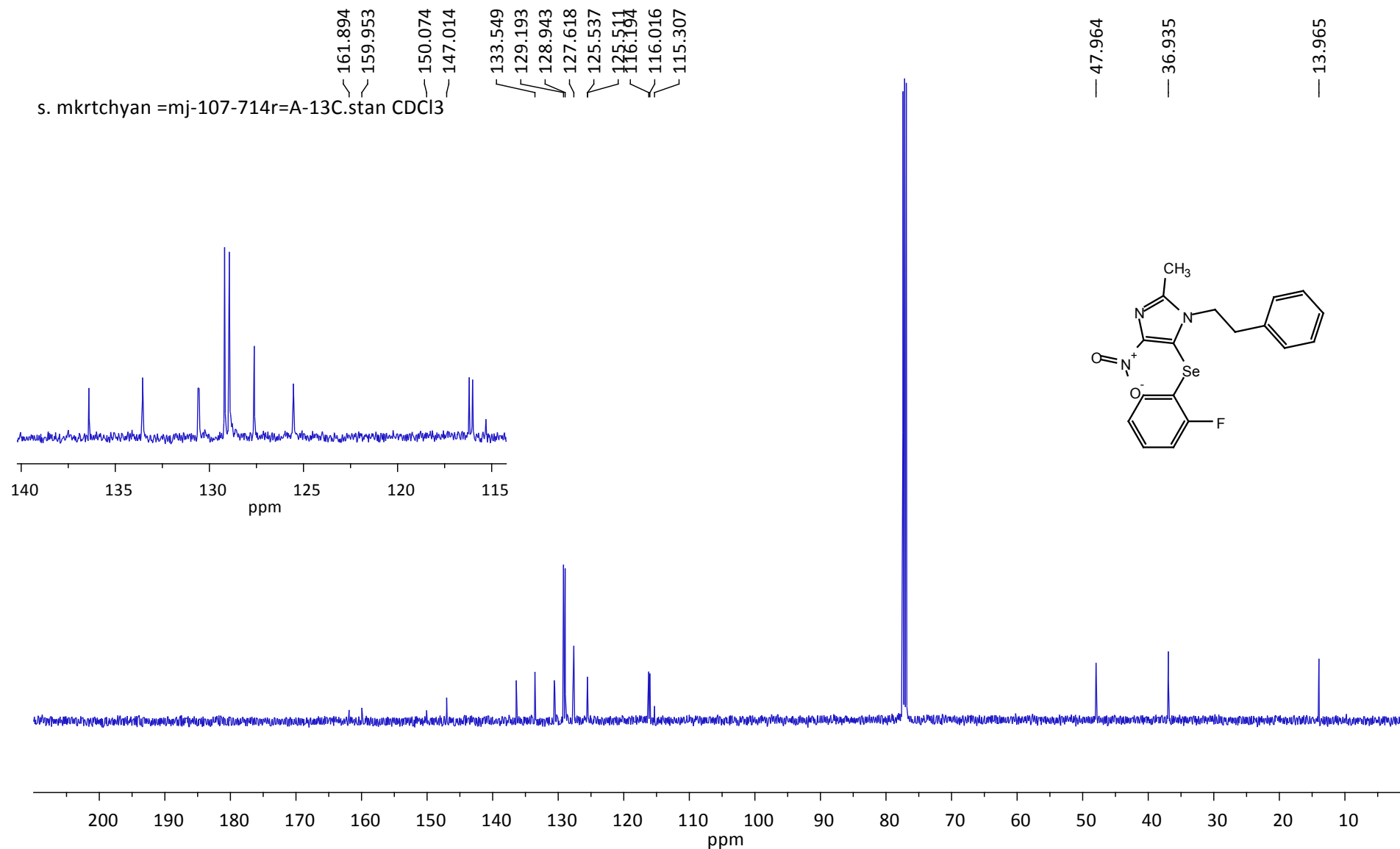
— 2.212

s. mkrtyan =mj107-714=1H.stan CDCl3



Comment s. mkrtyan =mj107-714=1H.stan CDCl3
Number of Scans 32
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 9a



Comment	s. mkrtyan =mj-107-714r=A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **9b**

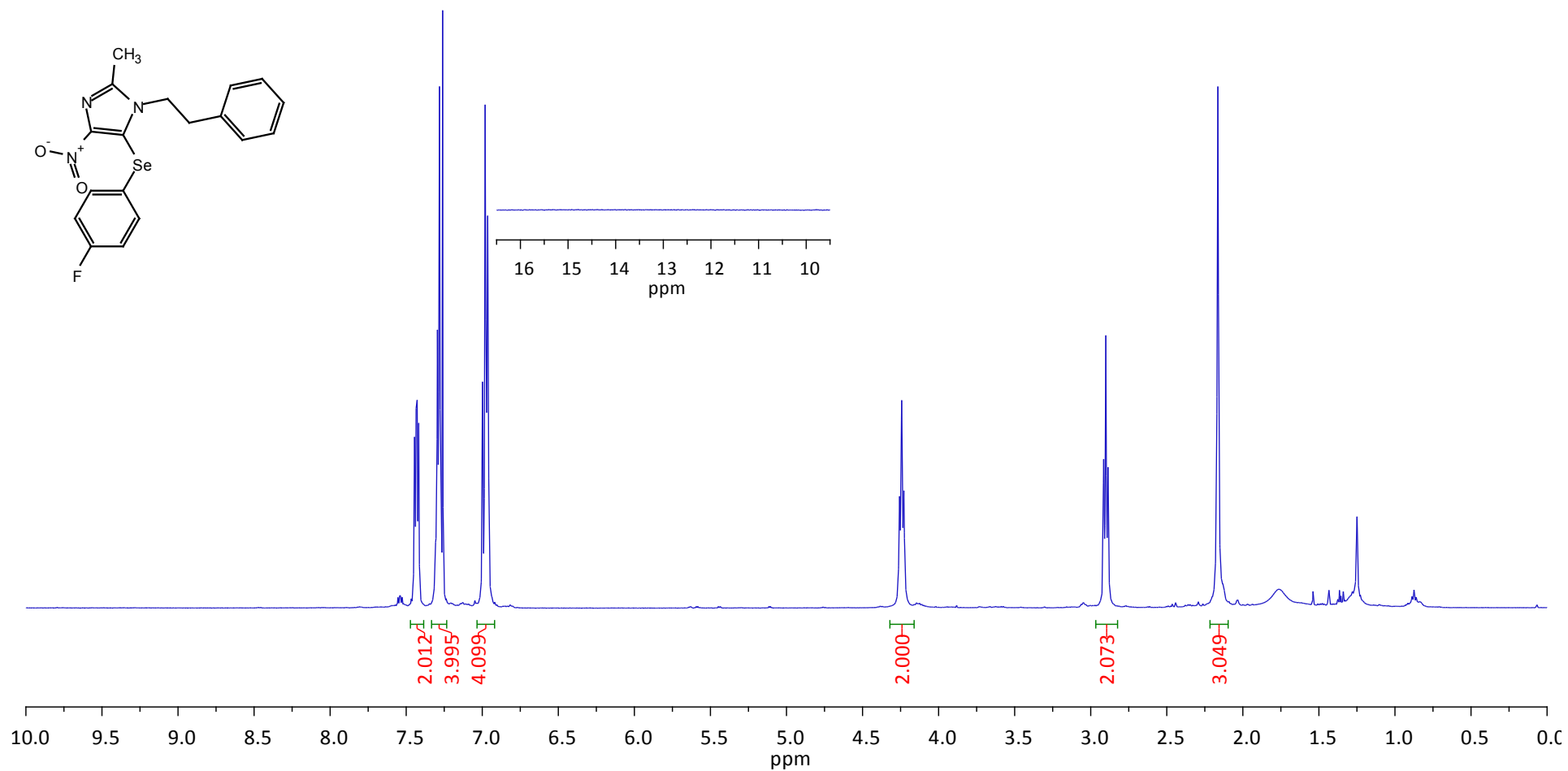
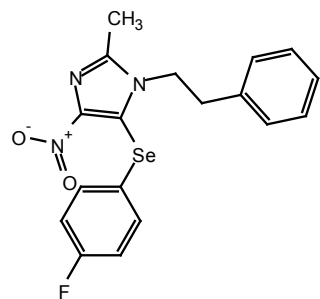
7.435
7.428
7.281
7.260
6.981

4.243

2.901

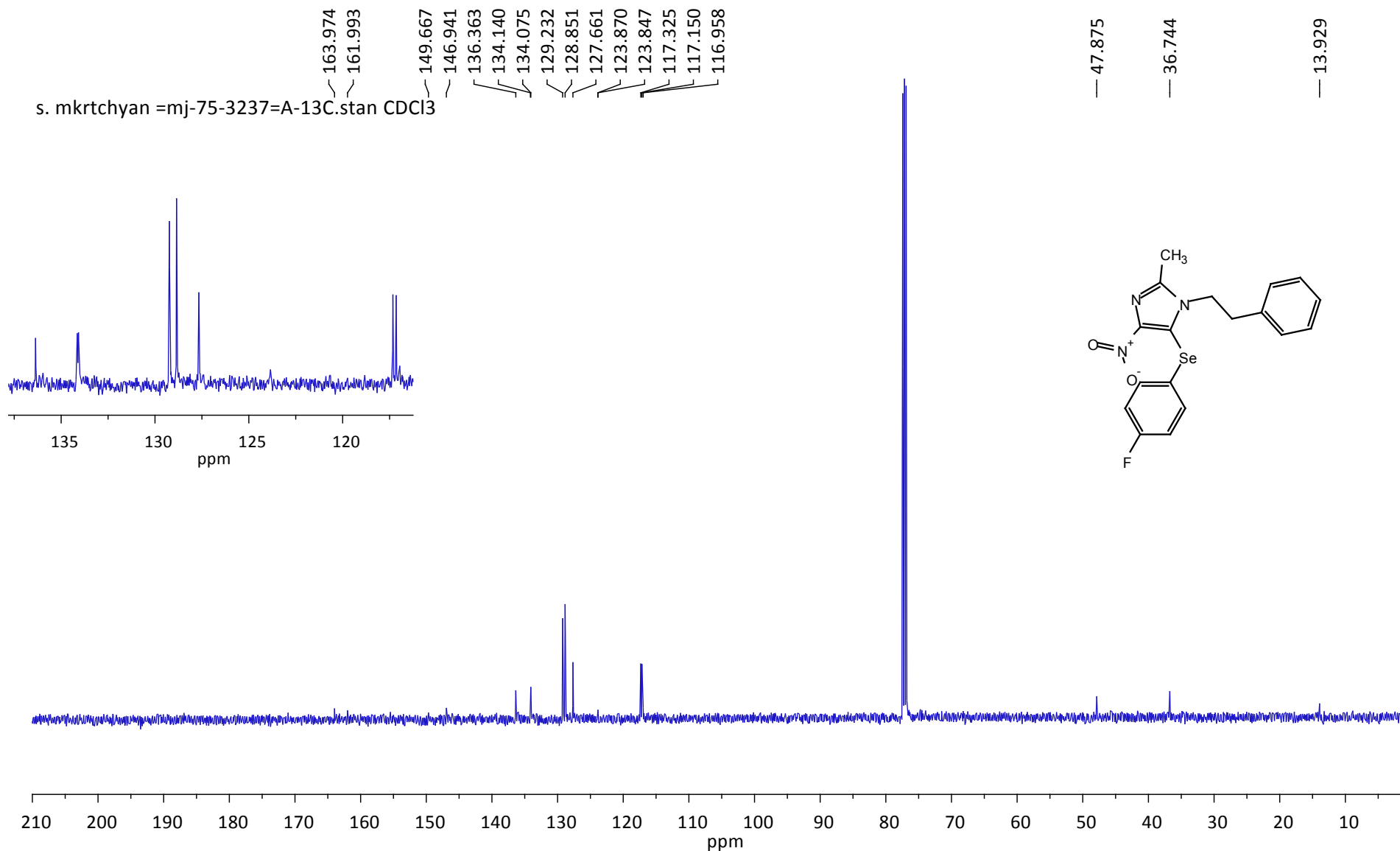
2.164

s. mkrtyan =mj-75-3237=1H.stan CDCl3



Comment s. mkrtyan =mj-75-3237=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **9b**



