Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Metal-Free, Room Temperature, Acid-$K_2S_2O_8$ Mediated Method for the Nitration of Olefins: An Easy Approach for the Synthesis of Nitroolefins

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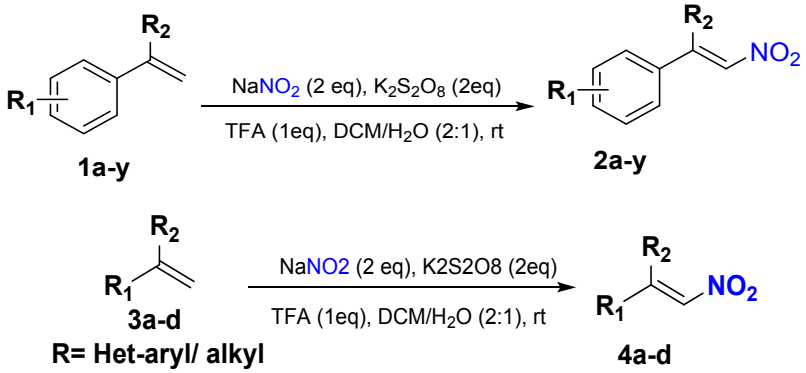
Materials and Methods

All reactions were performed under air atmosphere. Analytical thin layer chromatography was performed using TLC pre-coated silica gel 60 F_{254} (20 x 20 cm). TLC plates were visualized by exposing UV light or by iodine vapors or immersion in an acidic staining solution of p-anisaldehyde followed by heating on a hot plate. Organic solvents were concentrated by rotary evaporation. Column chromatography was performed on flash silica gel of 230-400 mesh size. Melting points were recorded on BUCHI Melting Point B-545 instrument and were uncorrected. ^{1}H NMR spectra were recorded with 400 and 500 MHz NMR instruments. Chemical data for protons are reported in parts per million (ppm, scale) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$: δ 7.26 or other solvents as mentioned). Mass spectra were recorded with LCMS-QTOF instrument. The coupling constant (J) are mentioned in Hz.

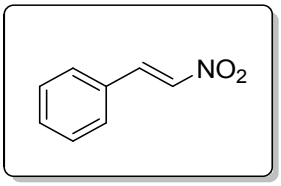
General Experimental Procedure for the Synthesis of Compounds in Table 2 and Table 3:

Styrene/alkene (1 mmol), $NaNO_2$ (2 mmol), $K_2S_2O_8$ (2 mmol) and TFA (1 mmol) in 4.5 ml of DCM/water (2:1) were stirred in open atmosphere at room temperature for 6 h. After completion of the reaction (reaction monitored by TLC) compound was extracted with DCM. The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude products were purified on a silica gel column using hexane/EtOAc to get the pure product and characterized by NMR and GC-MS.



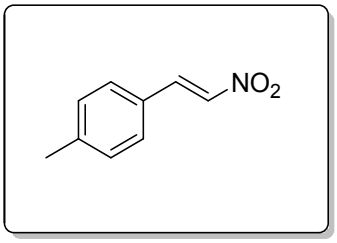
Characterization Data of Products

(*E*)-(2-Nitrovinyl)benzene (2a)



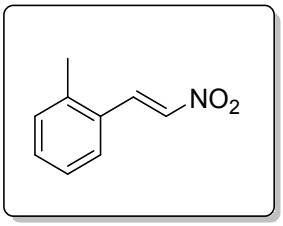
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 57-58 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-7.98 (d, J = 13.7 Hz, 1H), 7.61-7.57 (d, J = 13.7 Hz, 1H), 7.56–7.53 (m, 2H), 7.50-7.43 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.17, 137.11, 132.23, 130.06, 129.44, 129.21; GC-MS (m/z): 149.1 $[M]^+$.

***(E)*-1-Methyl-4-(2-nitrovinyl)benzene (2b)**



Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 221-223 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.94 (d, J = 13.6 Hz, 1H), 7.57-7.54 (d, J = 13.6 Hz, 1H), 7.44-7.42 (d, J = 8 Hz, 2H), 7.26-7.24 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.18 (1C), 139.20 (1C), 136.31 (1C), 130.19 (2C), 129.26 (2C), 127.32 (1C), 21.68 (1C) ; GC-MS (m/z): 163.10 $[M]^+$.

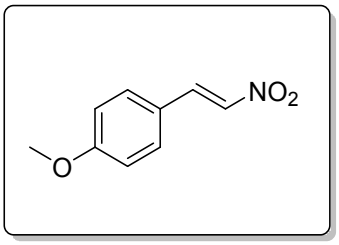
(*E*)-1-Methyl-2-(2-nitrovinyl)benzene (2c)



Light yellow liquid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30-8.27 (d, J = 13.6 Hz, 1H), 7.51–7.46 (m, 2H), 7.38-7.28 (m, 1H), 7.26-7.23 (m, 2H), 2.47

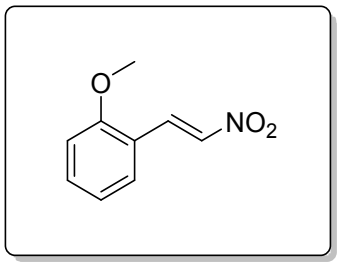
(s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.28, 137.60, 136.78, 132.00, 131.41, 128.92, 127.38, 126.80, 19.94; GC-MS (m/z): 163.10 $[M]^+$.

(*E*)-1-Methoxy-4-(2-nitrovinyl)benzene (2d)



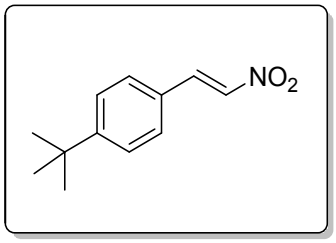
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 87-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.96 (d, J = 13.6 Hz, 1H), 7.54-7.50 (m, 3H), 6.97-6.95 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.97, 139.14, 135.01, 131.24, 122.54, 114.94, 55.58; GC-MS (m/z): 179.1 $[M]^+$.

(*E*)-1-Methoxy-2-(2-nitrovinyl)benzene (2e)



Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 84 - 86 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–8.11 (d, J = 13.6 Hz, 1H), 7.89–7.87 (d, J = 13.6 Hz, 1H), 7.48–7.43 (m, 2H), 7.04–6.97 (m, 2H), 3.95 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.53, 138.25, 135.60, 133.54, 132.56, 121.13, 119.09, 111.38, 55.67; GC-MS (m/z): 179.1 $[M]^+$.

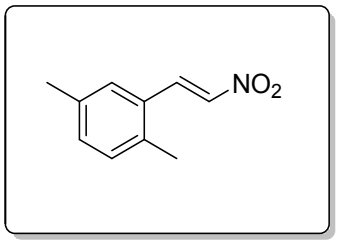
(*E*)-1-(Tert-butyl)-4-(2-nitrovinyl)benzene (2f)



Light yellow liquid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02–7.99 (d, J = 13.7 Hz, 1H), 7.61-7.58 (d, J = 13.7 Hz, 1H), 7.51–7.49 (d, J = 8.9 Hz, 2 H),

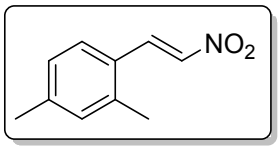
7.49-7.47 (d, J = 8.9 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.21, 139.15, 136.42, 129.16, 127.26, 126.48, 35.19, 31.07; GC-MS (m/z): 205.1 $[M]^+$.

(*E*)-1,4-Dimethyl-2-(2-nitrovinyl)benzene (2g)



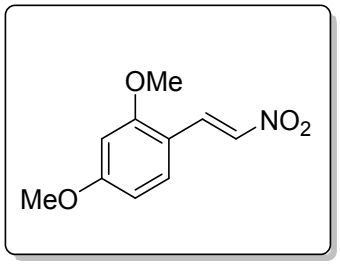
Light yellow liquid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29-8.26 (d, J = 13.6 Hz, 1H), 7.52-7.49 (d, J = 13.6 Hz, 1H), 7.32 (s, 1H), 7.21-7.15 (m, 2H), 2.43 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.39, 136.93, 136.31 (d, J = 5.2 Hz), 132.88, 131.29, 128.71, 127.82, 20.85, 19.42; GC-MS (m/z): 177.07 $[M]^+$.

(*E*)-2,4-dimethyl-1-(2-nitrovinyl)benzene (2h)



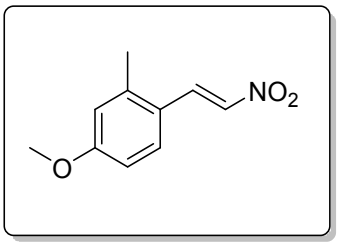
Light yellow solid; TLC (EtOAc:Hexane 1:9): R_f = 0.30; pale yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.19 (d, J = 13.6 Hz, 1H), 7.45-7.41 (d, J = 13.6 Hz, 1H), 7.36-7.34(d, J = 8 Hz, 1H), 7.03-6.98 (t, J = 8.4 Hz, 2H), 2.38 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.84 (1C), 139.36 (1C), 136.85 (1C), 136.74 (1C), 132.22 (1C), 127.64 (1C), 127.41 (1C), 126.06 (1C), 21.55 (1C), 19.90 (1C); GC-MS (m/z): 177.1$[M]^+$.

(*E*)-2,4-Dimethoxy-1-(2-nitrovinyl)benzene (2i)



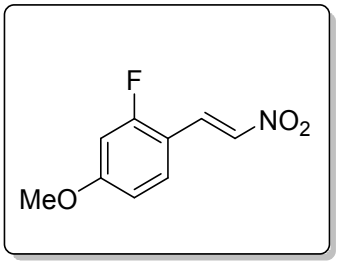
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 106-108 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.10-8.07 (d, J = 13.5 Hz, 1H), 7.84–7.81 (d, J = 13.5 Hz, 1H), 7.39–7.37 (d, J = 8.6 Hz, 1H), 6.57–6.54 (dd, J = 8.6, 2.3 Hz, 1H), 6.49–6.48 (d, J = 2.1 Hz, 1H), 3.93 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 161.2, 136.0, 135.7, 134.3, 112.4, 105.9, 98.6, 55.6; GC-MS (m/z): 209.1 $[M]^+$.

(*E*)-4-Methoxy-2-methyl-1-(2-nitrovinyl)benzene (2j)



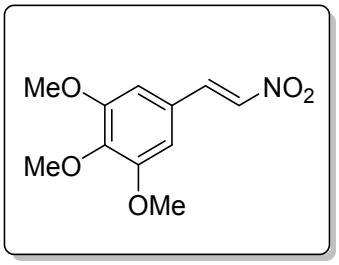
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 221-223 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.28–8.24 (d, J = 13.5 Hz, 1H), 7.51-7.46 (m, 2H), 6.79 (m, 2H), 3.85 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.66, 141.89, 136.64, 135.40, 129.39, 121.38, 116.48, 112.75, 55.46, 20.32; GCMS (m/z): 193.2 $[M]^+$.

(*E*)-2-Fluoro-4-methoxy-1-(2-nitrovinyl)benzene (2k)



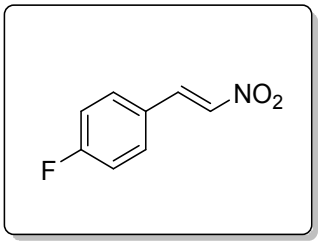
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 221-223 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.03–8.00 (d, J = 13.7 Hz, 1H), 7.68–7.64 (d, J = 13.7 Hz, 1H), 7.45–7.41 (t, J = 8.5 Hz, 1H), 6.80–6.77 (dd, J = 8.7, 2.4 Hz, 1H), 6.73–6.69 (dd, J = 12.6, 2.4 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.30-164.25 (d, J = 6.3 Hz), 164.20-162.21 (d, J = 250.74 Hz), 137.10-137.01 (d, J = 11.34 Hz), 132.84, 132.53-132.50 (d, J = 3.78 Hz), 111.41, 110.93-110.83 (d, J = 12.6 Hz), 102.57-102.37 (d, J = 25.2 Hz), 55.99; GC-MS (m/z): 197.1 $[M]^+$.

(*E*)-1,2,3-Trimethoxy-5-(2-nitrovinyl)benzene (2l)



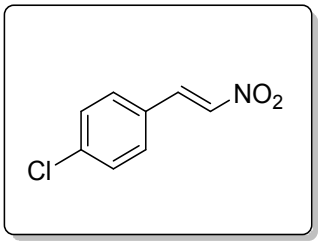
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 120-123 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.95–7.92 (d, *J* = 13.6 Hz, 1H), 7.57–7.54 (d, *J* = 13.6 Hz, 1H), 6.77 (s, 2H), 3.91 (d, *J* = 4.6 Hz, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.70, 141.82, 139.30, 136.38, 125.30, 106.51, 61.04, 56.29; GCMS (m/z): 239.1 $[M]^+$.

(*E*)-1-Fluoro-4-(2-nitrovinyl)benzene (2m)



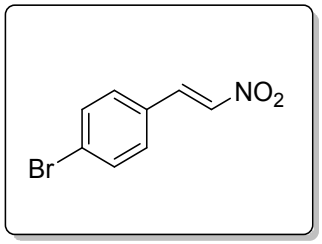
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 98-100 °C; ^1H NMR (400 MHz, $CDCl_3$) *δ* 8.09-7.97 (d, *J* = 13.7 Hz, 1H), 7.59–7.54 (m, 3H), 7.18-7.14 (d, *J* = 8.5 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -105.76 (qd, *J* = 8.3, 5.3 Hz); ^{13}C NMR (126 MHz, $CDCl_3$) *δ* 165.96-163.94 (d, *J*= 254.52), 137.95, 136.85, 131.41–131.34 (d, *J* = 8.82 Hz), 126.33, 116.89; GC-MS (m/z): 167.1 $[M]^+$.

(*E*)-1-Chloro-4-(2-nitrovinyl)benzene (2n)



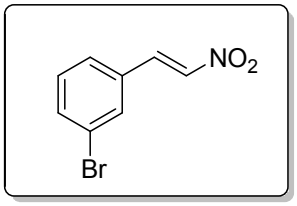
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 112-114 °C; ^1H NMR (400 MHz, $CDCl_3$) *δ* 7.99-7.95 (d, *J* = 13.7 Hz, 1H), 7.58-7.55 (d, *J* = 13.7 Hz, 1H), 7.51-7.49 (d, *J* = 8.5 Hz, 2H), 7.45-7.43 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 128.65, 129.87, 130.42, 137.53, 137.85, 138.43, 77.51, 77.20, 76.88; GC-MS (m/z): 183.1 $[M]^+$.

(*E*)-1-Bromo-4-(2-nitrovinyl)benzene (2o)



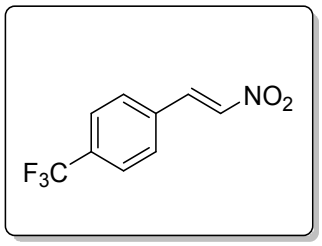
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 141-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.86 (d, J = 13.7 Hz, 1H), 7.54–7.49 (m, 3H), 7.36–7.33 (d, J = 8.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.86, 137.47, 132.78, 130.44, 128.94, 126.84; GC-MS (m/z): 226.9 $[M]^+$.

(*E*)-1-Bromo-3-(2-nitrovinyl)benzene (2p)



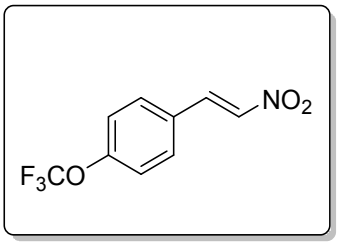
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 59-61 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 13.7 Hz, 1H), 7.70 (s, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 13.7 Hz, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.34 (t, J = 7.9 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.07, 137.43, 134.92, 132.07, 131.71, 130.91, 127.72, 123.45; GC-MS (m/z): 228.9 $[M]^+$.

(*E*)-1-(2-Nitrovinyl)-4-(trifluoromethyl)benzene (2q)



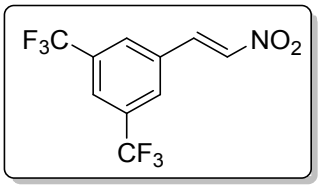
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 90-92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.01 (d, J = 13.7 Hz, 1H), 7.74-7.72 (d, J = 8.4 Hz, 2H), 7.70-7.68 (d, J = 8.4 Hz, 2H), 7.66-7.62 (d, J = 13.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.86, 137.20, 133.78-132.99 (q, J = 32.76, 30.24 Hz), 129.32, 126.31- 126.31 (q, J = 16.38, 3.78 Hz), 124.59, 122.43; GC-MS (m/z): 217.1 $[M]^+$.

(*E*)-1-(2-Nitrovinyl)-4-(trifluoromethoxy)benzene (2r)



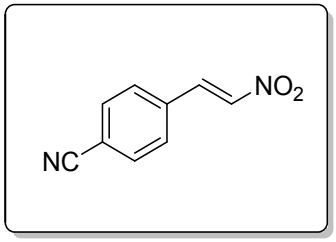
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 221-223 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.02-7.98 (d, J = 13.7 Hz, 1H), 7.62-7.60 (d, J = 8.7 Hz, 2H), 7.59-7.56 (d, J = 13.7 Hz, 1H), 7.32-7.30 (d, J = 8.7 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.72; ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.71-151.70(d, J = 1.01 Hz), 137.68, 137.33, 130.75, 128.56, 121.45, 119.00; GC-MS (m/z): 233.1 $[M]^+$.

(*E*)-1-(2-nitrovinyl)-3,5-bis(trifluoromethyl)benzene (2s)



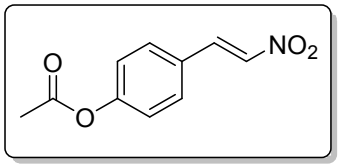
Pale yellow solid; TLC (EtOAc:Hexane 1:9): R_f = 0.30; mp 92-93°C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.08-8.05 (d, J = 14 Hz, 1H), 7.99 (s, 3H), 7.70-7.66 (d, J = 13.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.81 (s, 1C), 135.46 (s, 1C), 133.49-132.72(q, J= 30.24, 64.26Hz. 1C), 132.25 (s, 1C), 128.64-128.61 (d, J= 3.78Hz 1C), 125.17-125.06 (m, 1C), 123.75 (s, 1C), 121.58 (s, 1C); GC-MS (m/z): 285.0$[M]^+$.

(*E*)-4-(2-Nitrovinyl)benzonitrile (2t)



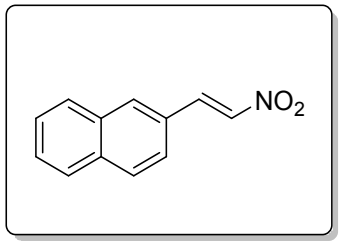
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 183-186 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 13.8 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 13.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.48, 136.67, 134.38, 133.06, 129.47, 117.89, 115.18; GC-MS (m/z): 174.1 $[M]^+$.

(*E*)-4-(2-nitrovinyl)phenyl acetate (2u)



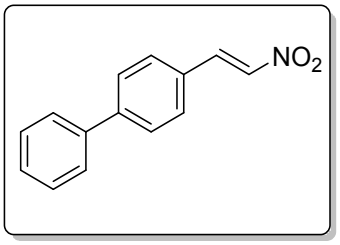
White solid; TLC (EtOAc:Hexane 1:9): R_f = 0.30; mp 176-178^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8 Hz, 1H), 7.59 (dd, *J* = 12, 12 Hz, 3H), 7.22 (d, *J* = 8 Hz, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.87 (1C), 153.54 (1C), 138.00 (1C), 137.17 (1C), 130.42 (2C), 127.69(1C), 122.78 (2C), 21.14(1C); GC-MS (m/z): 207.0$[M]^+$.

(*E*)-2-(2-Nitrovinyl)naphthalene (2v)



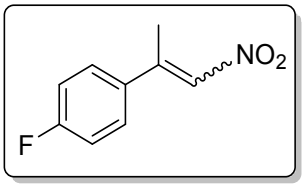
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 128-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.16-8.13 (d, *J* = 13.6 Hz, 1H), 8.00 (s, 1H), 7.90 –7.85 (m, 3H), 7.70-7.67 (d, *J* = 13.6 Hz, 1H), 7.61–7.54 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) *δ* 139.33, 137.13, 134.93, 133.15, 132.41, 129.40, 128.88, 128.45, 127.99, 127.54, 127.33, 123.32; GC-MS (m/z): 199.1 $[M]^+$.

(*E*)-4-(2-nitrovinyl)-1,1'-biphenyl (2w)



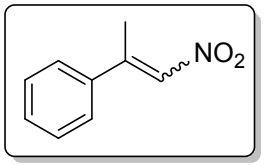
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.40; mp 190-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.44 (m, 5H), 7.41-7.38 (m, 2H), 7.30 –7.28 (m, 2H), 7.24-7.23 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.59, 137.10, 135.56, 134.41, 130.97, 129.37, 128.97, 128.93, 128.84, 128.55;.

(*E/Z*)-1-fluoro-4-(1-nitroprop-1-en-2-yl)benzene (2x)



Yellow oil; TLC (EtOAc:Hexane 1:9): R_f = 0.30; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 2H), 7.22-7.21 (d, *J* = 1.2 Hz, 1H), 7.10 – 7.04 (m, 2H), 2.57-2.56 (d, *J* = 1.4 Hz, 3H); ^{13}C NMR (126 MHz, CDCl3) δ 165.23 (1C), 163.16 (1C), 148.88 (1C), 136.29 (1C), 134.28 (1C), 128.91-128.84 (d, *J* = 8.75 Hz, 1C), 116.33 (1C), 116.15 (1C), 18.68 (1C).

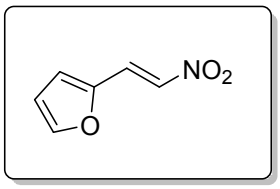
(*E/Z*)-(1-nitroprop-1-en-2-yl)benzene (2y)



Light yellow liquid; TLC (EtOAc:Hexane 1:9): R_f = 0.30; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (s, 5H), 7.24-7.23 (dd, *J* = 2.7,1.3 Hz, 1H), 2.579-2.575 (d, *J* = 1.6 Hz, 3H). ^{13}C NMR (101

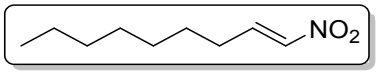
M(1C)Hz, $CDCl_3$) δ 149.94 (1C), 138.35, 136.38 (1C), 130.38 (1C), 129.06 (2C), 126.86 (2C), 18.60(1C); GC-MS (m/z): 163.1$[M]^+$

(*E*)-2-(2-Nitrovinyl)furan (4a)



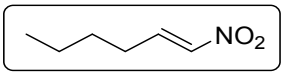
Light yellow solid; TLC (EtOAc:Hexane 2:8): R_f = 0.20; mp 77-79 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.80-7.77 (d, J = 13.2 Hz, 1H), 7.61 (s, 1H), 7.54-7.52 (d, J = 13.2 Hz, 1H), 6.92-6.91 (d, J = 3.5 Hz, 1H), 6.60-6.59 (dd, J = 3.5, 1.8 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.93, 146.62, 134.84, 125.53, 120.19, 113.43; GC-MS (m/z): 139.1 $[M]^+$.

(*E*)-1-nitronon-1-ene (4b)



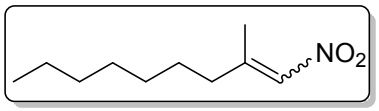
Yellow liquid; TLC (EtOAc:Hexane 1:9): R_f = 0.40; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 1H), 6.70-6.96 (dt, J = 13.4, 1.5 Hz, 1H), 2.29 – 2.23 (m, 2H), 1.55 – 1.47 (m, 2H), 1.34 – 1.28 (m, 9H), 0.90-0.86 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.83 (1C), 139.58 (1C), 31.65 (1C), 29.05 (1C), 28.92 (1C), 28.45 (1C), 27.74 (1C), 22.59 (1C), 14.03 (1C);

(*E*)-1-nitrohex-1-ene (4c)



Yellow liquid; TLC (EtOAc:Hexane 1:9): R_f = 0.40; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 1H), 6.99-6.96 (d, J = 13.2 Hz, 1H), 2.30 – 2.24 (m, 2H), 1.54 – 1.46 (m, 2H), 1.42 – 1.35 (m, 2H), 0.95-0.91 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.75 (1C), 139.58 (1C), 29.77 (1C), 28.10 (1C), 22.15 (1C), 13.63 (1C); ESI-MS (m/z) : 130.12$(M+H)^+$

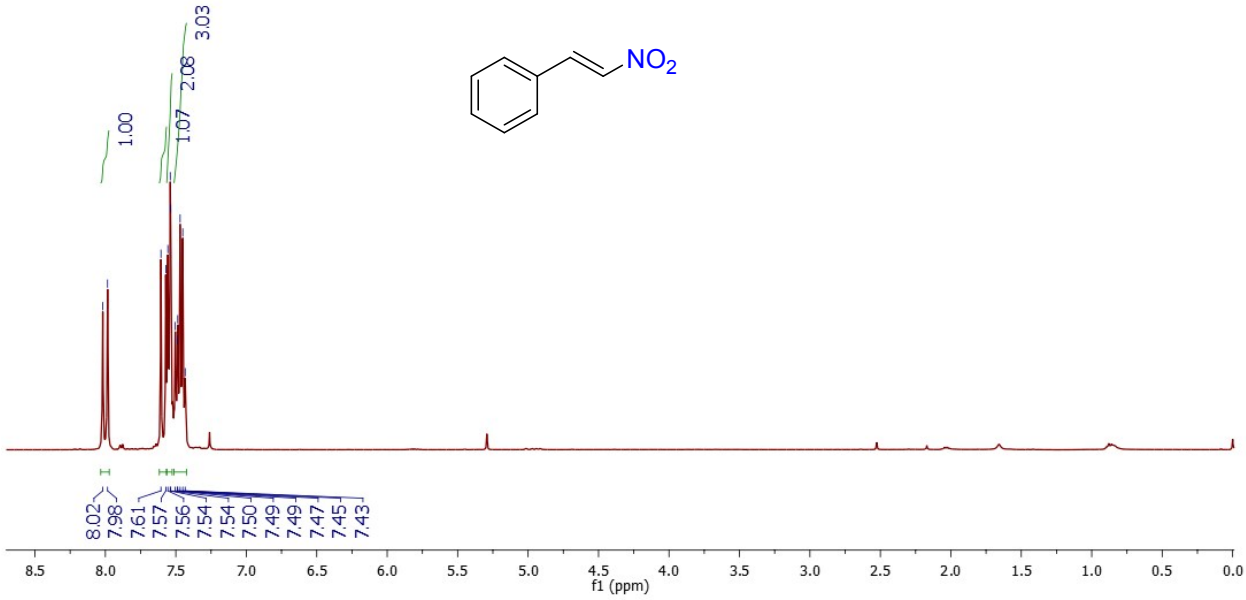
(*E/Z*)-2-methyl-1-nitronon-1-ene (4d)



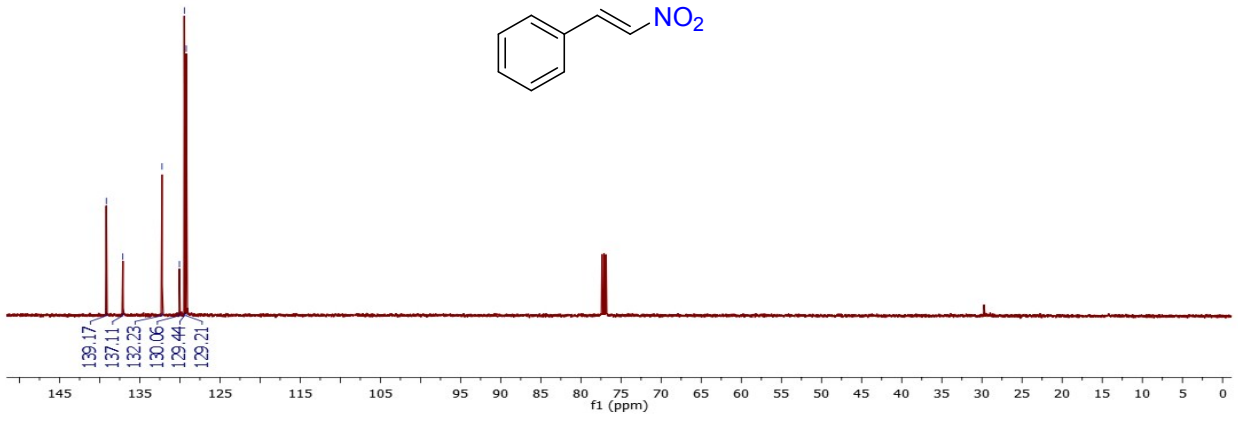
Yellow liquid; TLC (EtOAc:Hexane 1:15): R_f = 0.50; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.89 – 6.88 (m, 1H), 2.58-2.54 (t, *J* = 8 Hz, 1H), 2.17 – 2.16 (d, *J* = 1.2 Hz, 3H), 2.13-2.09 (m, 2H), 1.86 – 1.85 (d, *J* = 1.6 Hz, 1H), 1.48-1.41(m, 3H), 1.23-1.14(m, 12H), 0.83-0.80 (t, *J* = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.62 (1C), 135.16 (1C), 38.06 (1C), 31.66 (1C), 29.07 (1C), 28.97 (1C), 27.11 (1C), 22.59 (1C), 18.57 (1C), 14.06 (1C); HRMS (TOF MS ES-) : m/z 184.1332 calculated for $C_{10}H_{19}NO_2$ - H^+ (184.1338).

Spectras (^{1}H NMR, ^{13}C NMR, DEPT and GC-MS) of synthesized products

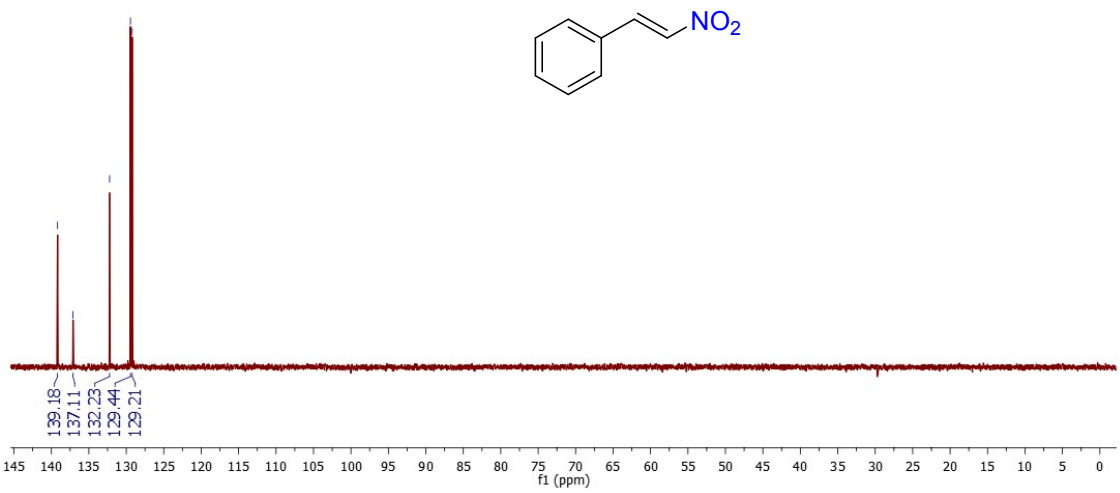
^{1}H NMR of (*E*)-(2-Nitrovinyl)benzene (2a)[1]



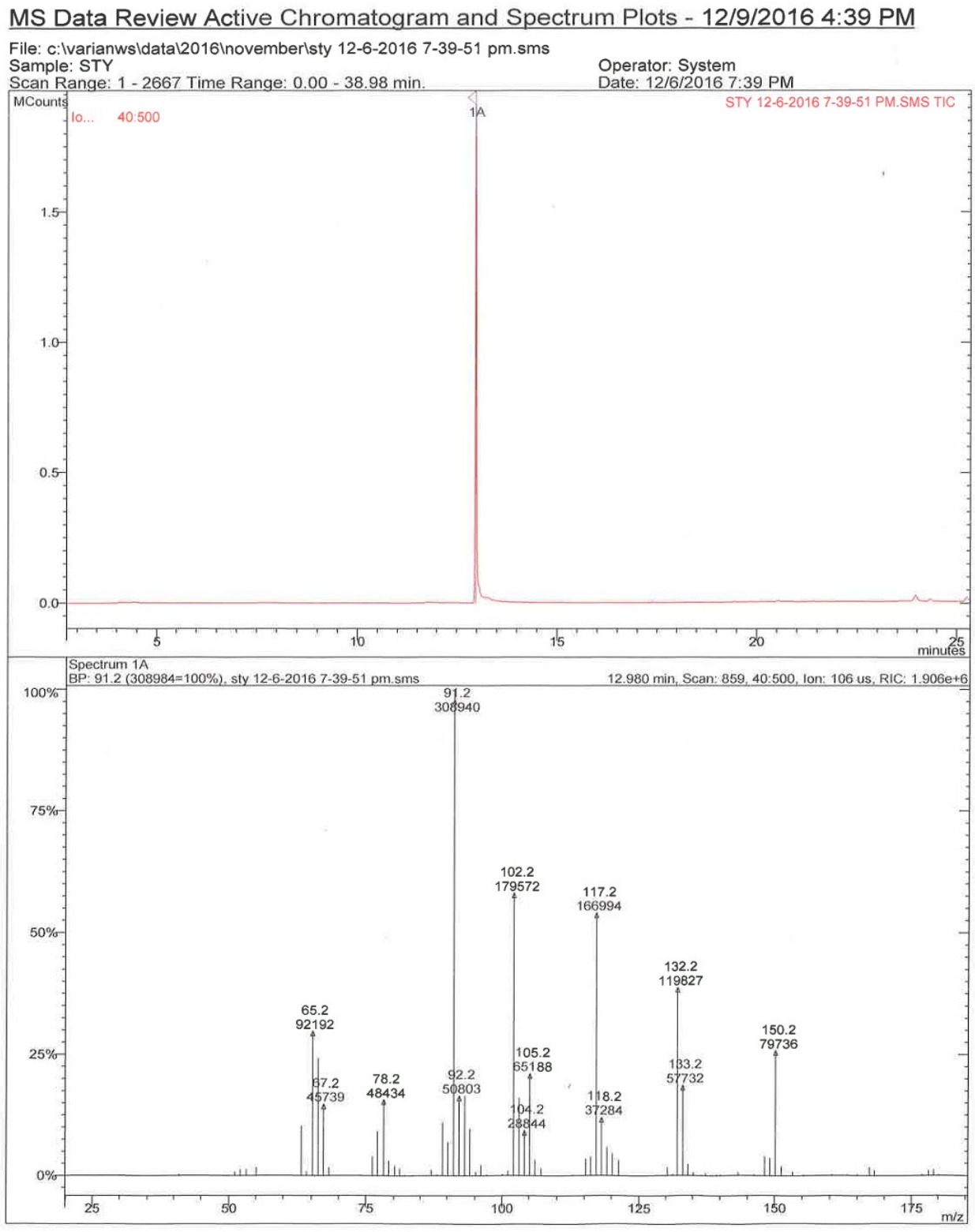
^{13}C NMR of (*E*)-(2-Nitrovinyl)benzene (2a)



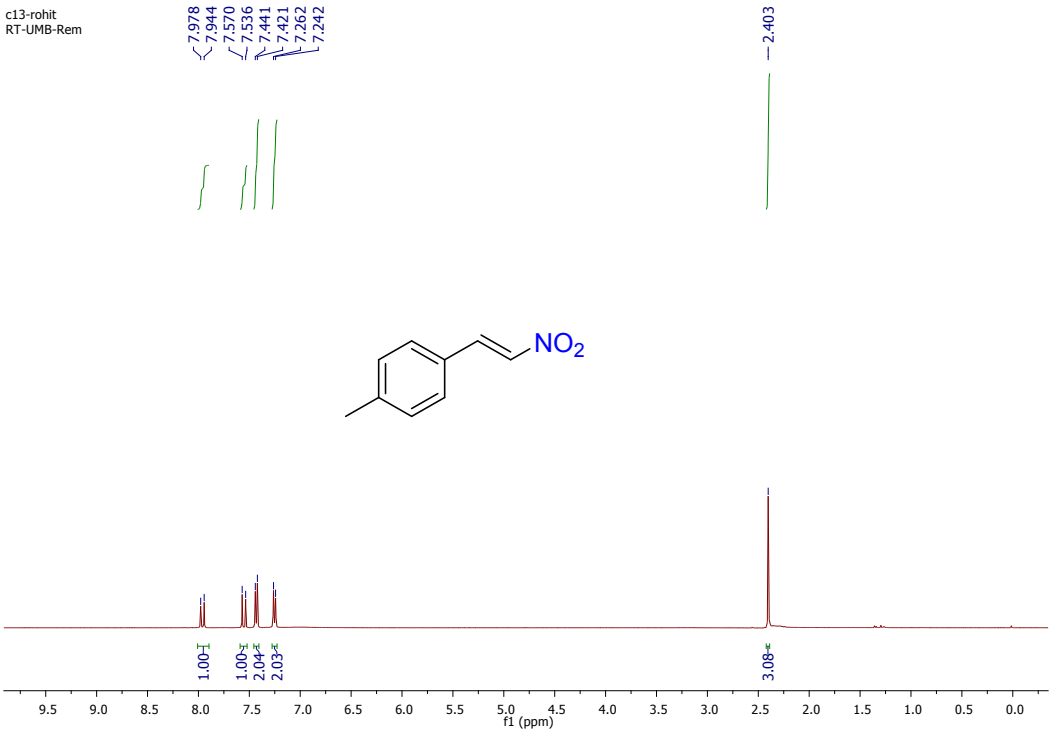
DEPT of (*E*)-(2-Nitrovinyl)benzene (2a)



