

One-pot Near-ambient Temperature Syntheses of Aryl(difluoroenol) Derivatives from Trifluoroethanol

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General Experimental

NMR spectra were recorded on a Bruker DPX-400 spectrometer. ^1H and ^{13}C NMR spectra were recorded using the deuterated solvent as the lock and the residual solvent as the internal reference. ^{19}F NMR spectra were recorded relative to chlorotrifluoromethane as the external standard. The multiplicities of the spectroscopic data are presented in the following manner: s = singlet, d = doublet, t = triplet, q = quartet and m = multiplet. Homocouplings (H–H, F–F) are given in Hertz and specified by J ; the nuclei involved in heteronuclear couplings are defined with the observed nucleus given first. Unless stated otherwise, all refer to 3J couplings. Chemical ionisation (CI) (ammonia or methane) and Electron Impact (EI) mass spectra were recorded on a VG Prospec, Kratos MS-80 mass spectrometer or an Agilent technologies 5975C mass spectrometer. A Micromass LCT mass spectrometer was used for low-resolution (ES-TOF) mass spectra (using methanol as the mobile phase) and HRMS measurements (using a lock mass incorporated into the mobile phase). HRMS measurements were also obtained from either the Thermofisher LTQ Orbitrap XL (NSI and APCI) and Finnigan MAT 900 XLT (CI) spectrometers (ESPRC Mass Spectrometry service) or a VG Autospec instrument. GC-MS spectra were carried out on an Agilent Technologies 5975C (CI) mass spectrometer fitted with an Agilent Technologies DB5MS UI column (30 m x 0.25 μm) with Helium carrier gas flow at 1 $\text{cm}^3 \text{ minute}^{-1}$. Thin layer chromatography was performed on pre-coated aluminium-backed silica gel plates (E.Merck, A.G.Darmstadt, Germany. Silica gel 60 F₂₅₄, thickness 0.2 mm). Visualisation was achieved using potassium permanganate staining and UV detection at 254 nm. Column chromatography was performed on silica gel (Zeochem, Zeoprep 60 HYD, 40-63 μm) using a Büchi Sepacore system. Elemental analyses were performed on a Perkin Elmer 2400 CHN analyser. IR spectra were

recorded on a Perkin Elmer Paragon 1000 FT-IR spectrometer using sodium chloride plates. Melting points were recorded on a Reichert hot stage melting point apparatus and are uncorrected. Phase separation was accomplished with Isolute SPE Accessories phase separators. Tetrahydrofuran was dried using a PureSolv system from Innovative Technology, Inc.. Light petroleum ether and hexane were distilled before chromatography. Alkylolithium reagents were titrated using the procedure of Duhamel and Plaquevent.³⁹ zinc(II) chloride was dried by fusing over a bunsen flame under vacuum (10 mmHg) and cooling under nitrogen. All materials were purchased from Aldrich or Acros (Fisher) and used as received unless otherwise stated. Commercial LDA (1.8 M solution THF/heptane/ethylbenzene) was purchased from Aldrich. 1-(*N,N*-Diethylcarbamoyloxy)-2,2,2-trifluoroethane was prepared according to the method of Howarth.²⁶ 1-(2'-methoxy-ethoxymethoxy)-2,2,2-trifluoroethane and 2,2-difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(tributylstannyl)ethene were prepared according to the method of Patel.²⁵ 1-Iodophenyl-4-trifluoromethanesulfonate was prepared according to the procedure of Stille.⁴⁰ *tetrakis*(Triphenylphosphino)palladium(0) was prepared according to the procedure of Coulson.⁴¹

General coupling procedure

Vinylzinc reagents **9a** and **9b** were prepared as described in the main text of the manuscript. Couplings were carried out following the procedures described for **12aa** and **12ba**, on a 1 mmole scale; 4.45 cm³ of a 0.22 M solution of vinylzinc reagent **9a** or 3.95 cm³ of a 0.25 M solution of vinylzinc **9b**, and 23 mg (0.02 mmol) of *tetrakis*(triphenylphosphino)palladium were used in each case. The reactions, work-up and purification were performed as described for **12aa** and **12ba**.

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(3''-methoxyphenyl) ethene 12ab