Comment s. mkrtyan =mj-75-3237=A-13C.stan CDCl₃

Number of Scans 512

Spectrometer Frequency 125.76

Spectral Width 36057.7

Spectral Size 65536

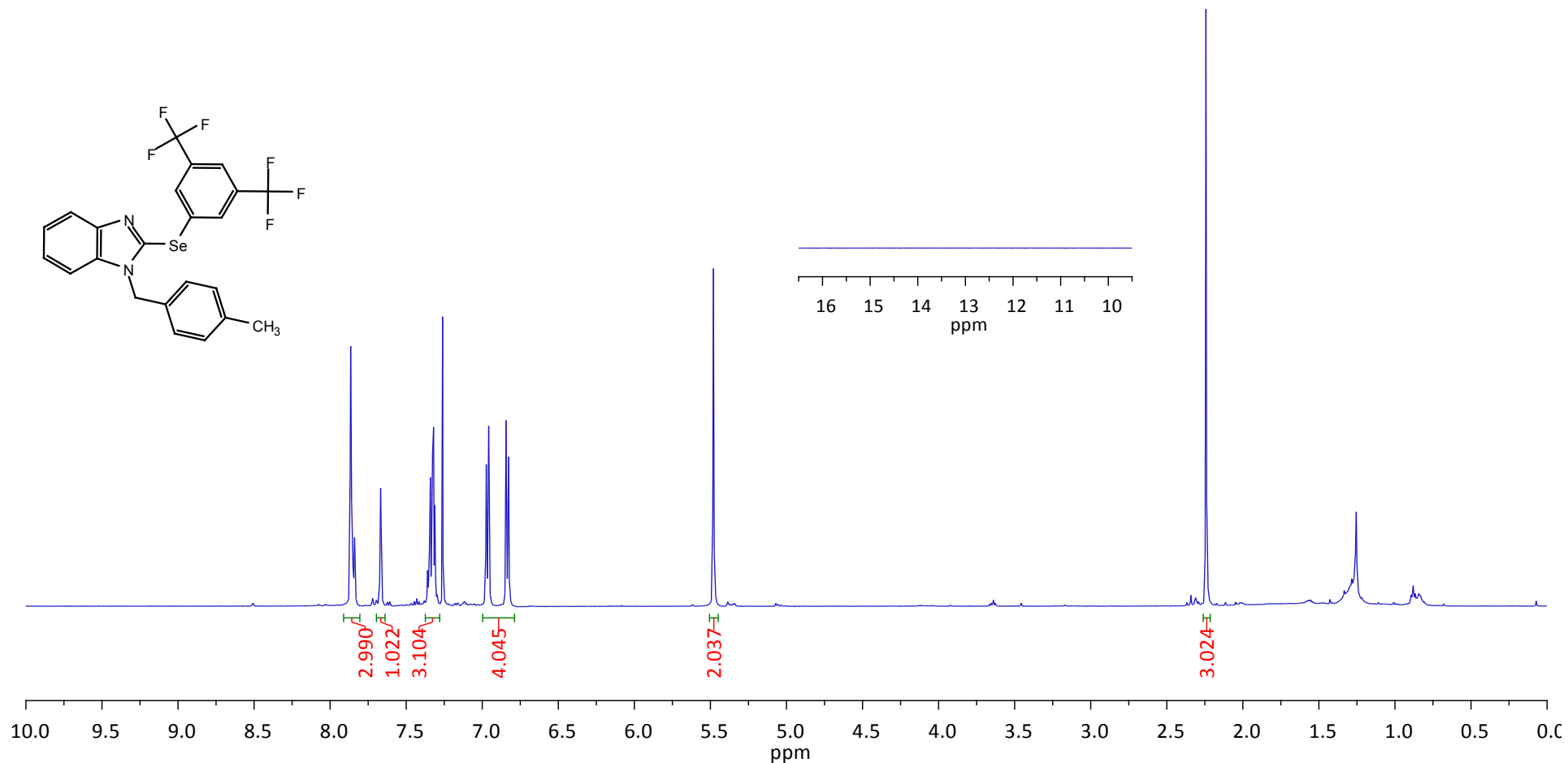
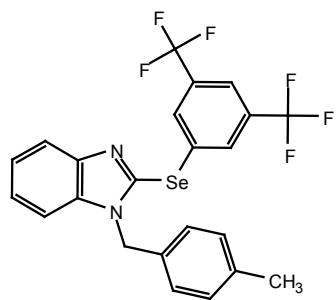
Compound 10a

7.865
7.668
7.320
7.260
7.260
6.958
6.843

5.480

2.242

s. mkrtyan mj-174-10251H.stan CDCl3

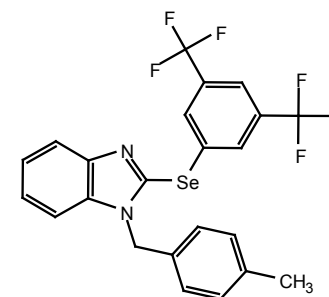
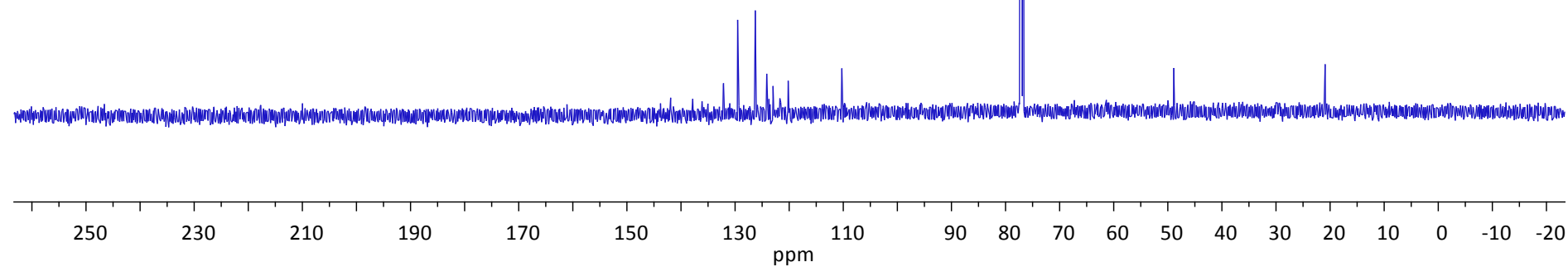
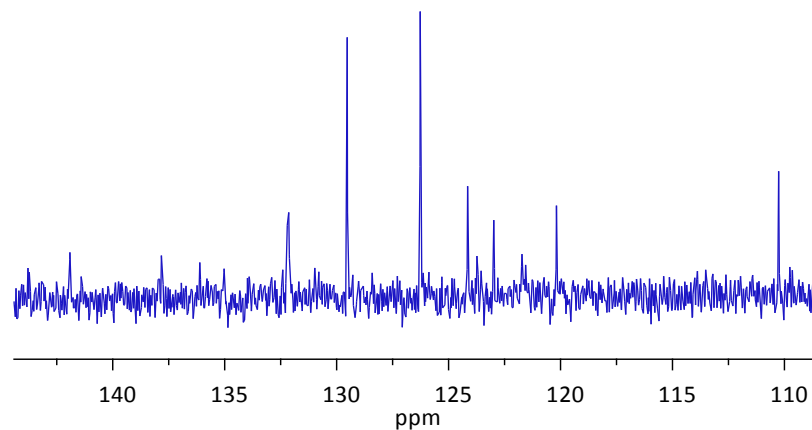


Comment s. mkrtyan mj-174-10251H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound 10a

141.911
137.826
136.114
132.405
132.255
132.139
130.975
129.529
126.266
124.152
122.980
121.724
120.181
110.260

s. mkrtyan mj-174-1025A-13C.stan CDCl3



— 48.897

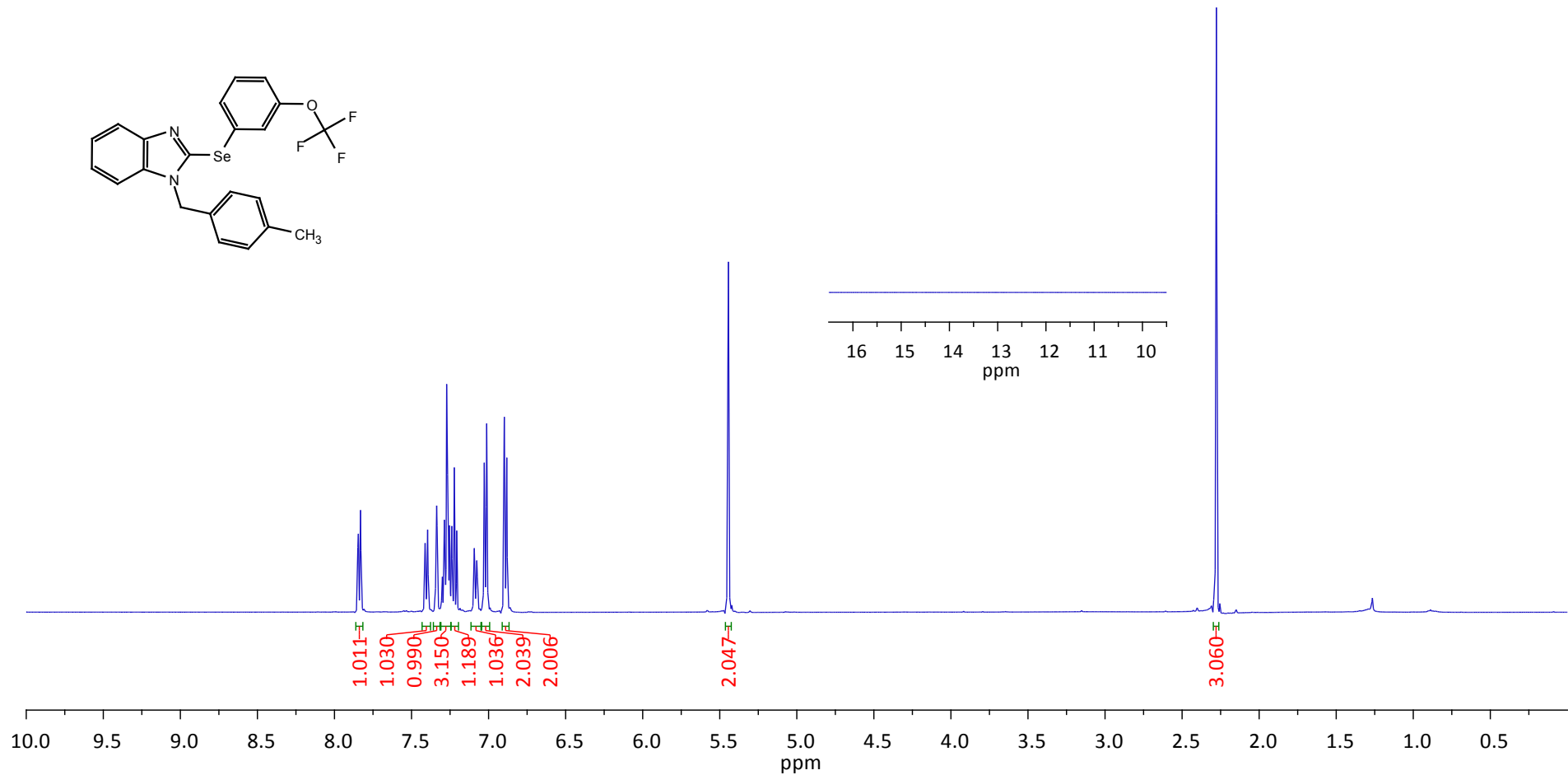
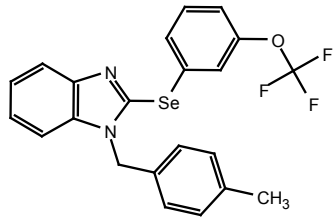
— 20.916

Comment s. mkrtyan mj-174-1025A-13C.stan CDCl3
Number of Scans 512
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