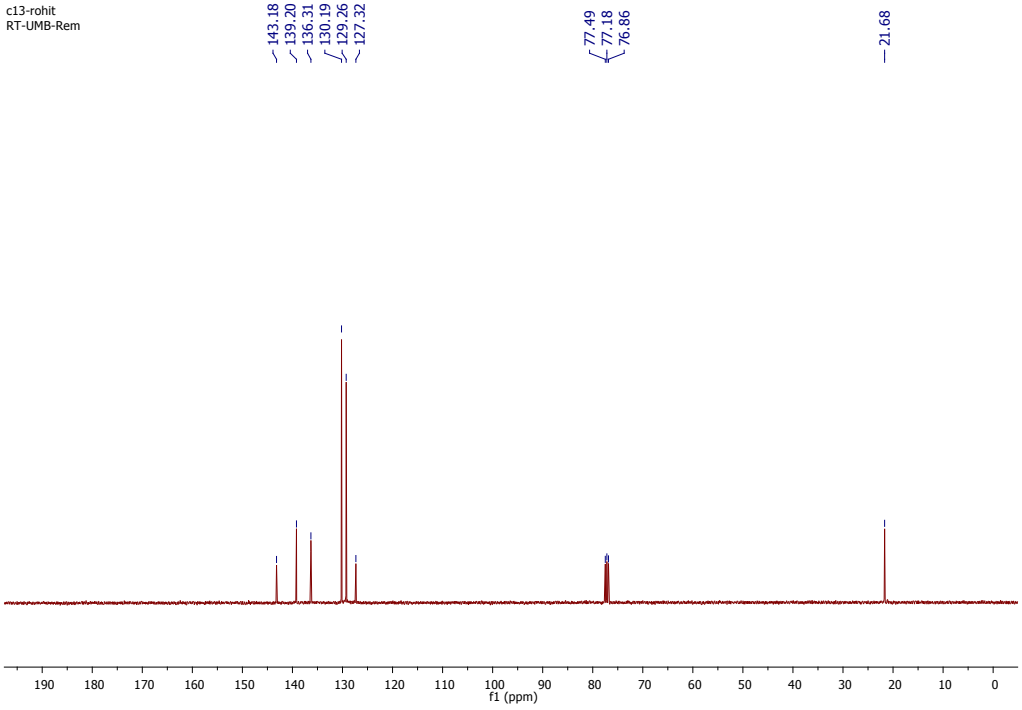
GC-MS of (*E*)-(2-Nitrovinyl)benzene (2a)



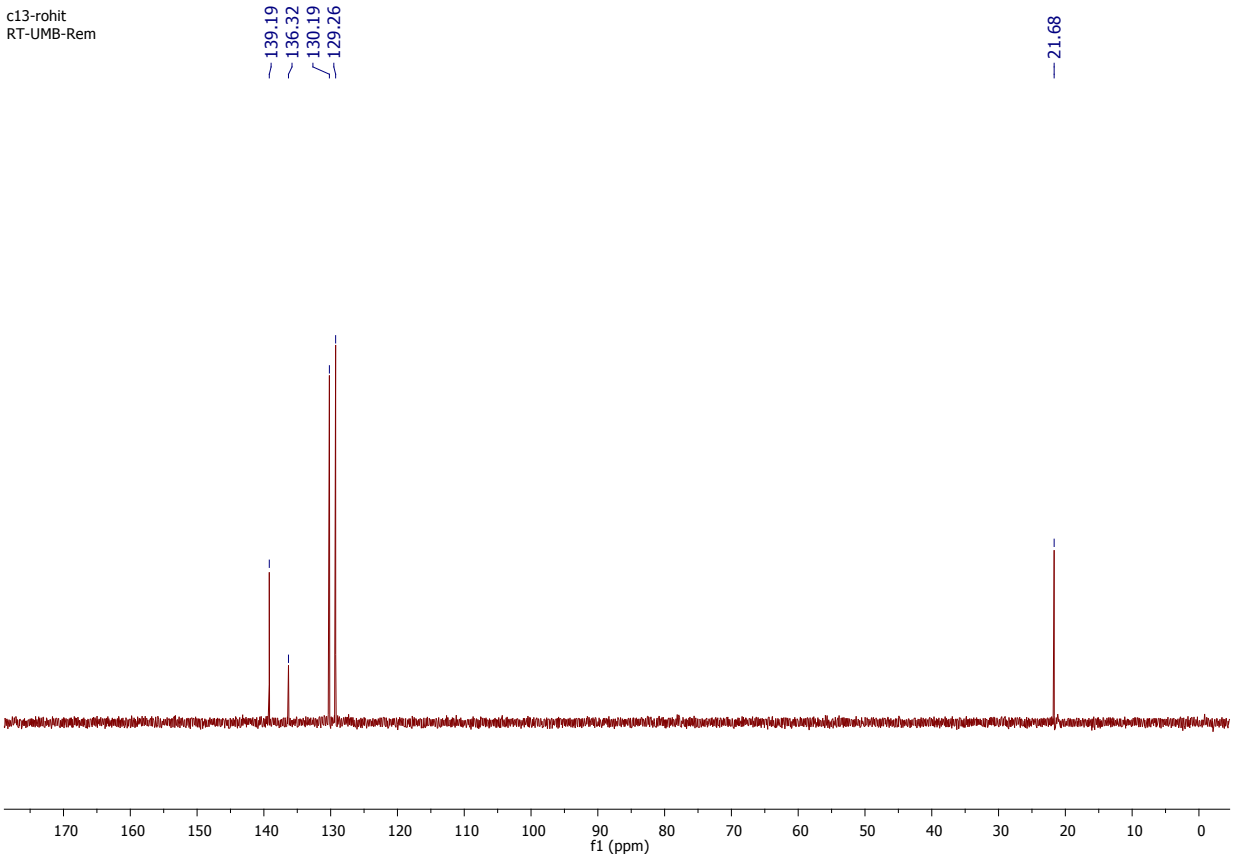
^{1}H NMR of (*E*)-4-Methyl-2-(2-nitrovinyl)benzene (2b)[1]



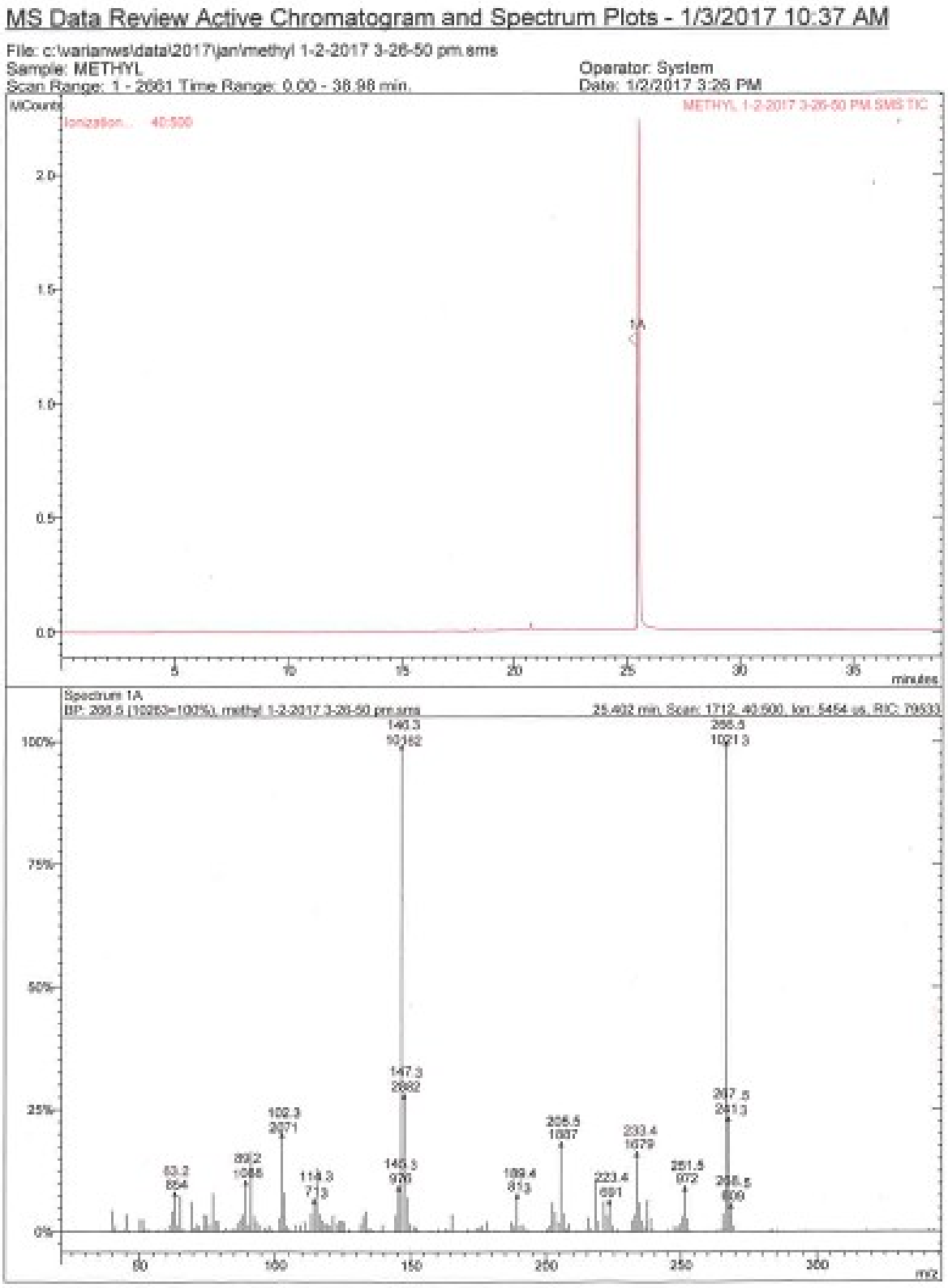
^{13}C NMR of (*E*)-4-Methyl-2-(2-nitrovinyl)benzene (2b)



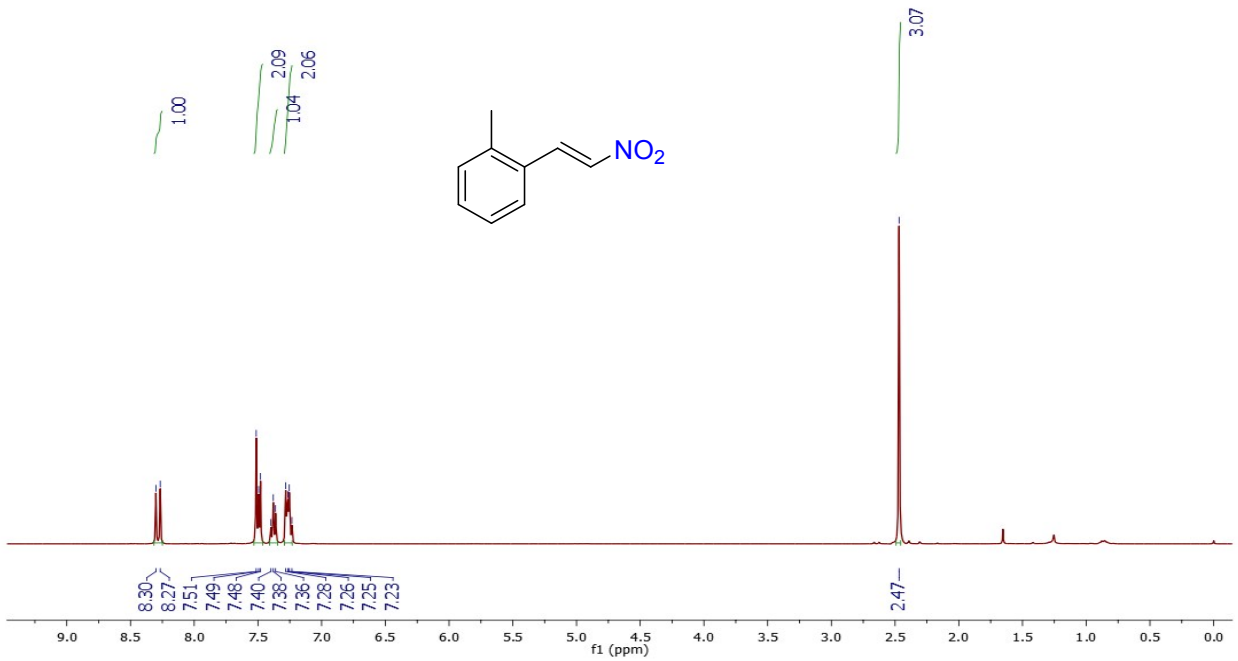
DEPT NMR of (*E*)-4-Methyl-2-(2-nitrovinyl)benzene (2b)



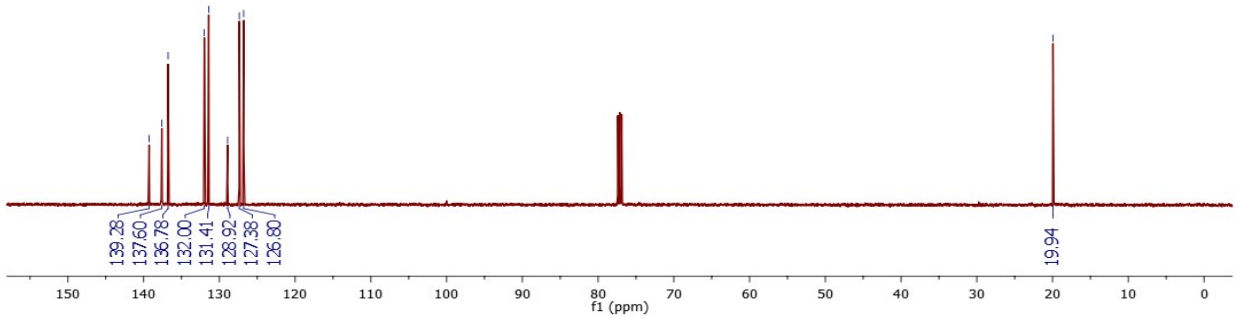
GC-MS of (*E*)-4-Methyl-2-(2-nitrovinyl)benzene (2b)



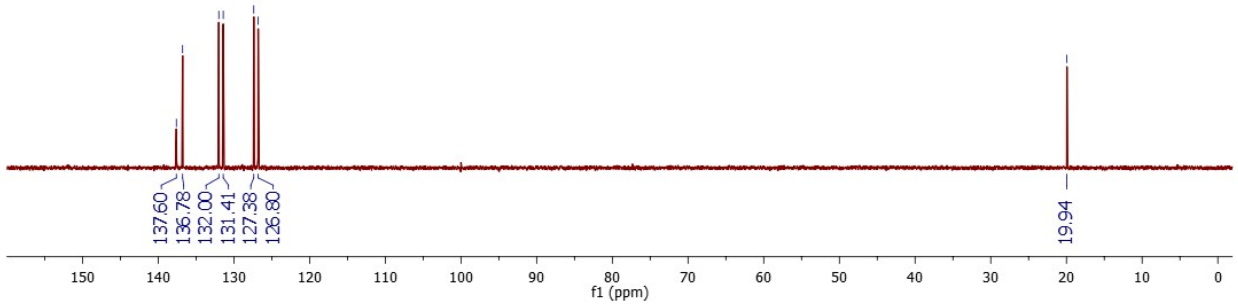
^{1}H NMR of (*E*)-1-Methyl-2-(2-nitrovinyl)benzene (2c)[2]



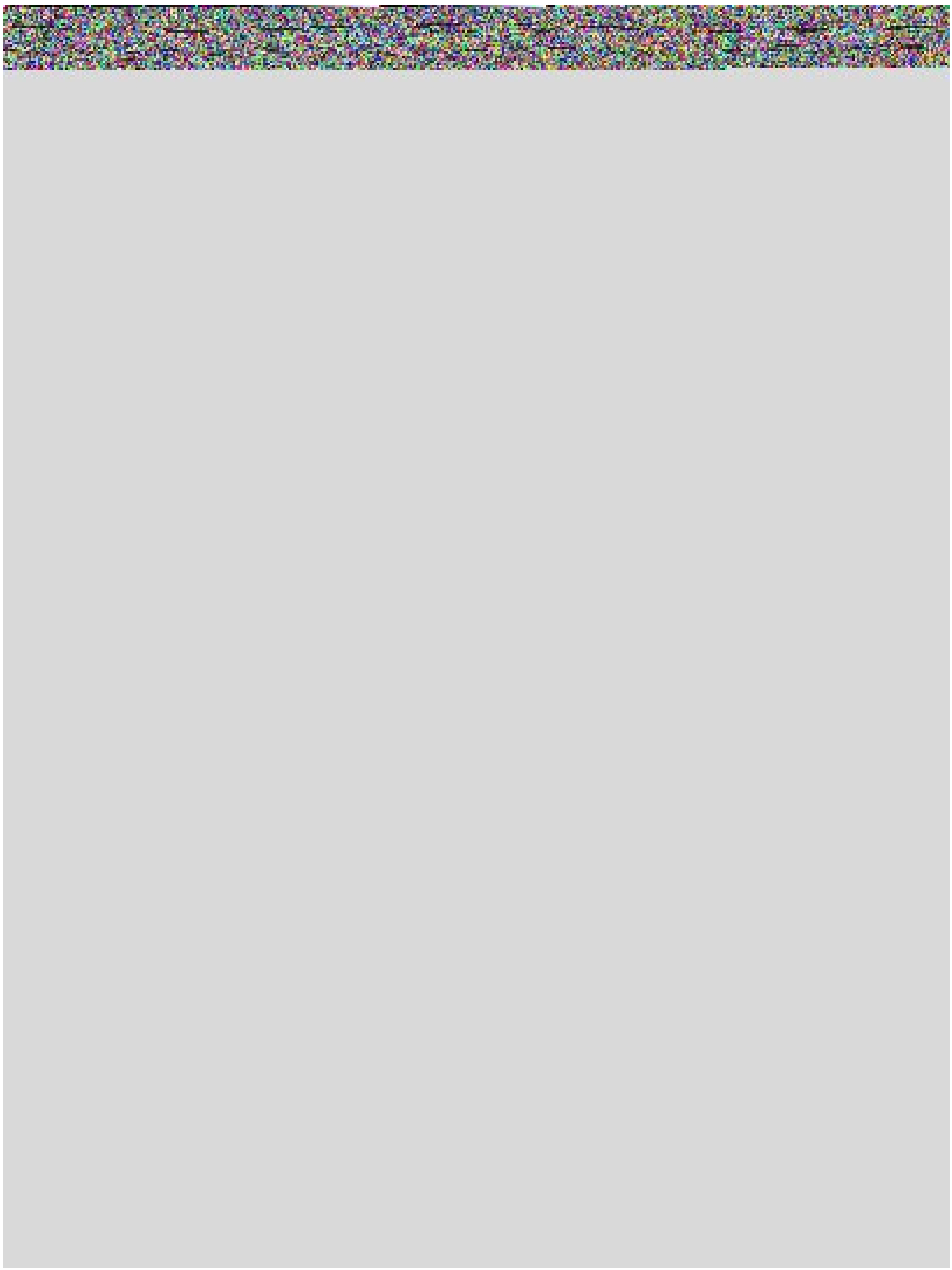
^{13}C NMR of (*E*)-1-Methyl-2-(2-nitrovinyl)benzene (2c)



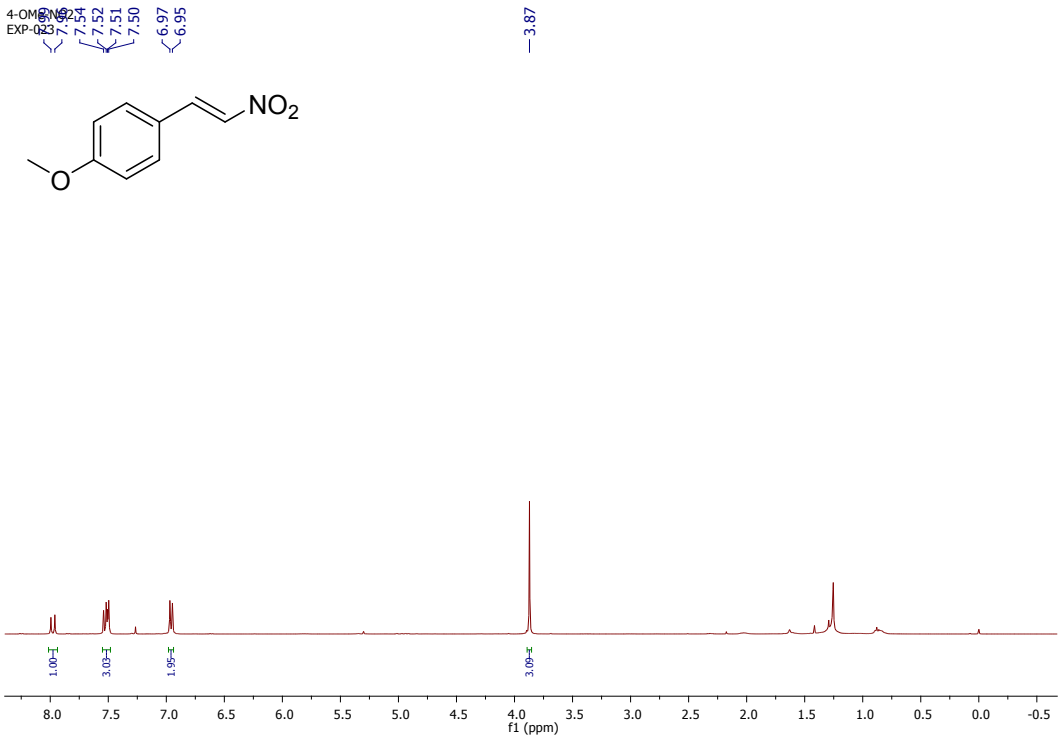
DEPT of (*E*)-1-Methyl-2-(2-nitrovinyl)benzene (2c)



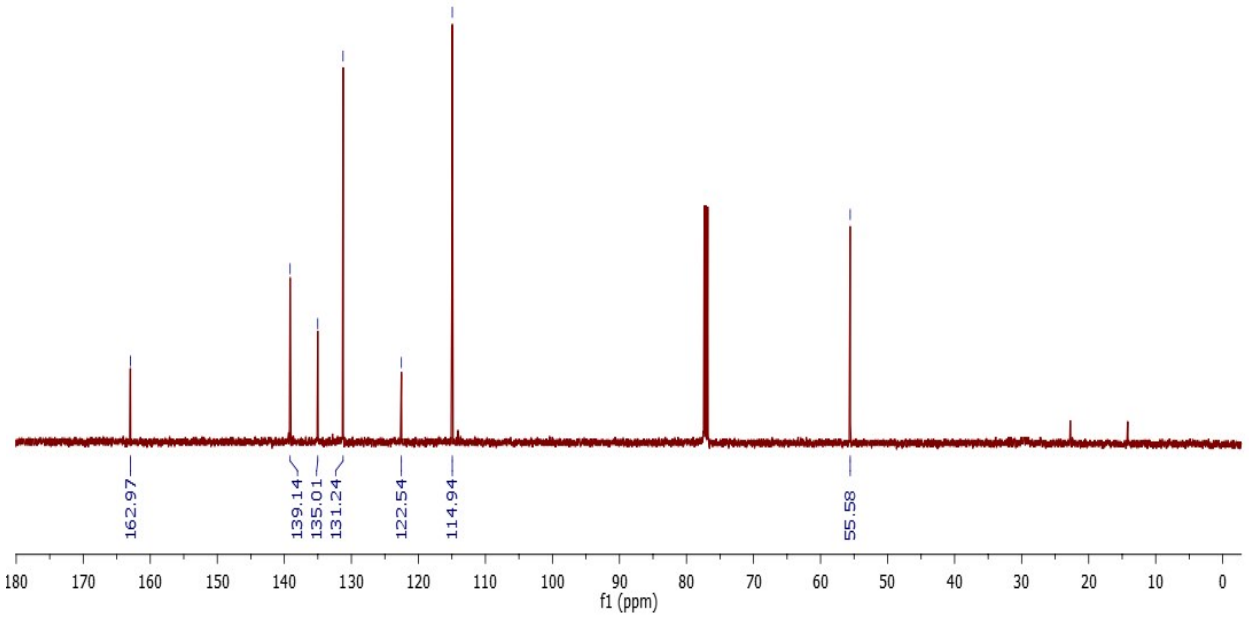
GC-MS of (*E*)-1-Methyl-2-(2-nitrovinyl)benzene (2c)



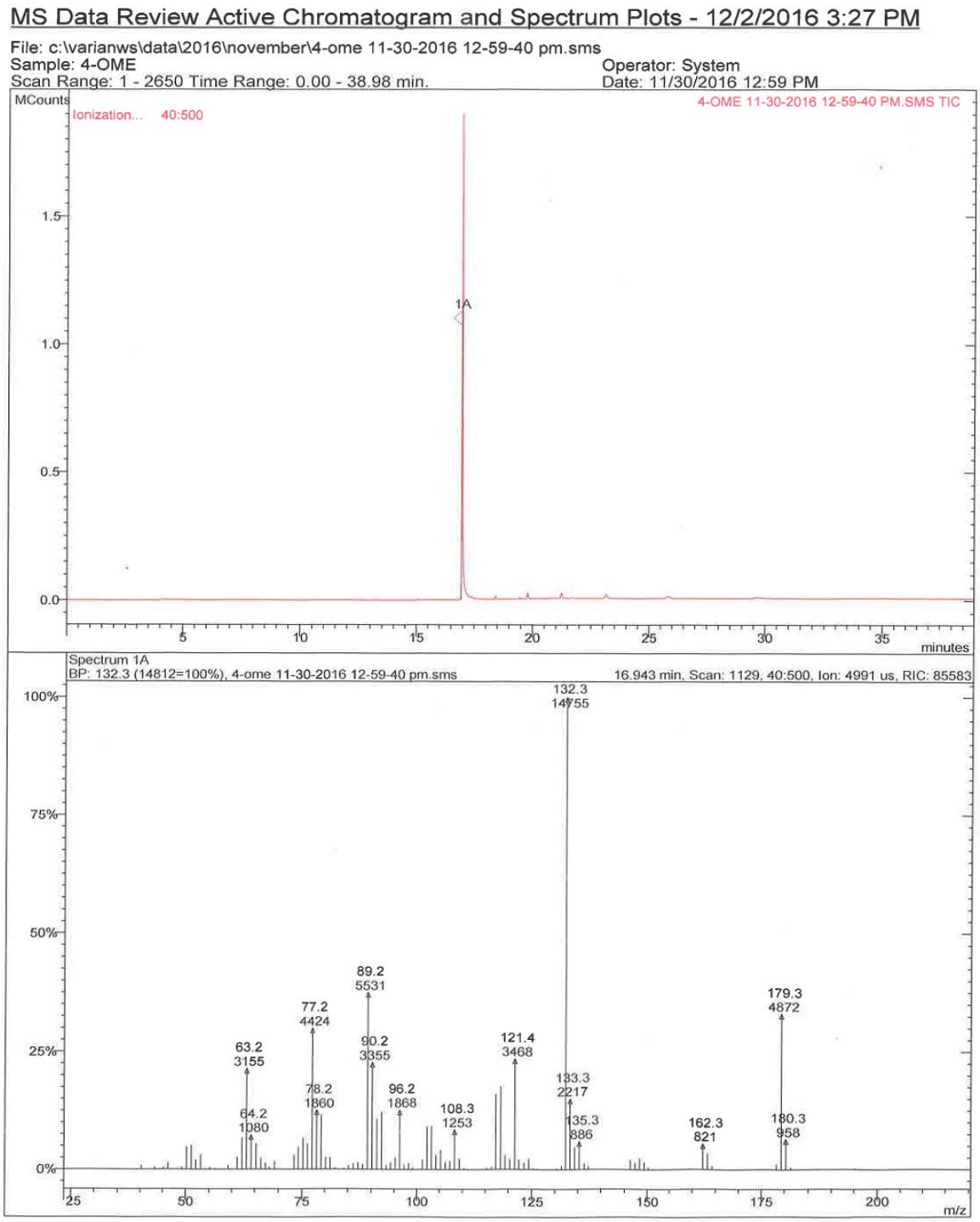
^{1}H NMR of (E)-1-methoxy-4-(2-nitrovinyl)benzene (2d)[1]



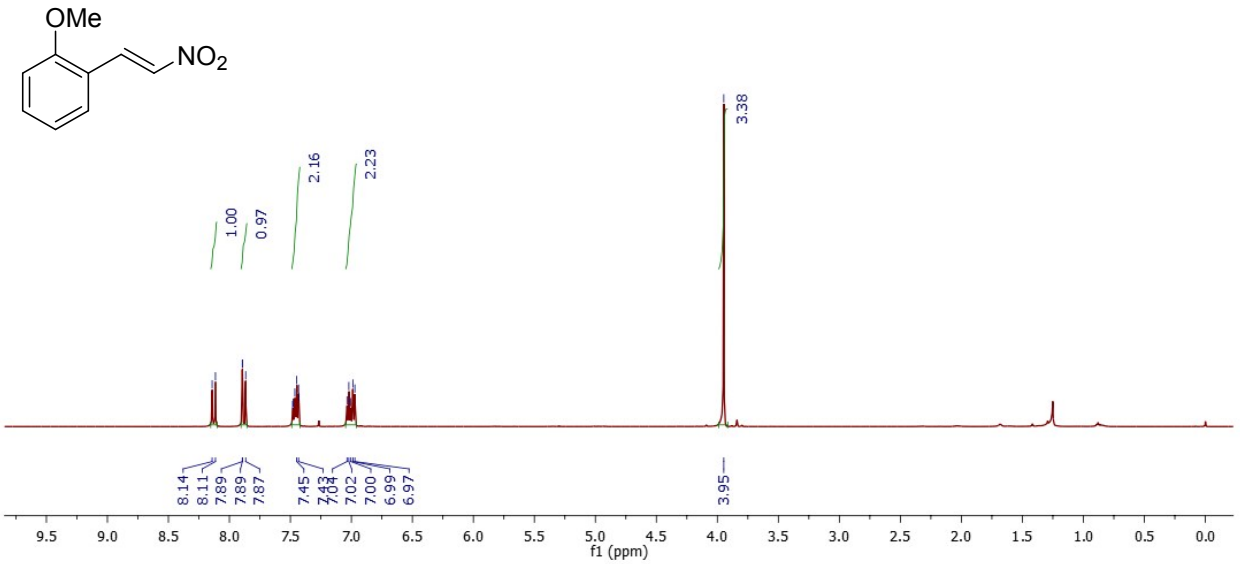
^{13}C NMR of (E)-1-methoxy-4-(2-nitrovinyl)benzene (2d)



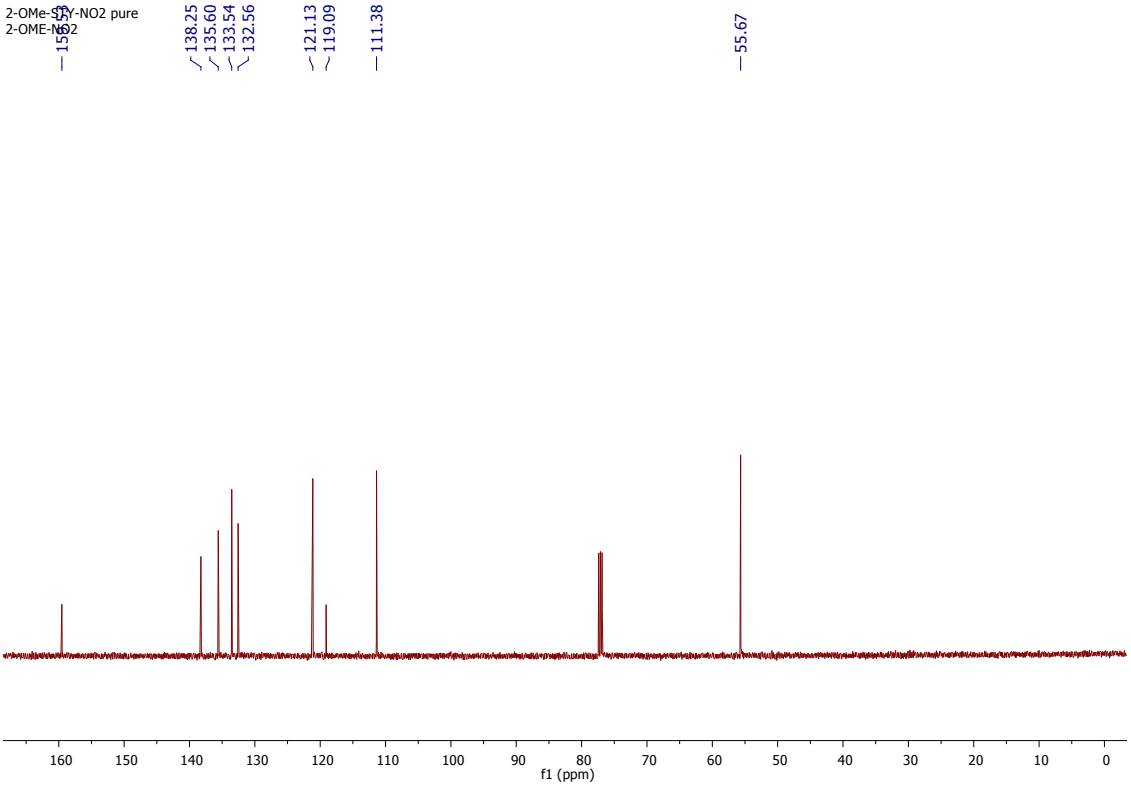
GC-MS of (E)-1-methoxy-4-(2-nitrovinyl)benzene (2d)



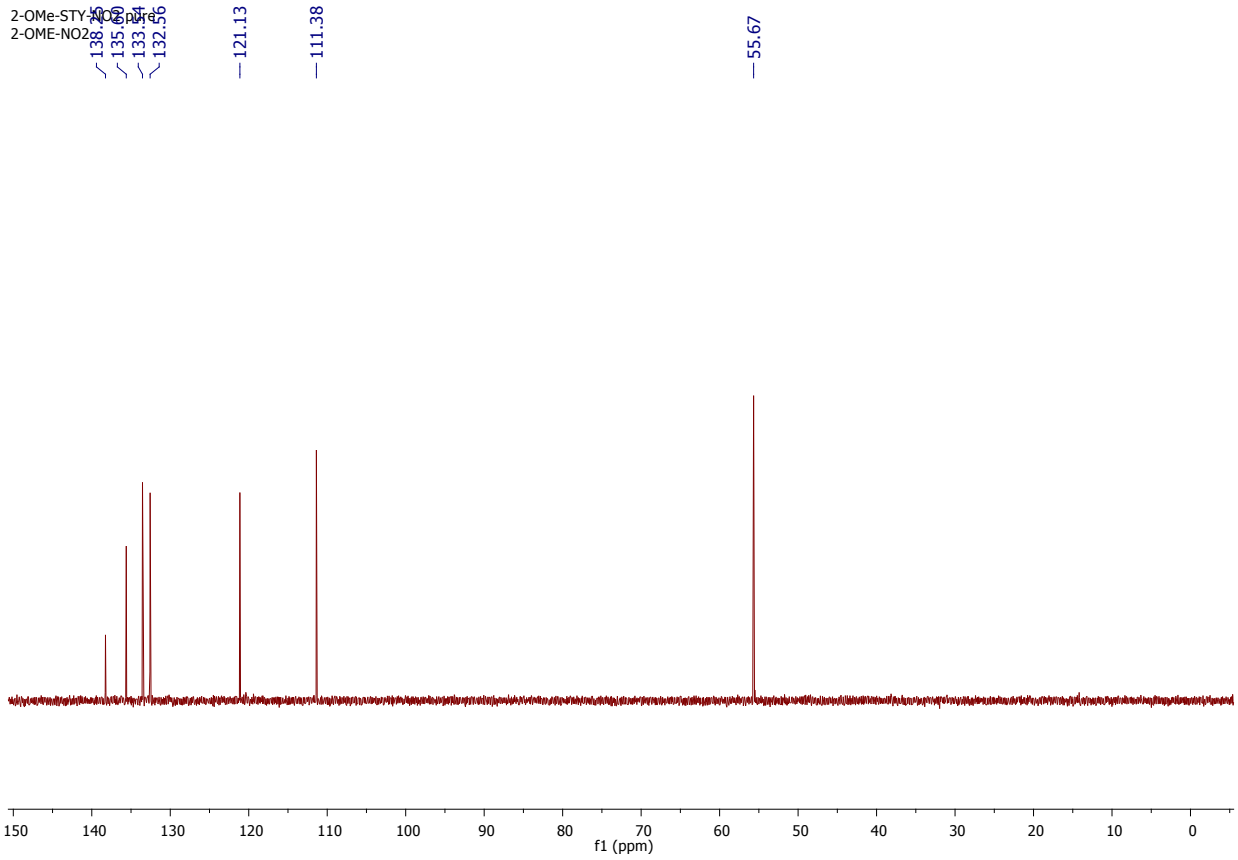
^{1}H NMR of (E)-1-methoxy-2-(2-nitrovinyl)benzene (2e)[3]



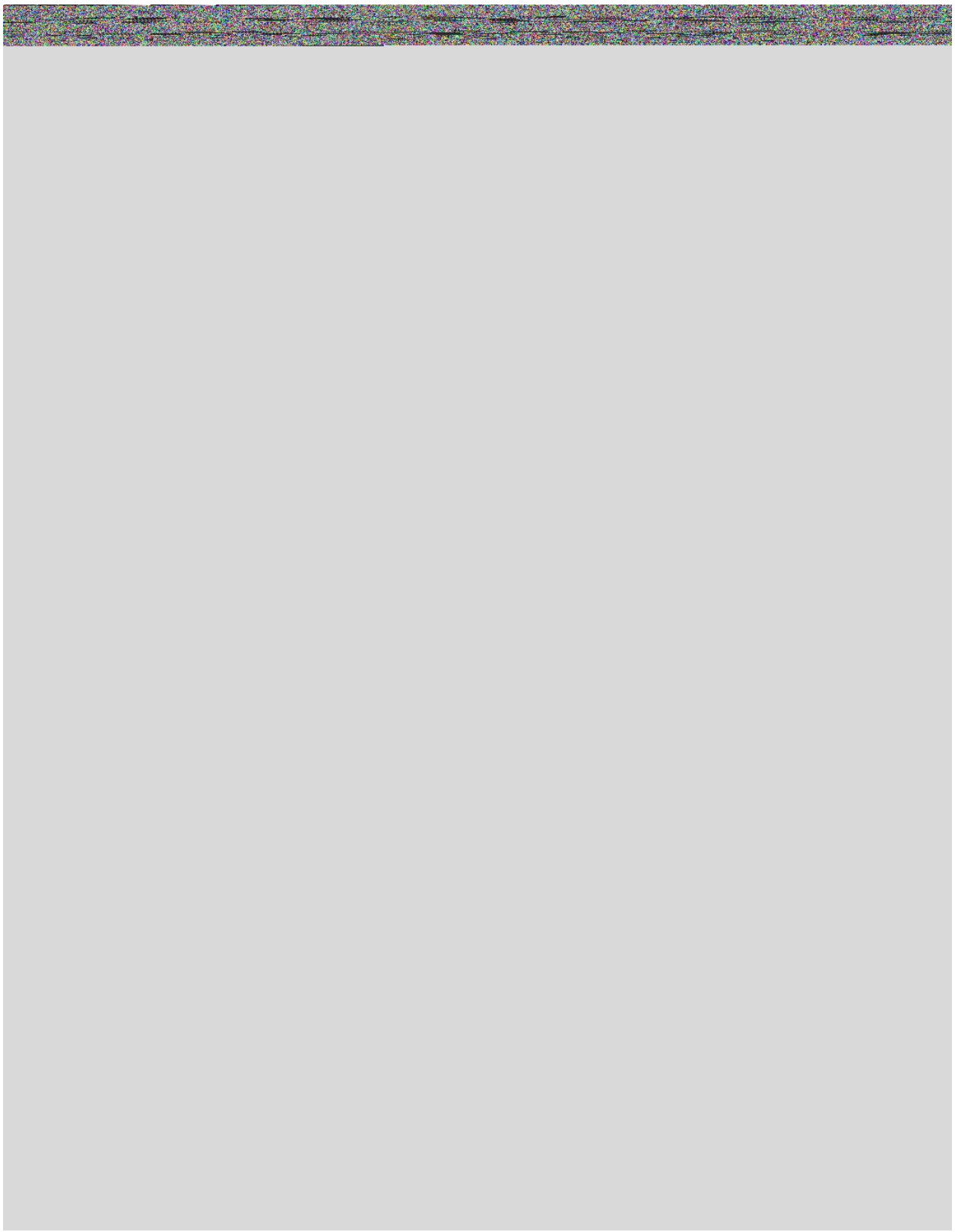
^{13}C NMR of (E)-1-methoxy-2-(2-nitrovinyl)benzene (2e)