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11b** (206 mg, 1.1 mmol) to afford **12ac** (199 mg, 73%) as a yellow oil; *R_f* (40% diethyl ether in light petroleum ether) 0.17; δ_{H} (400 MHz, CDCl₃) 3.40 (3 H, s, OCH₃), 3.56-3.60 (2 H, m, OCH₂CH₂O), 3.83 (3 H, s, ArOCH₃), 3.86-3.90 (2 H, m, OCH₂CH₂O), 4.90 (2 H, s, OCH₂O), 6.88 (1 H, br. dd, *J* 8.3, ⁴*J*_{H-H} 2.5, Ar*H*), 7.02-7.04 (1 H, m, Ar*H*), 7.08 (1 H, dq, *J* 7.8, ⁴*J*_{H-H} 1.3, Ar*H*), 7.31 (1 H, t, *J* 8.0, Ar*H*); δ_{C} (100 MHz, CDCl₃) 54.8, 58.5, 68.0, 71.1, 94.9 (t, ⁴*J*_{C-F} 3.1), 111.8 (dd, ⁴*J*_{C-F} 5.6, 3.6), 113.5, 115.0 (dd, ²*J*_{C-F} 35.4, 18.4), 118.8 (dd, ⁴*J*_{C-F} 5.6, 3.6), 129.1, 130.8 (br. d, ³*J*_{C-F} 6.0), 155.1 (app. t, ¹*J*_{C-F} 289.7), 159.2; δ_{F} (376 MHz, CDCl₃) -97.6 (1 F, d, ²*J*_{F-F} 55.3), -105.7 (1 F, d, ²*J*_{F-F} 55.3). These data are consistent with those reported by Katz and co-workers.¹

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-phenyl ethene 12ac

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11c** (172 mg, 1.1 mmol) to afford **12ac** (130 mg, 53%) as a yellow oil; *R_f* (40% diethyl ether in light petroleum ether) 0.33; ν_{max} (film)/cm⁻¹ 2929, 2884, 1735, 1449, 1265, 1201, 1177, 1153, 1103, 1070, 1032, 980, 948, 767, 715, 697; δ_{H} (400 MHz, CDCl₃) 3.40 (3 H, s, OCH₃), 3.56-3.60 (2 H, m, OCH₂CH₂O), 3.86-3.90 (2 H, m, OCH₂CH₂O), 4.90 (2 H, s, OCH₂O), 7.30-7.35 (1 H, m, Ar*H*), 7.37-7.42 (2 H, m, Ar*H*), 7.46-7.51 (2 H, m, Ar*H*); δ_{C} (100 MHz, CDCl₃) 58.5, 68.0, 71.1, 94.8 (t, ⁴*J*_{C-F} 3.0), 115.2 (dd, ²*J*_{C-F} 35.2, 18.3), 126.3 (dd, ⁴*J*_{C-F} 5.7, 3.2), 127.8, 128.0, 129.4 (br. d, ³*J*_{C-F} 6.1), 155.0 (app. t, ¹*J*_{C-F} 289.3); δ_{F} (376 MHz, CDCl₃) -98.0 (1 F, d, ²*J*_{F-F} 56.0), -106.5 (1 F, d, ²*J*_{F-F} 56.0); [HRMS (ES-TOF, [M + Na]⁺) Found: 267.0814. Calc. for C₁₂H₁₄O₃F₂Na:

267.0809]; m/z (CI) 245 (3%, $[M + H]^+$), 213 (5), 169 (25), 139 (10), 105 (20), 89 (100), 59 (50); GC (98) t_R 10.48 mins (70 – 320 °C, 20 °C min⁻¹).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-naphthyl ethene 12ad

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11d** (228 mg, 1.1 mmol) to afford **12ad** (142 mg, 48%) as a yellow oil; R_f (40% diethyl ether in light petroleum ether) 0.30; ν_{max} (film)/cm⁻¹ 2929, 2884, 2813, 1728, 1451, 1267, 1232, 1193, 1122, 1023, 954, 858, 840, 818, 749, 475; δ_H (400 MHz, CDCl₃) 3.41 (3 H, s, OCH₃), 3.58-3.61 (2 H, m, OCH₂CH₂O), 3.90-3.94 (2 H, m, OCH₂CH₂O), 4.96 (2 H, s, OCH₂O), 7.51-7.54 (2 H, m, ArH), 7.60 (1 H, dt, J 8.7, $^4J_{H-H}$ 1.7 ArH), 7.83-7.89 (3 H, m, ArH) 7.97 (1 H, br. s, ArH); δ_C (100 MHz, CDCl₃) 58.5, 68.1, 71.1, 95.0 (t, $^4J_{C-F}$ 3.0), 115.3 (dd, $^2J_{C-F}$ 35.2, 18.4), 123.6 (dd, $^4J_{C-F}$ 6.3, 2.7), 125.9 (app. t, $^4J_{C-F}$ 5.0), 126.0, 126.1, 126.8 (br. d, $^3J_{C-F}$ 6.0), 127.1, 127.7, 127.8, 132.5, 132.6, 155.2 (app. t, $^1J_{C-F}$ 291.1); δ_F (376 MHz, CDCl₃) -97.3 (1 F, d, $^2J_{F-F}$ 55.1), -106.1 (1 F, d, $^2J_{F-F}$ 55.1); [HRMS (NSI, $[M + NH_4]^+$) Found: 312.1409; calc. for C₁₆H₂₀F₂NO₃: 312.1411]; m/z (CI) 295 (5%, $[M + H]^+$), 219 (20), 189 (10), 155 (15), 89 (100), 59 (45); GC (98%) t_R 13.52 mins (70 – 320 °C, 20 °C min⁻¹).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(2''-methylphenyl) ethene 12ae