Compound **10b**

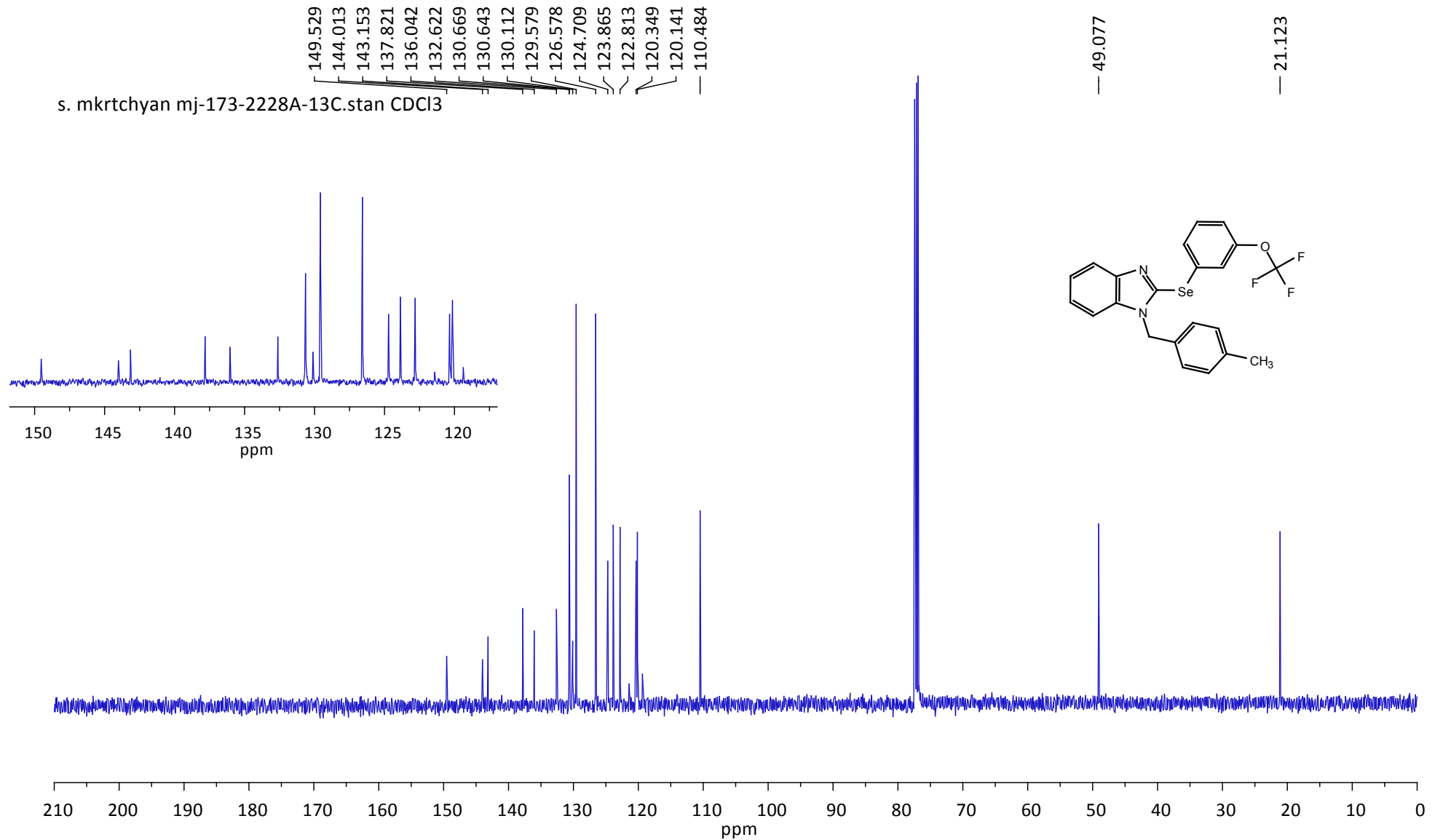
7.845
7.831
7.412
7.396
7.337
7.272
7.271
7.223
7.095
7.093
7.028
7.012
6.898
6.882
5.444

s. mkrtyan mj-173-22281H.stan CDCl3



Comment s. mkrtyan mj-173-22281H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

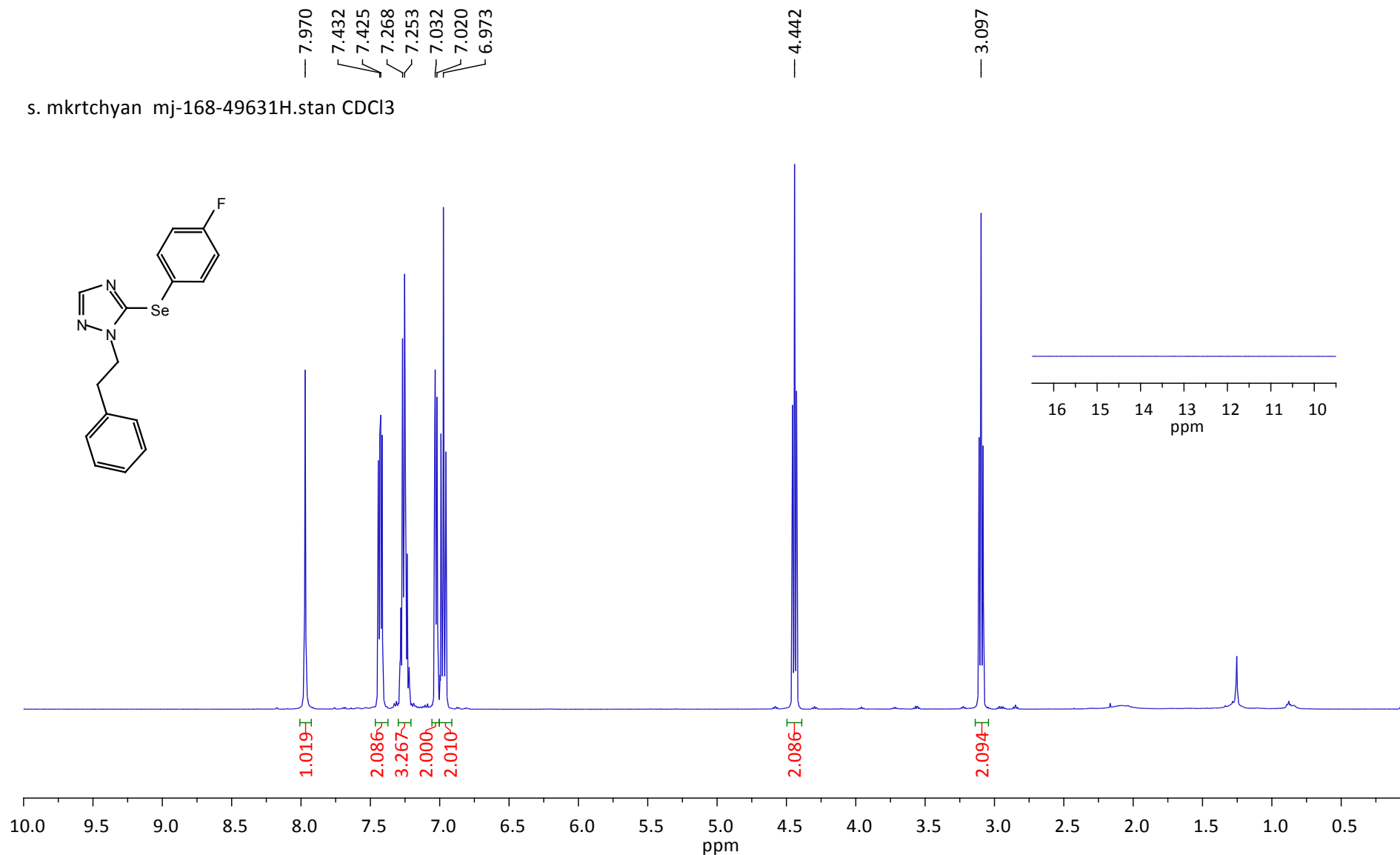
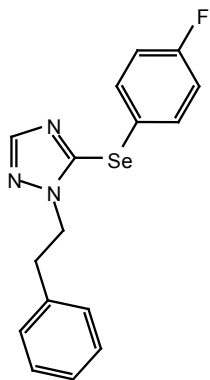
Compound 10b



Comment s. mkrтчyan mj-173-2228A-13C.stan CDCl3
Number of Scans 256
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

Compound **11**

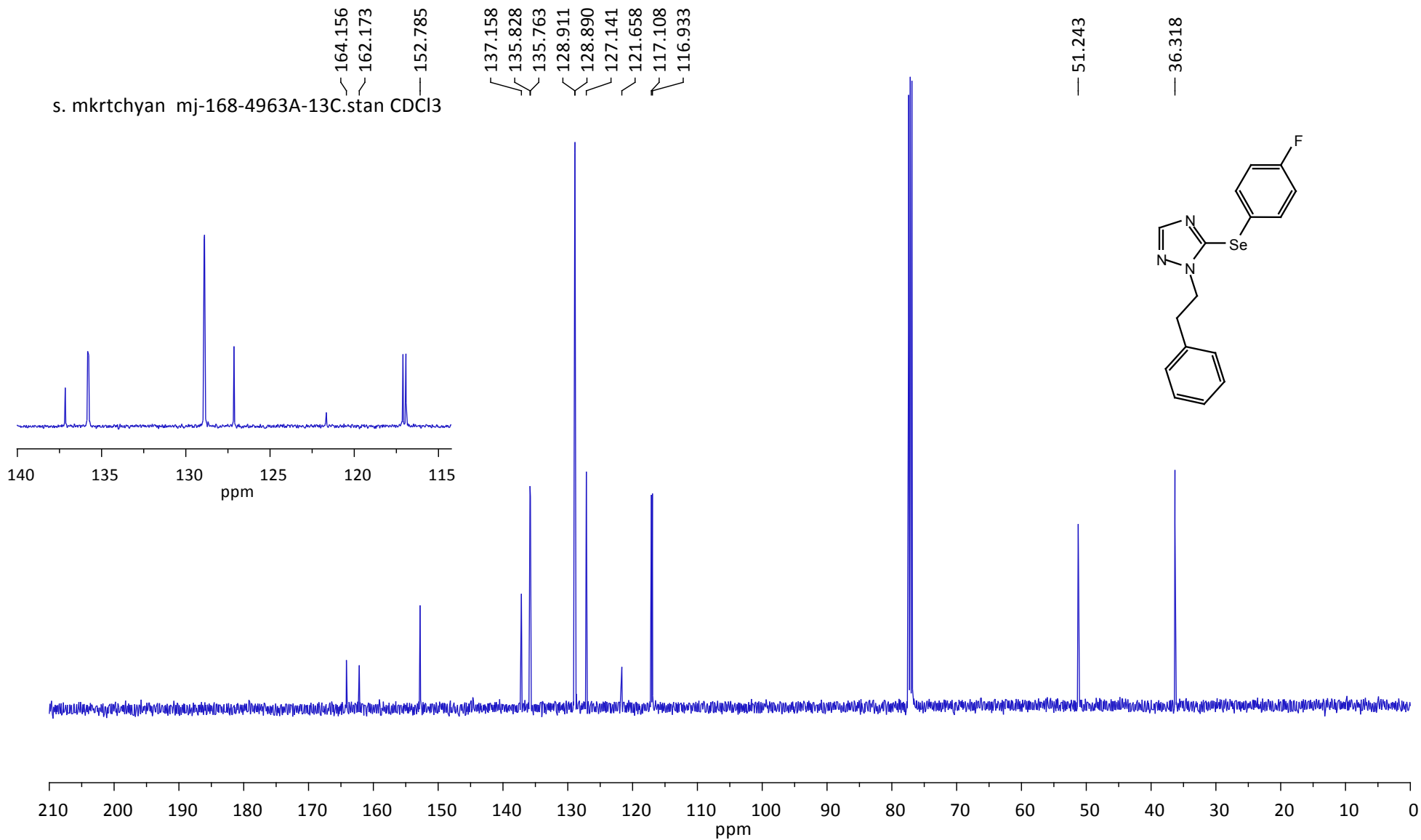
s. mkrтчyan mj-168-49631H.stan CDCl₃



Comment	s. mkrтчyan mj-168-49631H.stan CDCl ₃
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound 11

s. mkrtyan mj-168-4963A-13C.stan CDCl3



Comment s. mkrtyan mj-168-4963A-13C.stan CDCl3
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