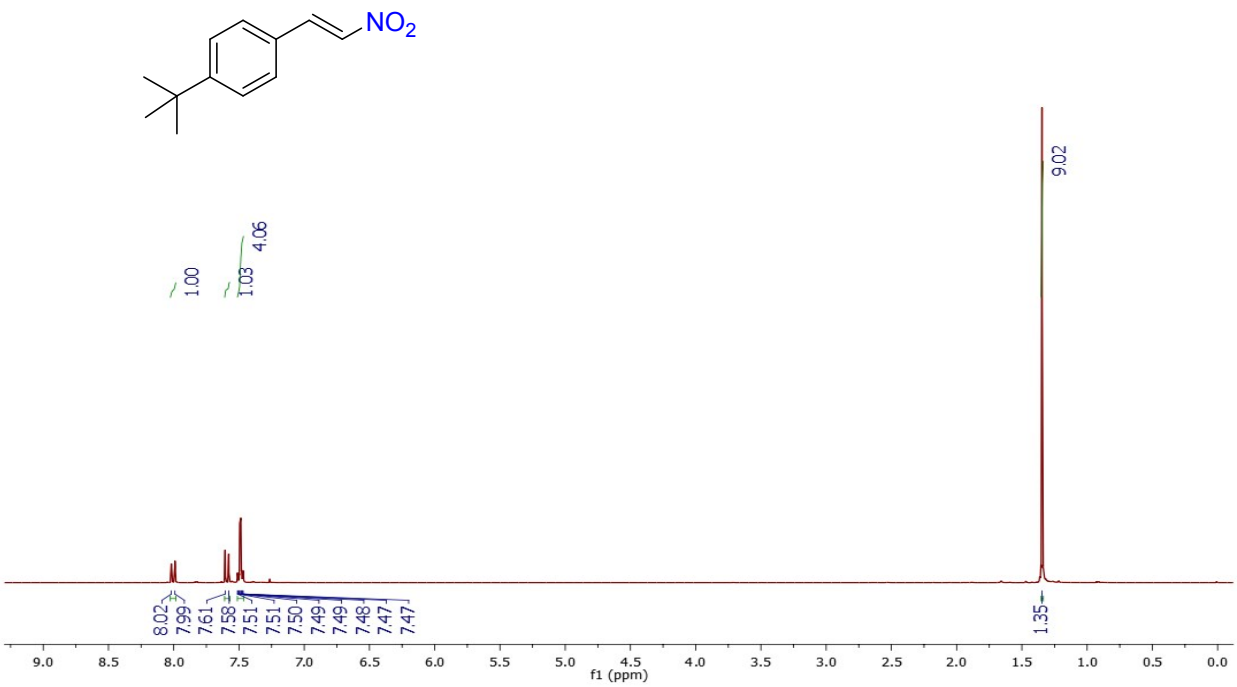
DEPT NMR of (E)-1-methoxy-2-(2-nitrovinyl)benzene (2e)



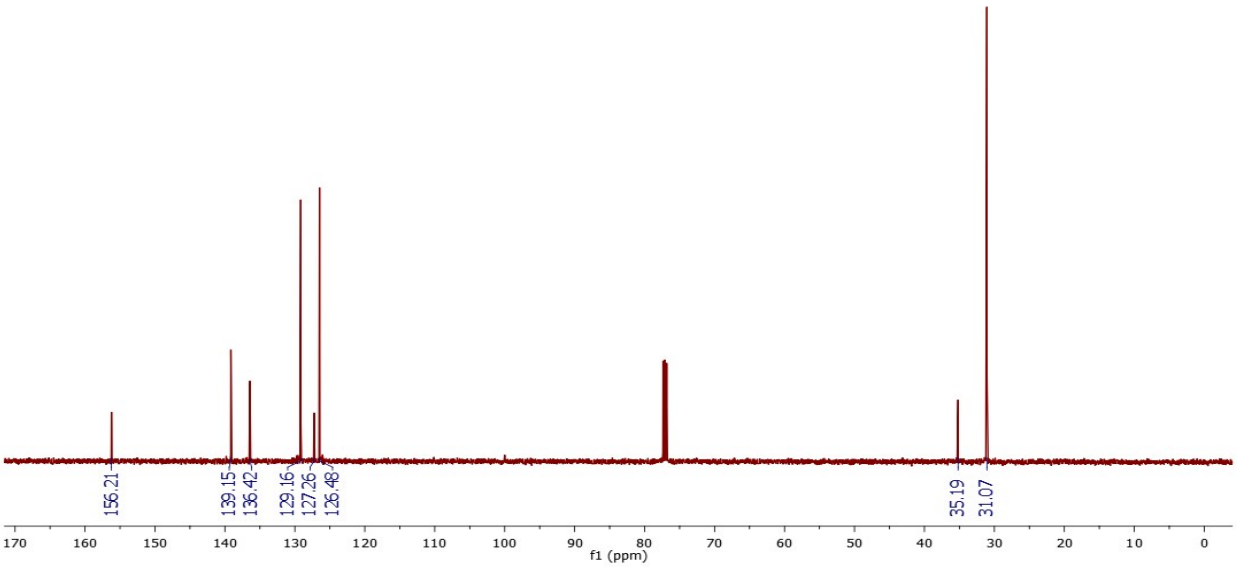
GC-MS of (E)-1-methoxy-2-(2-nitrovinyl)benzene (2e)



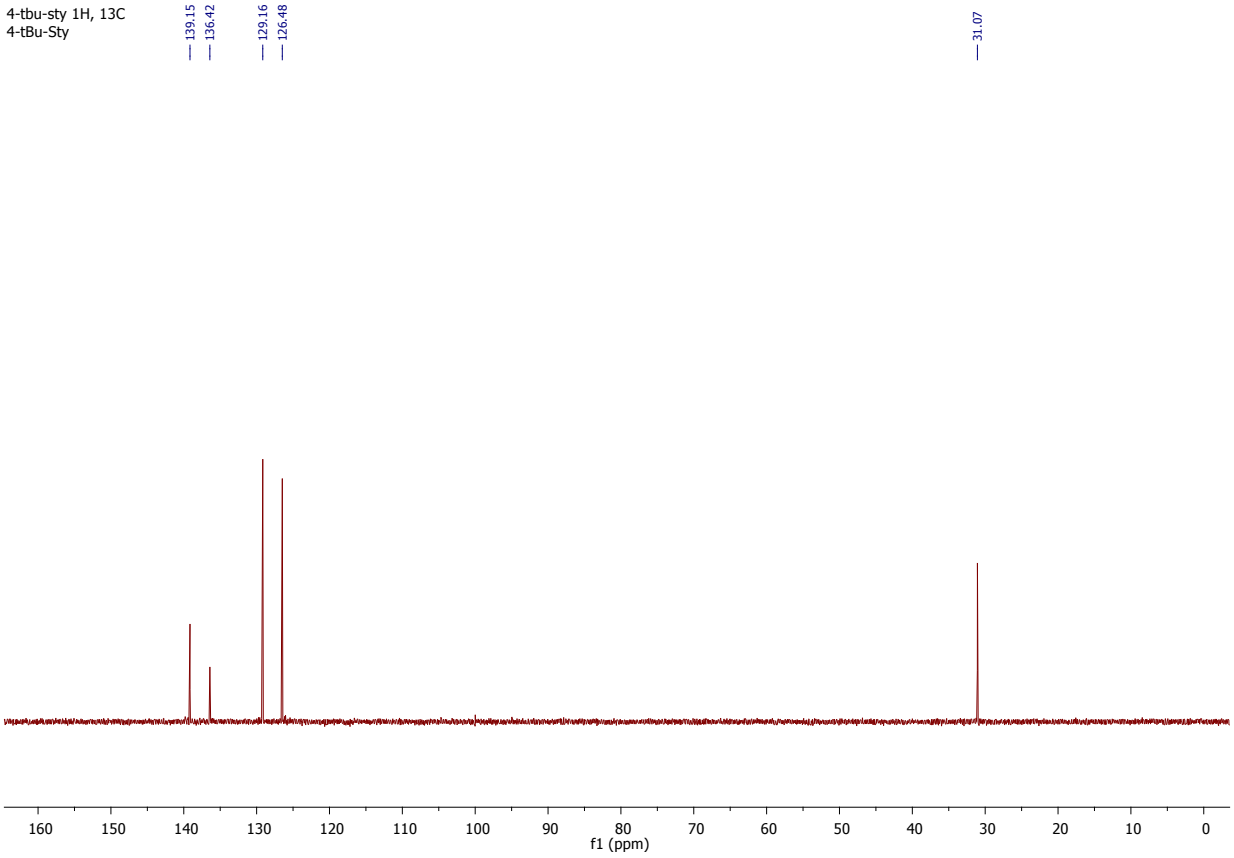
^{1}H NMR of (E)-1-(tert-butyl)-4-(2-nitrovinyl)benzene (2f)[4]



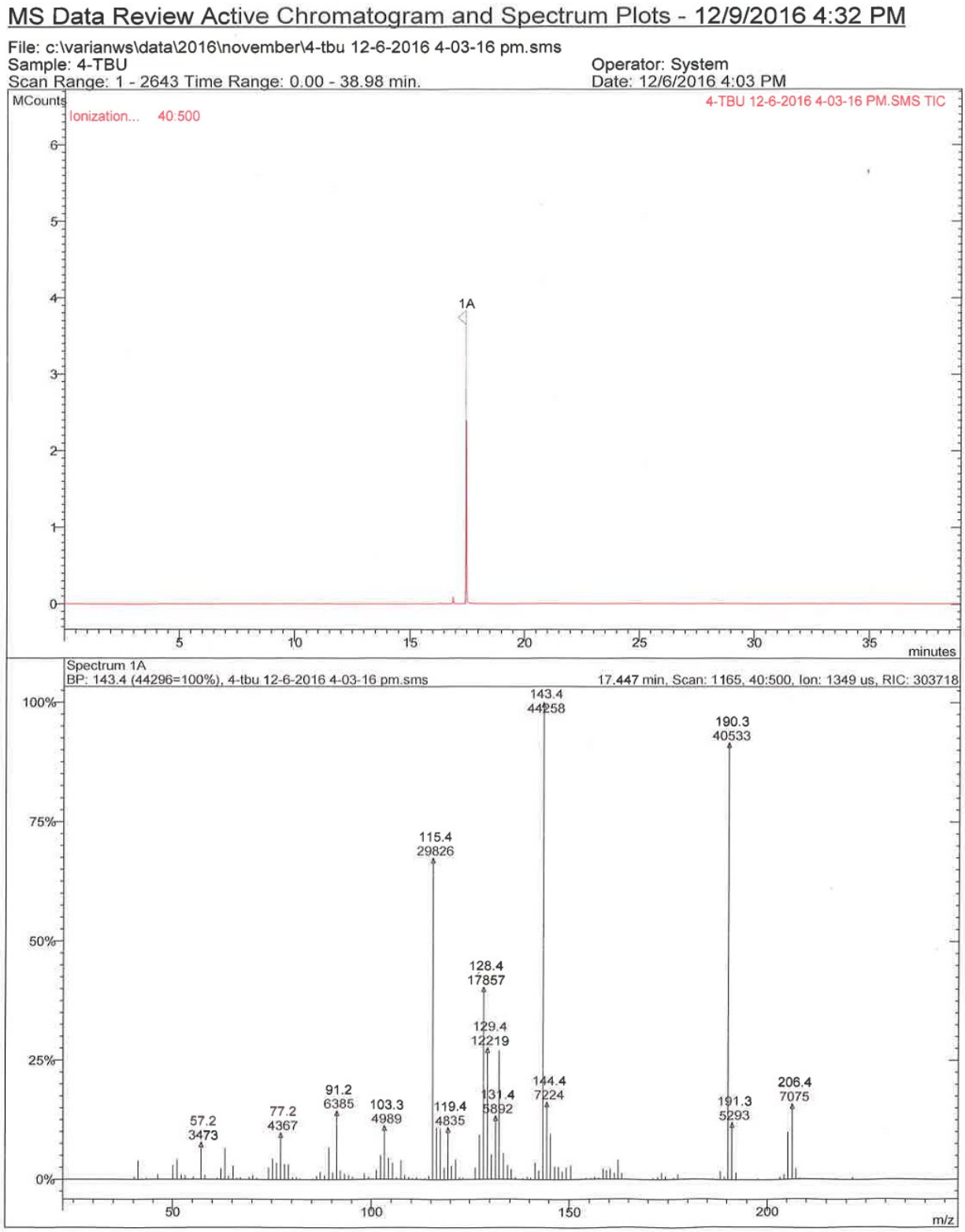
^{13}C NMR of (E)-1-(tert-butyl)-4-(2-nitrovinyl)benzene (2f)



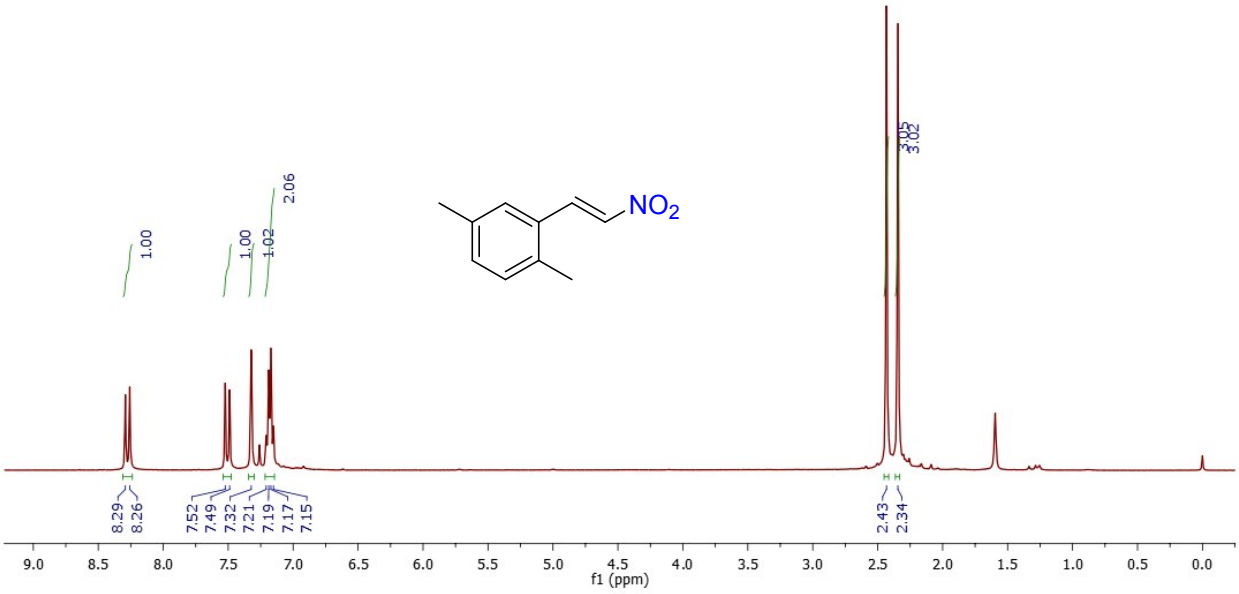
DEPT NMR of (E)-1-(tert-butyl)-4-(2-nitrovinyl)benzene (2f)



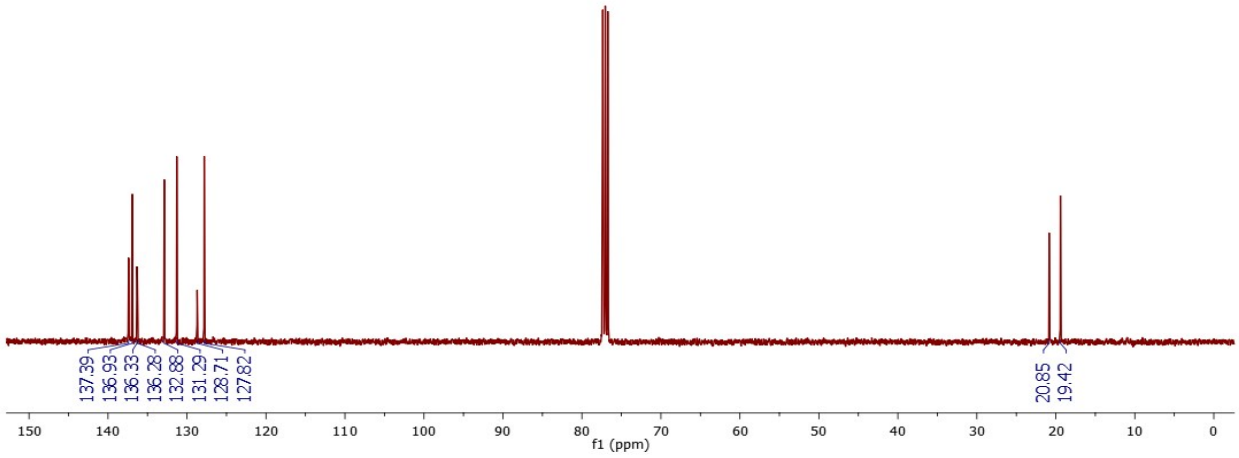
GC-MS of (E)-1-(tert-butyl)-4-(2-nitrovinyl)benzene (2f)



^{1}H NMR of (E)-1,4-dimethyl-2-(2-nitrovinyl)benzene (2g)[5]

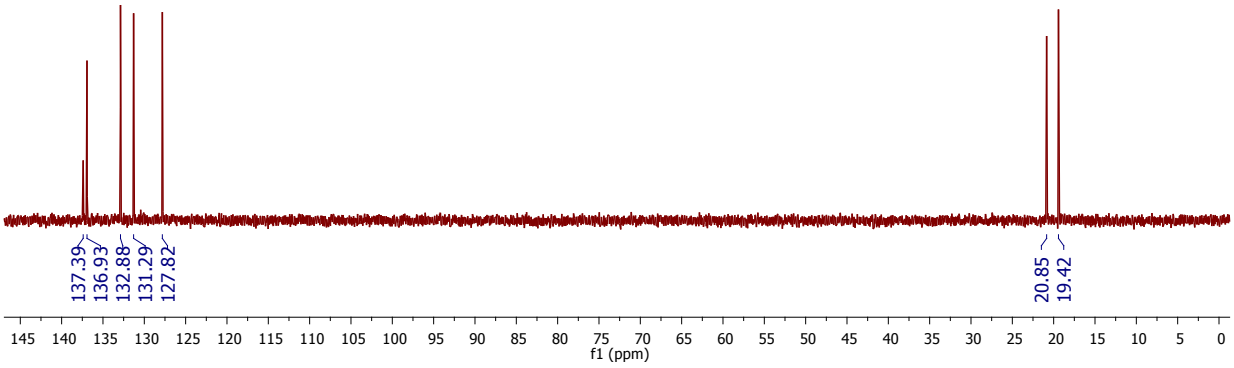


^{13}C NMR of (E)-1,4-dimethyl-2-(2-nitrovinyl)benzene (2g)

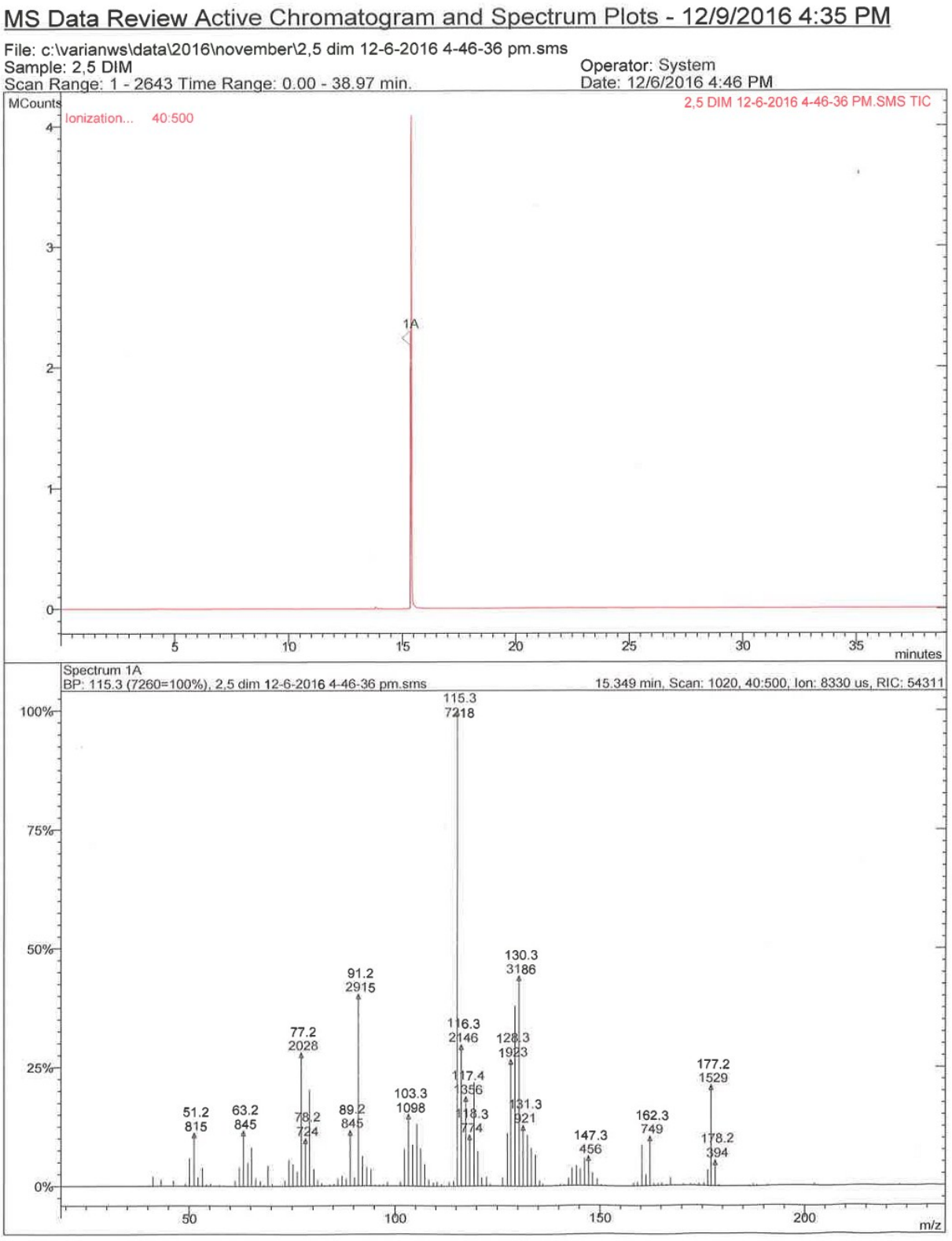


DEPT NMR of (E)-1,4-dimethyl-2-(2-nitrovinyl)benzene (2g)

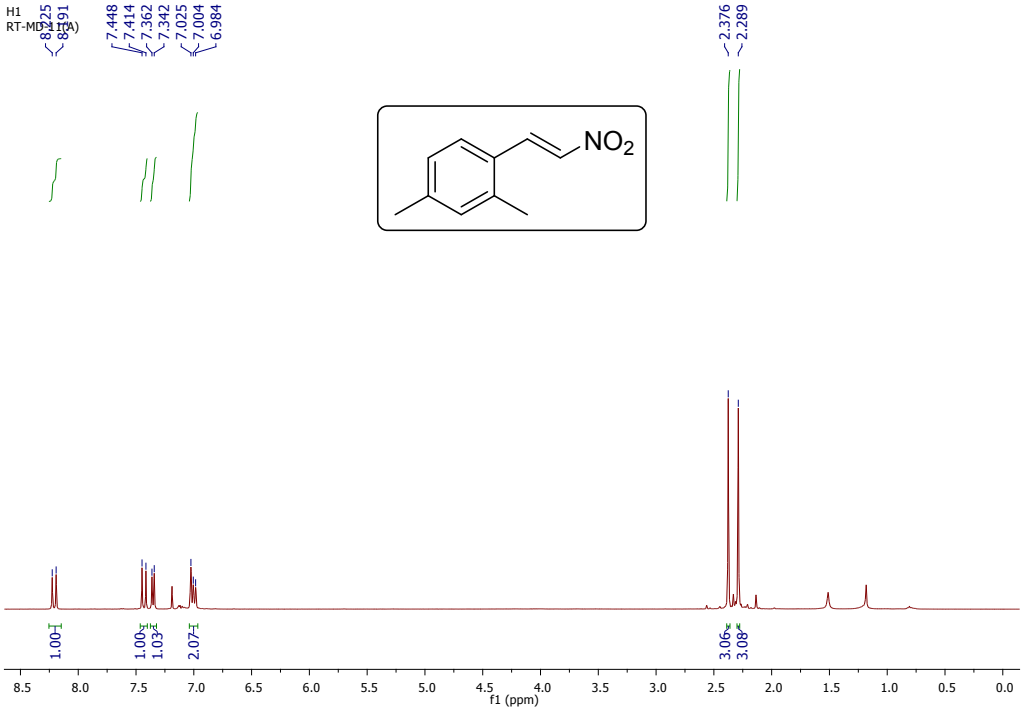
G-101, C-13
G-101



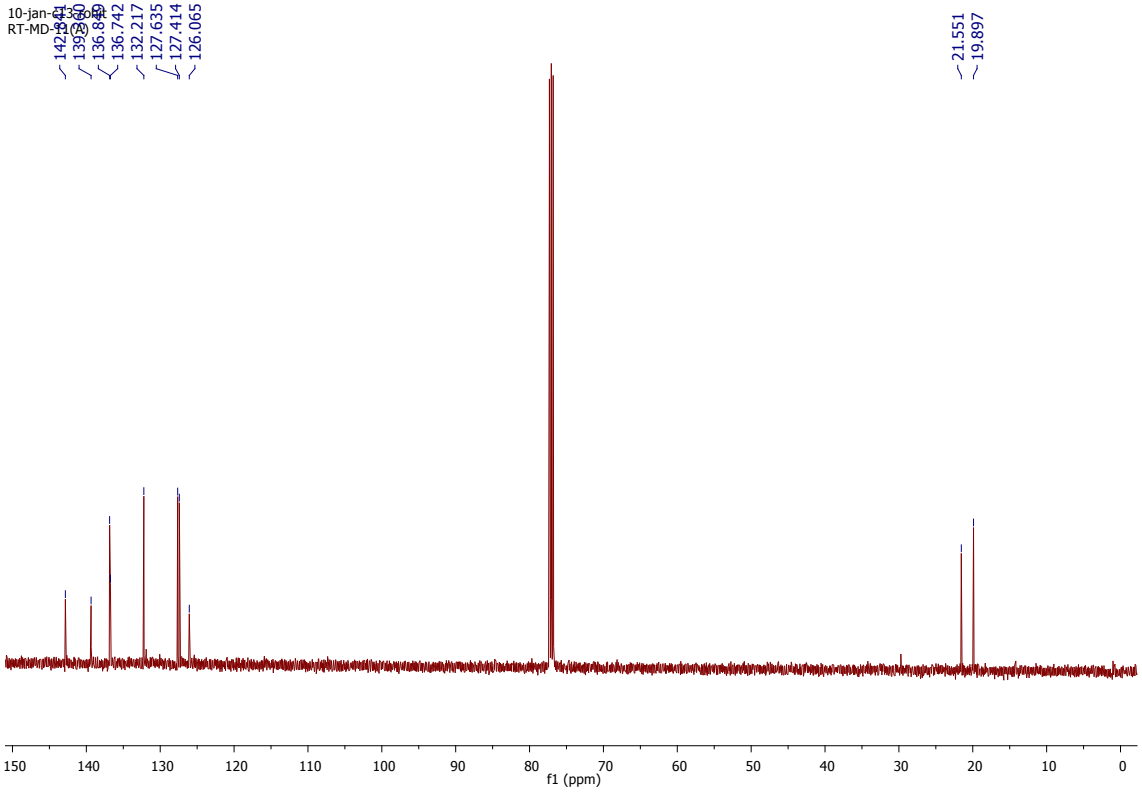
GC-MS of (E)-1,4-dimethyl-2-(2-nitrovinyl)benzene (2g)



^{1}H NMR spectra of (E)-2,4-dimethyl-1-(2-nitrovinyl)benzene (2h)[6]



^{13}C NMR Spectra of (E)-2,4-dimethyl-1-(2-nitrovinyl)benzene (2h)

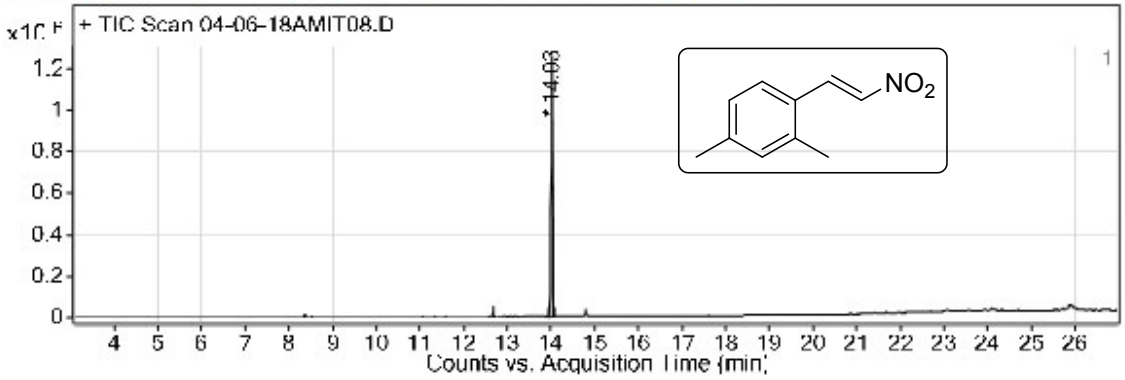


GC-MS of compound(E)-2,4-dimethyl-1-(2-nitrovinyl)benzene(2h)

Data Filename	04-06-18AMIT08.D	**Sample Name**	MD-11 A
Sample Type	Sample	**Position**	8
Instrument Name	GCMS	**User Name**	manager
Acq Method	AMIT.M	**Acquired Time**	6/5/2018 7:45:39 PM
IRM Calibration Status	Not Applicable	**DA Method**	Default.m
Comment			
Expected Barcode		**Sample Amount**	
Vial	8	**SeqPath**	C:\msdchem\1\sequence\june 4.s
TuneName	12 atune.u	**TunePath**	C:\msdchem\1\5975\
TuneDateStamp	43251.42431	**OperatorName**	manager
RunCompletedFlag	TRUE		

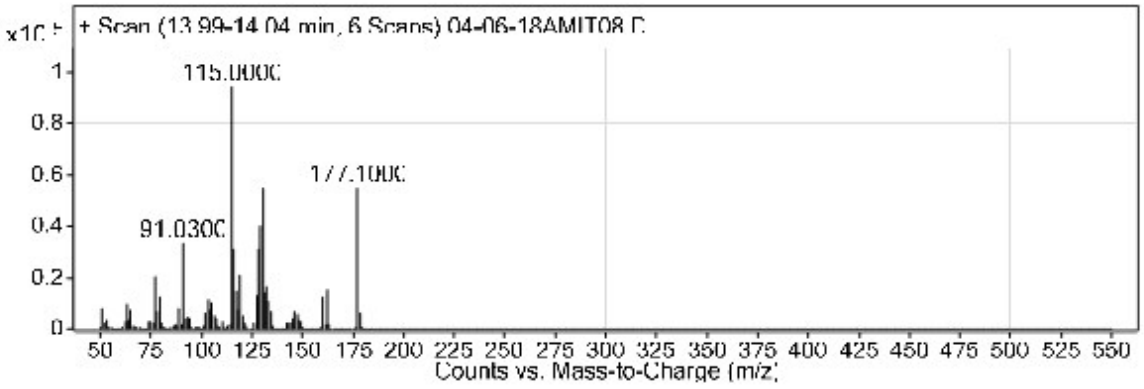
User Chromatograms

Fragmentor Voltage 0 **Collision Energy** 0 **Ionization Mode** Unspecified

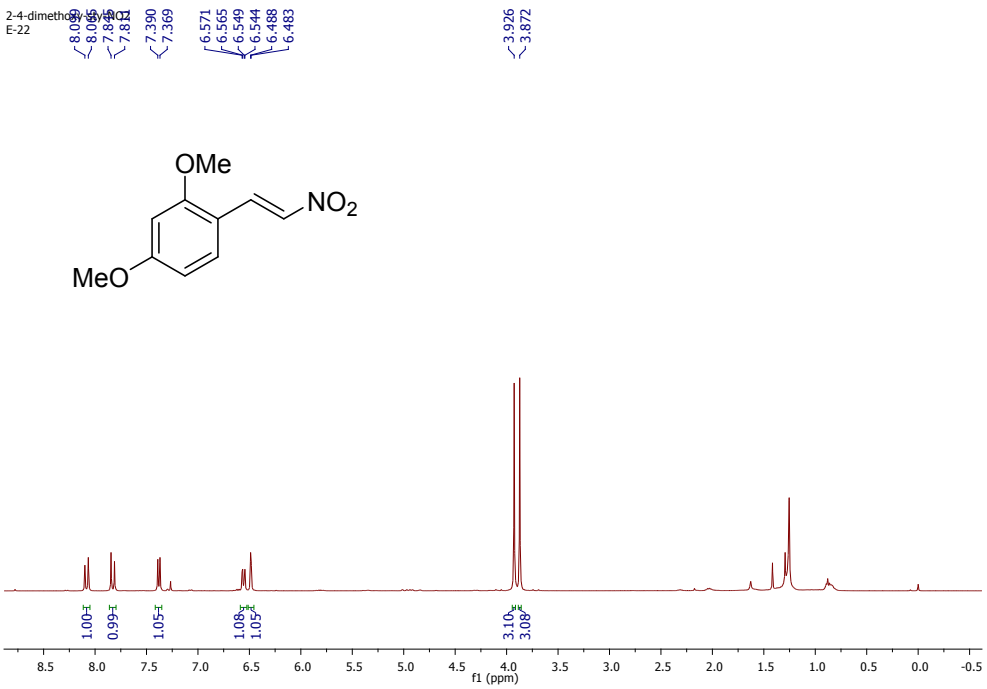


User Spectra

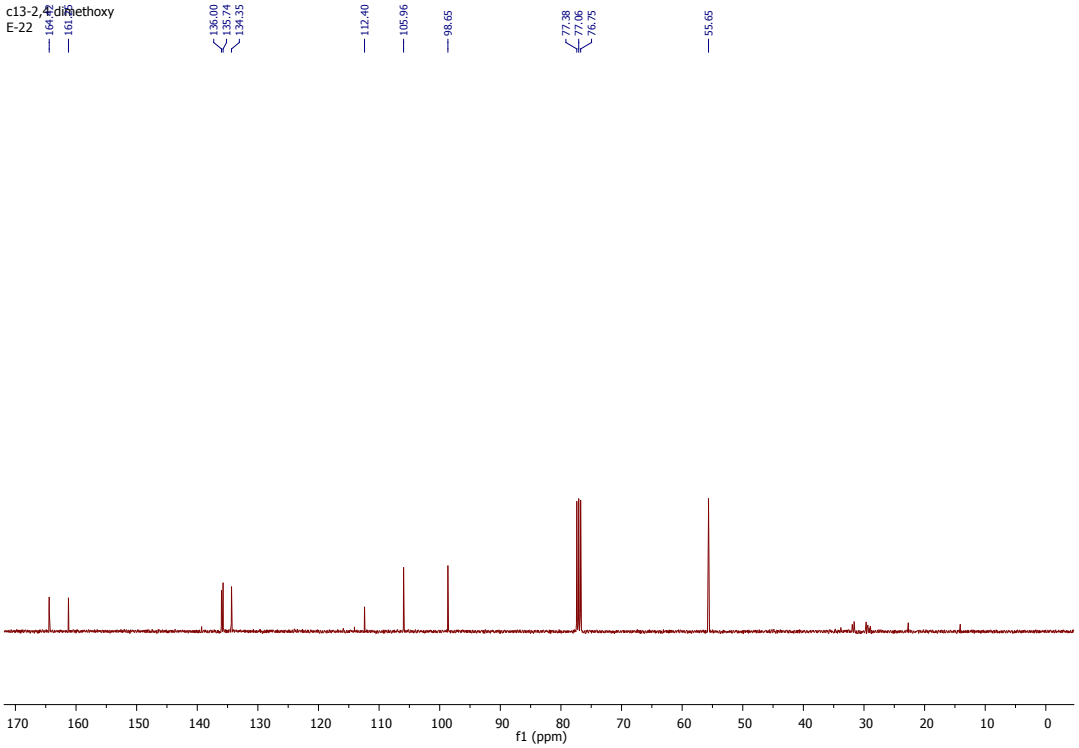
Spectrum Source	Fragmentor Voltage	Collision Energy	Ionization Mode
Peak (1) in "+ TIC Scan - 04-06-18AMIT08.D"	0	0	Unspecified