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11e** (188 mg, 1.1 mmol) to afford **12ae** (103 mg, 40%) as a yellow oil; R_f (20% diethyl ether in light petroleum ether) 0.23; δ_H (400 MHz, CDCl₃) 2.37 (3 H, s, ArCH₃) 3.40 (3 H, s, OCH₃), 3.54-3.58 (2 H, m, OCH₂CH₂O), 3.79-3.83 (2 H, m, OCH₂CH₂O), 4.73 (2 H, d, $^5J_{H-F}$ 0.67, OCH₂O), 7.19-7.37 (4 H, m, ArH); δ_C (100 MHz, CDCl₃) 19.4, 59.0, 67.8, 71.6, 93.3, 114.3 (dd, $^2J_{C-F}$ 42.0, 17.9), 125.7, 128.0, 129.5, 130.4, 130.7 (br. t, $^4J_{C-F}$ 2.8), 138.4 (br. d, $^3J_{C-F}$ 2.3), 154.2 (dd, $^1J_{C-F}$ 290.2, 280.3); δ_F (376 MHz, CDCl₃) -102.2 (1 F, d, $^2J_{F-F}$ 64.1), -109.2 (1 F, d, $^2J_{F-F}$ 64.1); m/z

(CI) 259 (1%, $[M + H]^+$), 227 (5), 183 (17), 153 (15), 119 (7), 89 (100), 59 (33); GC (98%) t_R 10.57 mins (70 – 320 °C, 20 °C min⁻¹). These data are consistent with those reported by Katz and co-workers.¹

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(4''-chlorophenyl) ethene 12af

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11f** (192 mg, 1.1 mmol) to afford **12af** (151 mg, 54%) as a yellow oil; R_f (40% diethyl ether in light petroleum ether) 0.49; ν_{max} (film)/cm⁻¹ 2929, 2882, 2821, 1729, 1493, 1263, 1151, 1092, 1027, 979, 939, 832, 832; δ_H (400 MHz, CDCl₃) 3.40 (3 H, s, OCH₃), 3.56-3.59 (2 H, m, OCH₂CH₂O), 3.85-3.89 (2 H, m, OCH₂CH₂O), 4.88 (2 H, s, OCH₂O), 7.36-7.44 (4 H, m, ArH); δ_C (100 MHz, CDCl₃) 58.5, 68.1, 71.1, 95.0 (t, $^4J_{C-F}$ 3.0), 114.5 (dd, $^2J_{C-F}$ 35.3, 19.2), 127.5 (dd, $^4J_{C-F}$ 6.0, 3.4), 128.0 (br. d, $^3J_{C-F}$ 5.8), 128.3, 133.6, 155.0 (app. t, $^1J_{C-F}$ 290.3); δ_F (376 MHz, CDCl₃) -97.0 (1 F, d, $^2J_{F-F}$ 54.5), -105.4 (1 F, d, $^2J_{F-F}$ 54.5); [HRMS (EI, M⁺) Found: 278.05201; Calc. for C₁₂H₁₃(³⁵Cl)F₂O₃: 278.05213]; m/z (CI) 279 (1%, $[M + H]^+$), 247 (5), 203 (10), 173 (8), 138 (8), 89 (100), 59 (54); GC (98%) t_R 11.55 mins (70 – 320 °C, 20 °C min⁻¹).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-[4''-(trifluoromethanesulfonyloxy)phenyl] ethene 12ag

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11g** (387 mg, 1.1 mmol) to afford **12af** (97 mg, 25%) as a yellow oil; R_f (40% diethyl ether in hexane) 0.32; ν_{max} (film)/cm⁻¹ 1731, 1504, 1428, 1271, 1251, 1215, 1179, 1142, 1103, 984, 941, 889, 847; δ_H (400 MHz, CDCl₃) 3.40 (3 H, s, OCH₃), 3.55-3.58 (2 H, m, OCH₂CH₂O), 3.85-3.89 (2 H, m, OCH₂CH₂O), 4.91 (2 H, s, OCH₂O), 7.32 (2 H, br. d, J 8.9, ArH), 7.59 (2 H, br. d, J 8.9, ArH); δ_C (100 MHz, CDCl₃) 58.5, 68.2, 71.0, 95.3 (t, $^4J_{C-F}$ 3.1), 114.1 (dd, $^2J_{C-F}$ 35.1, 19.8),