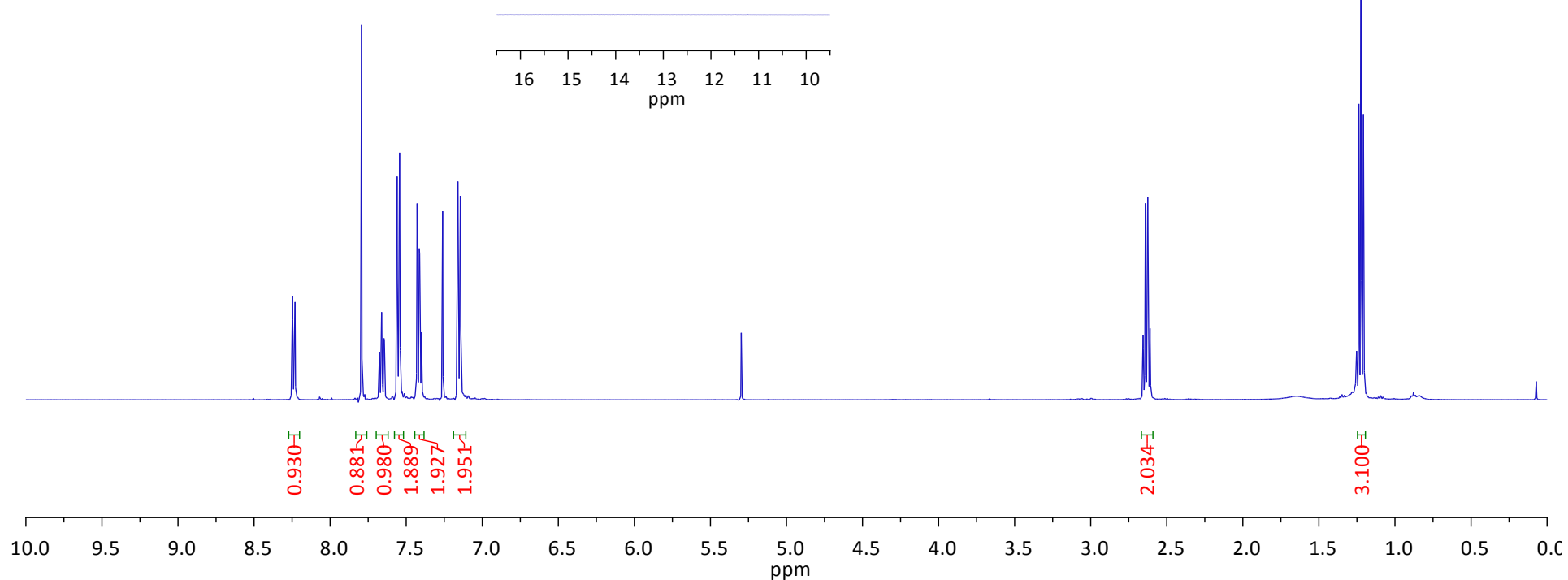
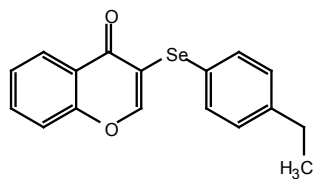
Compound **12a**

8.247
8.234
8.231
7.793
7.662
7.560
7.544
7.428
7.414
7.411
7.260
7.160
7.144

2.640
2.625

1.222

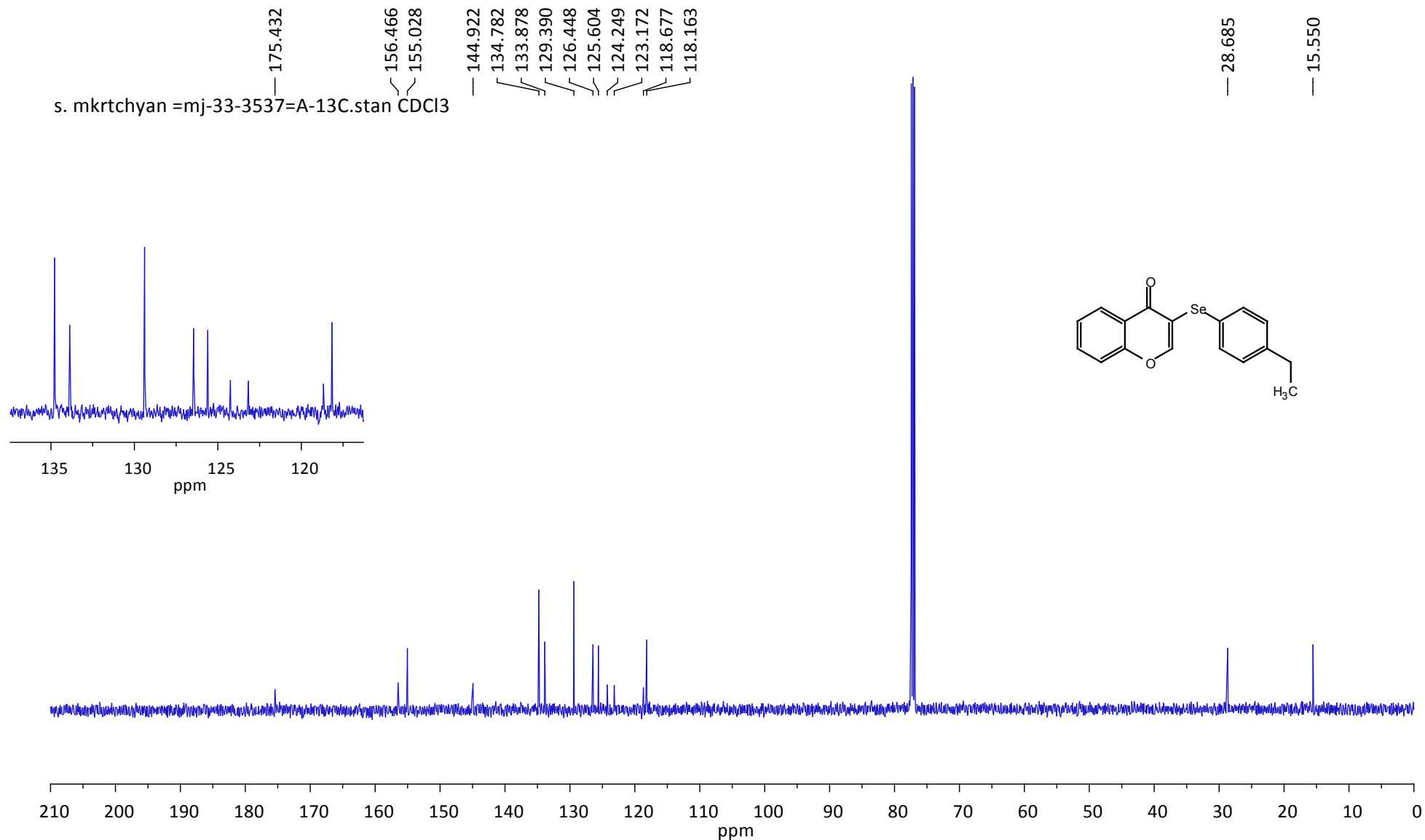
s. mkrtyan =mj-33-3537=1H.stan CDCl3



Comment s. mkrtyan =mj-33-3537=1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **12a**

s. mkrtchyan =mj-33-3537=A-13C.stan CDCl₃



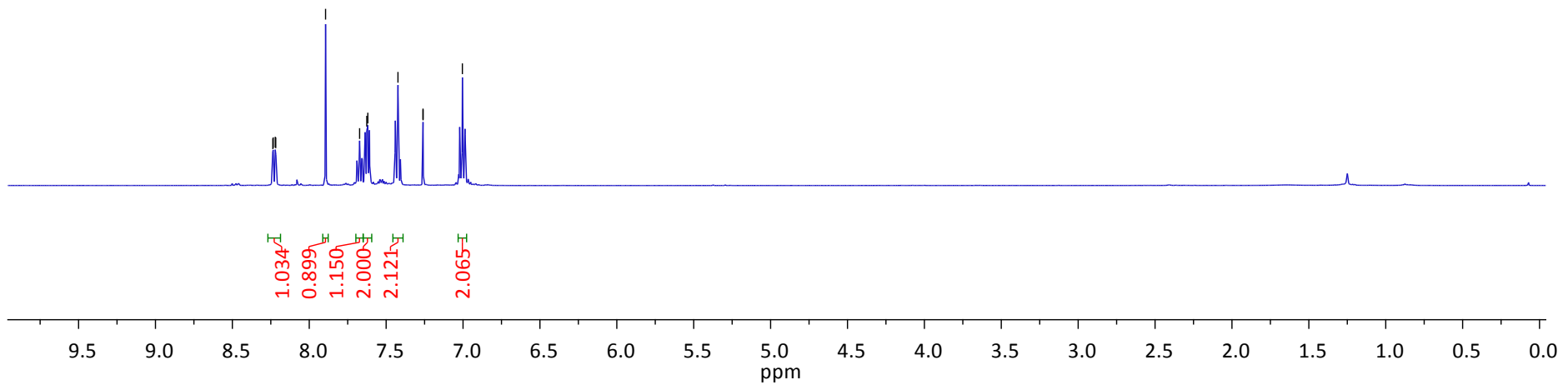
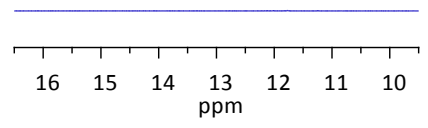
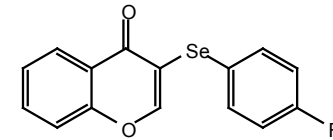
Comment	s. mkrtchyan =mj-33-3537=A-13C.stan CDCl ₃
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound 12b

s. mkrtychyan =mj-37-3739=1H.stan CDCl3

8.237
8.234
8.221
8.218
7.894
7.673
7.626
7.619
7.423
7.260
7.260
7.004

Chloroform-d



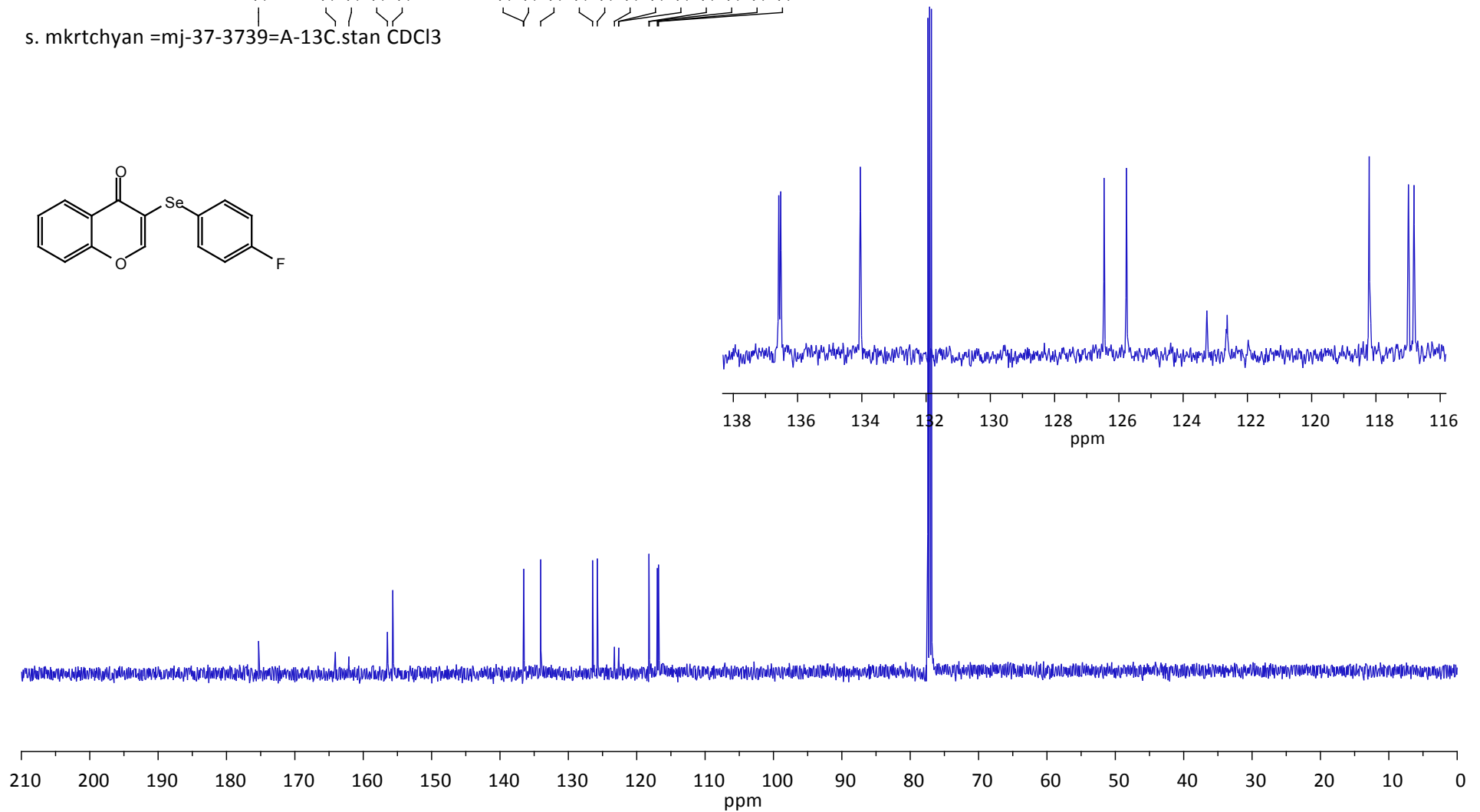
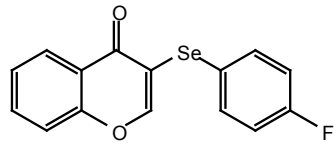
Comment s. mkrtychyan =mj-37-3739=1H.stan CDCl3
Number of Scans 32
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 12b

s. mkrtyan =mj-37-3739=A-13C.stan CDCl3

136.585
136.521
134.045
126.457
125.763
123.261
122.653
122.626
118.208
118.170
116.986
116.814