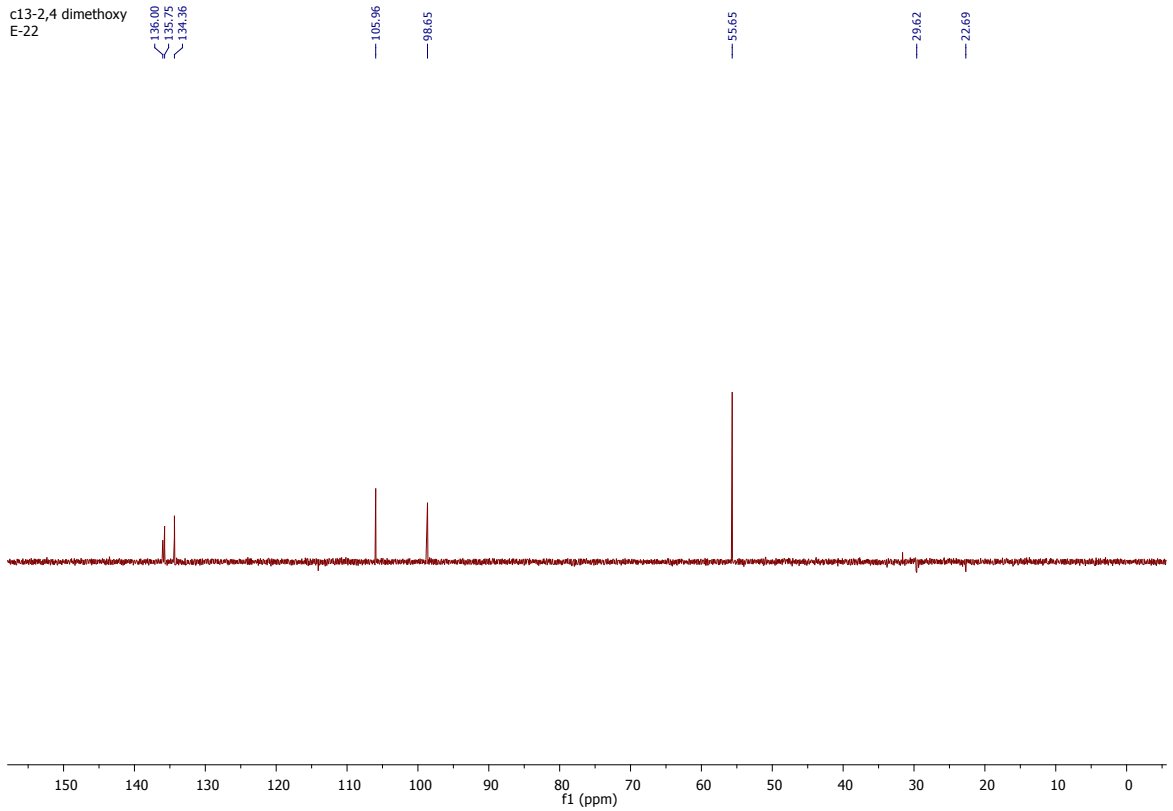
^{1}H NMR of (E)-2,4-dimethoxy-1-(2-nitrovinyl)benzene (2i)[7]



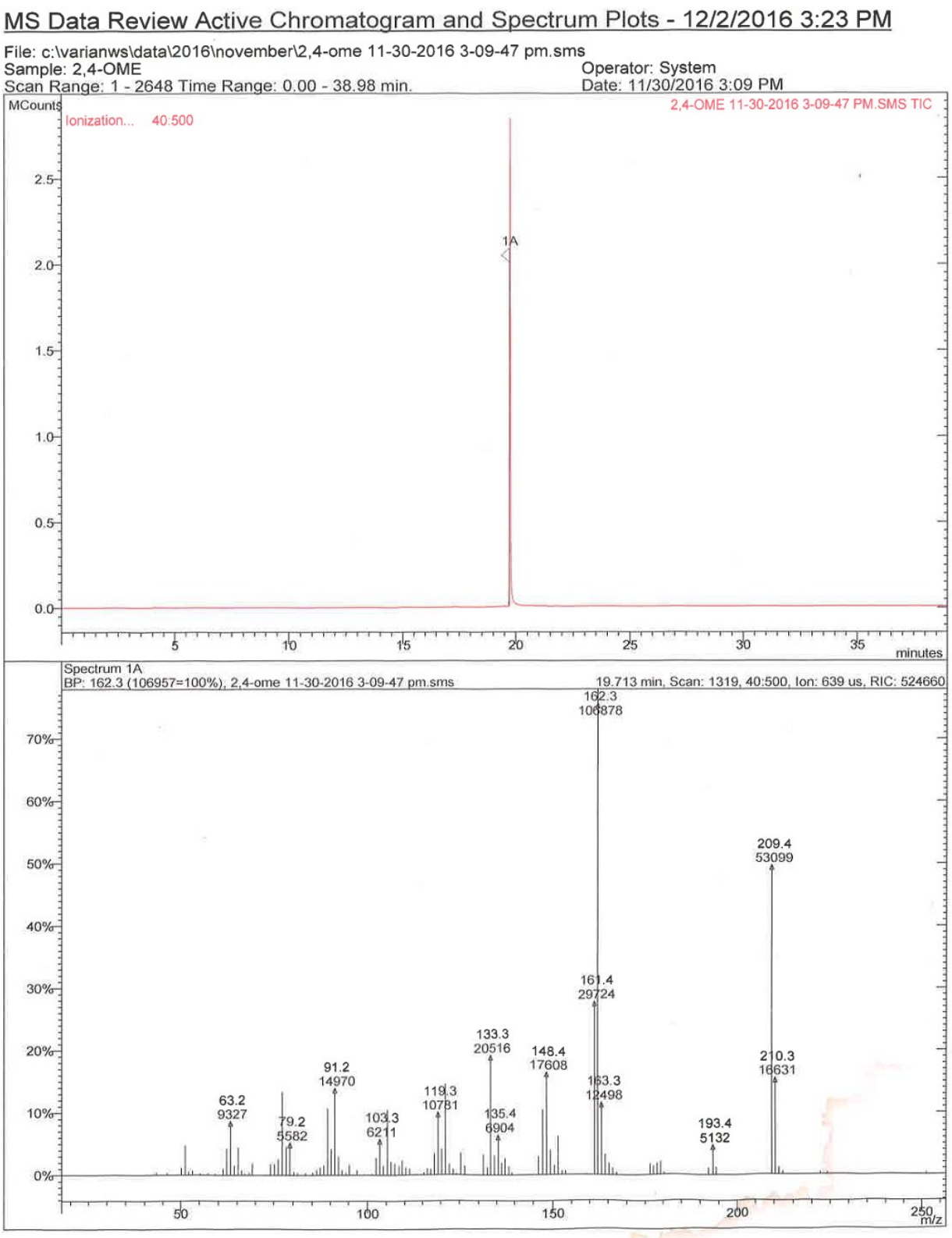
^{13}C NMR (E)-2,4-dimethoxy-1-(2-nitrovinyl)benzene (2i)



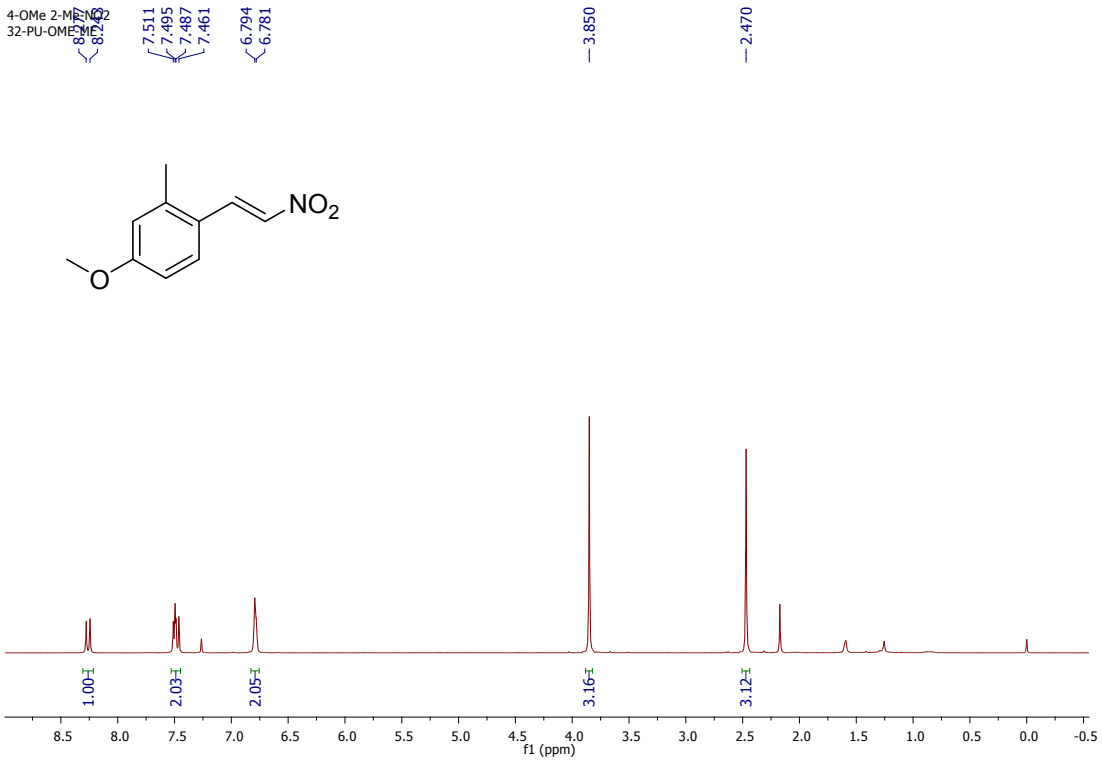
DEPT of (E)-2,4-dimethoxy-1-(2-nitrovinyl)benzene (2i)



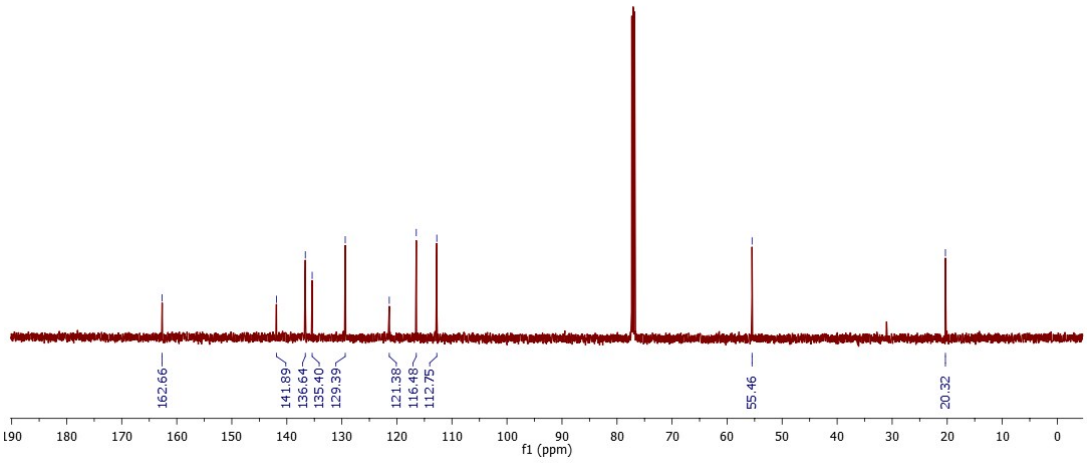
GC-MS of (E)-2,4-dimethoxy-1-(2-nitrovinyl)benzene (2i)



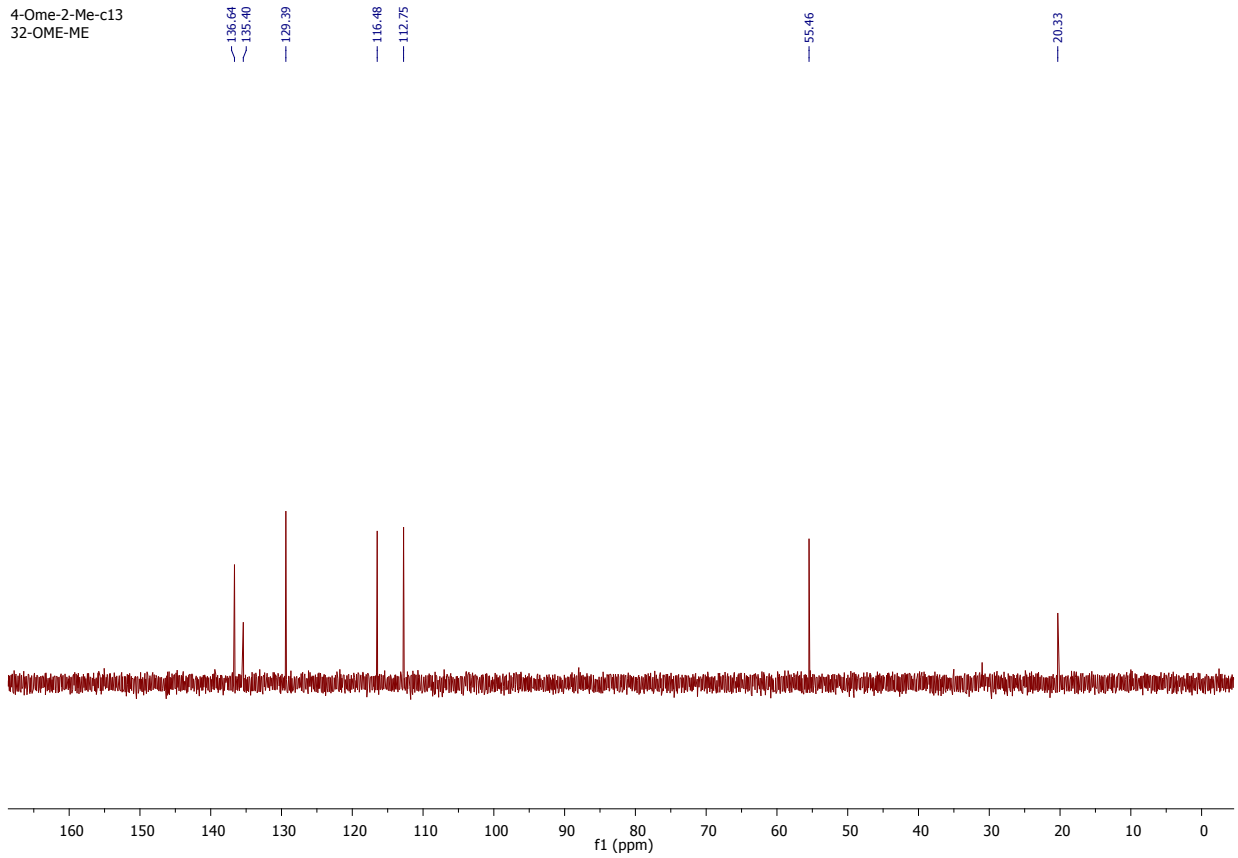
^{1}H NMR of (E)-4-methoxy-2-methyl-1-(2-nitrovinyl)benzene (2j)[8]



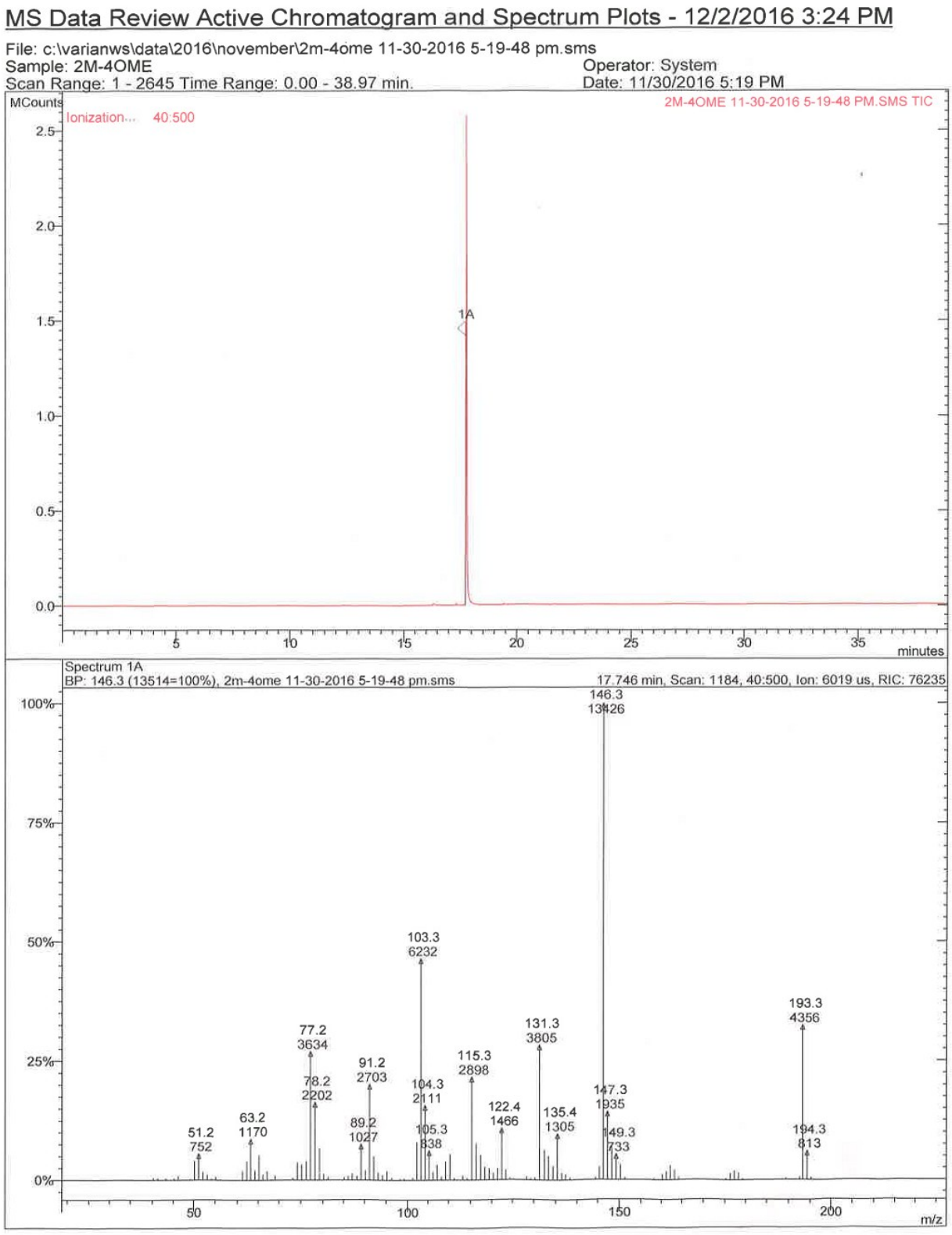
^{13}C NMR of (E)-4-methoxy-2-methyl-1-(2-nitrovinyl)benzene (2j)



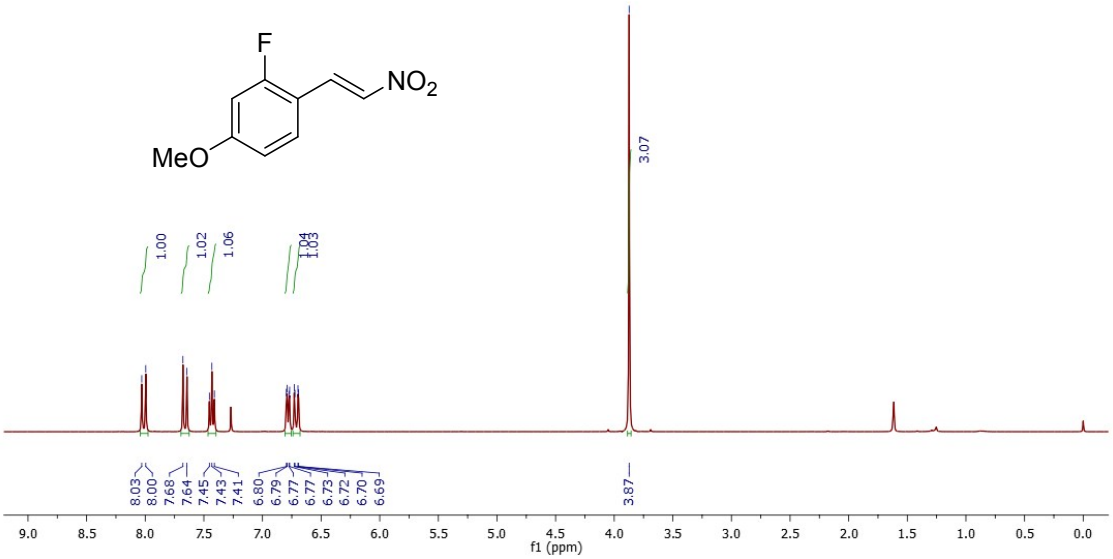
DEPT NMR of (E)-4-methoxy-2-methyl-1-(2-nitrovinyl)benzene (2j)



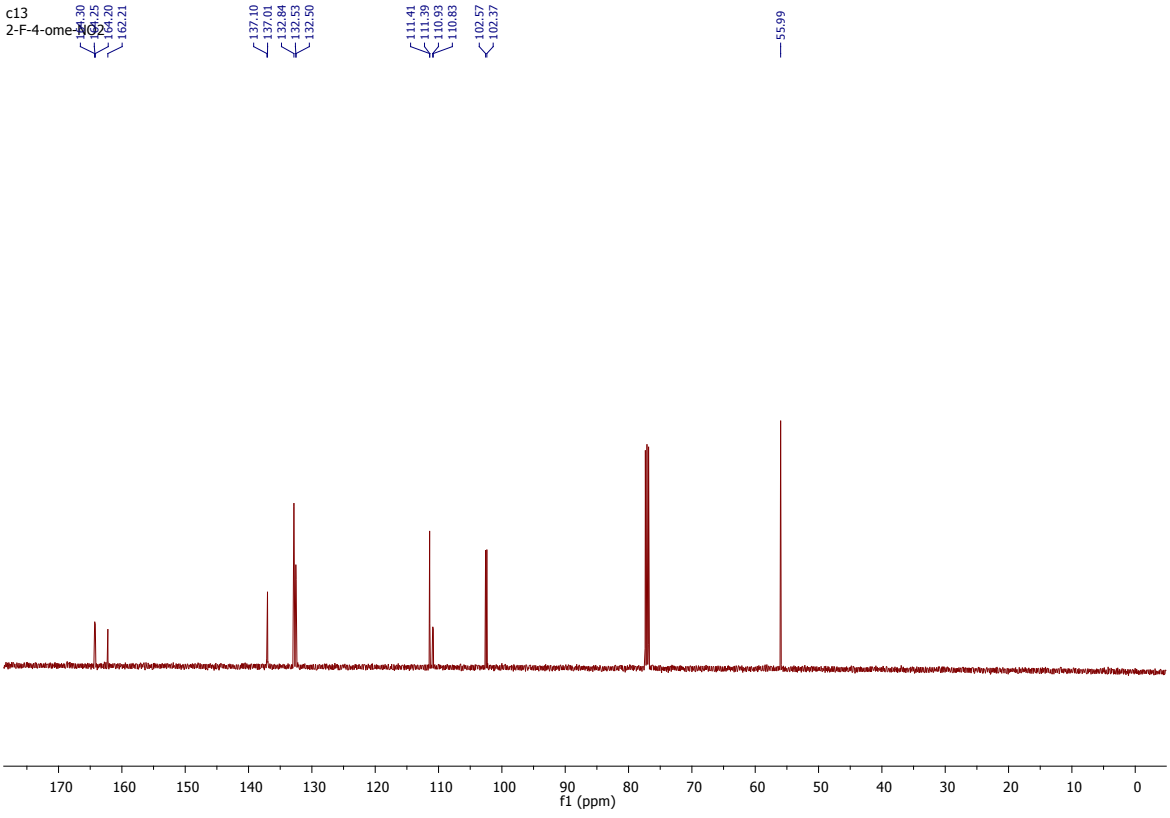
GC-MS of (E)-4-methoxy-2-methyl-1-(2-nitrovinyl)benzene (2j)



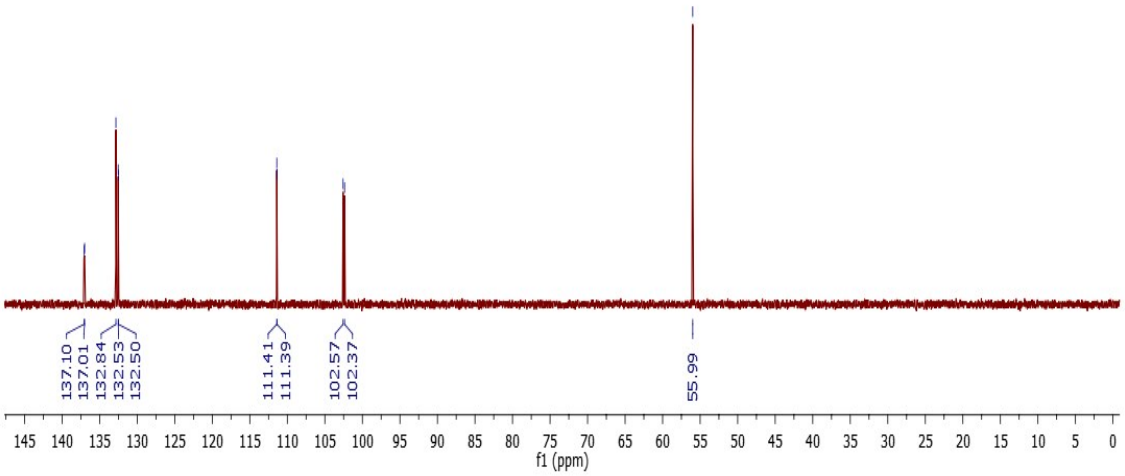
^{1}H NMR of (E)-2-fluoro-4-methoxy-1-(2-nitrovinyl)benzene (2k)[9]



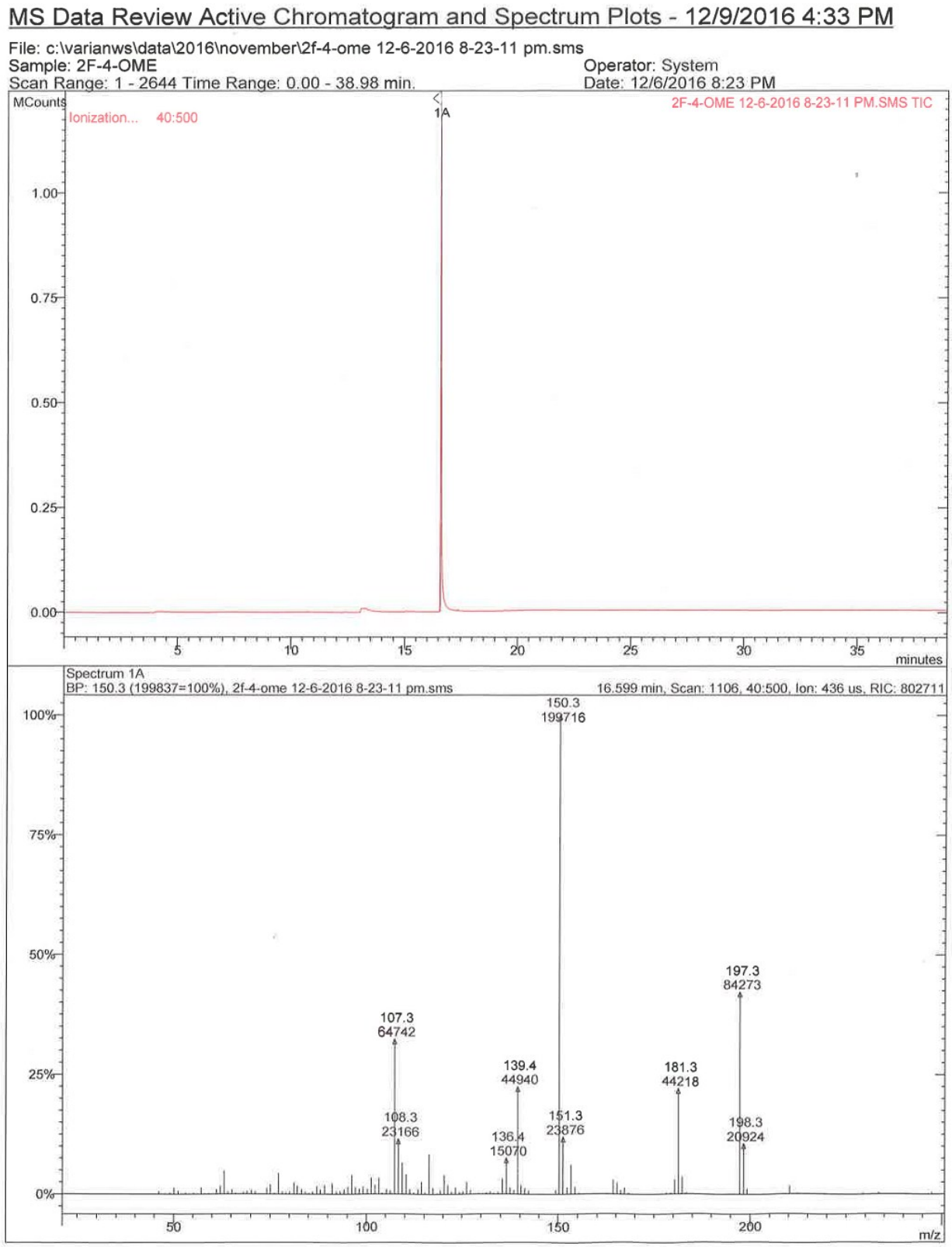
^{13}C NMR of (E)-2-fluoro-4-methoxy-1-(2-nitrovinyl)benzene (2k)



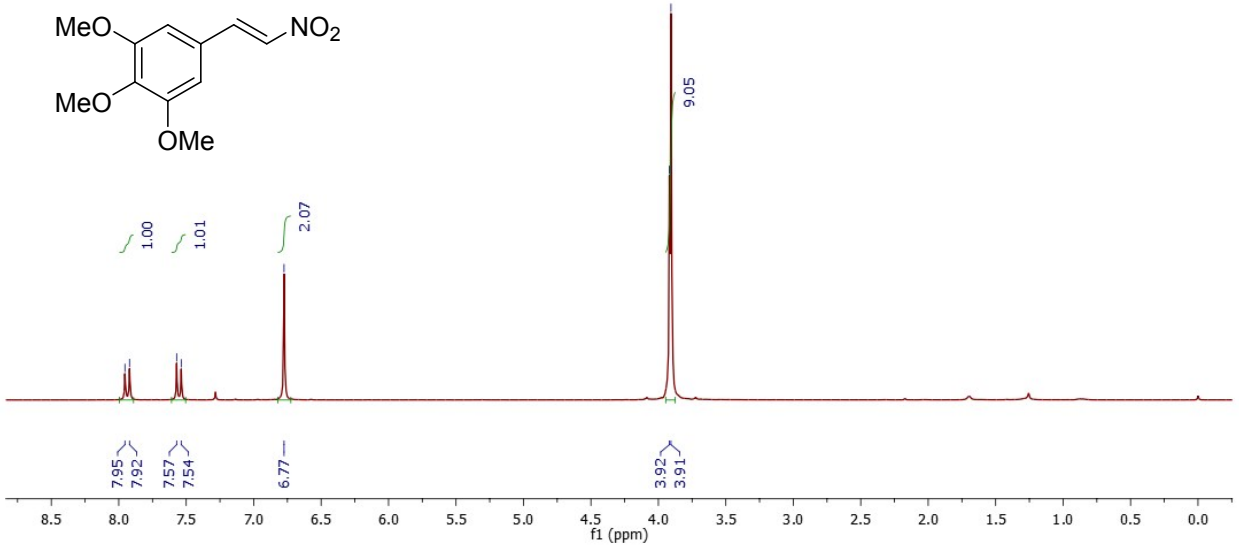
DEPT NMR of (E)-2-fluoro-4-methoxy-1-(2-nitrovinyl)benzene (2k)



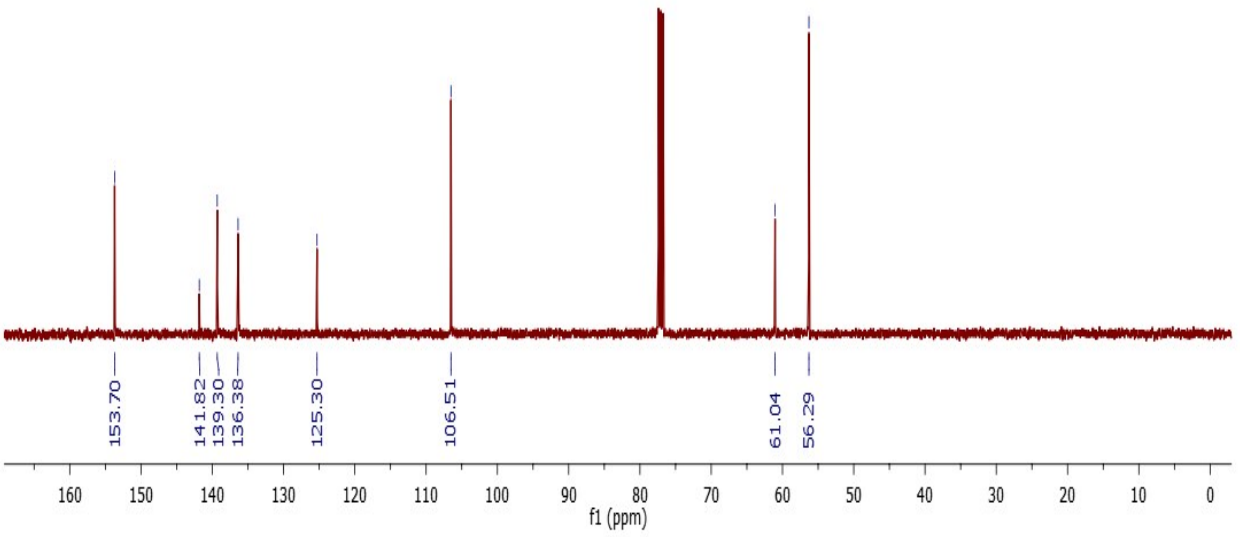
GC-MS of (E)-2-fluoro-4-methoxy-1-(2-nitrovinyl)benzene (2k)



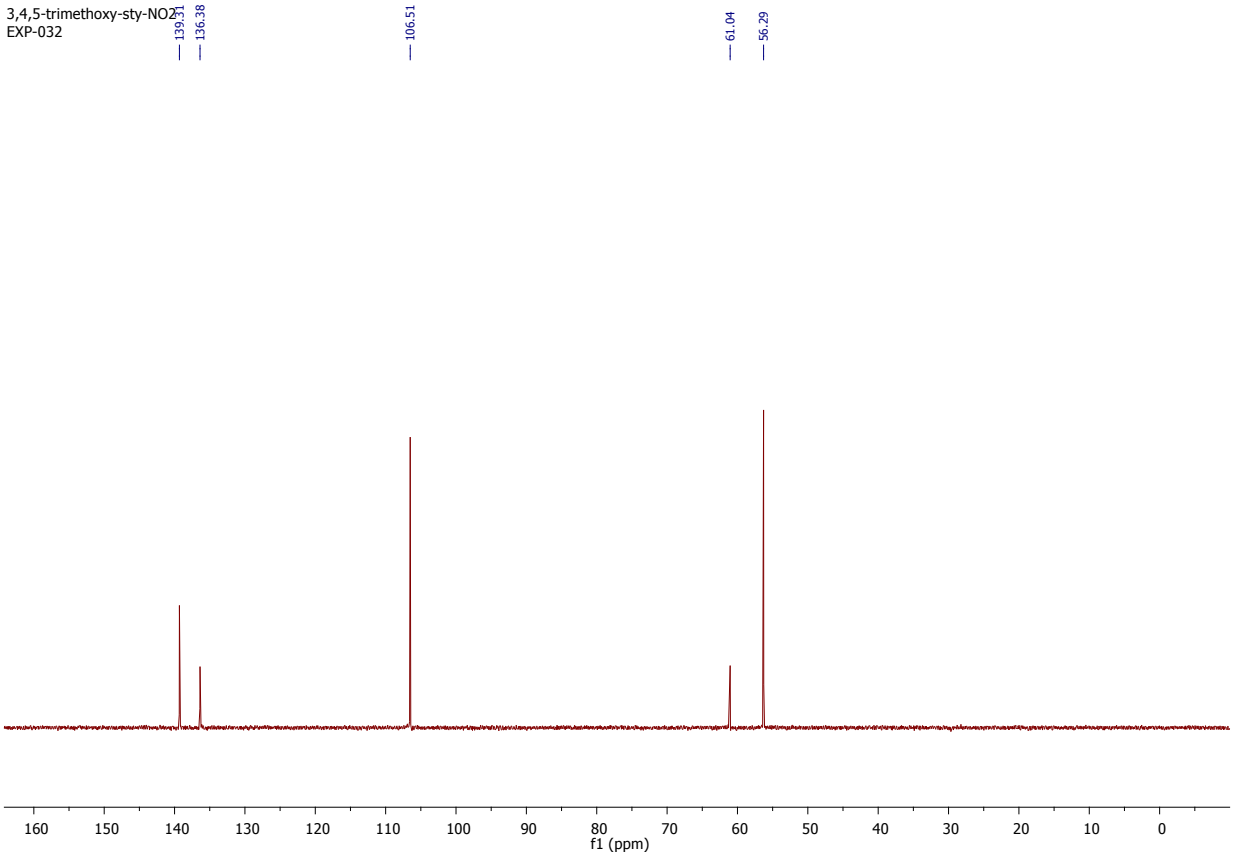
^{1}H NMR of (E)-1,2,3-trimethoxy-5-(2-nitrovinyl)benzene (2l)[10]



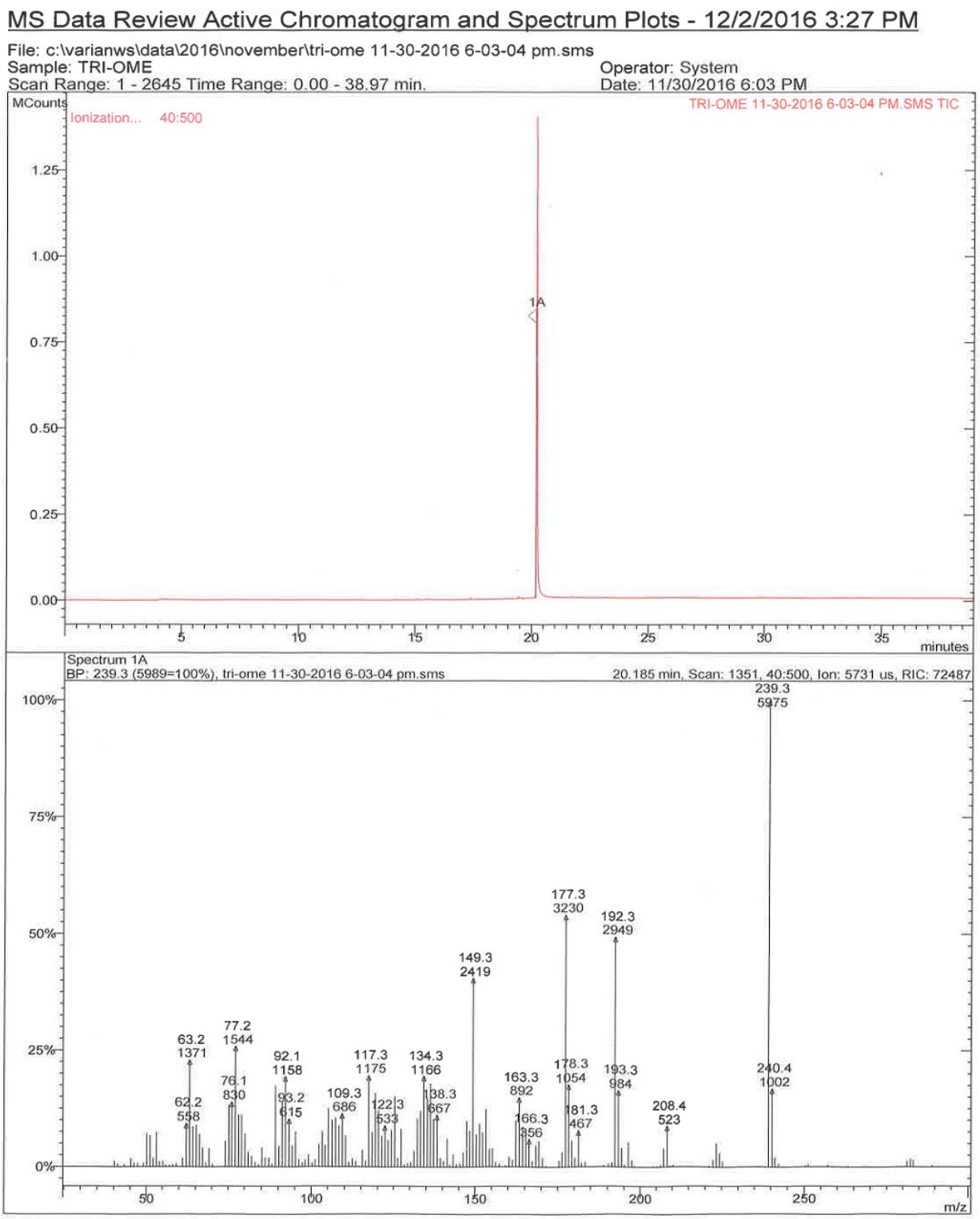
^{13}C NMR of (E)-1,2,3-trimethoxy-5-(2-nitrovinyl)benzene (2l)