118.2 (q, $^1J_{\text{C-F}}$ 320.1), 121.1, 128.0 (dd, $^4J_{\text{C-F}}$ 6.3, 3.4), 130.3 (br. d, $^3J_{\text{C-F}}$ 6.3), 148.4, 155.3 (app. t, $^1J_{\text{C-F}}$ 291.7); δ_{F} (376 MHz, CDCl_3) -72.8 (3 F, s), -95.6 (1 F, d, $^2J_{\text{F-F}}$ 51.8), -104.4 (1 F, d, $^2J_{\text{F-F}}$ 51.8); [HRMS (ES-TOF, $[\text{M} + \text{Na}]^+$) Found: 415.0247; Calc. for $\text{C}_{13}\text{H}_{13}\text{O}_6\text{F}_5\text{SNa}$: 415.0251]; m/z (CI) 393 (2%, $[\text{M} + \text{H}]^+$), 89 (100), 59 (30); GC (98%) t_{R} 11.87 mins (70 – 320 °C, 20 °C min $^{-1}$).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(4'-trifluoromethylbenzene) ethene 12ah

Was prepared from **9a** (4.45 cm 3 of a 0.22 M solution) and **11h** (248 mg, 1.1 mmol) to afford **12ah** (103 mg, 41%) as a yellow oil; R_{f} (20% diethyl ether in light petroleum ether) 0.15; δ_{H} (400 MHz, CDCl_3) 3.39 (3 H, s, OCH_3), 3.54-3.58 (2 H, m, $\text{OCH}_2\text{CH}_2\text{O}$), 3.85-3.89 (2 H, m, $\text{OCH}_2\text{CH}_2\text{O}$), 4.90 (2 H, s, OCH_2O), 7.61 (2 H, br. d, J 8.6, ArH), 7.67 (2 H, br. d, J 8.6, ArH); δ_{C} (100 MHz, CDCl_3) 58.5, 68.2, 71.0, 95.4 (t, $^4J_{\text{C-F}}$ 3.0), 114.5 (dd, $^2J_{\text{C-F}}$ 34.2, 19.3), 123.4 (q, $^1J_{\text{C-F}}$ 271.8), 125.0 (q, $^3J_{\text{C-F}}$ 3.0), 126.3 (dd, $^4J_{\text{C-F}}$ 6.5, 3.5), 129.7 (q, $^2J_{\text{C-F}}$ 32.5), 133.4 (br. d, $^3J_{\text{C-F}}$ 6.4), 155.0 (app. t, $^1J_{\text{C-F}}$ 291.9); δ_{F} (376 MHz, CDCl_3) -62.8 (3 F, s) -94.9 (1 F, d, $^2J_{\text{F-F}}$ 50.0), -103.6 (1 F, d, $^2J_{\text{F-F}}$ 50.0); m/z (CI) 313 (1%, $[\text{M} + \text{H}]^+$), 293 (67), 237 (13), 173 (5), 89 (100), 59 (50); GC (98%) t_{R} 10.28 mins (70 – 320 °C, 20 °C min $^{-1}$). These data are consistent with those reported by Katz and co-workers.¹

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(3''-trifluoromethylphenyl) ethene 12aj

Was prepared from **9a** (4.45 cm 3 of a 0.22 M solution) and **11j** (248 mg, 1.1 mmol) to afford **12aj** (63 mg, 20%) as a yellow oil; R_{f} (40% diethyl ether in hexane) 0.33; δ_{H} (400 MHz, CDCl_3) 3.40 (3 H, s, OCH_3), 3.55-3.58 (2 H, m, $\text{OCH}_2\text{CH}_2\text{O}$), 3.86-3.90 (2 H, m, $\text{OCH}_2\text{CH}_2\text{O}$), 4.92 (2 H, s, OCH_2O), 7.53 (1 H, t, J 7.8, ArH), 7.59 (1 H, br. d, J 7.8, ArH), 7.68 (1 H, br. d, J 7.8, ArH) 7.76 (1 H, br. s, ArH); δ_{C} (100 MHz, CDCl_3) 58.5, 68.2, 71.0, 95.4 (t, $^4J_{\text{C-F}}$ 3.2), 114.4 (dd, $^2J_{\text{C-F}}$ 34.6, 19.3), 122.8 – 123.1 (m, includes signals for (Ar)C-

H), 123.37 (q, $^1J_{C-F}$ 272.6), 124.4 (d, $^3J_{C-F}$ 3.5), 128.6, 129.3 (br. d, $^4J_{C-F}$ 4.0), 130.6 (q, $^2J_{C-F}$ 32.6), 130.7 (br. d, $^3J_{C-F}$ 6.4), 155.0 (app. t, $^1J_{C-F}$ 291.3); δ_F (376 MHz, $CDCl_3$) -62.8 (3 F, s) - 95.7 (1 F, d, $^2J_{F-F}$ 51.9), -104.5 (1 F, d, $^2J_{F-F}$ 51.9); [HRMS (APCI, $[M + NH_4]^+$) Found: 330.11327; Calc. for $C_{13}H_{17}F_5NO_3$: 330.11286]. m/z (CI) 313 (2%, $[M + H]^+$), 249 (30), 236 (15), 216 (10), 89 (100), 59 (30), 41 (25); GC (97%) t_R 10.17 mins (70 – 250 °C, 20 °C min $^{-1}$).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(4''-cyanophenyl) ethene 12ak