175.310
164.076
162.100
156.466
155.677



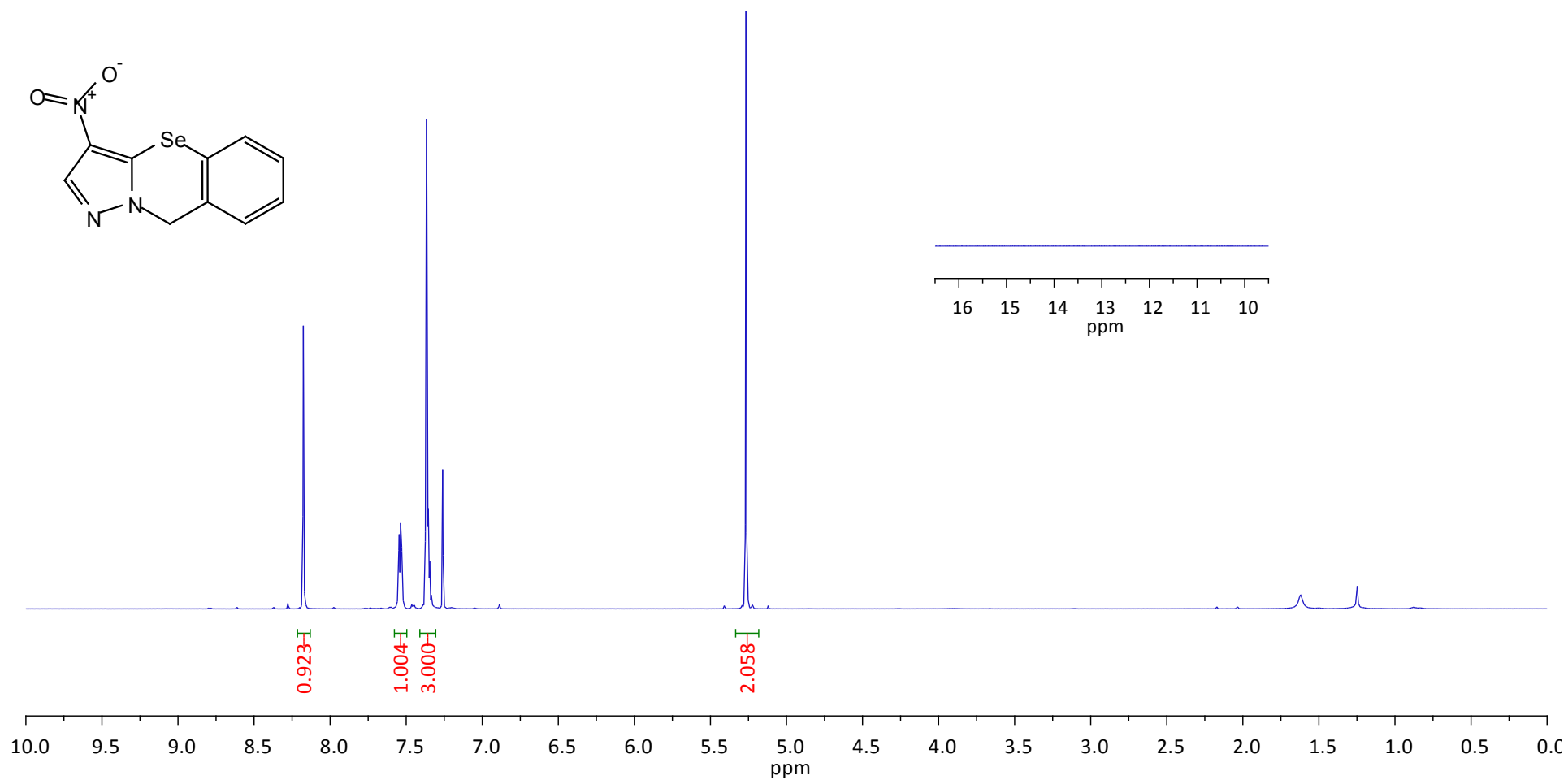
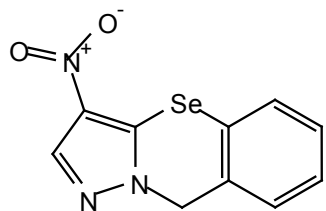
Comment s. mkrtyan =mj-37-3739=A-13C.stan CDCl3
Number of Scans 256
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

Compound **13a**

— 8.176
~ 7.537
~ 7.366
~ 7.260

— 5.267

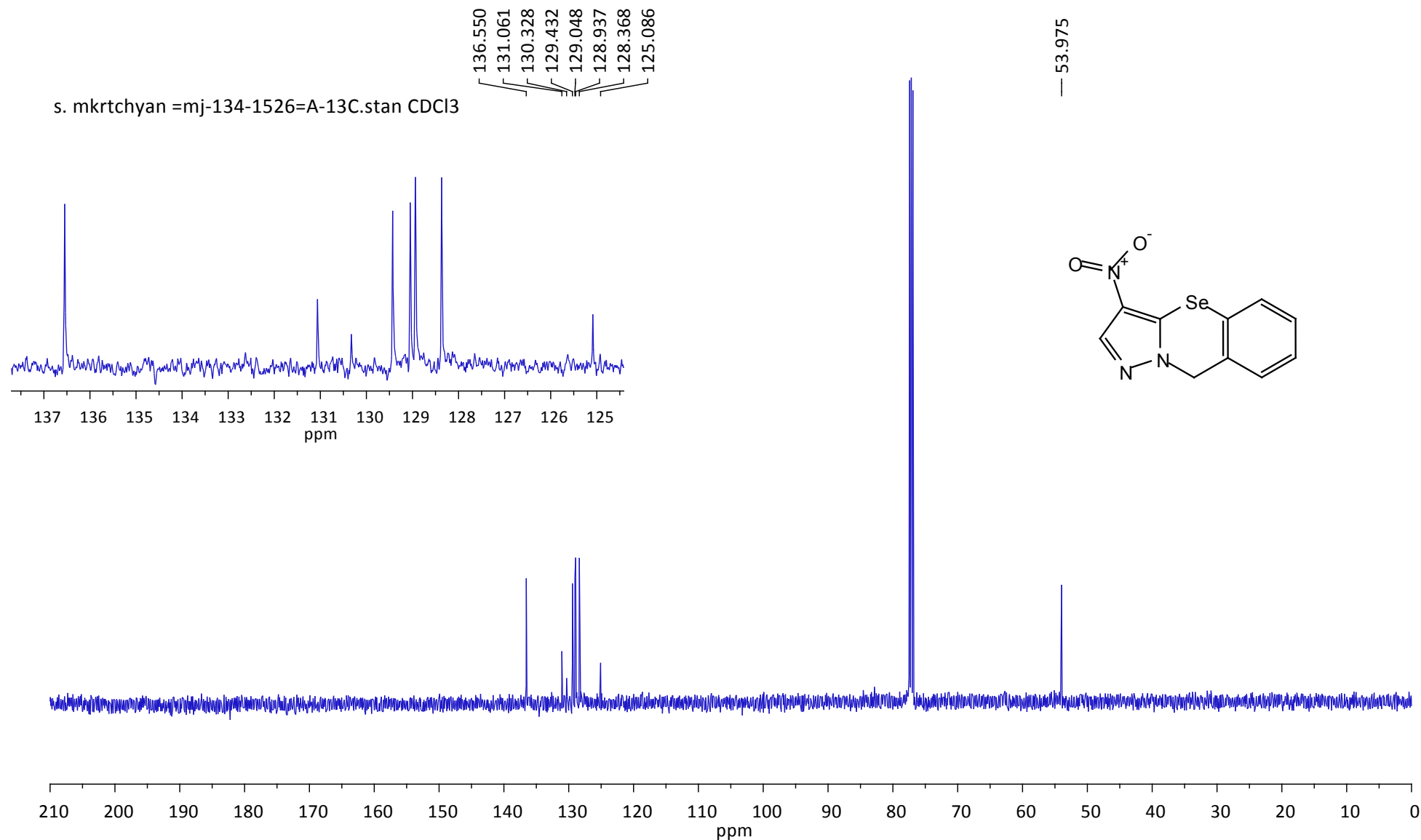
s. mkrtyan =mj-134-1526=1H.stan CDCl3



Comment s. mkrtyan =mj-134-1526=1H.stan CDCl3
Number of Scans 24
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound 13a

s. mkrtchyan =mj-134-1526=A-13C.stan CDCl3



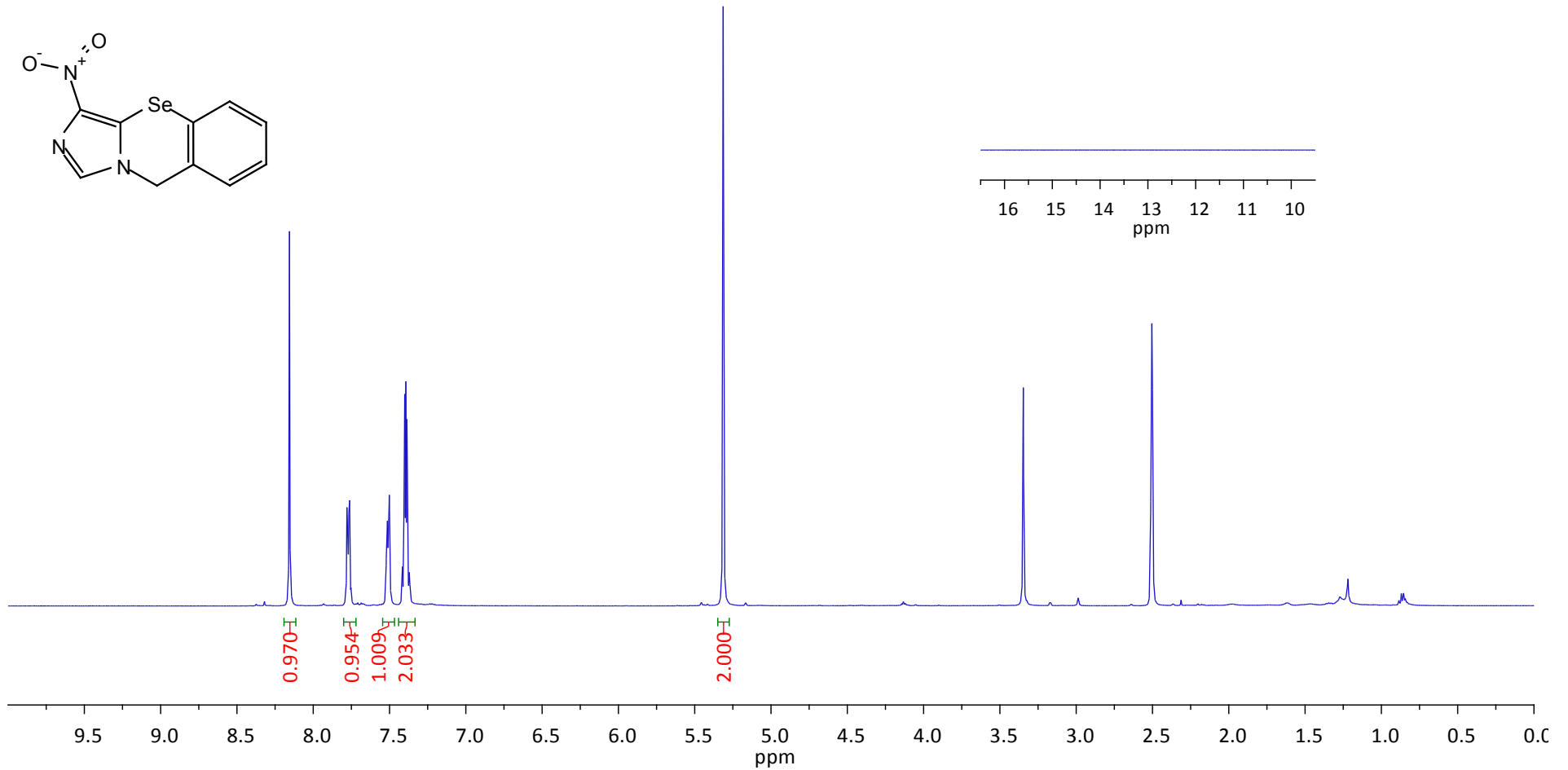
Comment	s. mkrtchyan =mj-134-1526=A-13C.stan CDCl3
Number of Scans	256
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