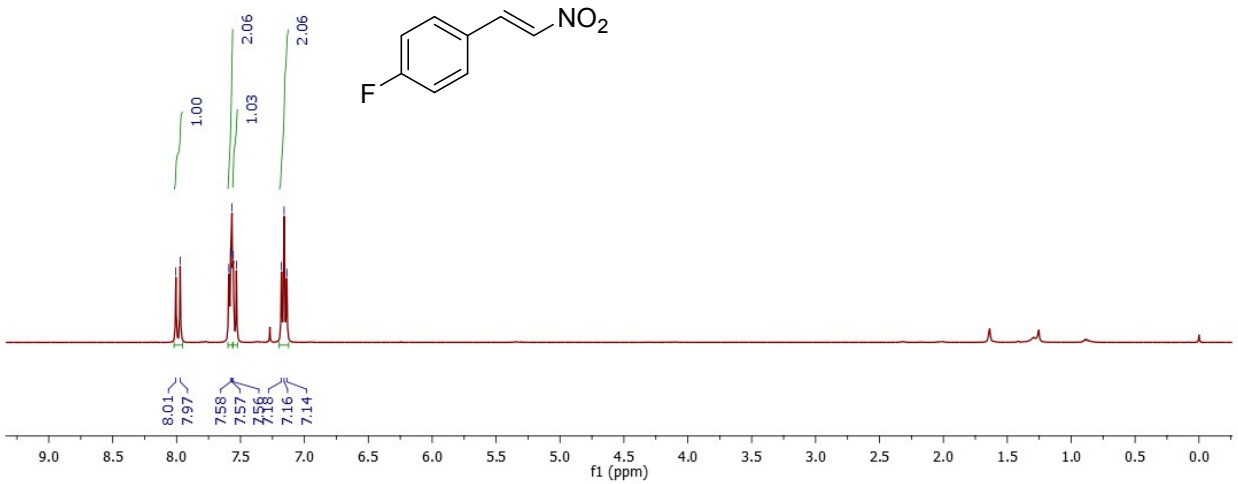
DEPT NMR of (E)-1,2,3-trimethoxy-5-(2-nitrovinyl)benzene (2l)



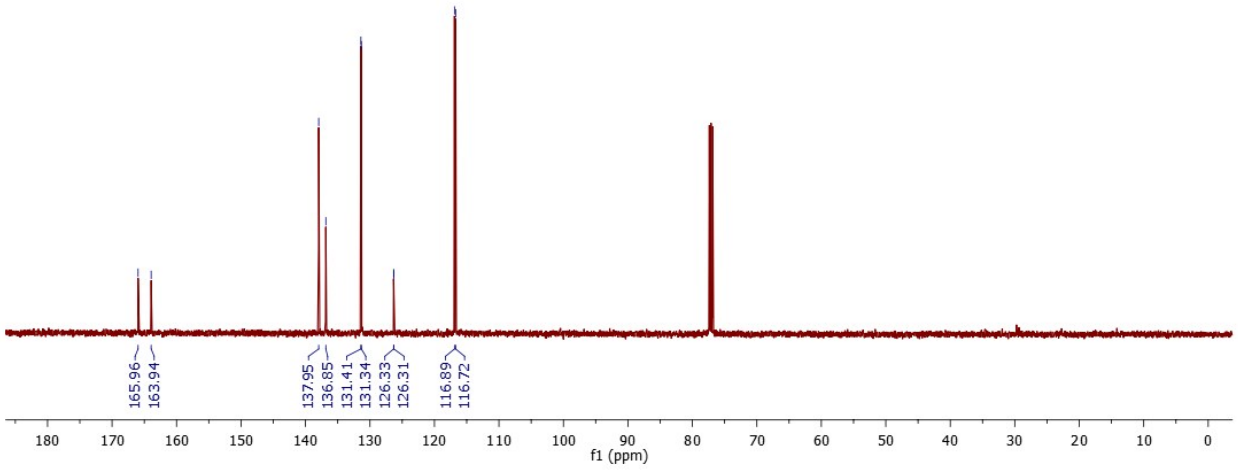
GC-MS of (E)-1,2,3-trimethoxy-5-(2-nitrovinyl)benzene (2l)



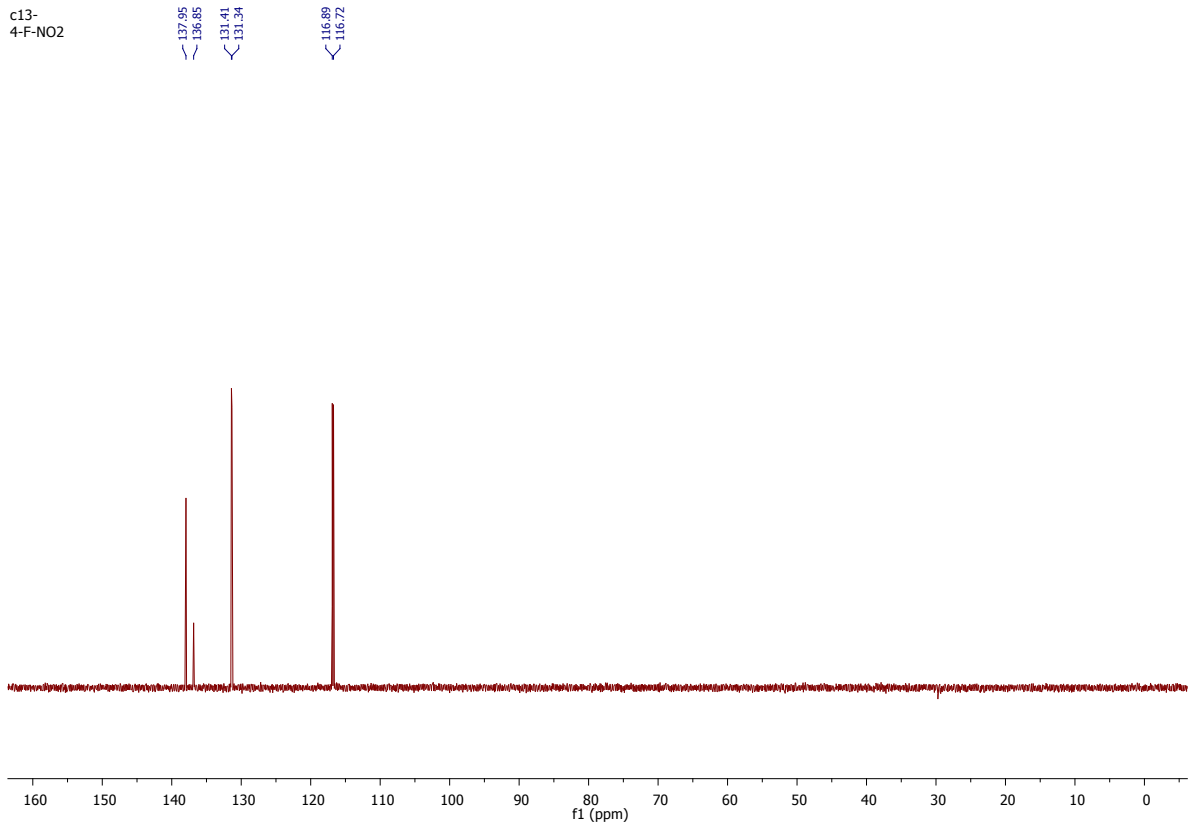
^{1}H NMR of (E)-1-fluoro-4-(2-nitrovinyl)benzene (2m)[11]



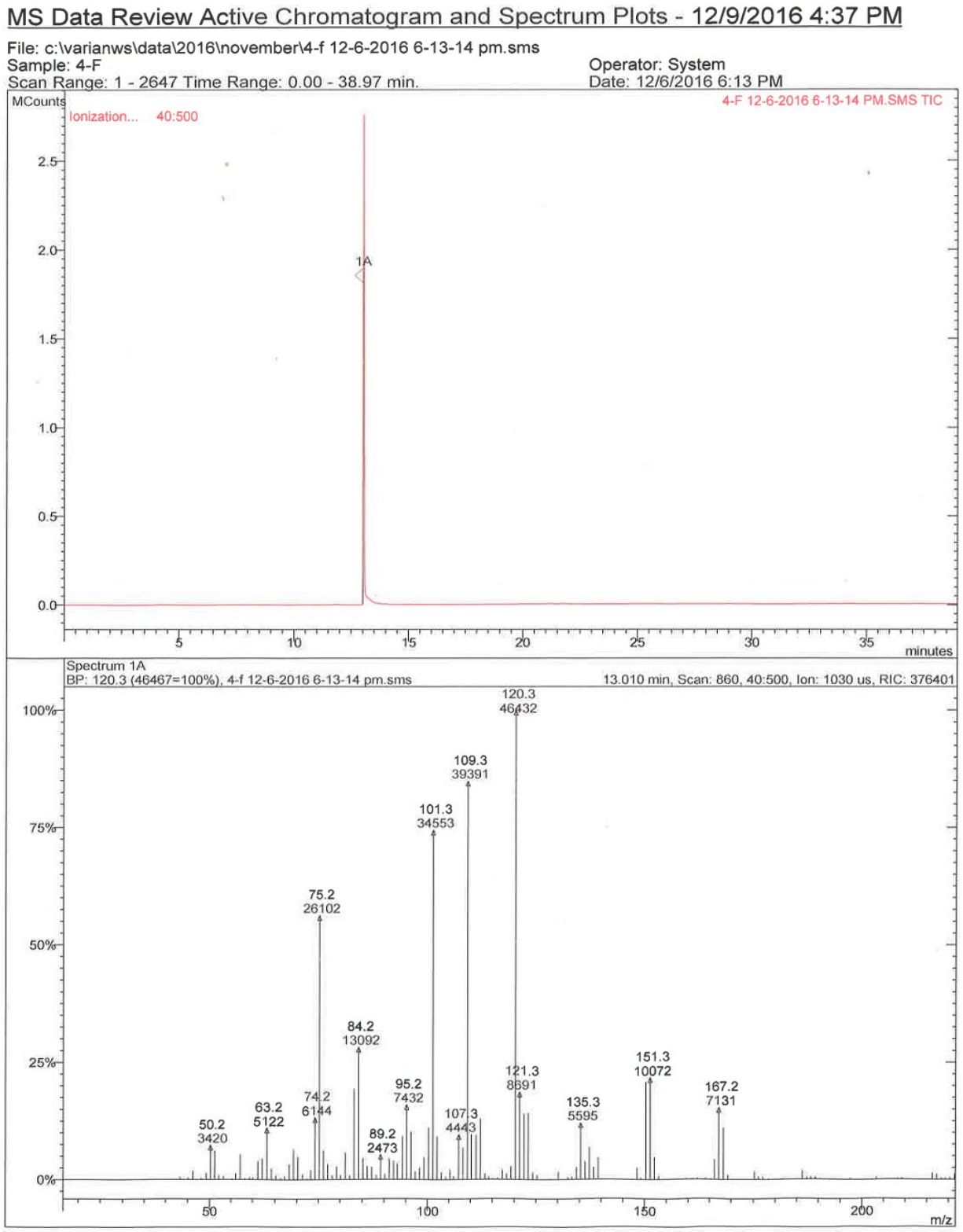
^{13}C NMR of (E)-1-fluoro-4-(2-nitrovinyl)benzene (2m)



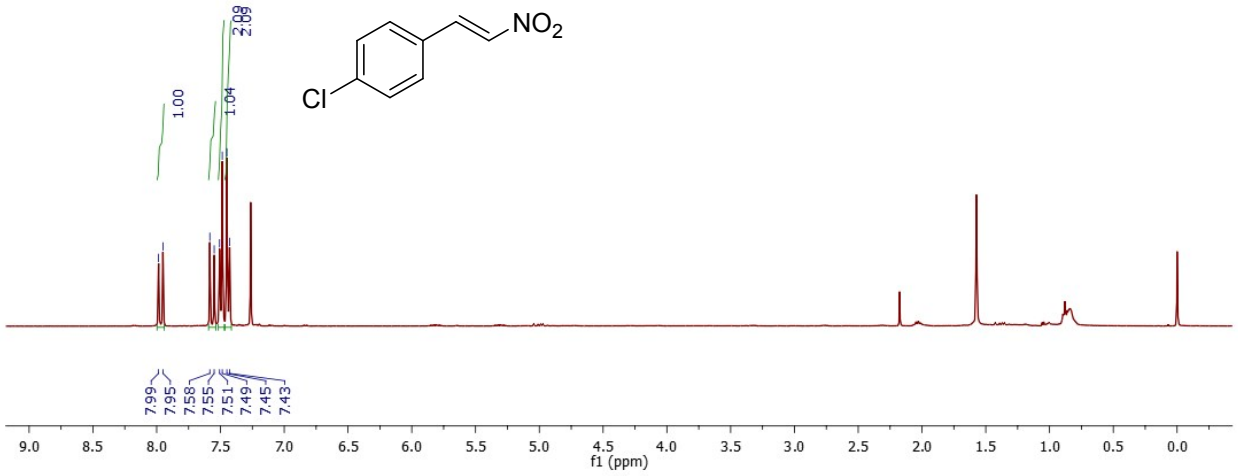
DEPT NMR of (E)-1-fluoro-4-(2-nitrovinyl)benzene (2m)



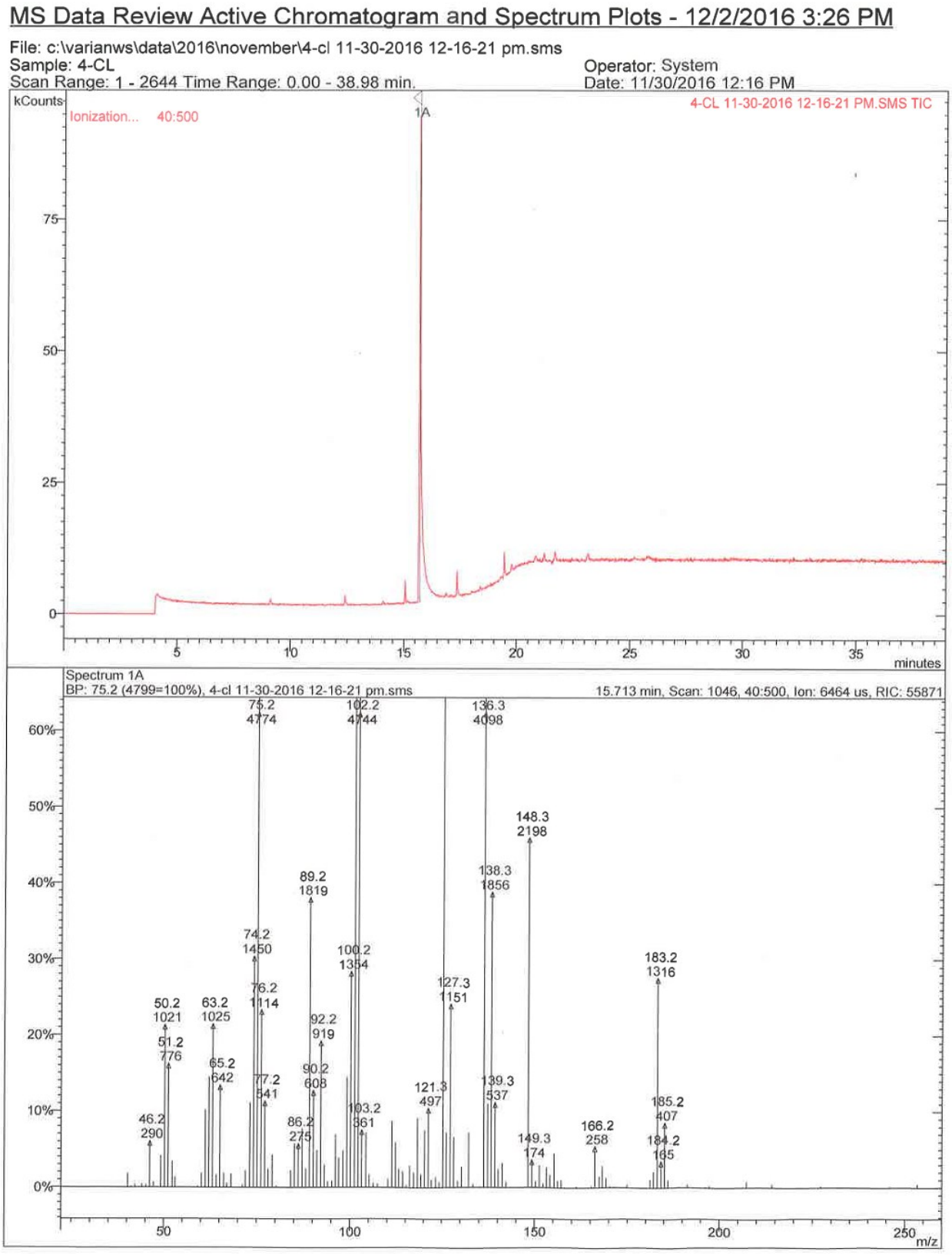
GC-MS of (E)-1-fluoro-4-(2-nitrovinyl)benzene (2m)



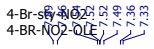
^{1}H NMR of (E)-1-chloro-4-(2-nitrovinyl)benzene (2n)[11]

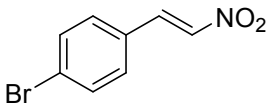


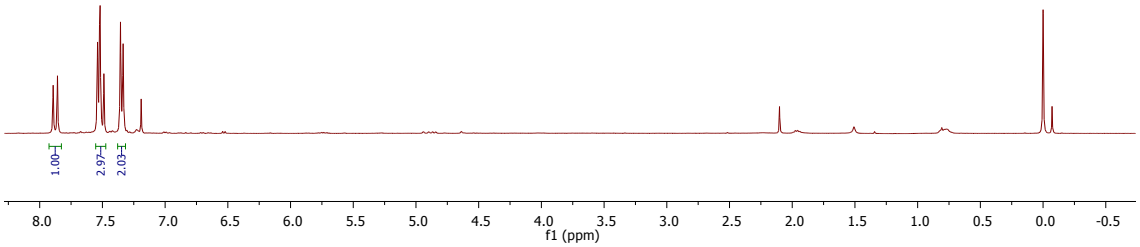
GC-MS of (E)-1-chloro-4-(2-nitrovinyl)benzene (2n)



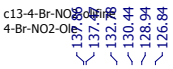
^{1}H NMR of (E)-1-bromo-4-(2-nitrovinyl)benzene (2o)[11]

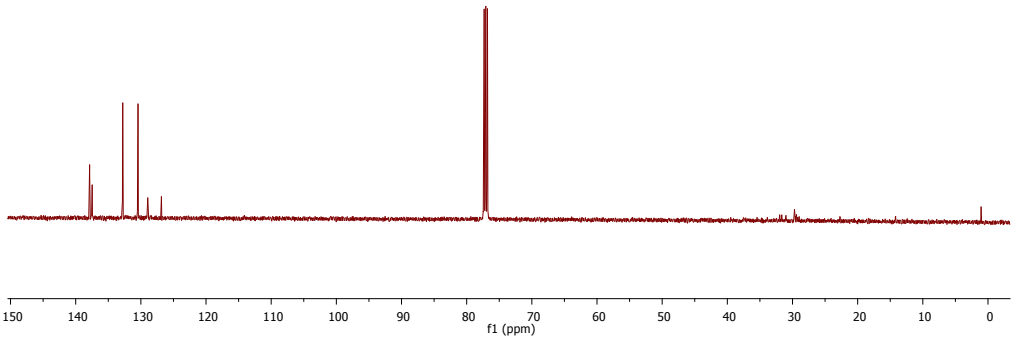




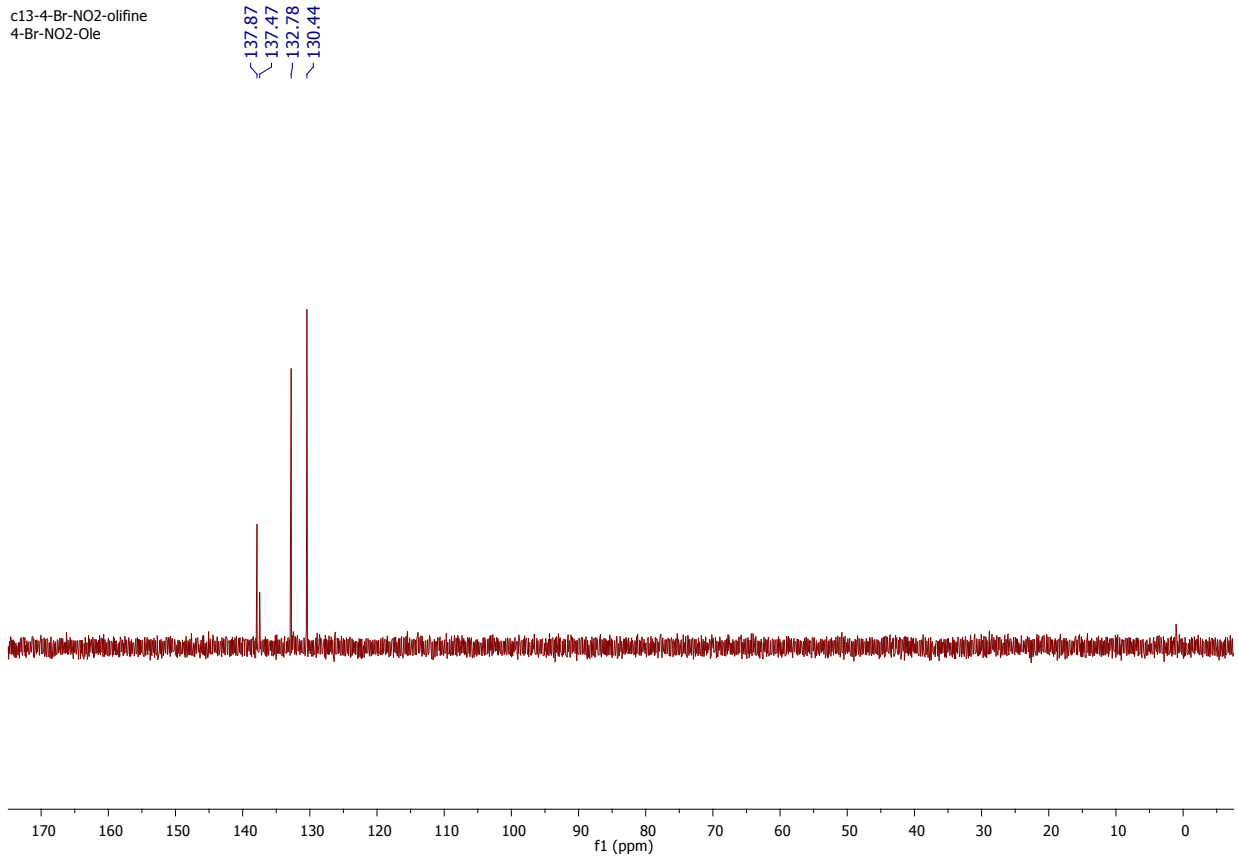


^{13}C NMR of (E)-1-bromo-4-(2-nitrovinyl)benzene (2o)

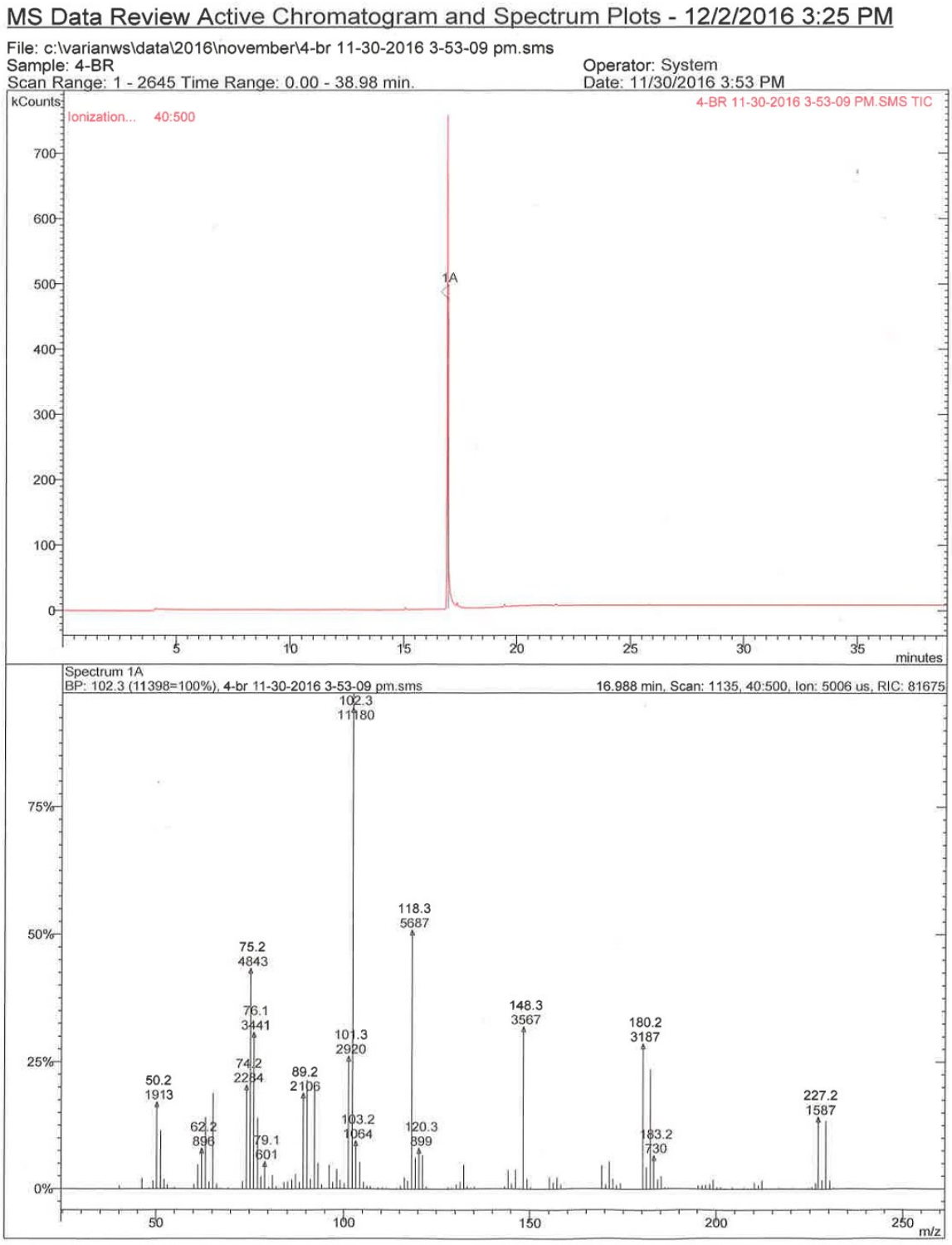




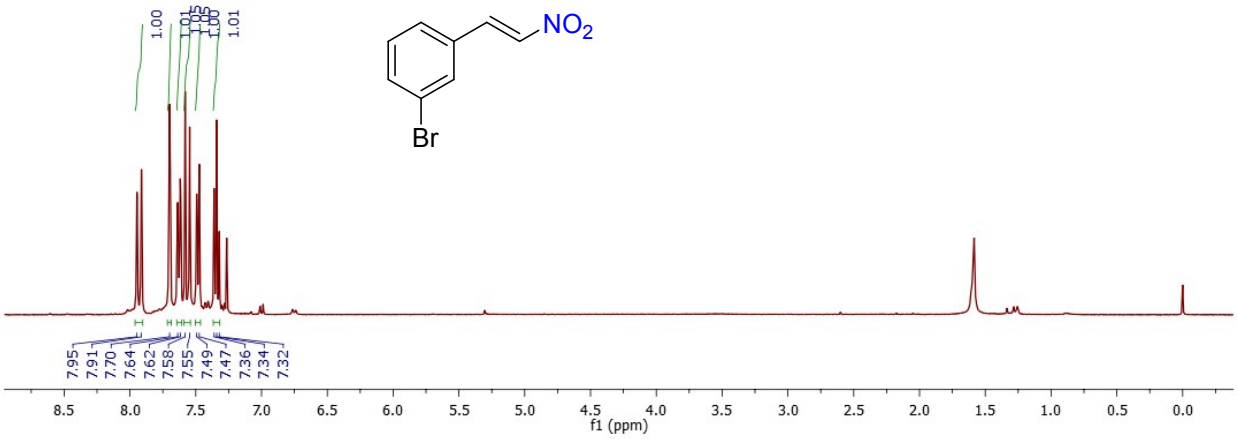
DEPT NMR of (E)-1-bromo-4-(2-nitrovinyl)benzene (2o)



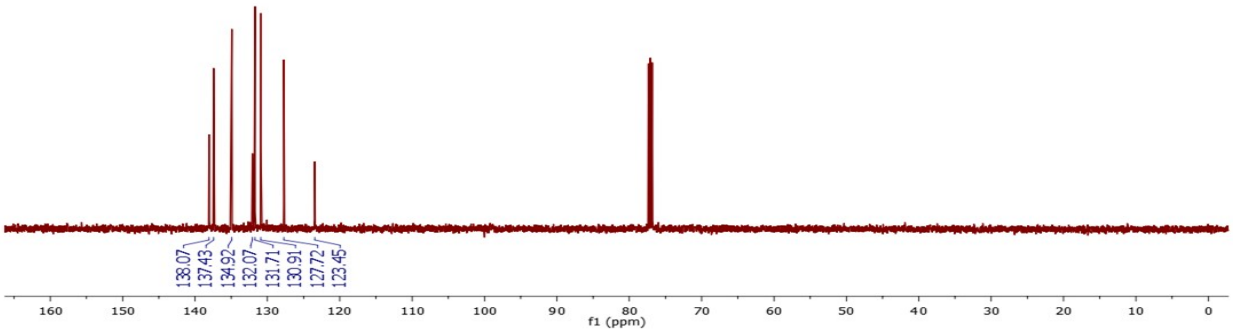
GC-MS of (E)-1-bromo-4-(2-nitrovinyl)benzene (2o)



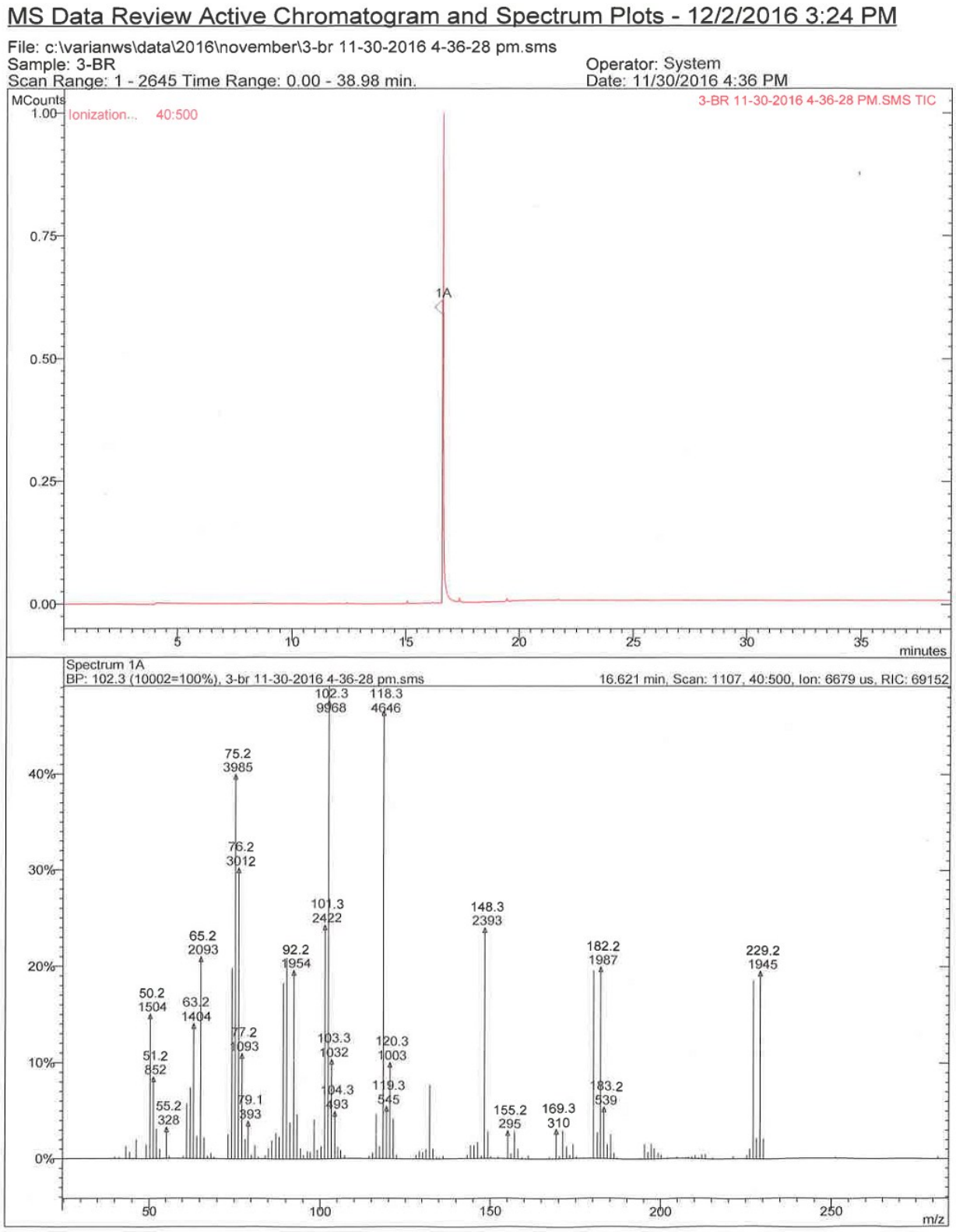
^{1}H NMR of (E)-1-bromo-3-(2-nitrovinyl)benzene (2p)[16]



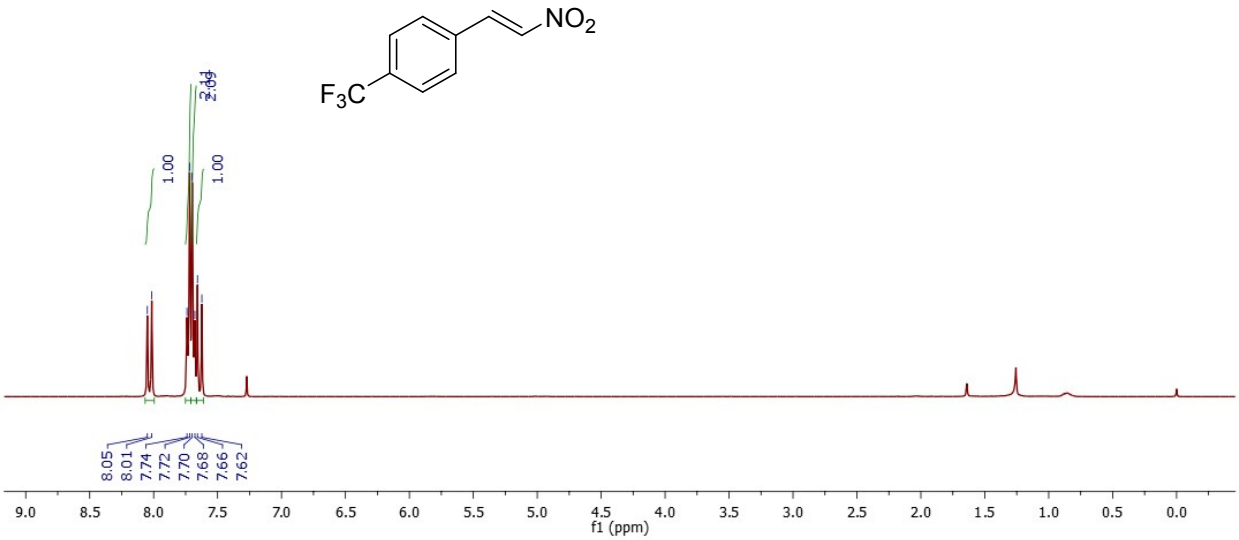
^{13}C NMR of (E)-1-bromo-3-(2-nitrovinyl)benzene (2p)



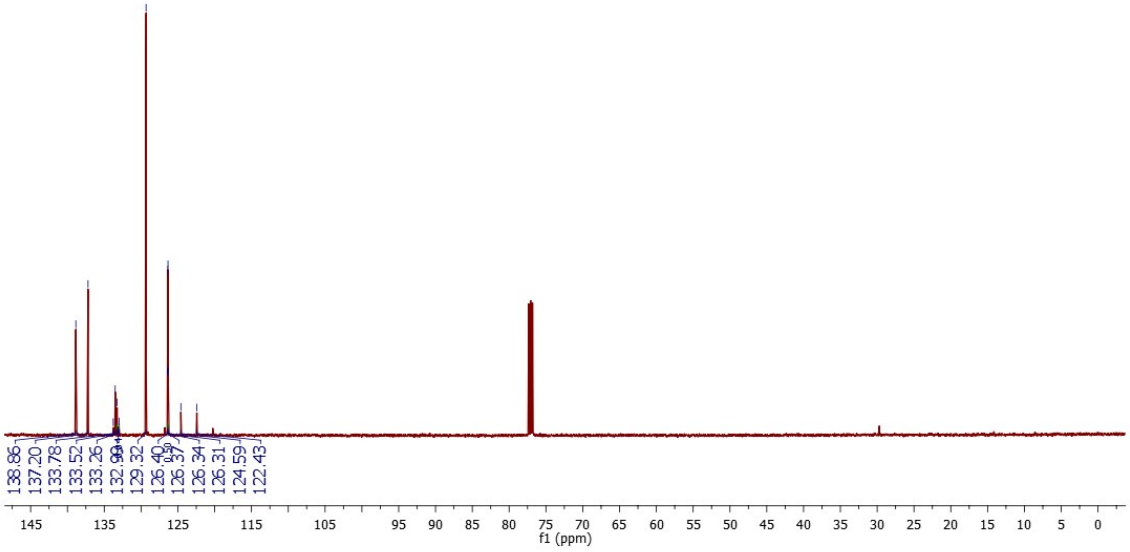
GC-MS of (E)-1-bromo-3-(2-nitrovinyl)benzene (2p)