Was prepared from **9a** (4.45 cm 3 of a 0.22 M solution) and **11k** (200 mg, 1.1 mmol) to afford **12af** (68 mg, 25%) as a yellow oil; R_f (40% diethyl ether in hexane) 0.11; ν_{max} (film)/cm $^{-1}$ 2885, 2822, 2229, 1717, 1608, 1267, 1153, 1099, 1074, 980, 932, 844; δ_H (400 MHz, $CDCl_3$) 3.39 (3 H, s, OCH_3), 3.54-3.57 (2 H, m, CH_2O), 3.85-3.89 (2 H, m, CH_2O), 4.90 (2 H, s, OCH_2O), 7.60 (2 H, d, J 8.6, ArH), 7.69 (2 H, d, J 8.6, ArH); δ_C (100 MHz, $CDCl_3$) 58.6, 68.3, 71.0, 95.7, 111.2, 114.4 (dd, $^2J_{C-F}$ 32.8, 19.3), 117.9, 126.4 (dd, $^4J_{C-F}$ 6.9, 3.5), 131.8, 134.6 (br. d, $^3J_{C-F}$ 6.5), 155.6 (app. t, $^1J_{C-F}$ 293.3); δ_F (376 MHz, $CDCl_3$) -93.1 (1 F, d, $^2J_{F-F}$ 45.5), -101.6 (1 F, d, $^2J_{F-F}$ 45.5); [HRMS (ES-TOF, $[M + NH_4]^+$) Found: 287.1205; Calc. for $C_{13}H_{17}F_2N_2O_3$: 287.1202]. m/z (CI) 328 (5), 310 (5), 298 (40%, $[M + C_2H_5]^+$), 89 (100), 59 (40), 41 (35); GC (98%) t_R 12.26 mins (70 – 250 °C, 20 °C min $^{-1}$).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(3''-cyanophenyl) ethene 12al

Was prepared from **9a** (4.45 cm 3 of a 0.22 M solution) and **11l** (200 mg, 1.1 mmol) to afford **12al** (89 mg, 33%) as a yellow oil; Yellow oil; R_f (40% diethyl ether in light petroleum ether) 0.13; δ_H (400 MHz, $CDCl_3$) 3.40 (3 H, s, OCH_3), 3.53-3.58 (2 H, m, OCH_2CH_2O), 3.84-3.90 (2 H, m, OCH_2CH_2O), 4.91 (2 H, s, OCH_2O), 7.49-7.80 (4 H, envelope, ArH); δ_C (100 MHz,

CDCl₃) 58.5, 68.3, 71.0, 95.5 (t, ⁴J_{C-F} 3.3), 112.6, 114.0 (dd, ²J_{C-F} 34.6, 19.5), 117.8, 129.0, 129.5 (dd, ⁴J_{C-F} 6.0, 3.5), 130.2 (dd, ⁴J_{C-F} 6.7, 3.5), 131.1, 131.4 (br. d, ³J_{C-F} 6.2), 155.4 (app. t, ¹J_{C-F} 292.8); δ_F(376 MHz, CDCl₃) -94.6 (1 F, d, ²J_{F-F} 50.1), -103.6 (1 F, d, ²J_{F-F} 50.1); [HRMS (APCI, [M + NH₄]⁺) Found: 287.1201; Calc. for C₁₃H₁₇F₂N₂O₃: 287.1207]. *m/z* (CI) 328 (10), 310 (10), 270 (2%, [M + H]⁺), 194 (5), 89 (100), 59 (30), 41 (20); GC (97%) t_R 12.12 mins (70 – 250 °C, 20 °C min⁻¹).

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(4''-nitrophenyl) ethene 12am

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11m** (274 mg, 1.1 mmol) to afford **12am** (119 mg, 41%) as orange needles; mp 35.5-38 °C; (Found: C, 60.9; H, 6.0; N, 5.3; C₁₃H₁₅F₂NO₂ requires C, 61.2; H, 5.9; N, 5.5%); R_f (40% diethyl ether in light petroleum ether) 0.13; ν_{max}(film)/cm⁻¹ 2920, 2891, 2818, 1709, 1594, 1505, 1457, 1346, 1331, 1266, 1180, 1159, 1100, 1081, 1032, 980, 914, 851, 757, 729, 698, 672; δ_H(400 MHz, CDCl₃) 3.39 (3 H, s, OCH₃), 3.54-3.58 (2 H, m, OCH₂CH₂O), 3.86-3.90 (2 H, m, OCH₂CH₂O), 4.92 (2 H, s, OCH₂O), 7.64-7.69 (2 H, m, ArH), 8.23-8.27 (2 H, m, ArH); δ_C(100 MHz, CDCl₃) 58.5, 68.4, 71.0, 95.7 (t, ⁴J_{C-F} 3.1), 114.4 (dd, ²J_{C-F} 33.5, 19.7), 123.3, 126.5 (dd, ⁴J_{C-F} 7.0, 3.6), 136.5 (br. d, ³J_{C-F} 6.7), 146.7, 155.8 (app. t, ¹J_{C-F} 294.6); δ_F(376 MHz, CDCl₃) -92.3 (1 F, d, ²J_{F-F} 43.6), -100.8 (1 F, d, ²J_{F-F} 43.6); [HRMS (CI, [M+NH₄]⁺) Found: 307.1101; Calc. for C₁₂H₁₇N₂F₂O₅: 307.1100].