Compound **13b**

— 8.156
└─ 7.779
└─ 7.762
└─ 7.502
└─ 7.400
└─ 7.393

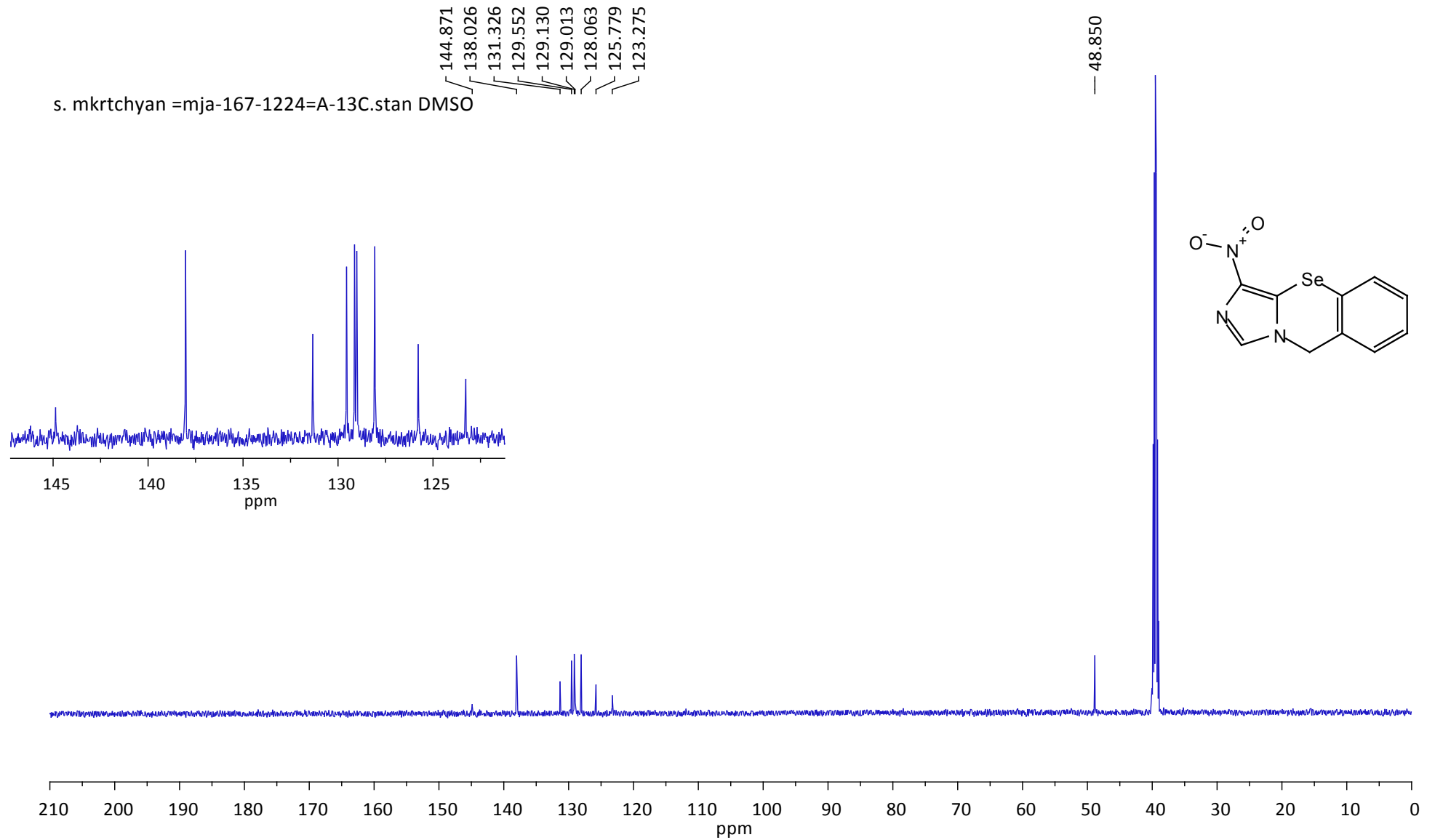
— 5.313

s. mkrtyan =mja-167-1224=1H.stan DMSO



Comment s. mkrtyan =mja-167-1224=1H.stan DMSO
Number of Scans 39
Spectrometer Frequency 500.13
Spectral Width 12335.5
Spectral Size 65536

Compound **13b**



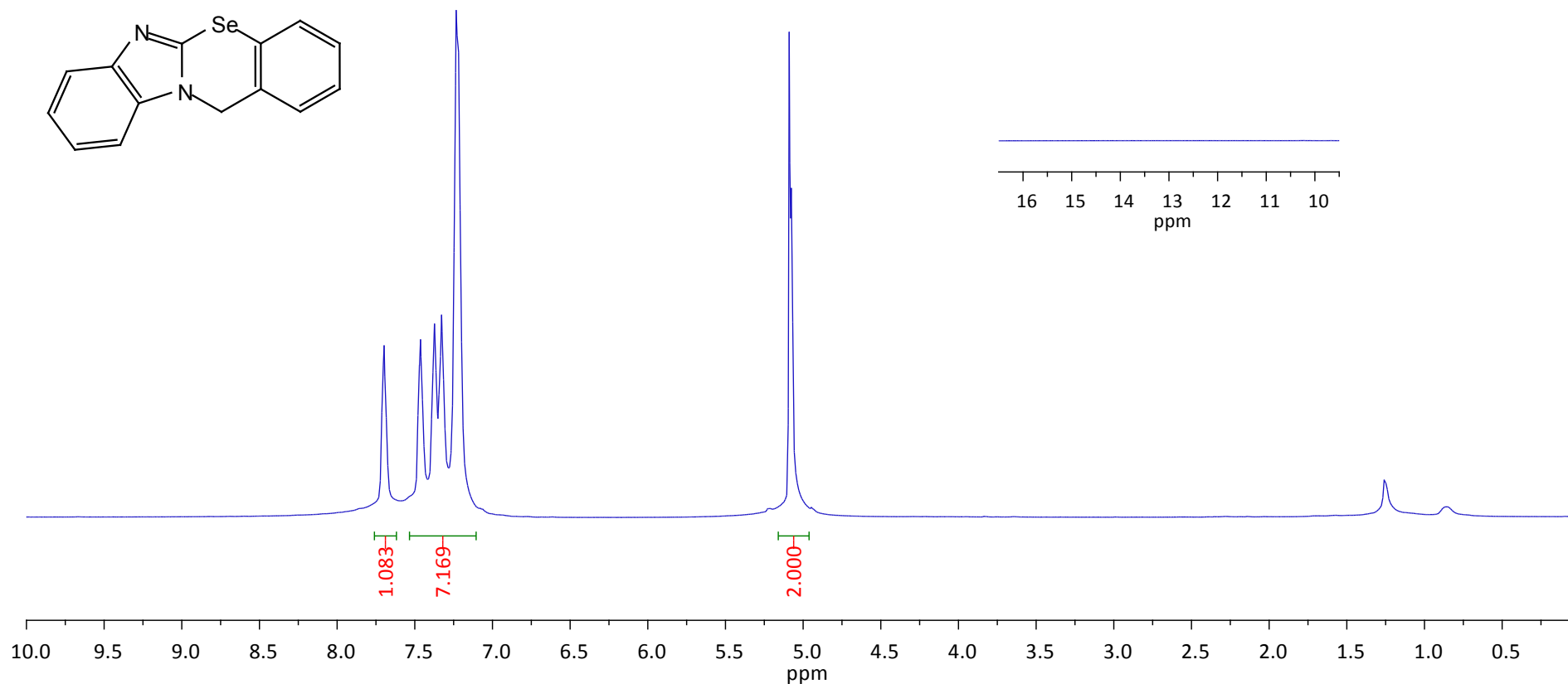
Comment s. mkrтчhуа =mja-167-1224=A-13C.stan DMSO
Number of Scans 512
Spectrometer Frequency 125.76
Spectral Width 36057.7
Spectral Size 65536

Compound **13c**

7.698
7.463
7.373
7.327
7.234
7.229
7.222

5.090

s. mkrtyan =mj-145-613=1H.stan CDCl3



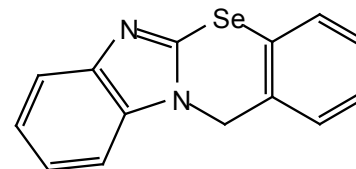
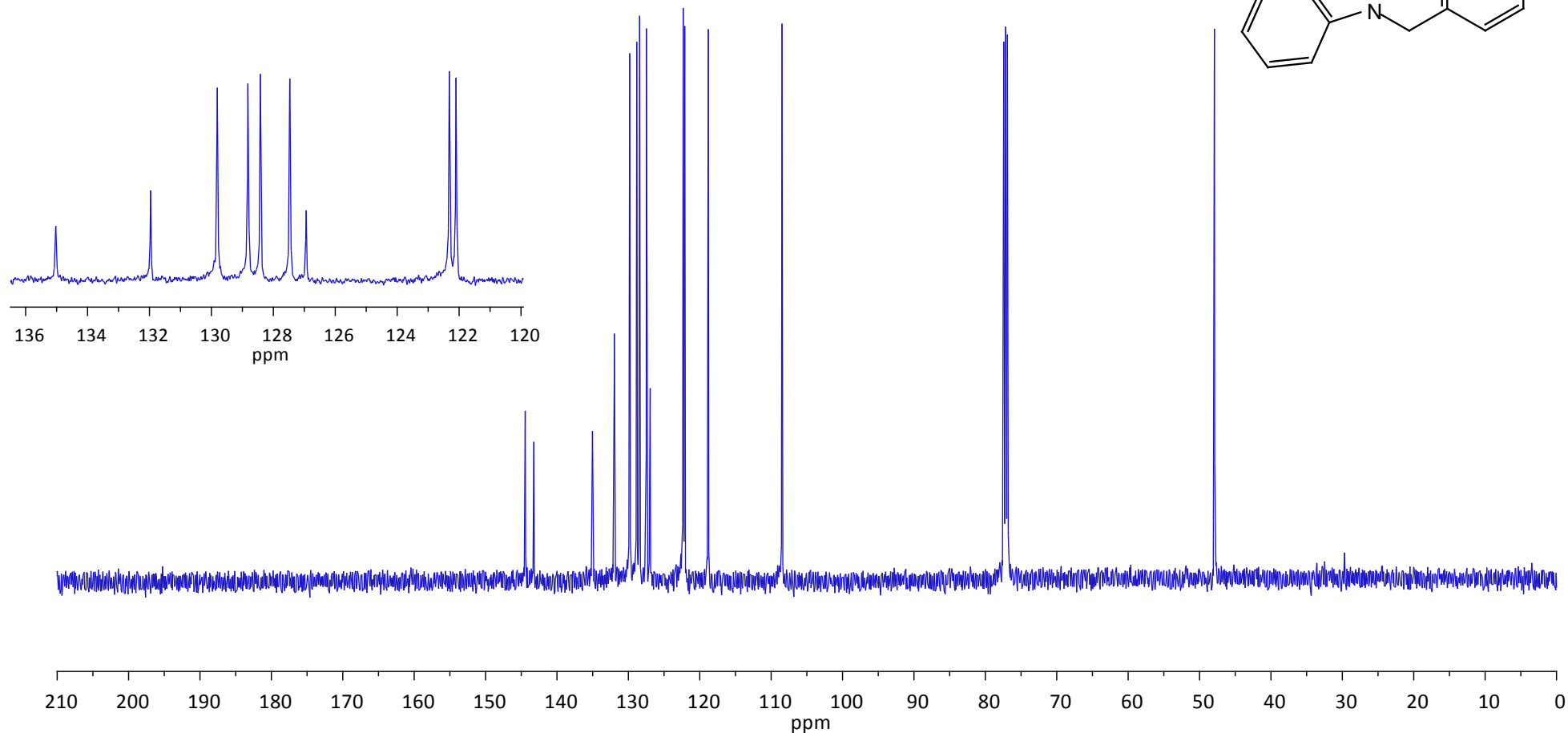
Comment	s. mkrtyan =mj-145-613=1H.stan CDCl3
Number of Scans	24
Spectrometer Frequency	500.13
Spectral Width	12335.5
Spectral Size	65536