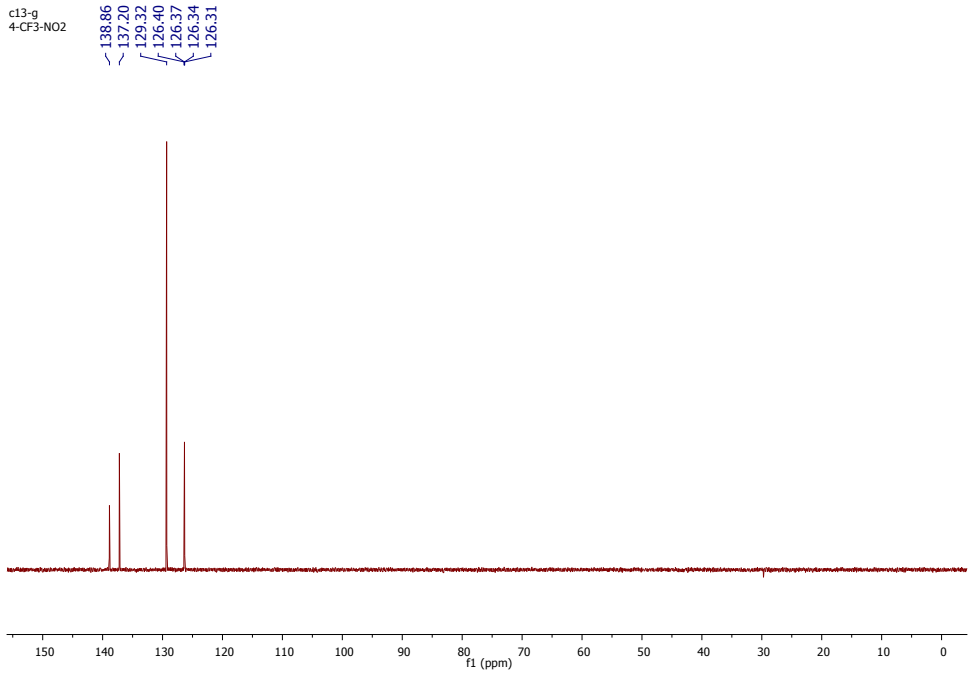
^{1}H NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethyl)benzene (2q)[12]



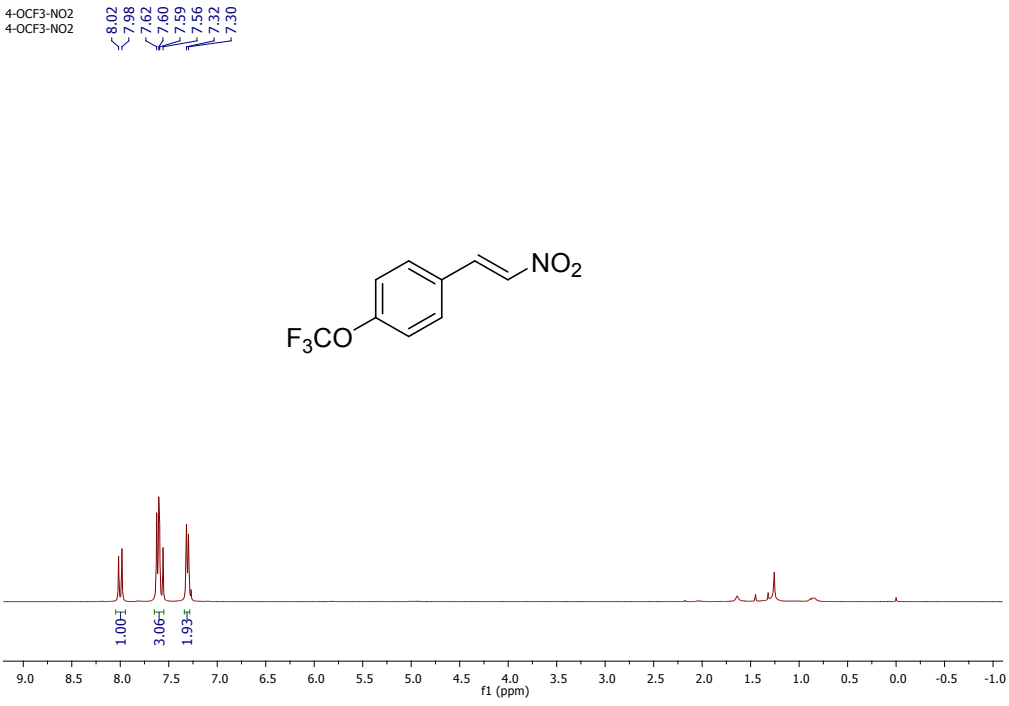
^{13}C NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethyl)benzene (2q)



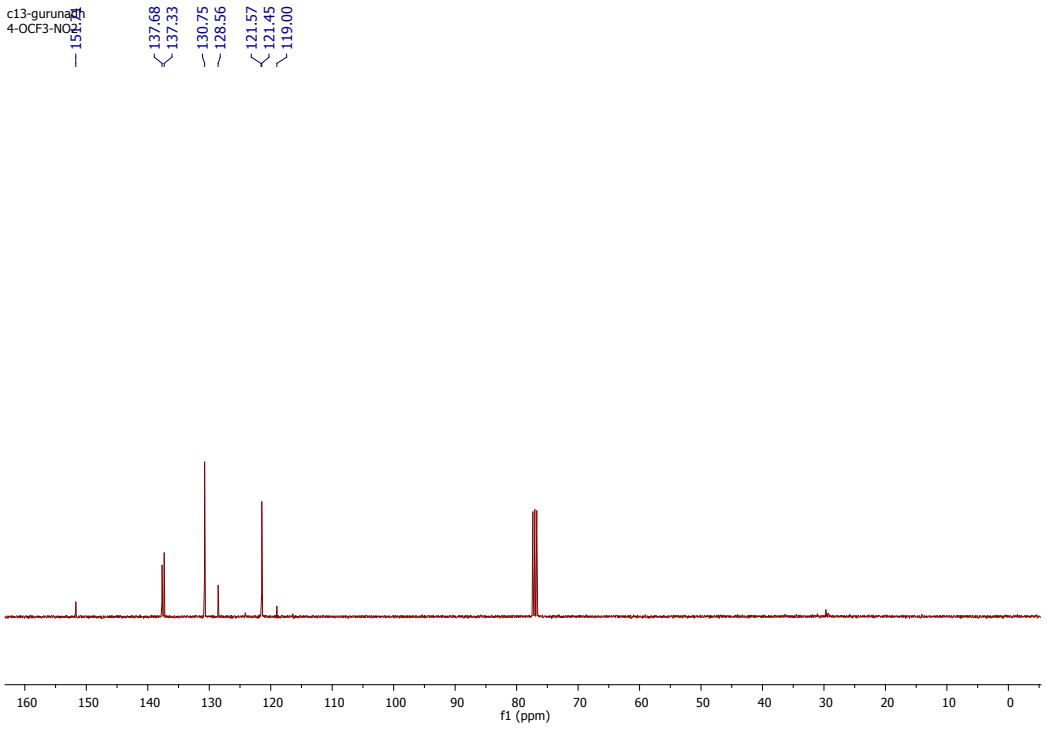
DEPT NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethyl)benzene (2q)



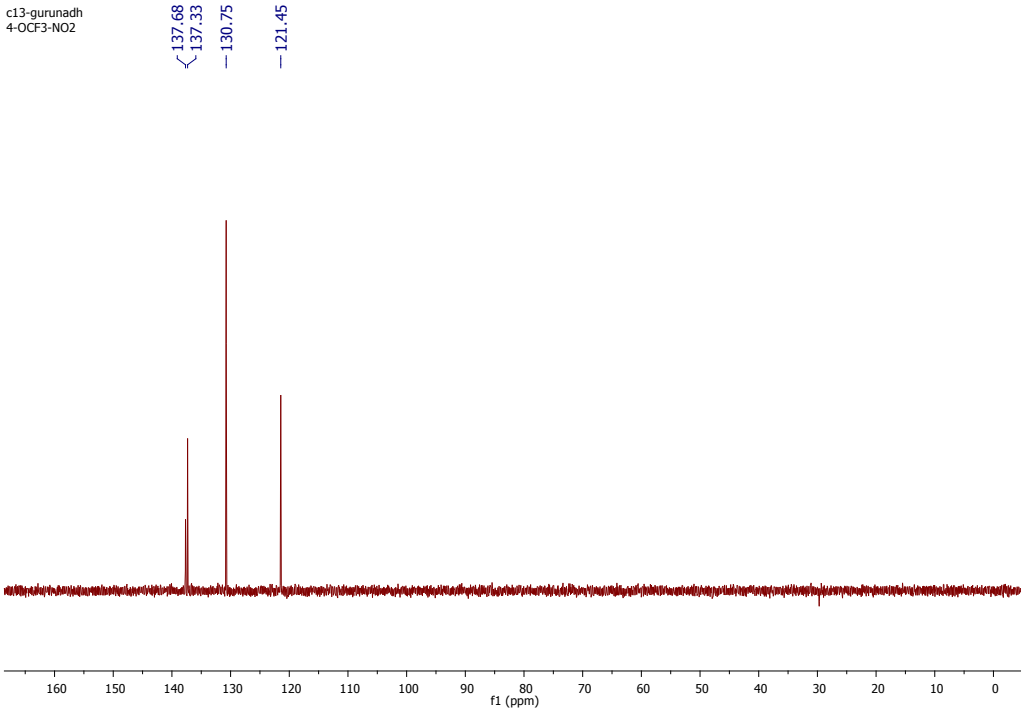
^{1}H NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethoxy)benzene (2r)[11]



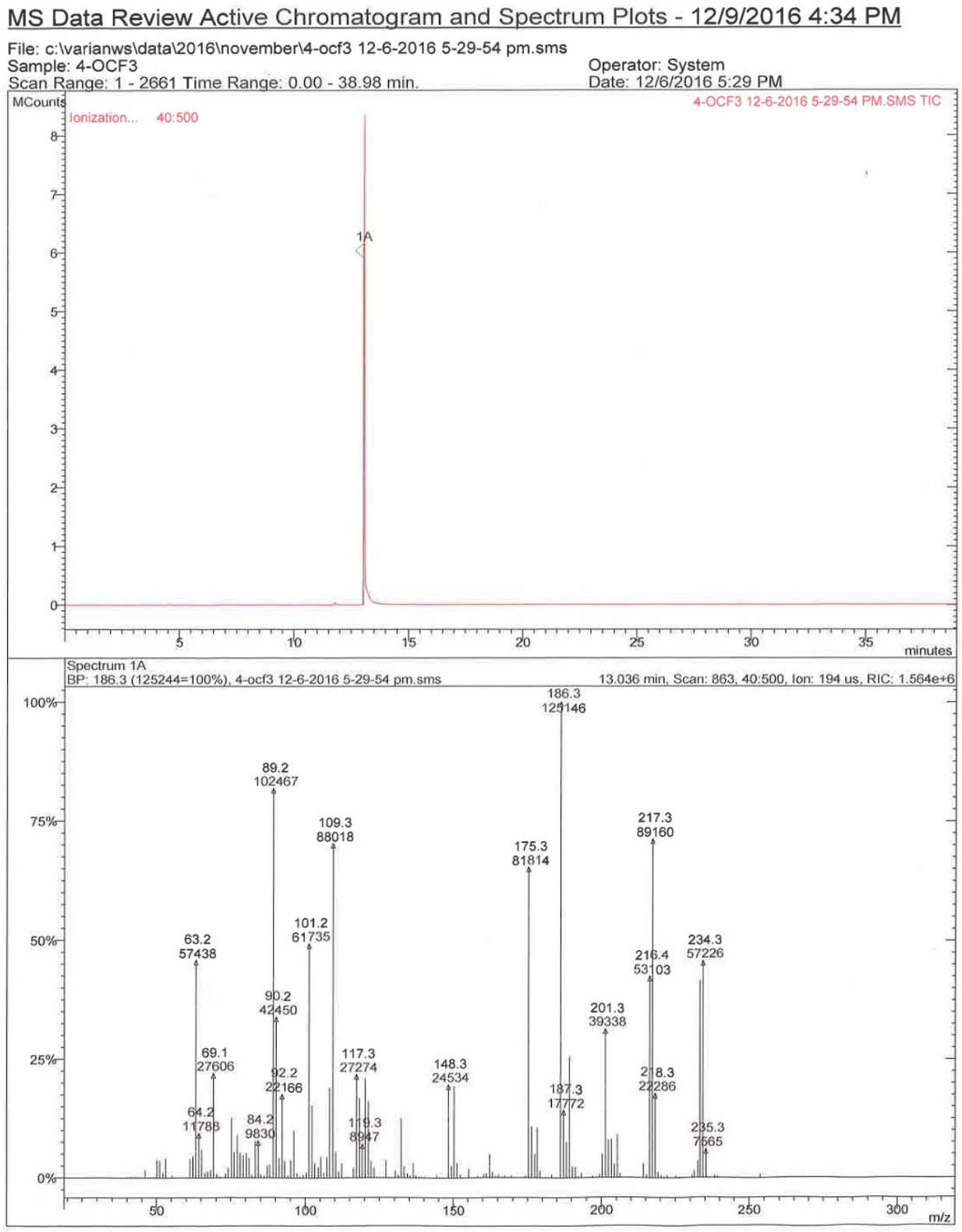
^{13}C NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethoxy)benzene (2r)



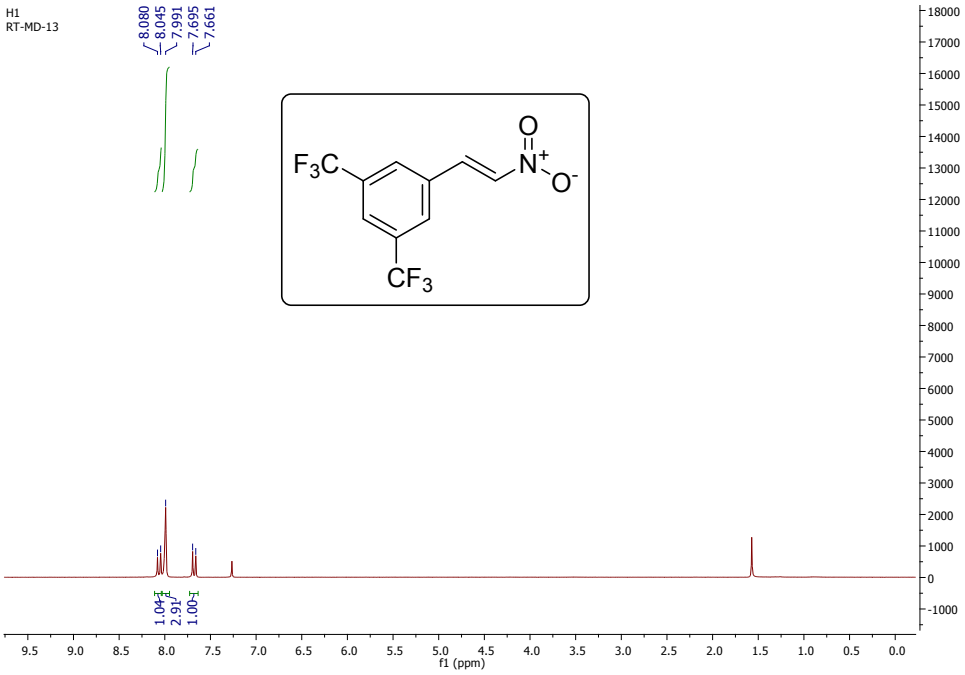
DEPT NMR of (E)-1-(2-nitrovinyl)-4-(trifluoromethoxy)benzene (2r)



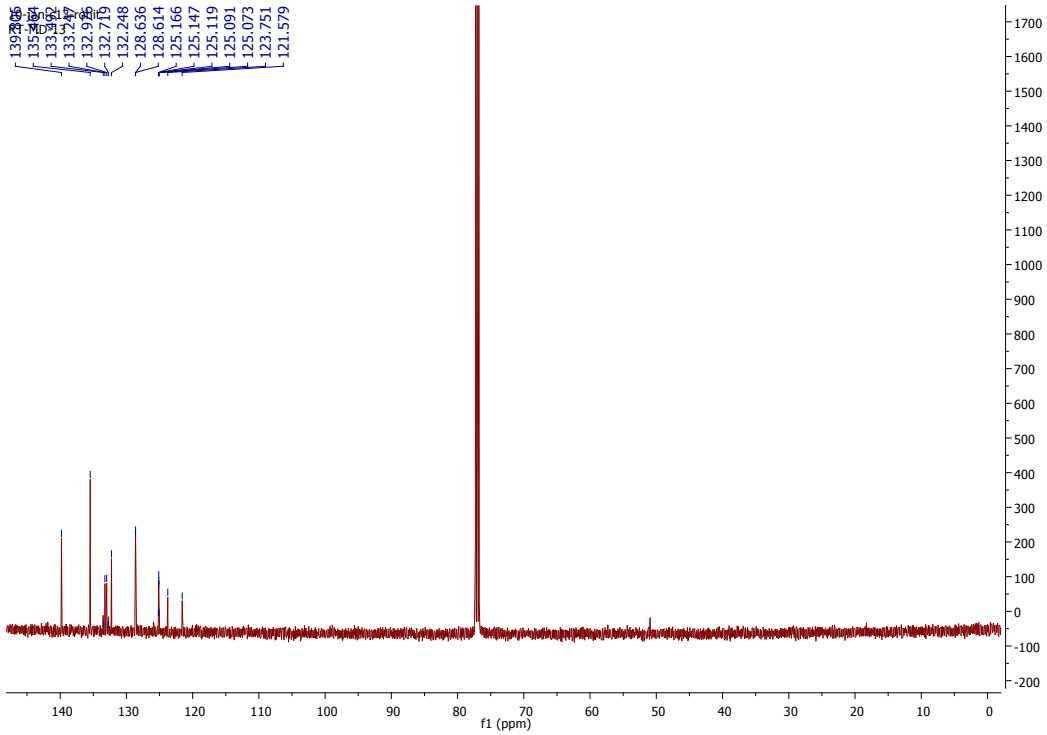
GC-MS of (E)-1-(2-nitrovinyl)-4-(trifluoromethoxy)benzene (2r)



^{1}H NMR of (E)-1-(2-nitrovinyl)-3,5-bis(trifluoromethyl)benzene (2s)[12]

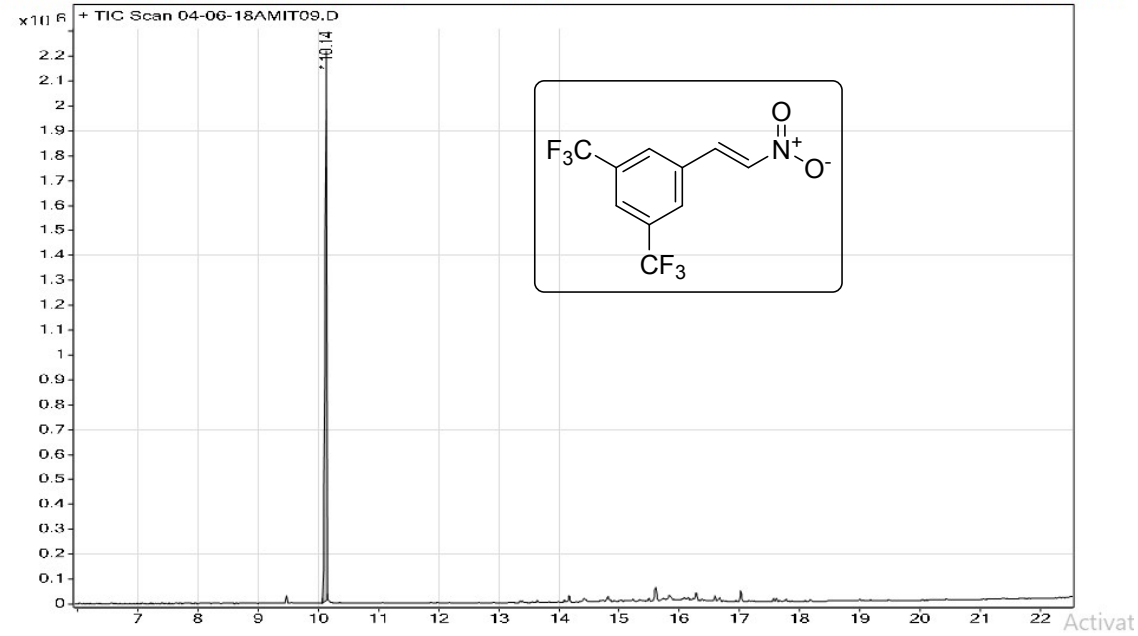


^{13}C of (E)-1-(2-nitrovinyl)-3,5-bis(trifluoromethyl)benzene (2s)

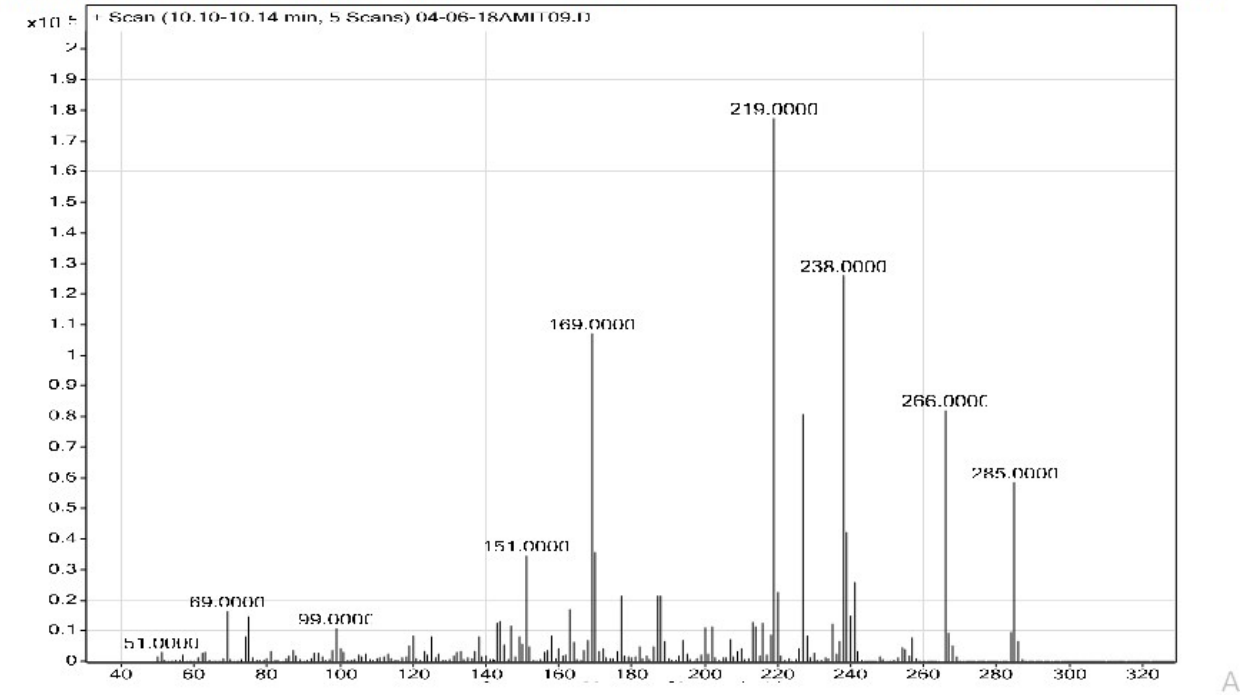


GC-MS Spectra of (E)-1-(2-nitrovinyl)-3,5-bis(trifluoromethyl)benzene (2s)

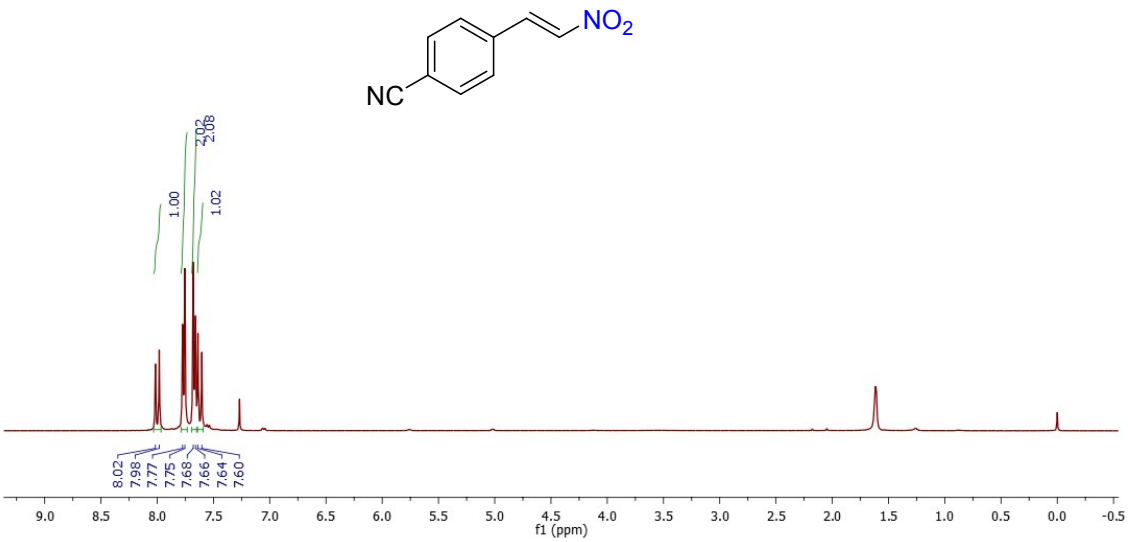
Sample Name	MD-13	**Position**	9	**Instrument Name**	GCMS	**User Name**	manager
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	04-06-18AMIT09.D	**ACQ Method**	AMIT.M	**Comment**		**Acquired Time**	6/5/2018 7:45:46 PM



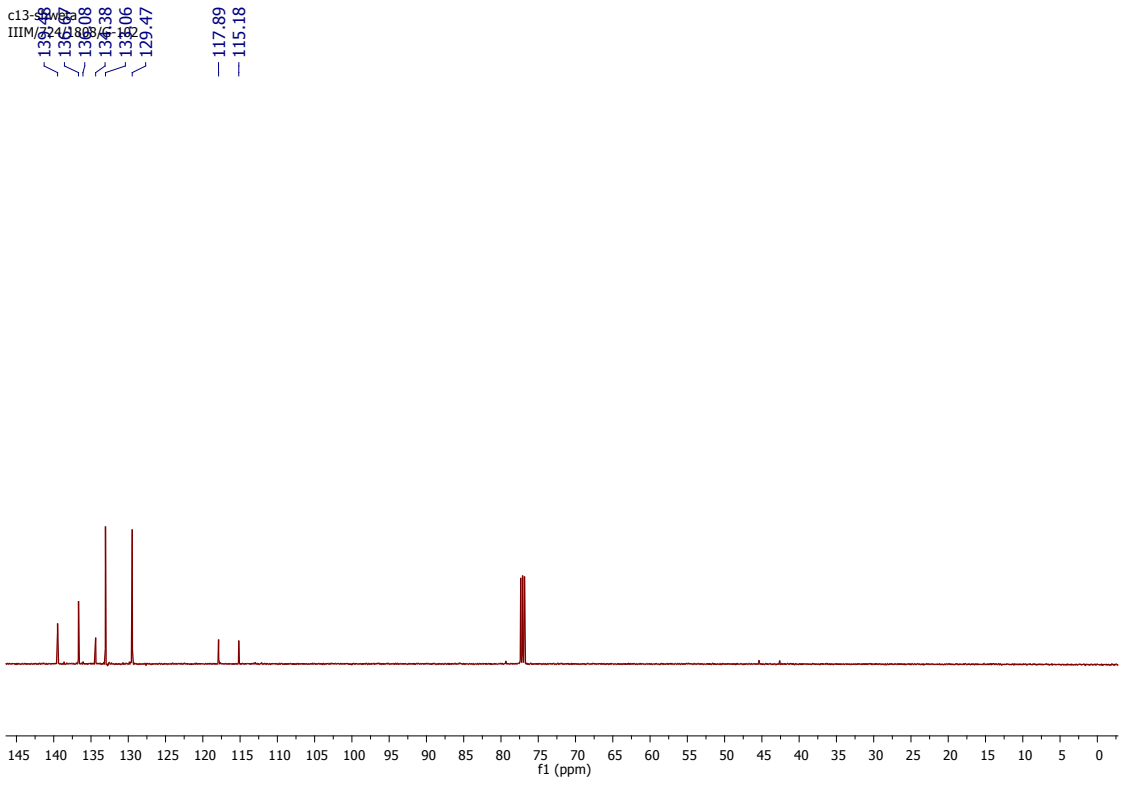
Sample Name	MD-13	**Position**	9	**Instrument Name**	GCMS	**User Name**	manager
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	04-06-18AMIT09.D	**ACQ Method**	AMIT.M	**Comment**		**Acquired Time**	6/5/2018 7:45:46 PM



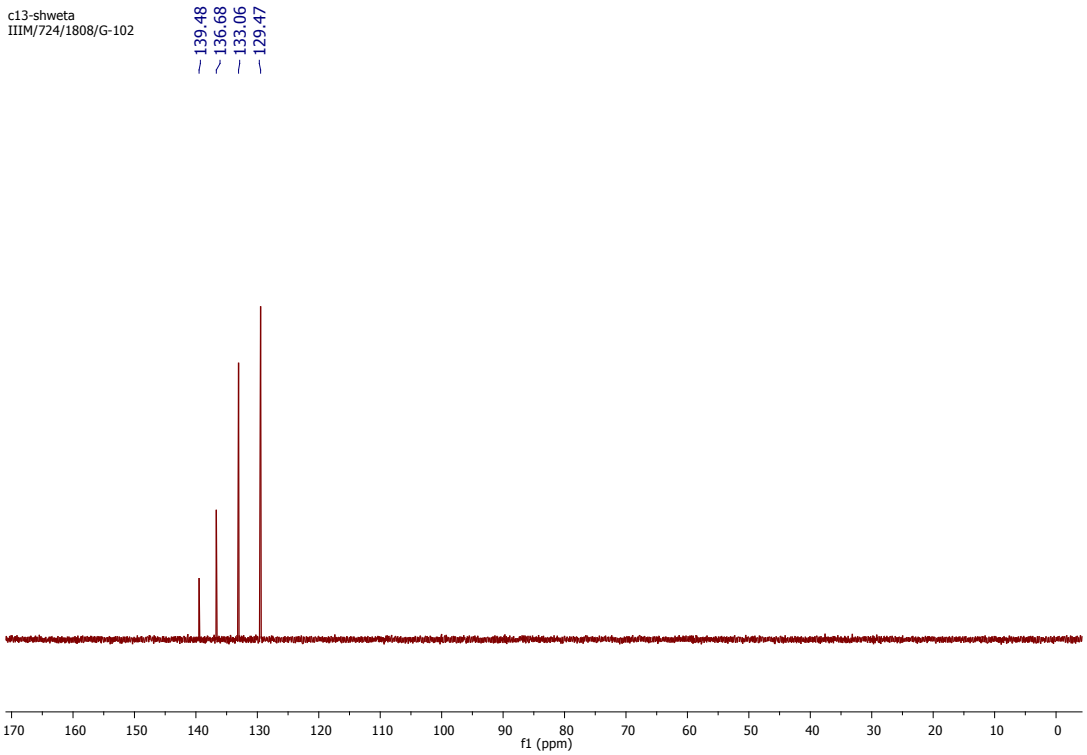
^{1}H NMR of (E)-4-(2-nitrovinyl)benzonitrile (2t)[13]



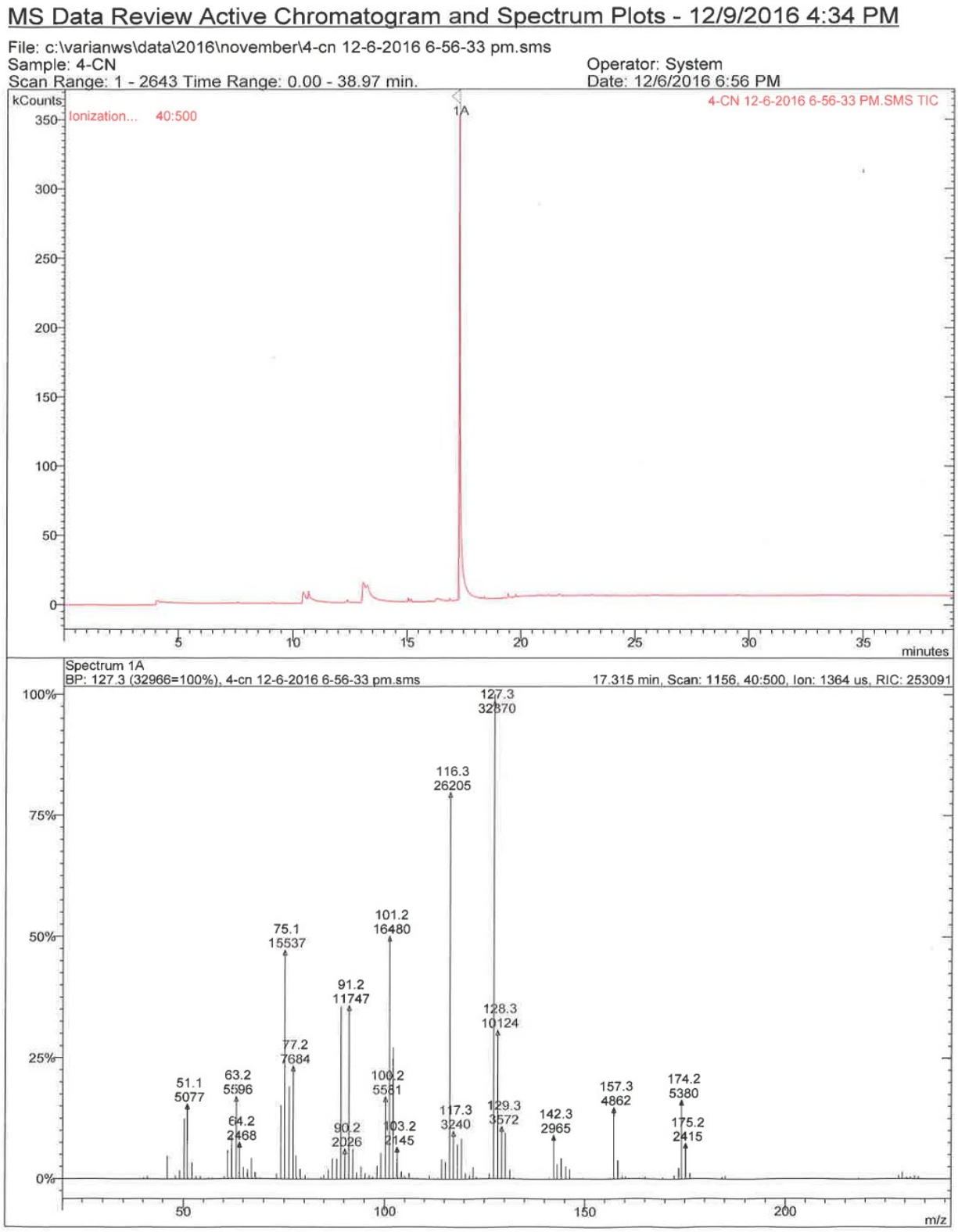
^{13}C NMR of (E)-4-(2-nitrovinyl)benzonitrile (2t)



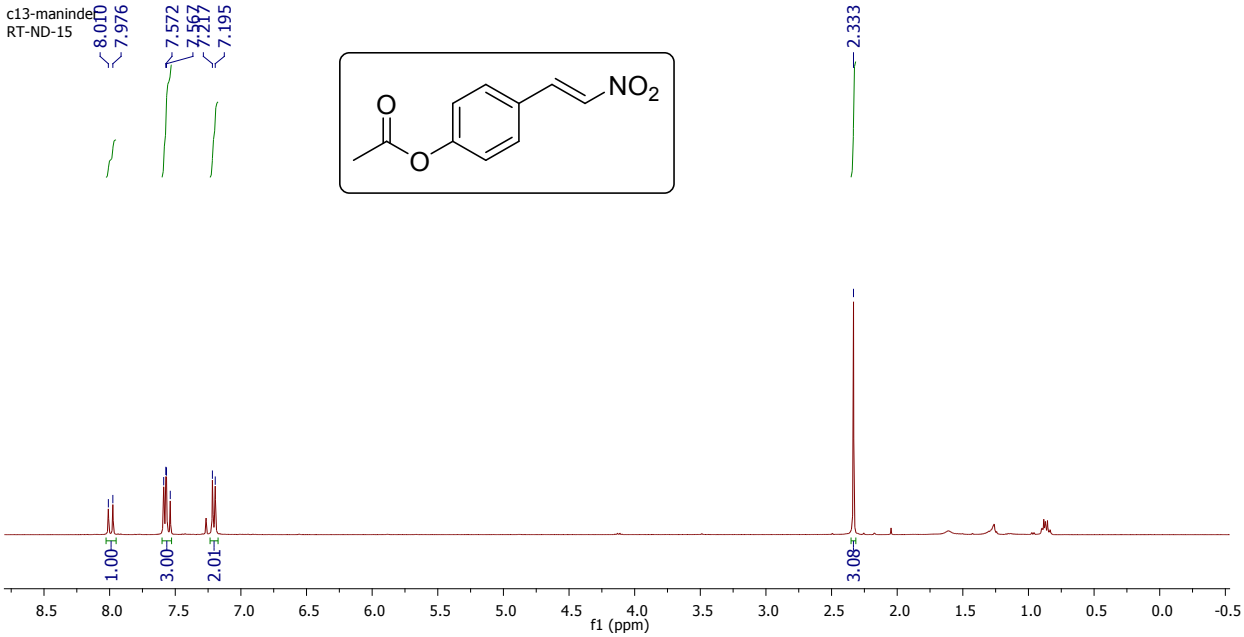
DEPT NMR of (E)-4-(2-nitrovinyl)benzonitrile (2t)