2,2-Difluoro-1-(2'-methoxy-ethoxymethoxy)-1-(3''-nitrophenyl) ethene 12an

Was prepared from **9a** (4.45 cm³ of a 0.22 M solution) and **11n** (222 mg, 1.1 mmol) to afford **12an** (91 mg, 31%) as a yellow oil; R_f (40% diethyl ether in hexane) 0.13; δ_H(400 MHz, CDCl₃) 3.40 (3 H, s, OCH₃), 3.56-3.60 (2 H, m, OCH₂CH₂O), 3.88-3.92 (2 H, m, OCH₂CH₂O), 4.95 (2 H, s, OCH₂O), 7.59 (1 H, t, *J* 8.0), 7.83 (1 H, dq, *J* 7.8, ⁴J_{H-H} 1.3, ArH),

8.18 (1 H, br. dd, J 8.0, $^4J_{\text{H-H}}$ 2.0, ArH), 8.37 (1 H, t, 4J 2.0); δ_{C} (100 MHz, CDCl_3) 58.5, 68.3, 71.0, 95.7 (t, $^4J_{\text{C-F}}$ 3.1), 114.1 (dd, $^2J_{\text{C-F}}$ 34.3, 19.3), 121.0 (dd, $^4J_{\text{C-F}}$ 6.0, 3.6), 122.4, 129.1, 131.7 (dd, $^4J_{\text{C-F}}$ 7.2, 3.4), 131.9 (br. d, $^3J_{\text{C-F}}$ 6.7), 148.1, 155.5 (app. t, $^1J_{\text{C-F}}$ 293.2); δ_{F} (376 MHz, CDCl_3) -94.1 (1 F, d, $^2J_{\text{F-F}}$ 49.0), -103.0 (1 F, d, $^2J_{\text{F-F}}$ 49.0); m/z (CI) 318 (10%, $[\text{M} + \text{C}_2\text{H}_5]^+$), 258 (5), 213 (10), 198 (5), 89 (100), 59 (40), 41 (70); GC (98%) t_{R} 12.66 mins (70 – 250 °C, 20 °C min⁻¹). These data are consistent with those reported by Katz and co-workers.¹

1-(*N,N*-diethylcarbamoyloxy)-2,2-difluoro-1-(3'-methoxyphenyl) ethene 12bb

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11b** (206 mg, 1.1 mmol) to afford **12b** (179 mg, 63%) as a pale yellow oil; R_{f} (40% diethyl ether in light petroleum ether) 0.31; ν_{max} (film)/cm⁻¹ 2977, 2939, 1733, 1602, 1581, 1422, 1382, 1270, 1219, 1142, 1096, 1043, 1007, 952, 931, 843, 782, 755, 690; δ_{H} (400 MHz, CDCl_3) 1.20 (3 H, t, J 7.1, NCH_2CH_3), 1.29 (3 H, t, J 7.1, NCH_2CH_3), 3.38 (2 H, q, J 7.1, NCH_2CH_3), 3.47 (2 H, q, J 7.1, NCH_2CH_3), 3.83 (3 H, s, OCH_3), 6.87 (1 H, dd, J 8.35, $^4J_{\text{H-H}}$ 2.55, ArH), 6.98 (1 H, s, ArH), 7.04 (1 H, d, J 7.65, ArH), 7.31 (1 H, t, J 8.02, ArH); δ_{C} (100 MHz, CDCl_3) 12.8, 13.7, 41.5, 42.1, 54.7, 110.8 (dd, $^4J_{\text{C-F}}$ 6.6, 3.5), 111.8 (dd, $^2J_{\text{C-F}}$ 38.0, 19.3), 113.2, 117.4 (dd, $^4J_{\text{C-F}}$ 6.6, 3.5), 129.1, 131.1 (br. d, $^3J_{\text{C-F}}$ 6.6), 152.4, 154.5 (app. t, $^1J_{\text{C-F}}$ 290.4), 159.2; δ_{F} (376 MHz, CDCl_3) -93.5 (1 F, d, $^2J_{\text{F-F}}$ 48.4), -103.2 (1 F, d, $^2J_{\text{F-F}}$ 48.4); [HRMS (ES-TOF, $[\text{M} + \text{Na}]^+$) Found: 308.1059; Calc. for $\text{C}_{14}\text{H}_{17}\text{NO}_3\text{F}_2\text{Na}$: 308.1074]; m/z (CI) 303 (100%, $[\text{M} + \text{NH}_4]^+$), 286 (48%, $[\text{M} + \text{H}]^+$), 74 (53), 72 (20), 52 (9) and 44 (16).