Compound **13c**

144.446
143.237
131.965
129.811
128.820
128.420
127.468
122.317
122.100
118.898

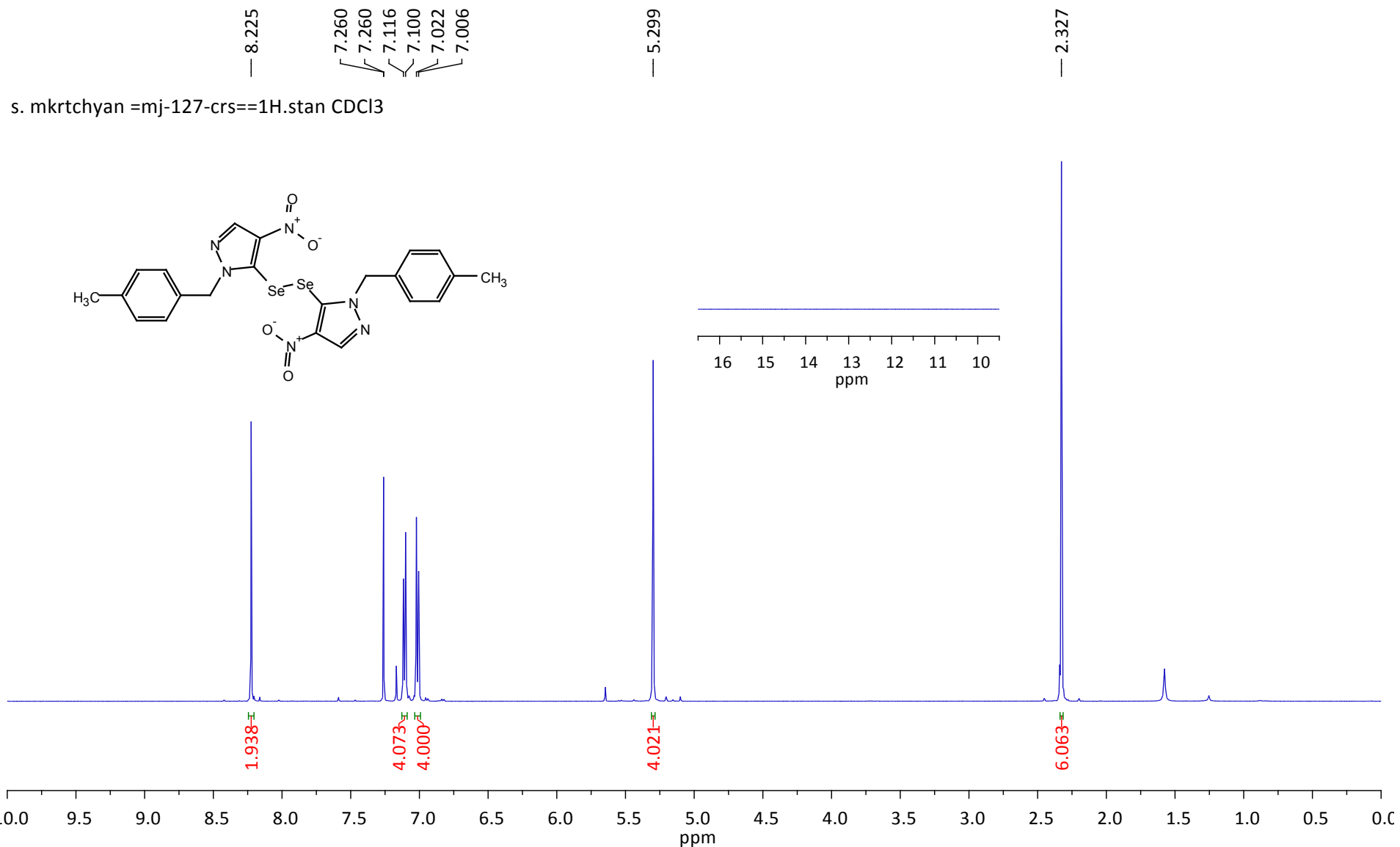
— 47.919

s. mkrtchyan =mj-145-613=A-13C.stan CDCl₃



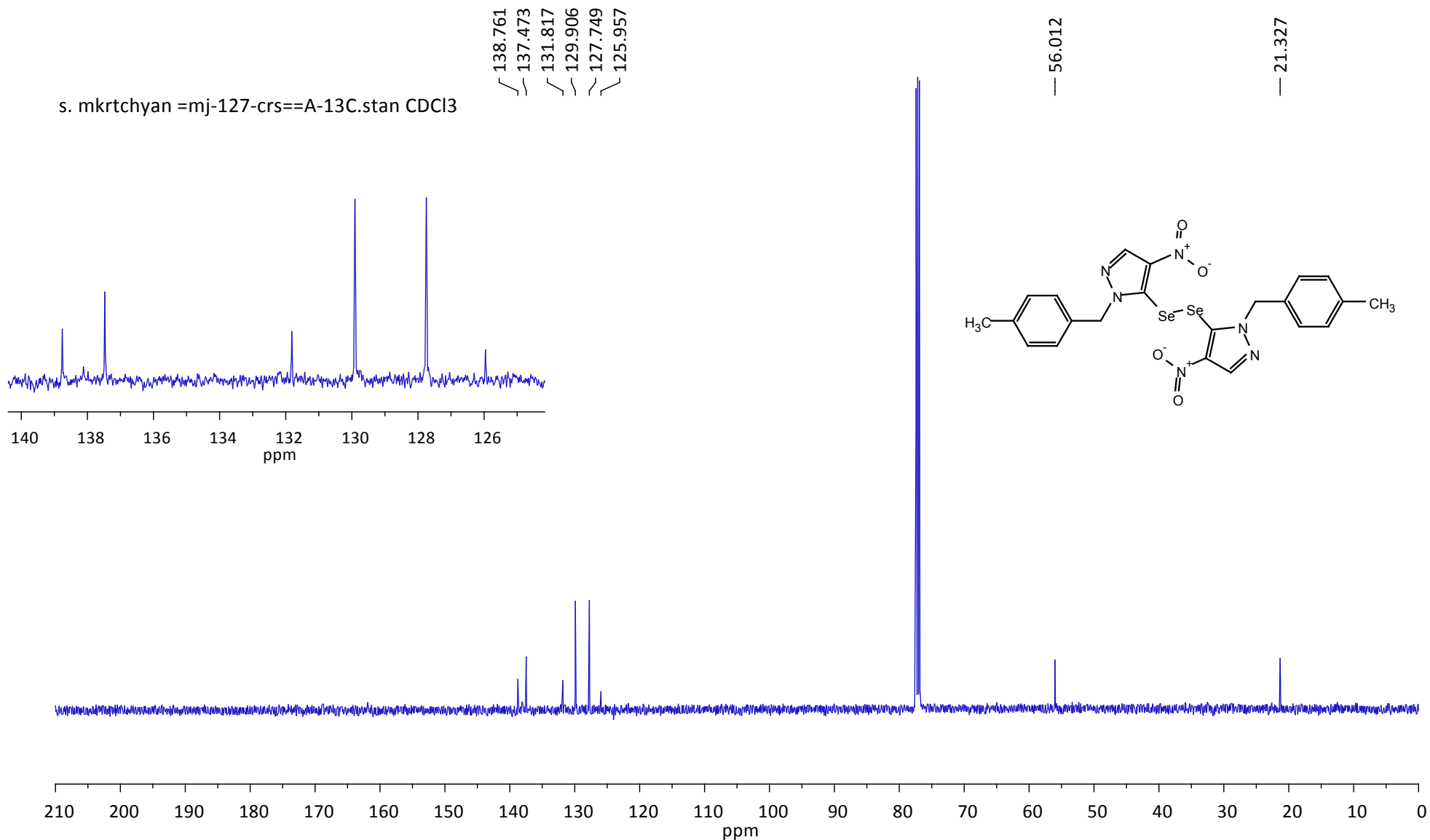
Comment s. mkrtchyan =mj-145-613=A-13C.stan CDCl₃
 Number of Scans 512
 Spectrometer Frequency 125.76
 Spectral Width 36057.7
 Spectral Size 65536

Compound **1by**



Comment s. mkrtyan =mj-127-crs==1H.stan CDCl3
 Number of Scans 24
 Spectrometer Frequency 500.13
 Spectral Width 12335.5
 Spectral Size 65536

Compound **1by**



Comment	s. mkrtchyan =mj-127-crs==A-13C.stan CDCl3
Number of Scans	512
Spectrometer Frequency	125.76
Spectral Width	36057.7
Spectral Size	65536

(D) X-ray single crystal analysis of compounds **1c**, **2f**, **5b**, **5d**, **5f**, **5i**, **5k** and **5m**.

CCDC 1922898-1922905 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/structures. Figures presenting molecular structures of all structurally determined compounds, tables containing crystals data and data refinement as well as details of X-ray diffraction experiments are given in SI file.

X-ray diffraction experimental details

Data for single crystals suitable for diffraction experiments of the compounds **1c**, **2f**, **5b**, **5d**, **5f**, **5i**, **5k** and **5m** were collected at room temperature on a Gemini A Ultra Diffractometer (Rigaku Oxford Diffraction) with mirror monochromated Mo/K α radiation ($\lambda = 0.71073 \text{ \AA}$). Data collection and data reduction were performed in the CrysAlisPro program [1]. The empirical absorption corrections using spherical harmonics implemented in multi-scan scaling algorithm were applied. To solve and refine the structure OLEX-2 version 1.2 [2] with incorporated SHELXT [3] (direct methods) and SHELXL (the full-matrix least-squares technique) programs [4] was used. All non-hydrogen atoms were refined with anisotropic temperature factors. The H-atoms were placed in calculated positions with fixed isotropic thermal parameters ($U_{\text{iso}}(\text{H}) = 1.2 \times [U_{\text{eq}}(\text{C})]$ or $1.5 \times [U_{\text{eq}}(\text{C})]$ for aromatic or aliphatic carbon atoms, respectively). In **1c** symptoms of disorder were detected. For the most influenced fragments i.e. seleno atom and nitro groups, two positions were considered with free occupancy factors that equalled to 0.79(2) for the major component at the final stage of the refinement. In **5d** the -CF₃ group showed rotational disorder and the final model contains two most probable position of the group with s.o.f. for major component refined to 0.624(14). Crystal data for the investigated compounds are collected in Tables S1a and S1b.

¹ CrysAlisPro 1.171.38.46, Rigaku Oxford Diffraction, 2015.