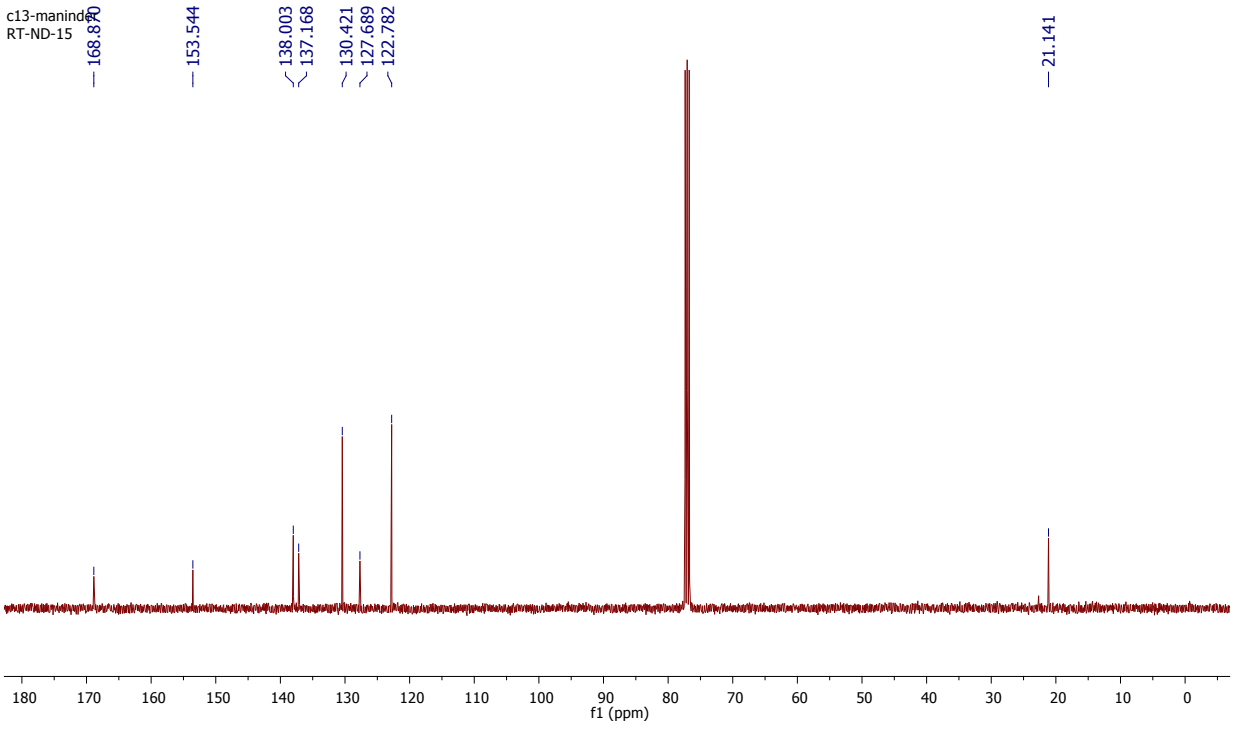
GC-MS of (E)-4-(2-nitrovinyl)benzonitrile (2t)



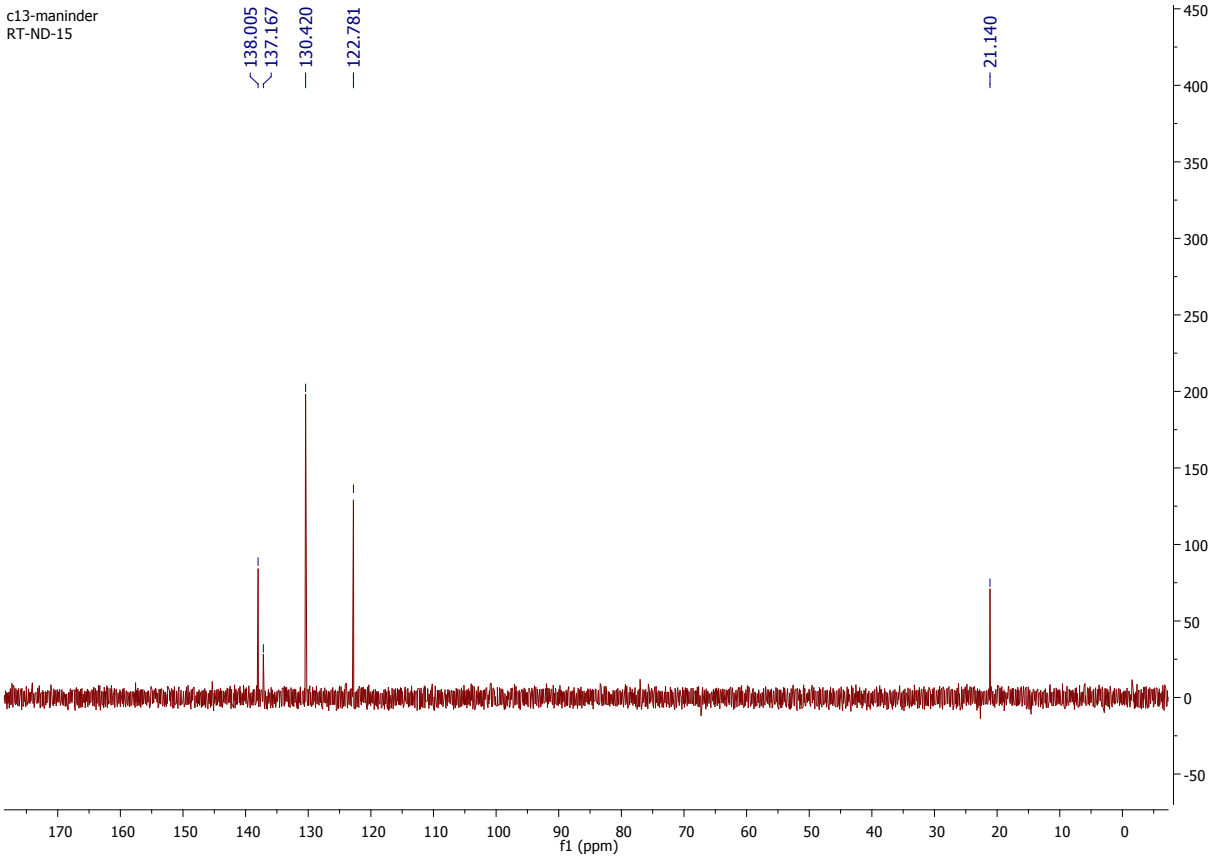
^{1}H NMR OF (E)-4-(2-nitrovinyl)phenyl acetate(2u)[14]



^{13}C NMR of (E)-4-(2-nitrovinyl)phenyl acetate(2u)

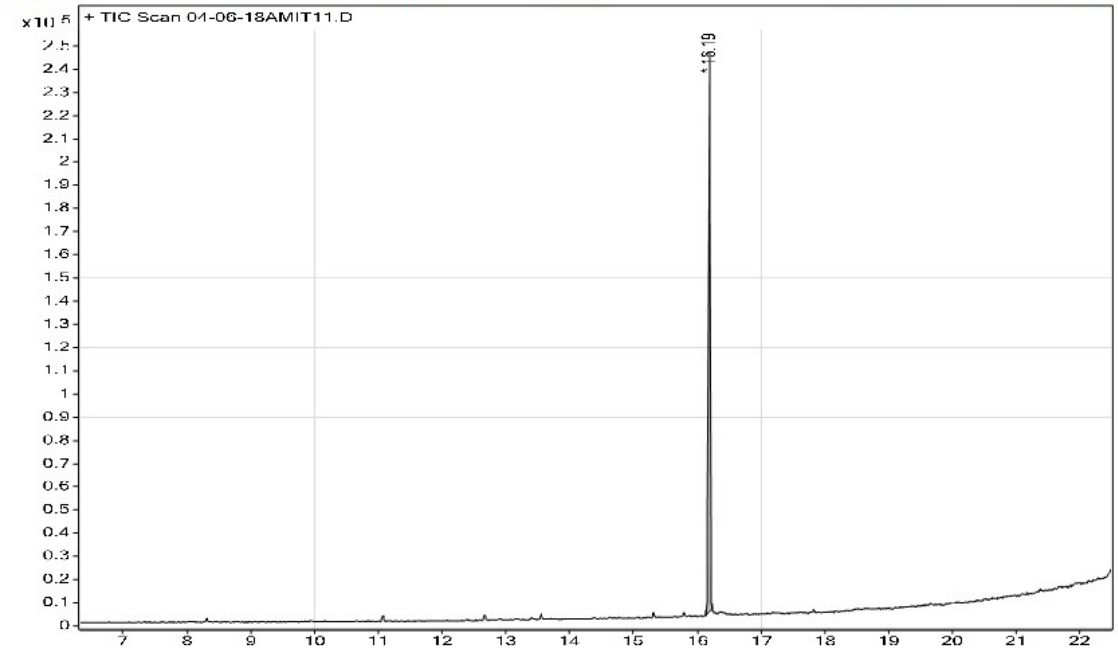


DEPT NMR of (E)-4-(2-nitrovinyl)phenyl acetate(2u)

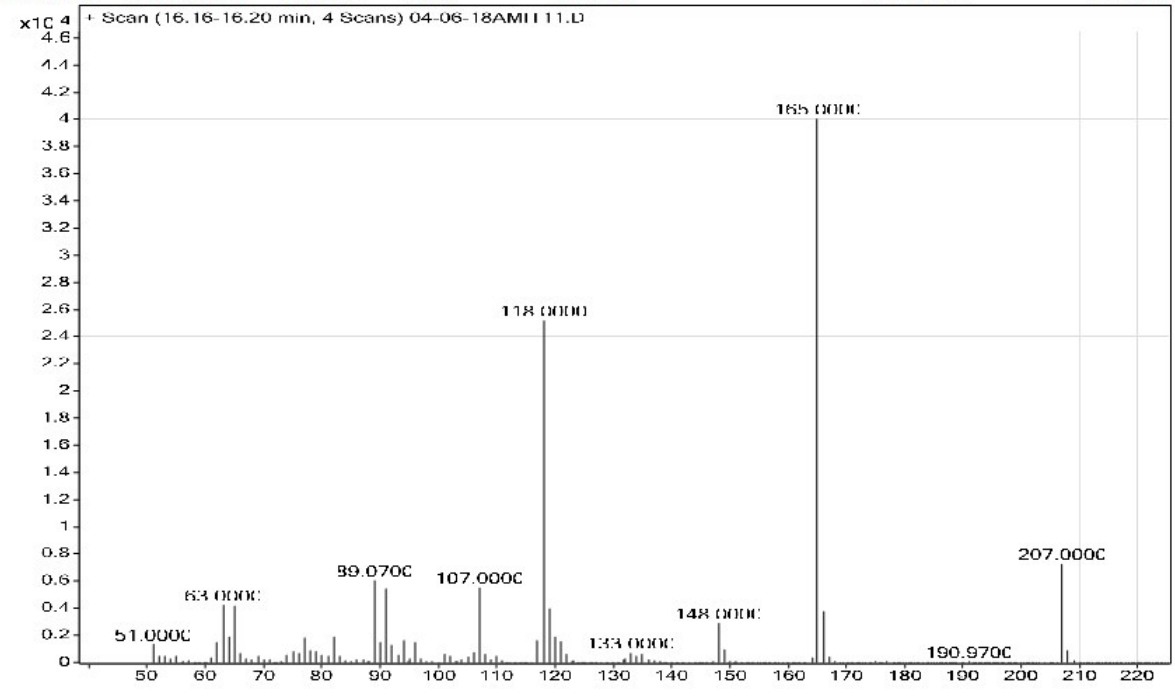


GC-MS spectra of (E)-4-(2-nitrovinyl)phenyl acetate(2u)

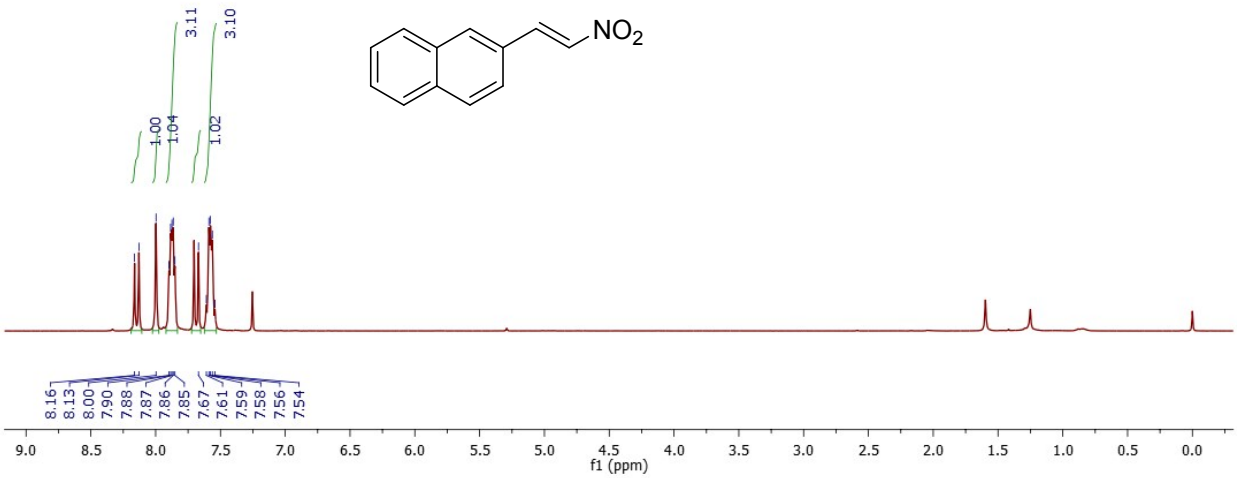
Sample Name	MD-15	**Position**	11	**Instrument Name**	GCMS	**User Name**	manager
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	04-06-18AMIT11.D	**ACQ Method**	AMIT.M	**Comment**		**Acquired Time**	6/5/2018 7:46:02 PM



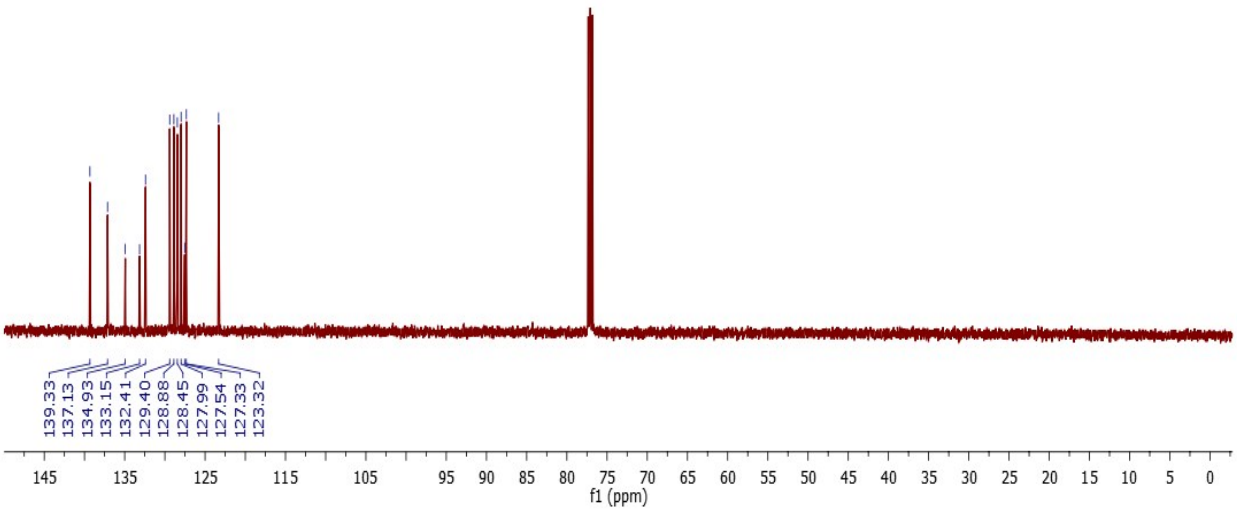
Sample Name	MD-15	**Position**	11	**Instrument Name**	GCMS	**User Name**	manager
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	04-06-18AMIT11.D	**ACQ Method**	AMIT.M	**Comment**		**Acquired Time**	6/5/2018 7:46:02 PM



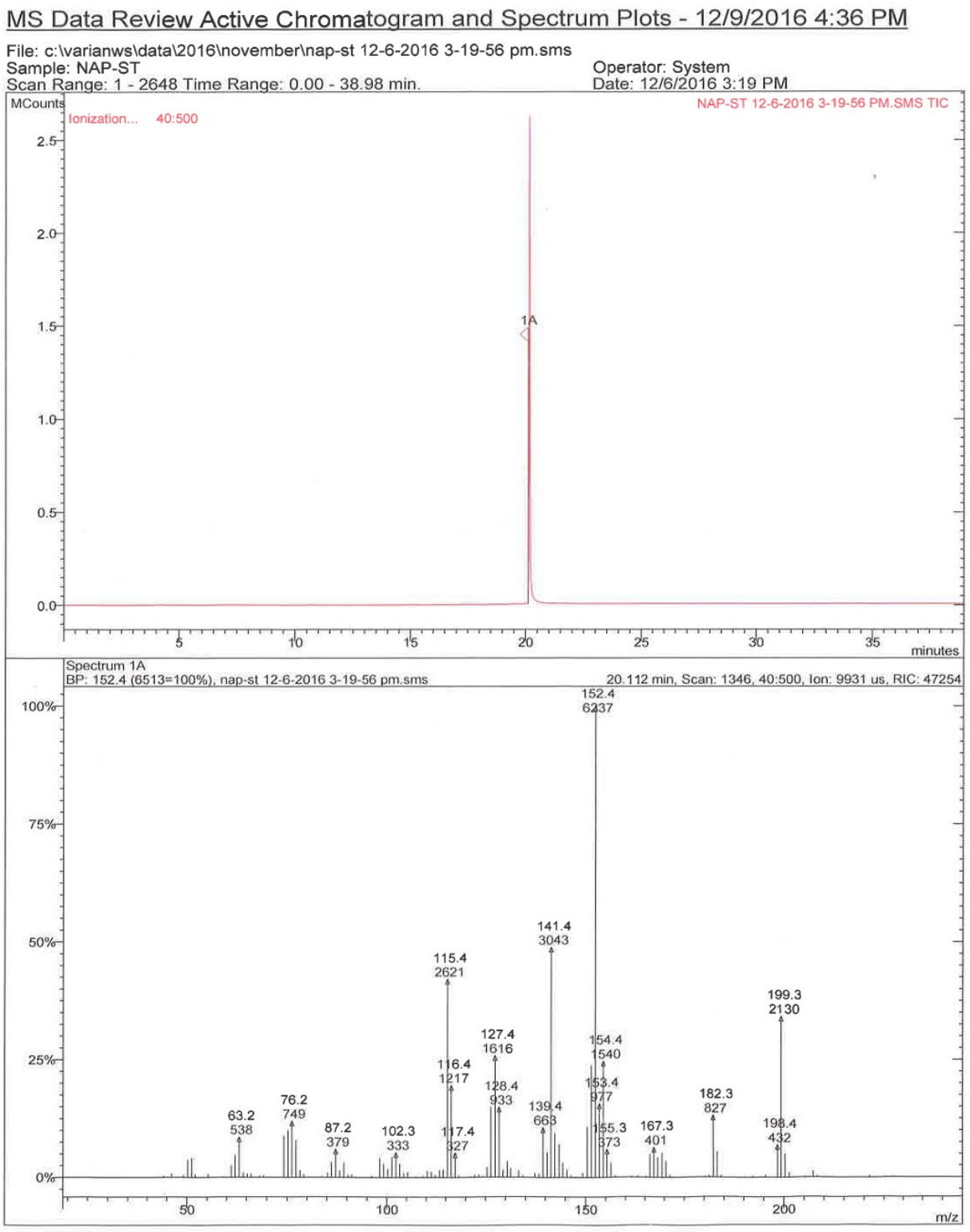
^{1}H NMR of (E)-2-(2-nitrovinyl)naphthalene (2v)[15]



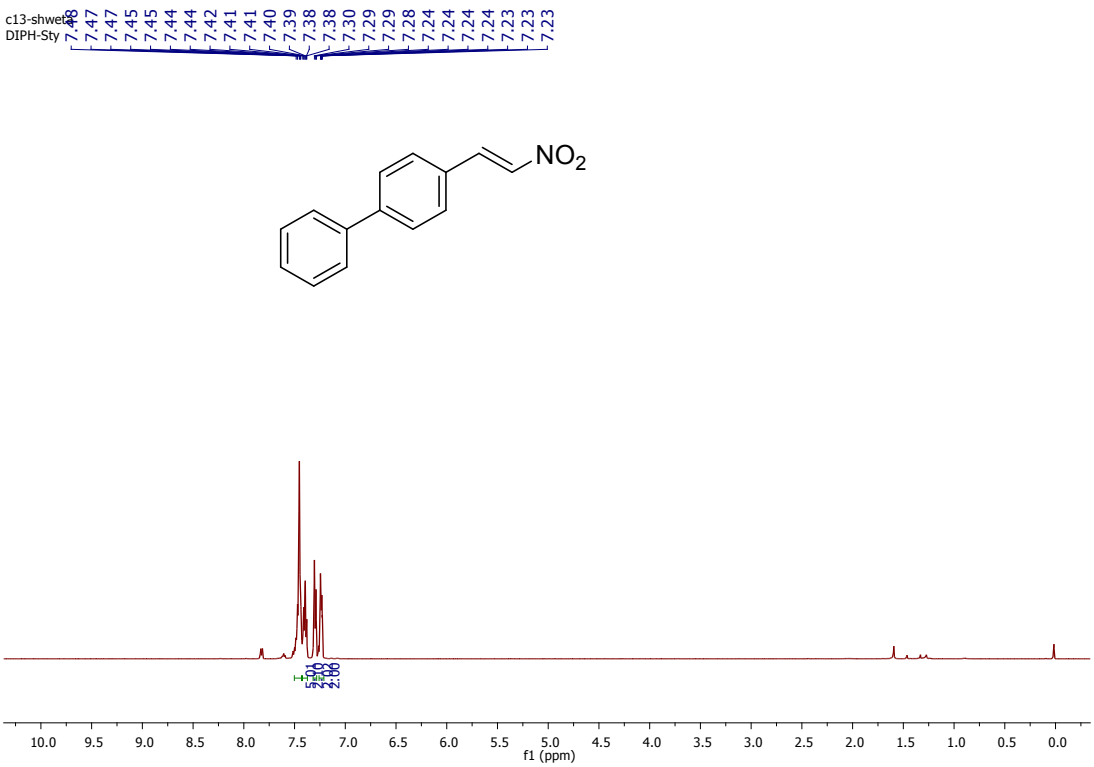
^{13}C NMR of (E)-2-(2-nitrovinyl)naphthalene (2v)



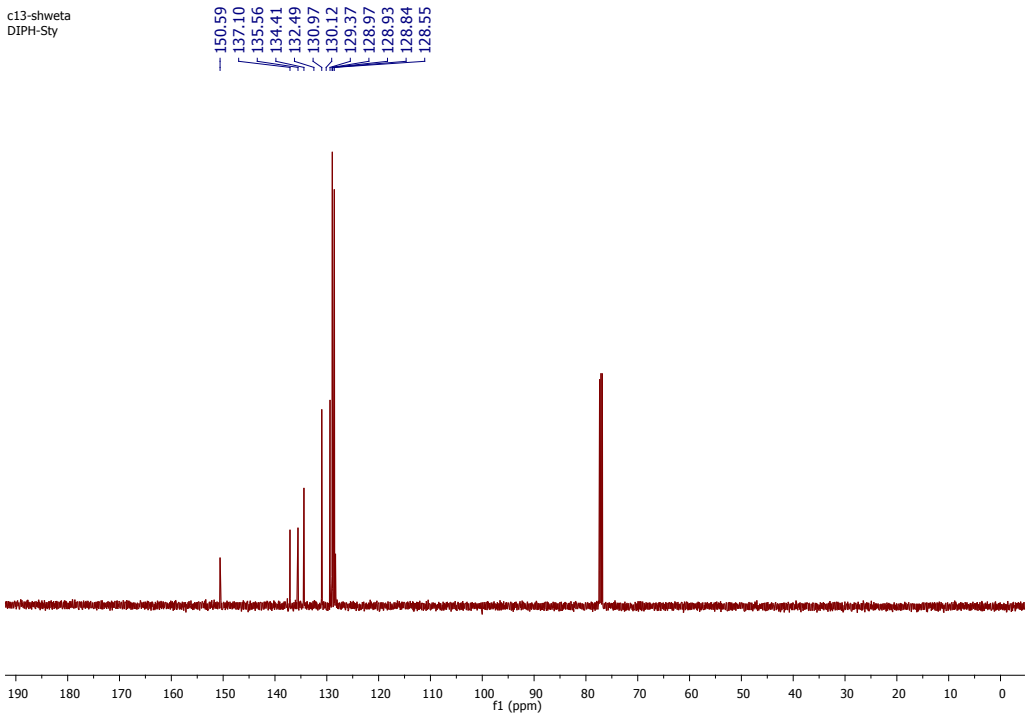
GC-MS of (E)-2-(2-nitrovinyl)naphthalene (2v)



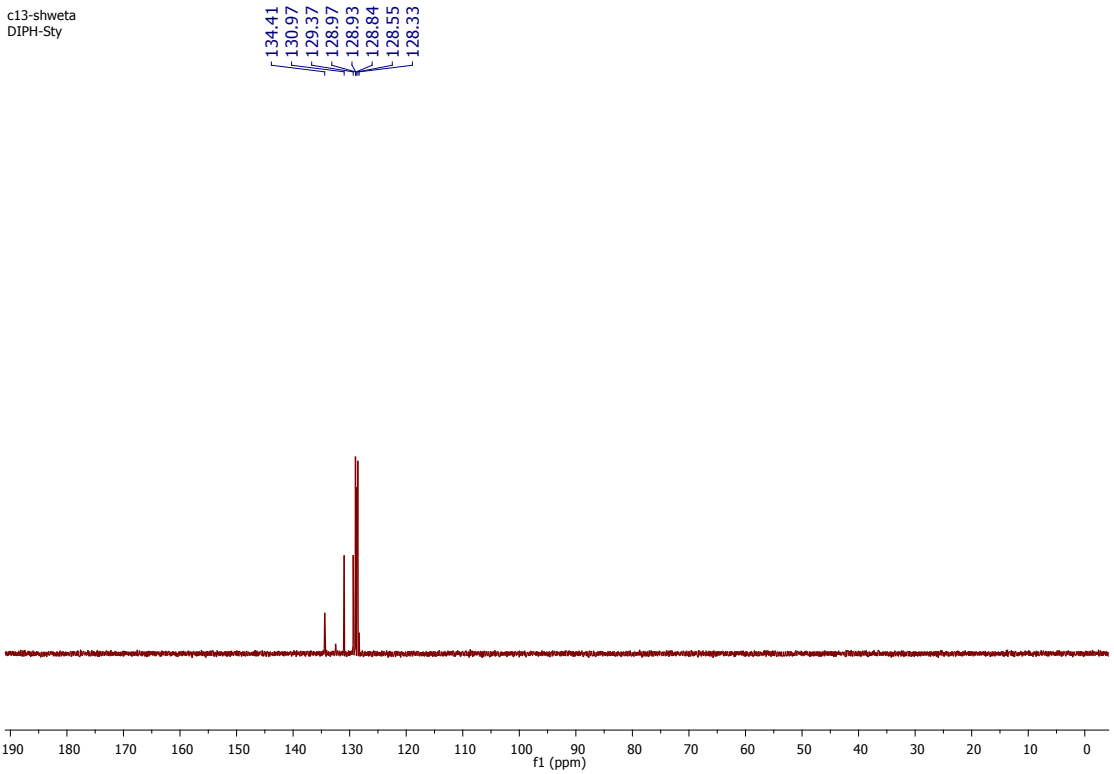
^{1}H NMR of (E)-4-(2-nitrovinyl)-1,1'-biphenyl (2w)[16]



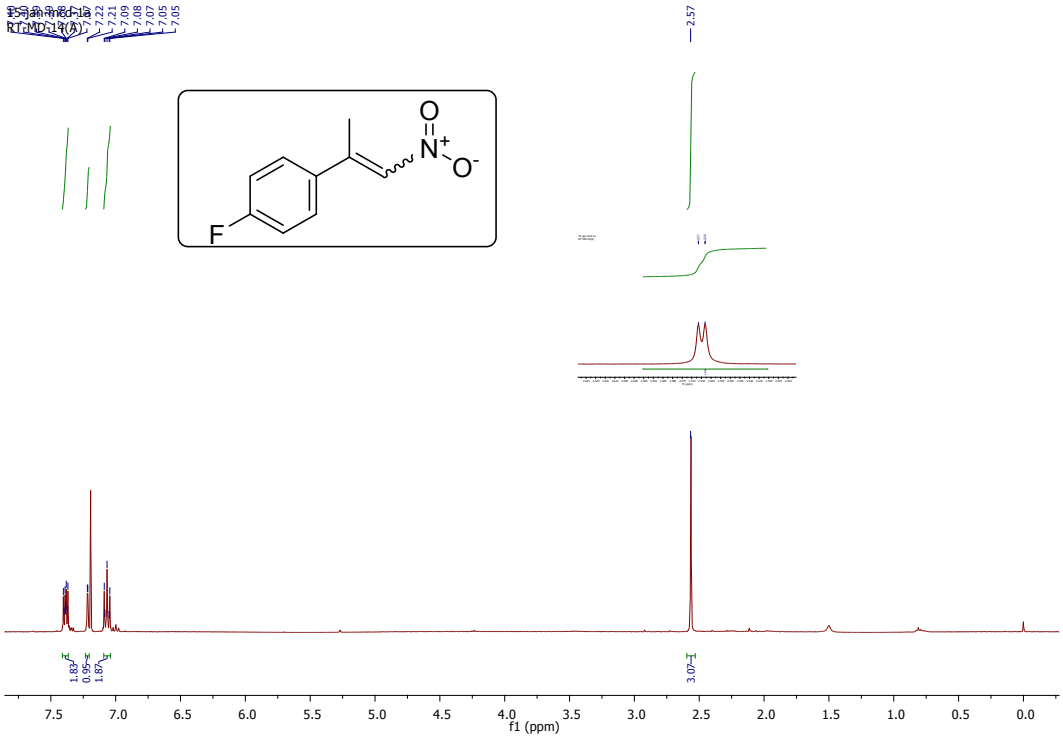
^{13}C NMR of (E)-4-(2-nitrovinyl)-1,1'-biphenyl (2w)



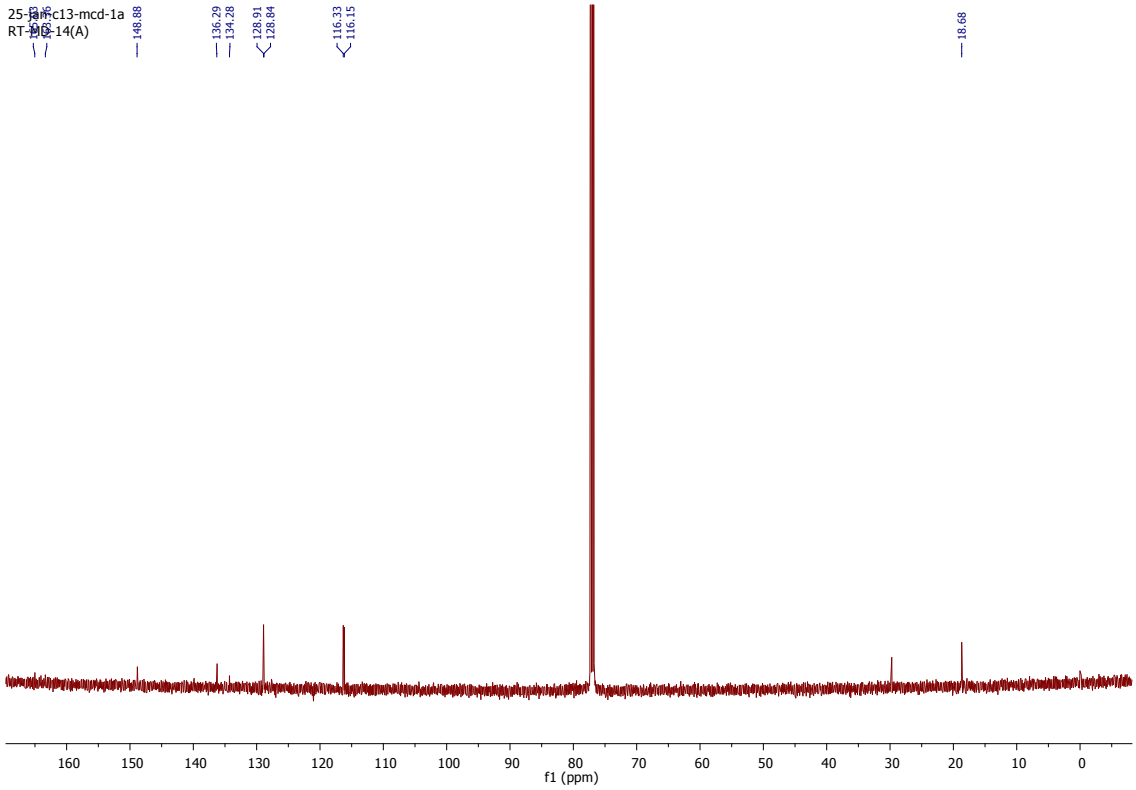
DEPT NMR of (E)-4-(2-nitrovinyl)-1,1'-biphenyl (2w)



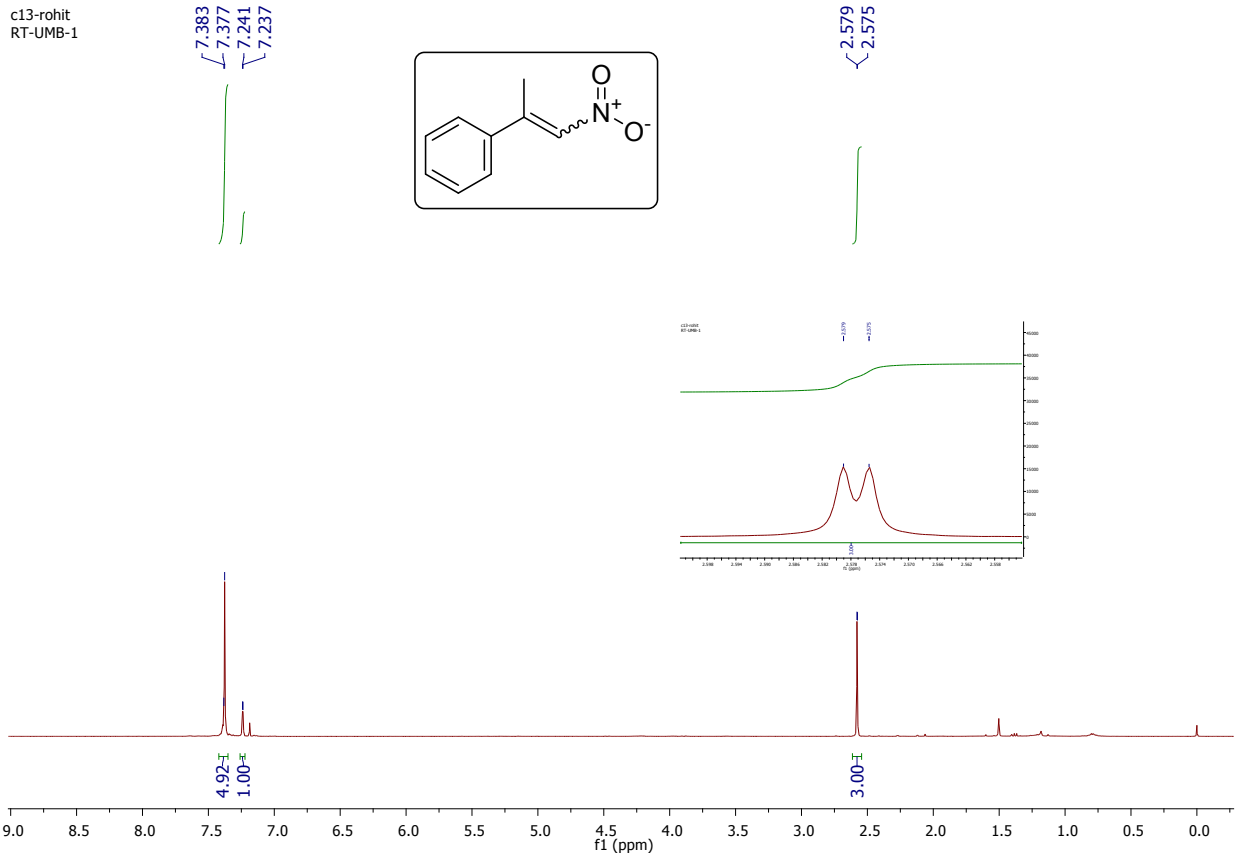
^{1}H NMR of (E/Z)-1-fluoro-4-(1-nitroprop-1-en-2-yl)benzene (2x) [17]



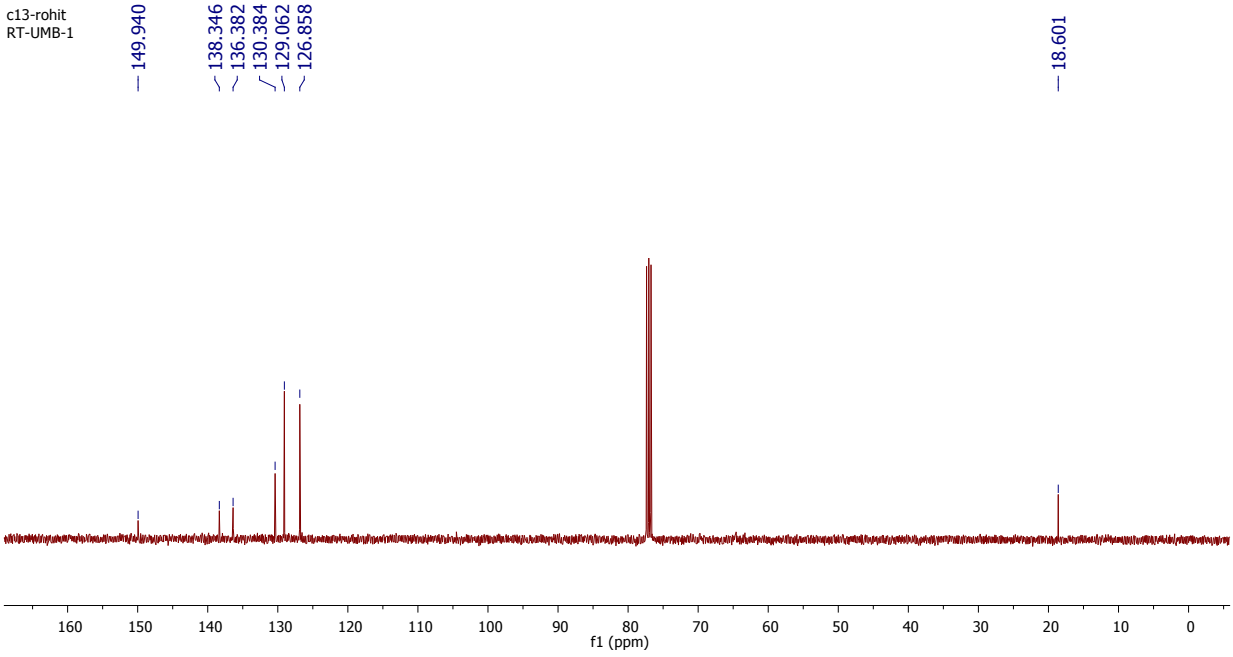
^{13}C NMR of (E/Z)-1-fluoro-4-(1-nitroprop-1-en-2-yl)benzene (2x) [17]