1-(*N,N*-diethylcarbamoyloxy)-2,2-difluoro-1-phenyl ethene 12bc

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11c** (172 mg, 1.1 mmol) to afford **12bc** (165 mg, 65%) as a yellow oil; R_{f} (40% diethyl ether in light petroleum ether) 0.31;

$\nu_{\text{max}}(\text{film})/\text{cm}^{-1}$ 1732, 1424, 1382, 1269, 1224, 1148, 984, 759, 693; $\delta_{\text{H}}(400 \text{ MHz, CDCl}_3)$ 1.20 (3 H, t, J 7.1, NCH_2CH_3), 1.29 (3 H, t, J 7.1, NCH_2CH_3), 3.38 (2 H, q, J 7.1, NCH_2CH_3), 3.47 (2 H, q, J 7.1, NCH_2CH_3), 7.29-7.34 (1 H, m, ArH), 7.38-7.46 (4 H, m, ArH); $\delta_{\text{C}}(100 \text{ MHz, CDCl}_3)$ 12.8, 13.7, 41.5, 42.1, 111.9 (dd, $^2J_{\text{C-F}}$ 38.40, 19.11), 125.0 (dd, $^4J_{\text{C-F}}$ 6.54, 3.47), 127.6, 128.0, 129.7 (br. d, $^3J_{\text{C-F}}$ 6.55), 152.4, 154.4 (app. t, $^1J_{\text{C-F}}$ 289.76); $\delta_{\text{F}}(376 \text{ MHz, CDCl}_3)$ -93.7 (1 F, d, $^2J_{\text{F-F}}$ 49.1), -103.7 (1F, d, $^2J_{\text{F-F}}$ 49.1); [HRMS (EI, M^+) Found: 255.106763; Calc. for $\text{C}_{13}\text{H}_{15}\text{F}_2\text{NO}_2$: 255.107085]; m/z (CI) 284 (8%, $[\text{M} + \text{C}_2\text{H}_5]^+$), 256 (60%, $[\text{M} + \text{H}]^+$), 100 (100); GC (98%) t_{R} 11.15 mins (70 – 320 °C, 20 °C min^{-1}).

1,1-Difluoro-2-(*N,N*-diethylcarbamoyloxy)-2-(2'-naphthyl) ethene 12bd

Was prepared from **9b** (3.95 cm^3 of a 0.25 M solution) and **11d** (228 mg, 1.1 mmol) to afford **12bd** (174 mg, 57%) as colourless plates; R_{F} (15% diethyl ether in hexane) 0.25; mp 57 – 57.5 °C; (Found: C, 66.7; H, 5.7; N, 4.4; $\text{C}_{13}\text{H}_{15}\text{F}_2\text{NO}_2$ requires C, 66.9; H, 5.6; N, 4.6%); $\delta_{\text{H}}(400 \text{ MHz, CDCl}_3)$ 1.22 (3 H, t, J 7.1, NCH_2CH_3), 1.34 (3 H, t, J 7.1, NCH_2CH_3), 3.41 (2 H, q, J 7.1, NCH_2CH_3), 3.53 (2 H, q, J 7.1, NCH_2CH_3), 7.48-7.54 (2 H, m, ArH), 7.58 (1 H, dt, J 8.7, $^4J_{\text{H-H}}$ 1.6 ArH), 7.82-7.92 (4 H, m, ArH); $\delta_{\text{C}}(100 \text{ MHz, CDCl}_3)$ 13.3, 14.2, 42.0, 42.6, 112.6 (dd, $^2J_{\text{C-F}}$ 38.1, 19.3), 123.0 (dd, $^4J_{\text{C-F}}$ 6.6, 2.8), 125.0 (t, $^4J_{\text{C-F}}$ 5.4), 126.5, 126.5, 127.6, 127.7 (br. d, $^3J_{\text{C-F}}$ 5.7), 128.3, 128.3, 132.9, 133.1, 153.0, 155.2 (app. t, $^1J_{\text{C-F}}$ 290.1); $\delta_{\text{F}}(376 \text{ MHz, CDCl}_3)$ -93.3 (1F, $^2J_{\text{F-F}}$ 48.1), -103.7 (1F, $^2J_{\text{F-F}}$ 48.1); [HRMS (CI, $[\text{M} + \text{NH}_4]^+$) Found: 323.158429; Calc. for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_2\text{F}_2$: 323.157110].