² O.V.Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, J. Appl. Cryst. 2009, **42**, 339-341. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. <http://dx.doi.org/10.1107/S0021889808042726>

³ G. M. Sheldrick, Acta Cryst. 2015, A71, 3–8. SHELXT - Integrated space-group and crystal-structure determination. <https://doi.org/10.1107/S2053273314026370>

⁴ G. M. Sheldrick, Acta Cryst. 2015, C71, 3–8. Crystal structure refinement with SHELXL. <https://doi.org/10.1107/S2053229614024218>

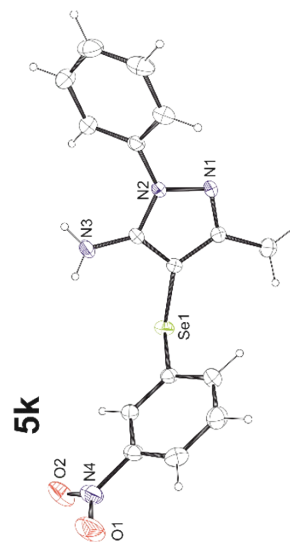
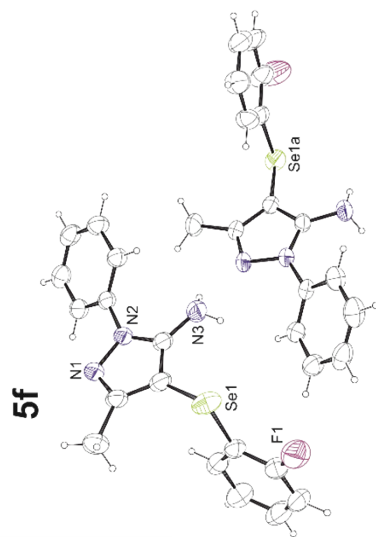
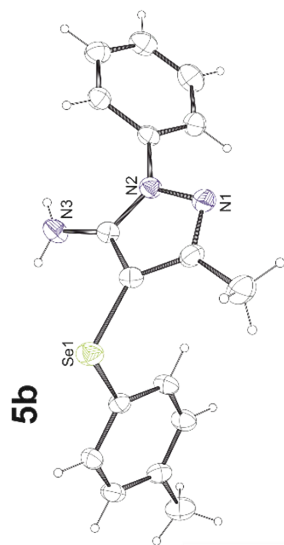
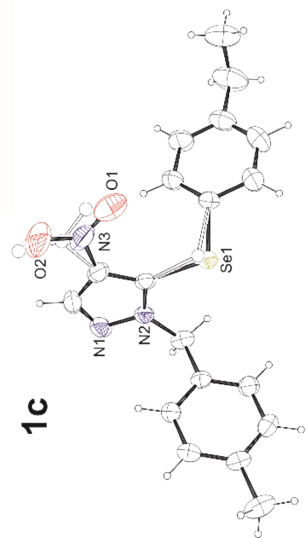
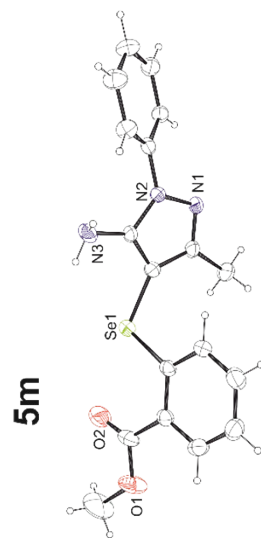
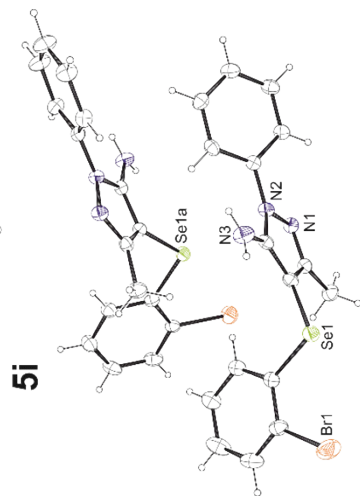
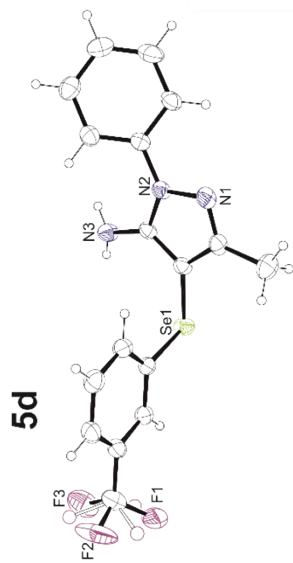
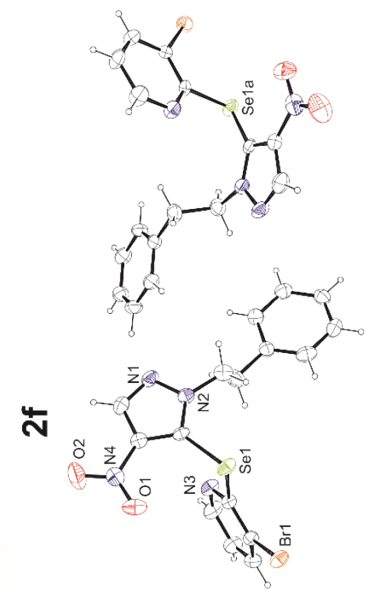


Figure 1. Ortep⁵ drawings of molecular structures. The thermal ellipsoids are drawn with 30% probability. Only the labels for atoms heavier than carbon atom are given. In the cases where two crystallographically molecules were found the labels of the second molecule correspond to the first one and are given with suffix “a”. Minor components of disordered groups are depicted with spheres of arbitrary radius.

Table S1a. Crystal data and data refinement for **1c**, **2f**, **5b** and **5d**

Compound	1c	2f	5b	5d
CCDC number	1922899	1922903	1922898	1922905
Empirical formula	C ₁₉ H ₁₉ N ₃ O ₂ Se	C ₁₆ H ₁₃ BrN ₄ O ₂ Se	C ₁₇ H ₁₇ N ₃ Se	C ₁₇ H ₁₄ F ₃ N ₃ Se
Formula weight	400.33	452.17	342.29	396.27
Temperature/K	293(2)	293(2)	293(2)	293(2)
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> /Å	4.8207(3)	7.8948(5)	12.5515(5)	5.7537(2)
<i>b</i> /Å	36.9783(15)	7.9369(6)	5.93199(19)	23.2453(8)
<i>c</i> /Å	10.4021(6)	31.3002(16)	21.5896(11)	12.4112(5)
α /°	90	83.404(5)	90	90
β /°	95.860(6)	89.627(5)	101.138(4)	90.937(4)
γ /°	90	60.612(7)	90	90
Volume/Å ³	1844.63(17)	1694.8(2)	1577.19(11)	1659.73(10)
<i>Z</i>	4	4	4	4
ρ_{calc} g/cm ³	1.442	1.772	1.442	1.586
μ /mm ⁻¹	2.052	4.590	2.378	2.296
<i>F</i> (000)	816.0	888.0	696.0	792.0
Crystal size/mm ³	0.35 × 0.08 × 0.05	0.5 × 0.3 × 0.3	0.7 × 0.4 × 0.2	0.8 × 0.2 × 0.2
Radiation	MoK α (λ = 0.71073 Å)			
2 θ range for data collection/°	6.612 to 62.856	6.562 to 62.636	6.616 to 54.994	6.566 to 50.992
Index ranges	-6 ≤ <i>h</i> ≤ 7, -53 ≤ <i>k</i> ≤ 49, -14 ≤ <i>l</i> ≤ 14	-11 ≤ <i>h</i> ≤ 10, -11 ≤ <i>k</i> ≤ 11, -44 ≤ <i>l</i> ≤ 45	-15 ≤ <i>h</i> ≤ 16, -7 ≤ <i>k</i> ≤ 7, -27 ≤ <i>l</i> ≤ 24	-6 ≤ <i>h</i> ≤ 6, -26 ≤ <i>k</i> ≤ 28, -15 ≤ <i>l</i> ≤ 15
Reflections collected	25566	24857	14178	9856
Independent reflections	5610 [<i>R</i> _{int} = 0.0730]	9838 [<i>R</i> _{int} = 0.0689]	3579 [<i>R</i> _{int} = 0.0392]	3036 [<i>R</i> _{int} = 0.0249]
Data/restraints/parameters	5610/21/266	9838/0/433	3579/2/200	3036/103/254
Goodness-of-fit on <i>F</i> ²	1.001	1.006	1.020	1.030
Final <i>R</i> indexes [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0516, <i>wR</i> ₂ = 0.0916	<i>R</i> ₁ = 0.0604, <i>wR</i> ₂ = 0.0631	<i>R</i> ₁ = 0.0365, <i>wR</i> ₂ = 0.0731	<i>R</i> ₁ = 0.0304, <i>wR</i> ₂ = 0.0670
Final <i>R</i> indexes	<i>R</i> ₁ = 0.1563, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.1642, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.0596, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.0408, <i>wR</i> ₂ =

⁵ L. J. Farrugia, J. Appl. Cryst. 2012, 45, 849–854. WinGX and ORTEP for Windows: an update. <https://doi.org/10.1107/S0021889812029111>.

[all data]	0.1215	0.0860	0.0819	0.0711
Largest diff. peak/hole / e Å ⁻³	0.28/-0.20	0.68/-0.56	0.37/-0.26	0.39/-0.38

Table S1a. Crystal data and data refinement for **5f**, **5i**, **5k** and **5m**

Compound	5f	5i	5k	5m
CCDC number	1922901	1922902	1922900	1922904
Empirical formula	C ₁₆ H ₁₄ FN ₃ Se	C ₁₆ H ₁₄ BrN ₃ Se	C ₁₆ H ₁₄ N ₄ O ₂ Se	C ₁₈ H ₁₇ N ₃ O ₂ Se
Formula weight	346.26	407.17	373.27	386.30
Temperature/K	293(2)	293(2)	293(2)	293(2)
Crystal system	triclinic	monoclinic	monoclinic	orthorhombic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>	<i>Pbca</i>
<i>a</i> /Å	10.7344(4)	9.4439(4)	8.0441(3)	12.6478(10)
<i>b</i> /Å	11.4734(4)	26.1410(11)	16.3997(6)	10.1017(8)
<i>c</i> /Å	13.5667(5)	12.8829(4)	12.5446(5)	26.833(3)
α /°	92.850(3)	90	90	90
β /°	109.342(3)	91.719(3)	106.994(4)	90
γ /°	97.713(3)	90	90	90
Volume/Å ³	1554.36(10)	3179.0(2)	1582.61(10)	3428.2(5)
Z	4	8	4	8
ρ_{calc} g/cm ³	1.480	1.701	1.567	1.497
μ /mm ⁻¹	2.422	4.872	2.387	2.206
F(000)	696.0	1600.0	752.0	1568.0
Crystal size/mm ³	0.42 × 0.36 × 0.28	0.4 × 0.1 × 0.1	0.8 × 0.6 × 0.4	0.28 × 0.26 × 0.08
Radiation	MoK α (λ = 0.71073 Å)			
2 θ range for data collection/°	7.02 to 53.994	6.518 to 52.998	6.792 to 56.484	6.442 to 62.878
Index ranges	-13 ≤ <i>h</i> ≤ 13, -14 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 17	-11 ≤ <i>h</i> ≤ 11, -32 ≤ <i>k</i> ≤ 32, -16 ≤ <i>l</i> ≤ 16	-10 ≤ <i>h</i> ≤ 10, -21 ≤ <i>k</i> ≤ 21, -16 ≤ <i>l</i> ≤ 16	-17 ≤ <i>h</i> ≤ 17, -9 ≤ <i>k</i> ≤ 14, -28 ≤ <i>l</i> ≤ 36
Reflections collected	35398	33276	29384	24626
Independent reflections	6775 [<i>R</i> _{int} = 0.0432]	6587 [<i>R</i> _{int} = 0.0735]	3906 [<i>R</i> _{int} = 0.0377]	5243 [<i>R</i> _{int} = 0.1042]
Data/restraints/ parameters	6775/4/397	6587/4/397	3906/2/217	5243/0/220
Goodness-of-fit on <i>F</i> ²	1.014	1.020	1.059	0.982
Final <i>R</i> indexes [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0407, <i>wR</i> ₂ = 0.0773	<i>R</i> ₁ = 0.0403, <i>wR</i> ₂ = 0.0647	<i>R</i> ₁ = 0.0262, <i>wR</i> ₂ = 0.0636	<i>R</i> ₁ = 0.0537, <i>wR</i> ₂ = 0.0992
Final <i>R</i> indexes	<i>R</i> ₁ = 0.0830, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.0859, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.0336, <i>wR</i> ₂ =	<i>R</i> ₁ = 0.1656, <i>wR</i> ₂ =

[all data]	0.0932	0.0772	= 0.0669	0.1373
Largest diff. peak/hole / e Å ⁻³	0.59/-0.51	0.42/-0.61	0.26/-0.32	0.65/-0.71