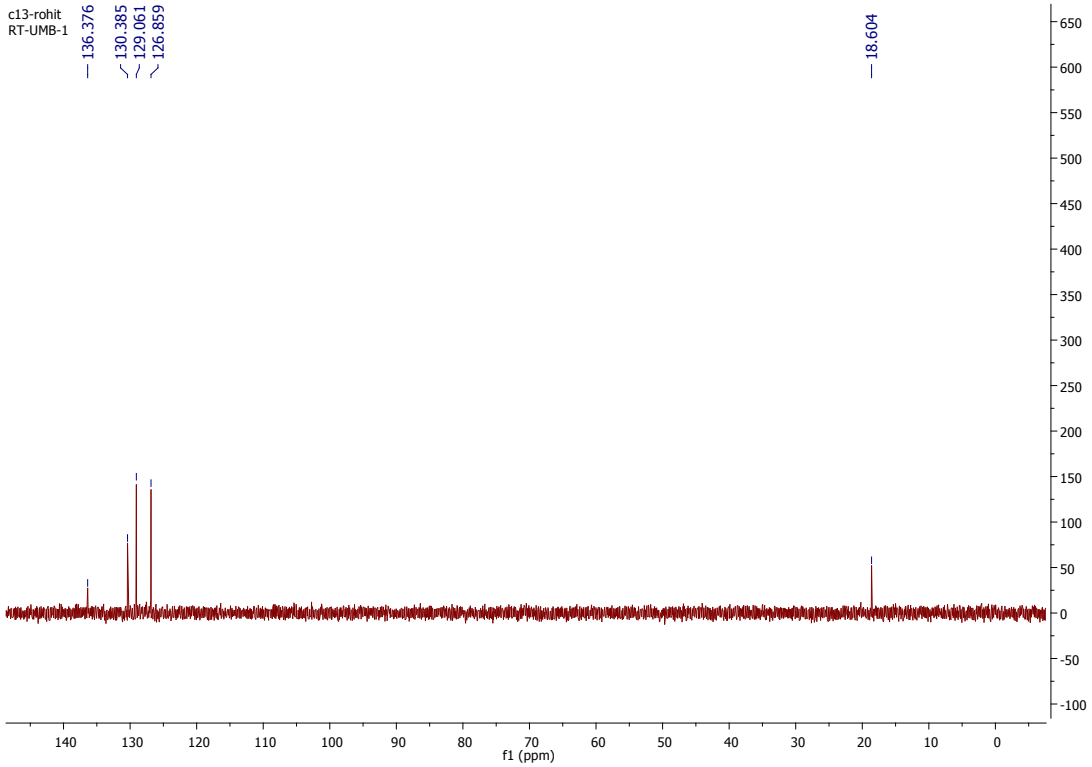
^{1}H NMR of (E/Z)-2-(1-nitroprop-1-en-2-yl)cyclohexa-1,3-diene (2y) [18]



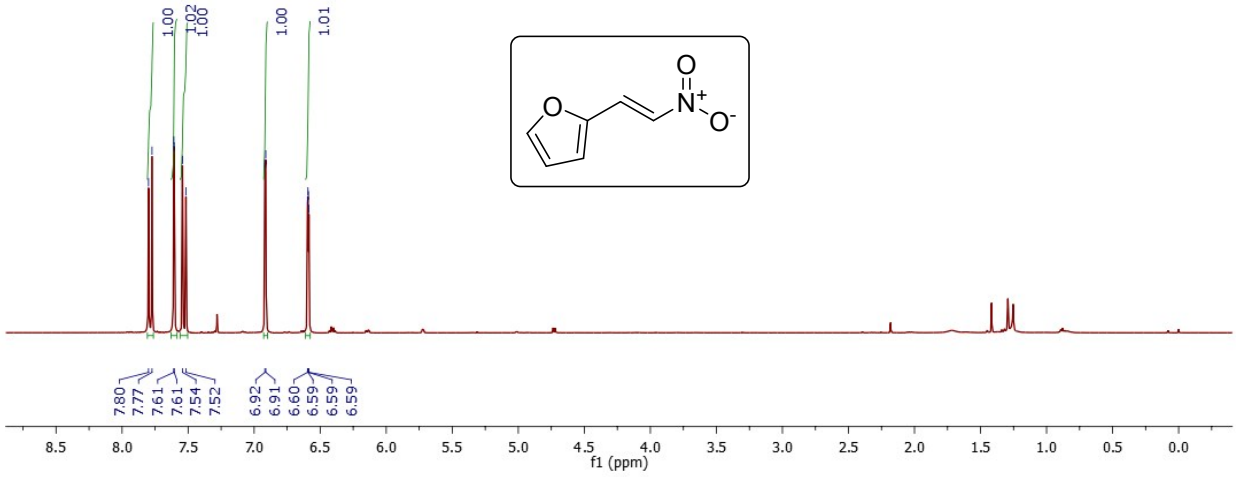
^{13}C NMR of (E/Z)-2-(1-nitroprop-1-en-2-yl)cyclohexa-1,3-diene (2y)



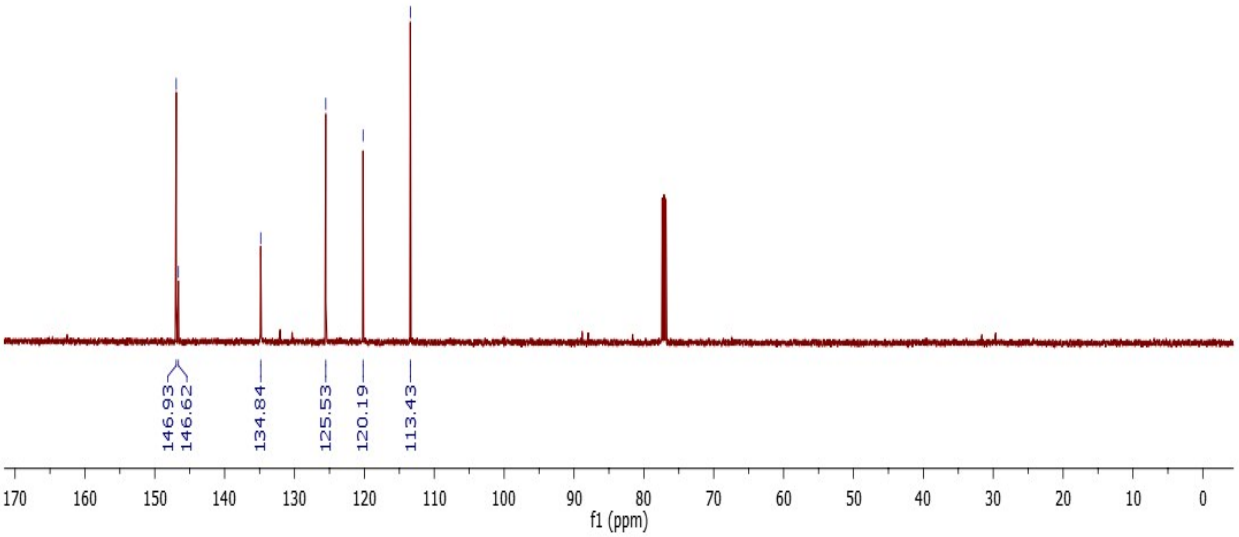
DEPT NMR of (E/Z)-2-(1-nitroprop-1-en-2-yl)cyclohexa-1,3-diene (2y)



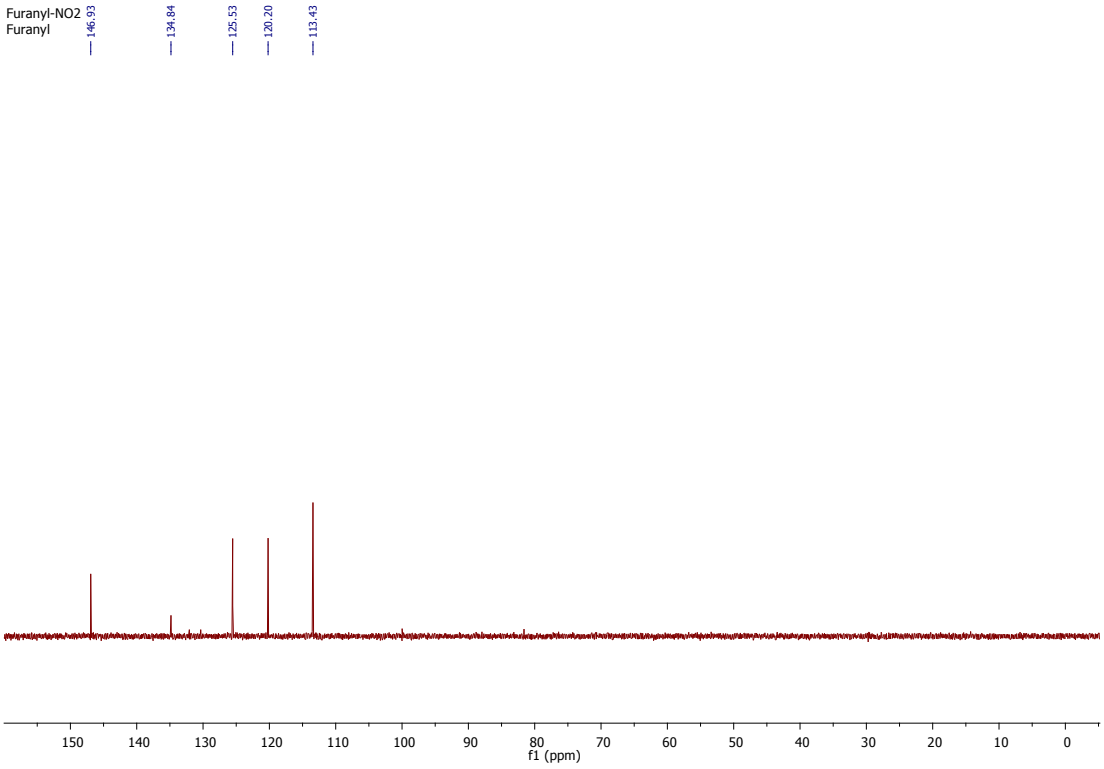
^{1}H NMR of (*E*)-2-(2-Nitrovinyl)furan (4a) [19]



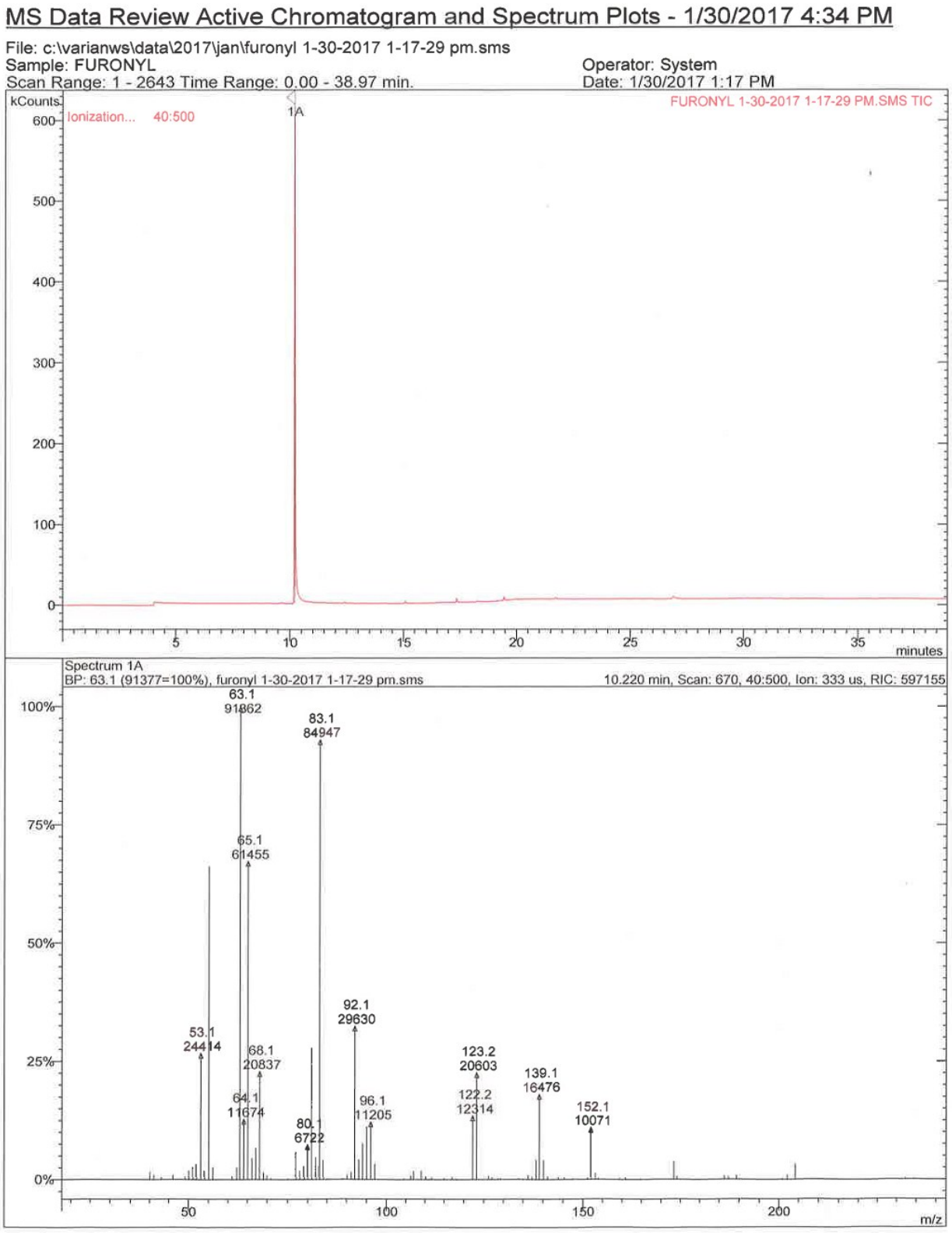
^{13}C NMR of (*E*)-2-(2-Nitrovinyl)furan (4a)



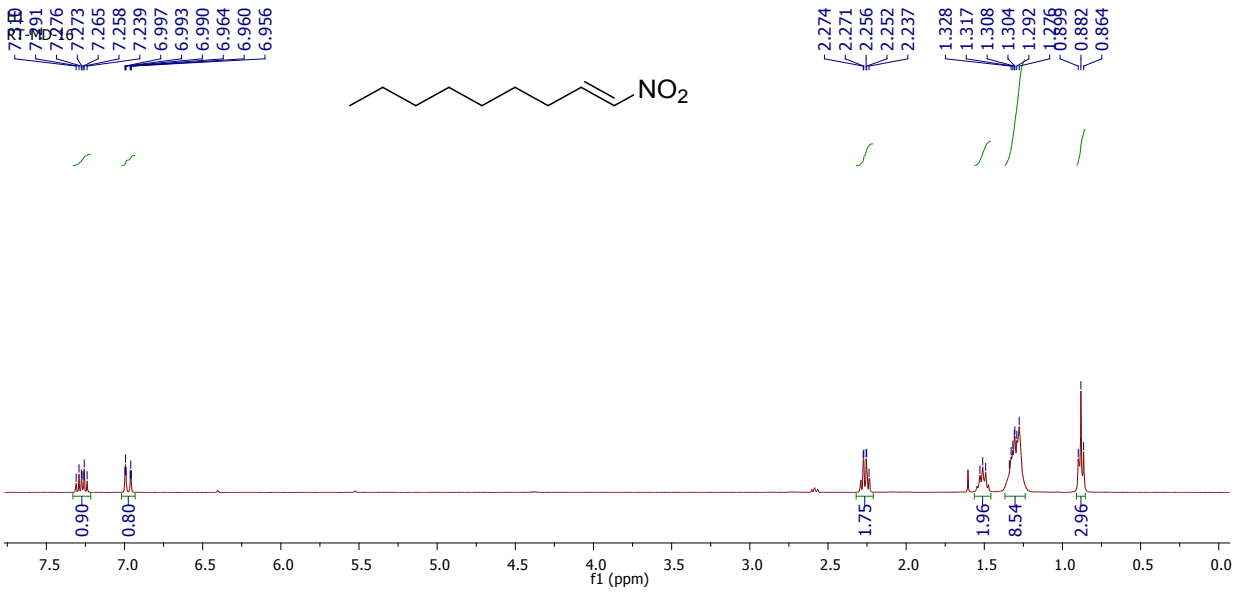
DEPT NMR of (*E*)-2-(2-Nitrovinyl)furan (4a)



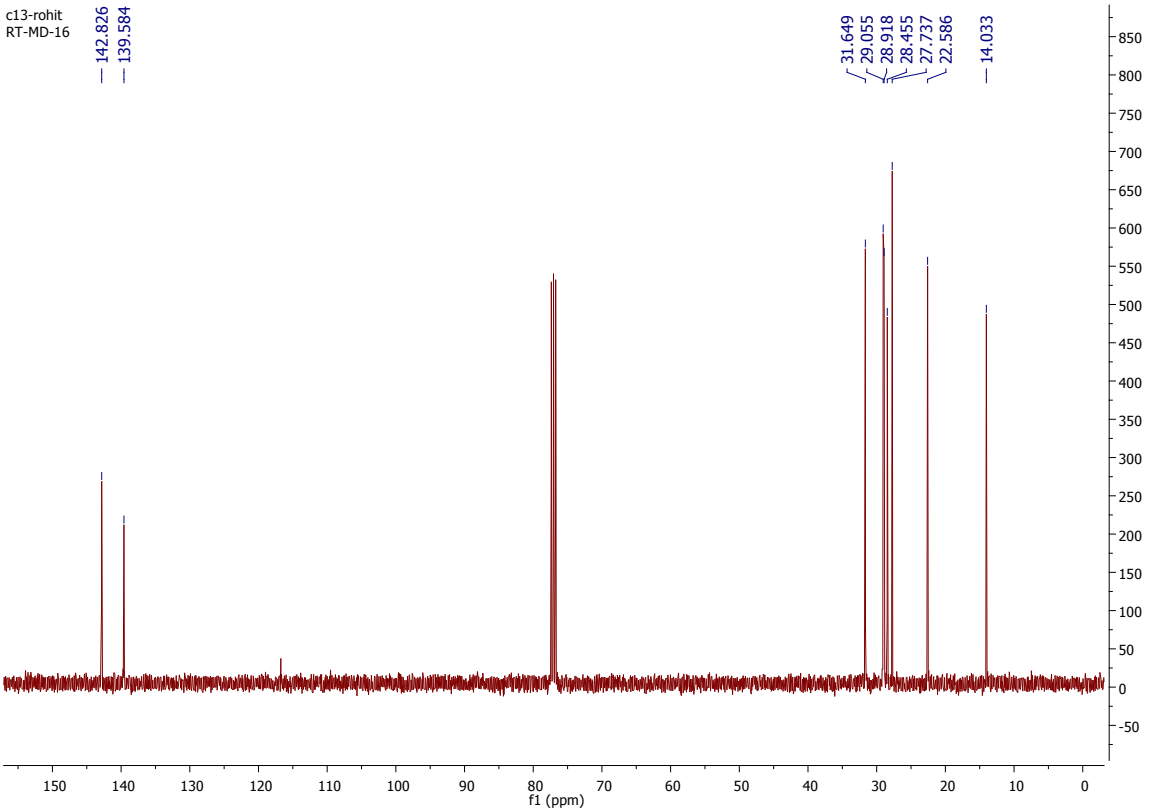
GC-MS of (*E*)-2-(2-Nitrovinyl)furan (4a)



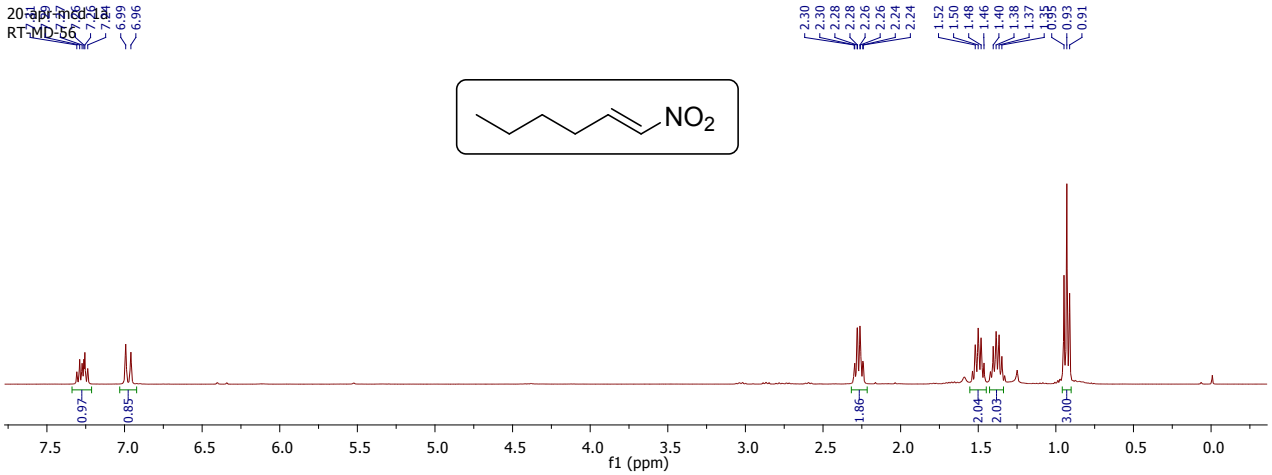
^{1}H NMR of (E)-1-nitronon-1-ene (4b)[20]



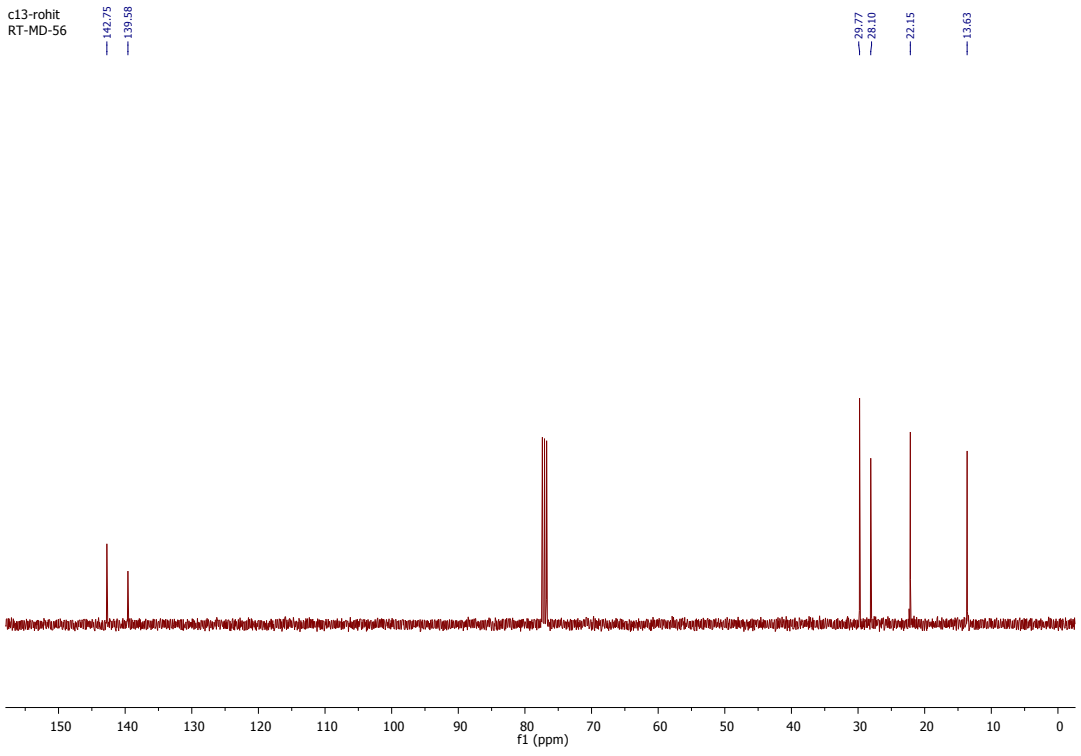
^{13}C NMR of (E)-1-nitronon-1-ene (4b)



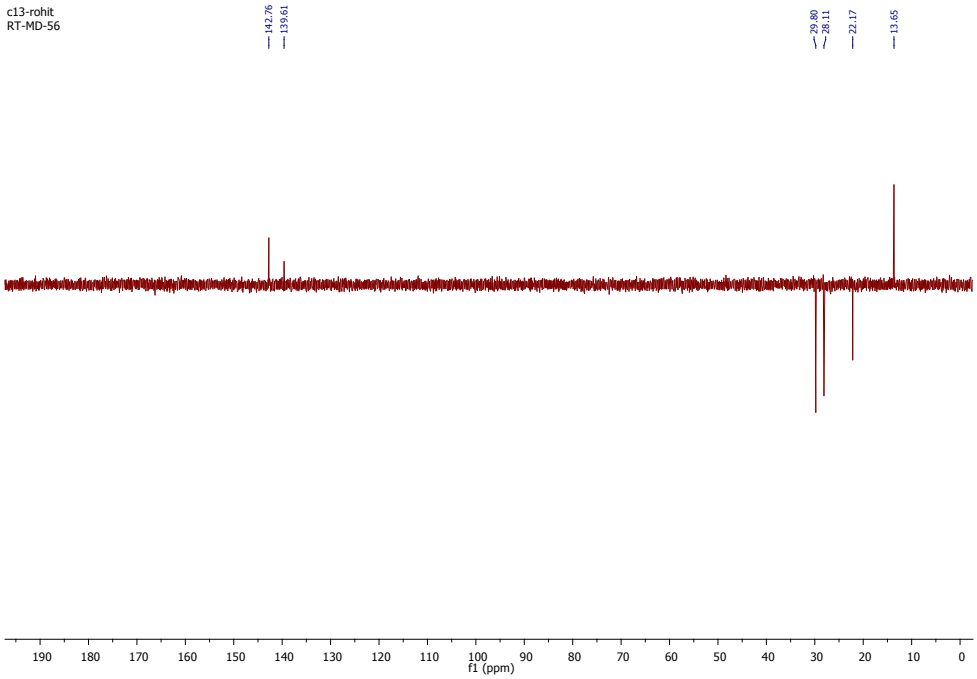
^{1}H NMR of (E)-1-nitrohex-1-ene (4c)[21]



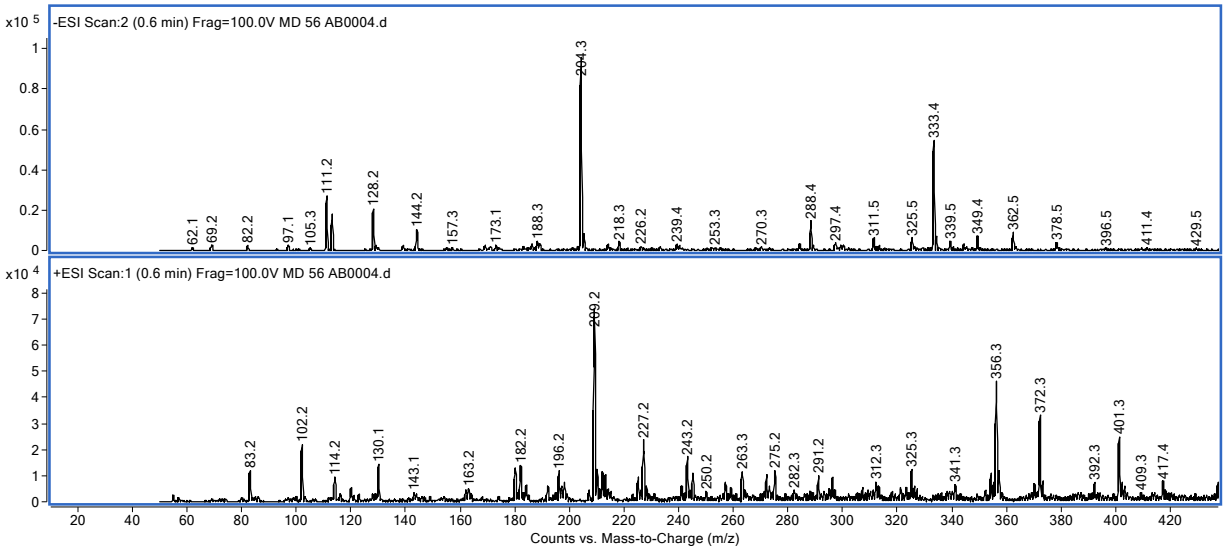
^{13}C NMR of (E)-1-nitrohex-1-ene (4c)



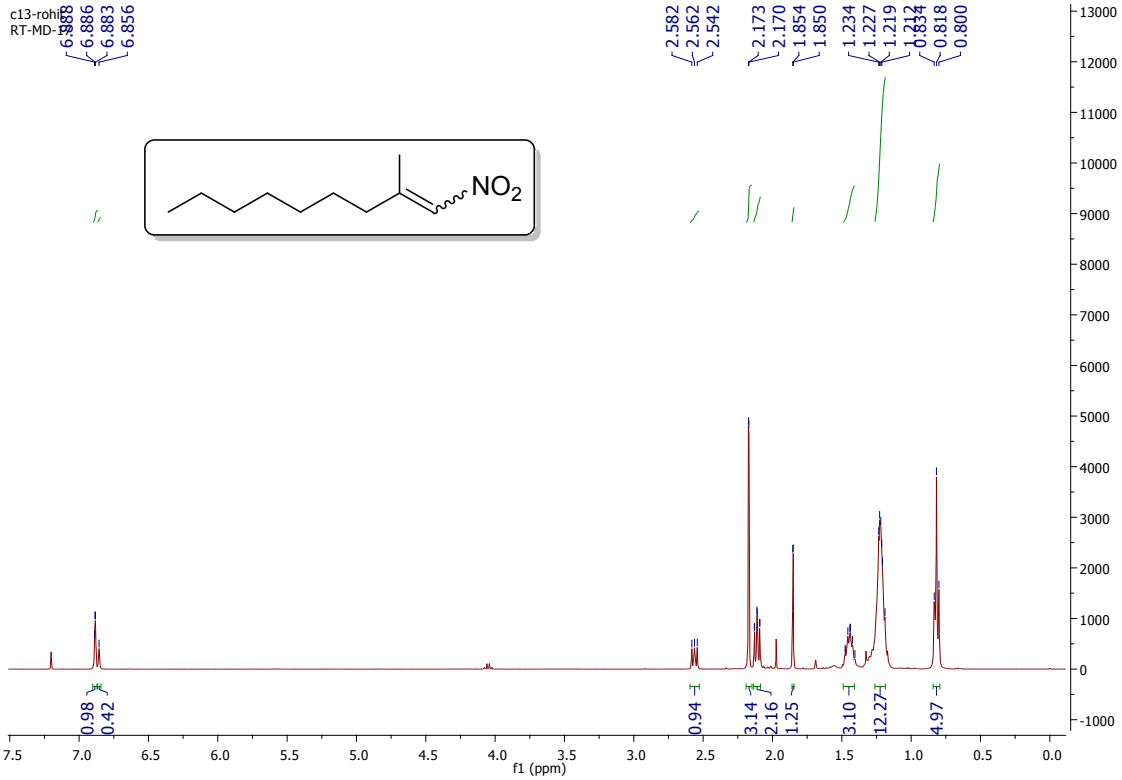
DEPT of (E)-1-nitrohex-1-ene (4c)



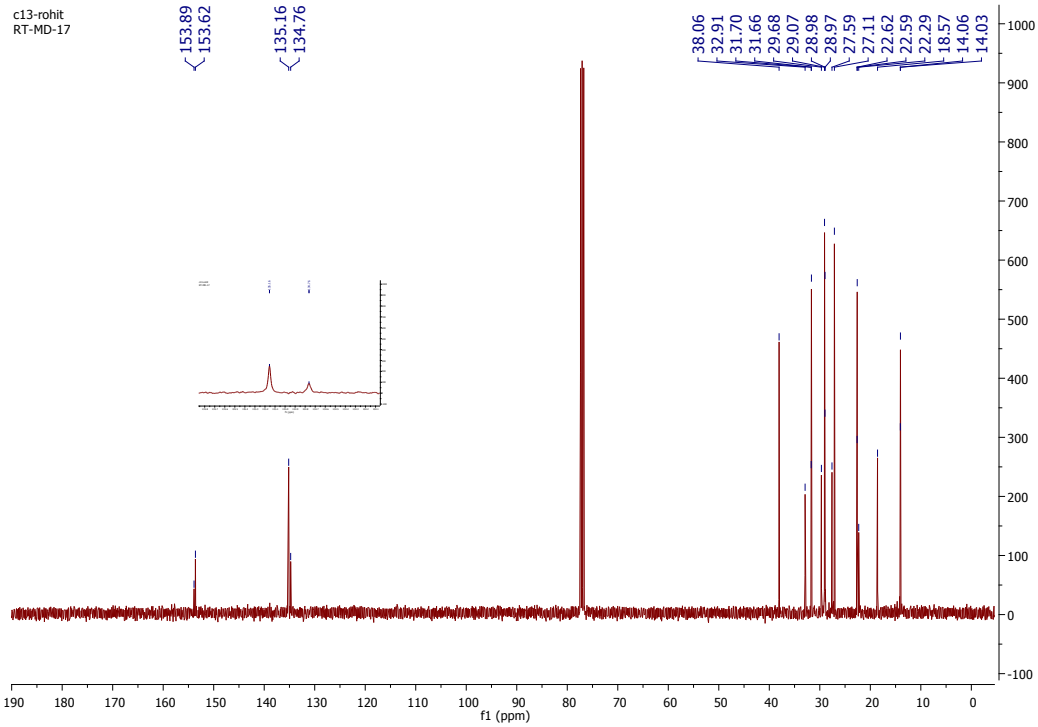
Mass spectra of (E)-1-nitrohex-1-ene 4(c)



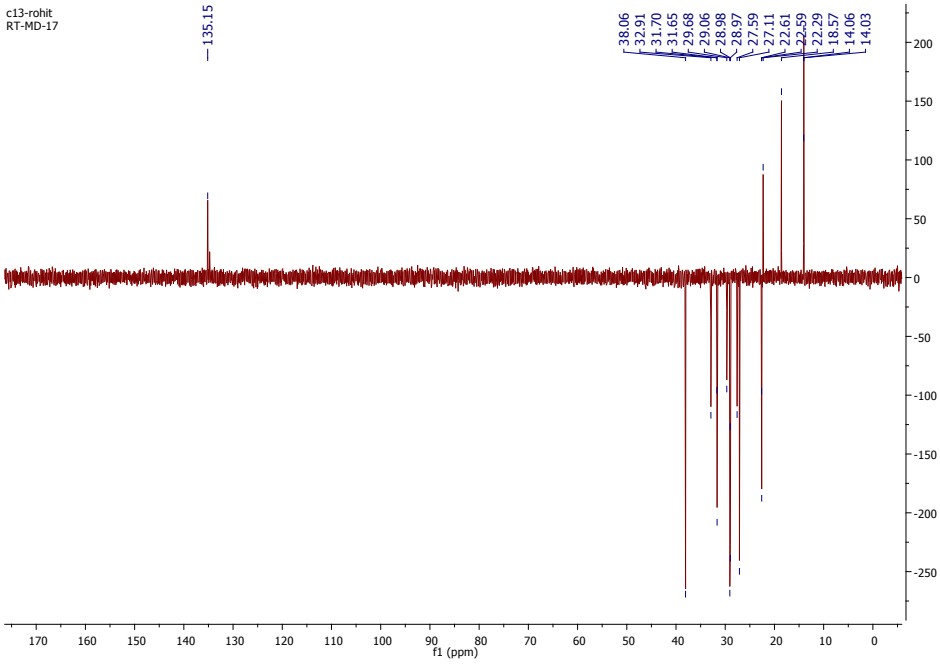
^{1}H NMR of (E/Z)-2-methyl-1-nitronon-1-ene (4d)[22]



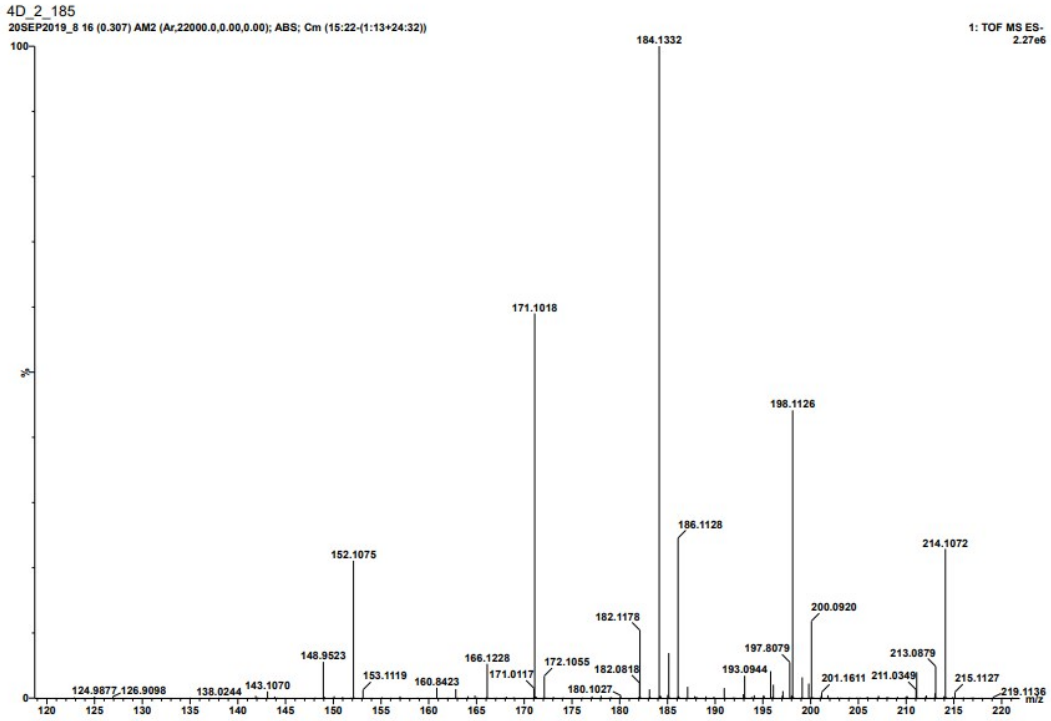
^{13}C NMR of (E/Z)-2-methyl-1-nitronon-1-ene (4d)



DEPT NMR of (*E/Z*)-2-methyl-1-nitronon-1-ene (4d)



HRMS of (*E/Z*)-2-methyl-1-nitronon-1-ene (4d)



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