1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-(4'-chlorophenyl)ethene 12bf

Was prepared from **9b** (3.95 cm^3 of a 0.25 M solution) and **11f** (192 mg, 1.1 mmol) to afford **12bd** (147 mg, 51%) as a pale yellow oil; R_{F} (40% diethyl ether in light petroleum ether) 0.39; $\nu_{\text{max}}(\text{film})/\text{cm}^{-1}$ 2982, 2939, 1727, 1499, 1424, 1260, 1140, 1094, 980, 818; $\delta_{\text{H}}(400$

MHz, CDCl₃) 1.20 (3 H, t, *J* 7.1, NCH₂CH₃), 1.28 (3 H, t, *J* 7.1, NCH₂CH₃), 3.38 (2 H, q, *J* 7.1, NCH₂CH₃), 3.46 (2 H, q, *J* 7.0, NCH₂CH₃), 7.37 (4 H, br. s, ArH); δ_C(100 MHz, CDCl₃); 12.8, 13.7, 41.5, 42.2, 111.3 (dd, ²*J*_{C-F} 38.0, 19.7), 126.3 (dd, ⁴*J*_{C-F} 6.5, 3.5), 128.3, 133.5, 152.3, 154.4 (app. t, ¹*J*_{C-F} 291.0); δ_F(376 MHz, CDCl₃) -93.1 (1F, ²*J*_{F-F} 48.0), -103.1 (1F, ²*J*_{F-F} 48.0); [HRMS (EI, M⁺) Found: 289.068714; Calc. for C₁₃H₁₅F₂NO₂F₂Cl: 289.068113]; *m/z* (CI) 318 (9%, [M + C₂H₅]⁺), 290 (50%, [M + H]⁺), 254 (10), 100 (100), 41 (20); GC (95%) t_R 12.02 mins (70 – 250 °C, 20 °C min⁻¹).

1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-[4''-(trifluoromethanesulfonyloxy)phenyl] ethene 12bg

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11g** (387 mg, 1.1 mmol) to afford **12bg** (240 mg, 60%) as a pale yellow oil; R_f (40% diethyl ether in hexane) 0.43; (Found: C, 41.72; H, 3.33; N, 3.82; C₁₄H₁₄F₅NO₅S requires C, 41.69; H, 3.50; N, 3.47%); ν_{max}(film)/cm⁻¹ 2982, 1736, 1598, 1505, 1426, 1275, 1216, 1146, 888; δ_H(400 MHz, CDCl₃) 1.21 (3 H, t, *J* 7.2, NCH₂CH₃), 1.29 (3 H, t, *J* 7.2, NCH₂CH₃), 3.39 (2 H, q, *J* 7.1, NCH₂CH₃), 3.47 (2 H, q, *J* 7.1, NCH₂CH₃), 7.30-7.34 (2 H, m, ArH), 7.50-7.55 (2 H, m, ArH); δ_C(100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.2, 110.8 (dd, ²*J*_{C-F} 38.2, 20.3), 118.2 (q, ¹*J*_{C-F} 320.9), 121.1, 126.9 (dd, ⁴*J*_{C-F} 6.9, 3.6), 130.3 (br. d, ³*J*_{C-F} 6.9), 148.3, 152.1, 154.6 (app. t, ¹*J*_{C-F} 291.8); δ_F(376 MHz, CDCl₃) -72.8 (3 F, s), -91.7 (1 F, d, ²*J*_{F-F} 44.9), -101.3 (1 F, d, ²*J*_{F-F} 44.9); [HRMS (ES-TOF, [M + Na]⁺) Found: 426.0413; Calc. for C₁₄H₁₄NO₅F₅Na: 426.0411). *m/z* (CI) 432 (13%, [M + C₂H₅]⁺), 404 (100%, [M + H]⁺), 271 (5), 100 (65), 57 (5); GC (98%) t_R 12.26 mins (70 – 320 °C, 20 °C min⁻¹).

1-(*N,N*-diethylcarbamoyloxy)-2,2-difluoro-1-(4'-trifluoromethylphenyl) ethene 12bh

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11h** (248 mg, 1.1 mmol) to afford **12bh** (172 mg, 53%) as a yellow oil; *R*_f (40% diethyl ether in light petroleum ether) 0.55; ν_{max} (film)/cm⁻¹ 2982, 2939, 1731, 1427, 1412, 1327, 1273, 1148, 1116, 1050, 980, 844, 822; δ_{H} (400 MHz, CDCl₃) 1.21 (3 H, t, *J* 7.2, NCH₂CH₃), 1.30 (3 H, t, *J* 7.2, NCH₂CH₃), 3.39 (2 H, q, *J* 7.2, NCH₂CH₃), 3.48 (2 H, q, *J* 7.2, NCH₂CH₃), 7.55 (2 H, br. d, *J* 8.3, Ar*H*), 7.66 (2 H, br. d, *J* 8.3, Ar*H*); δ_{C} (100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.2, 111.2 (dd, ²*J*_{C-F} 37.8, 19.9), 123.4 (q, ¹*J*_{C-F} 272.6), 125.0 – 125.2 (m), 129.5 (q, ²*J*_{C-F} 32.5), 133.5 (br. d, ³*J*_{C-F} 6.9), 152.2, 154.8 (app. t, ¹*J*_{C-F} 292.6); δ_{F} (376 MHz, CDCl₃) -62.9 (3 F, s), -91.1 (1 F, d, ²*J*_{F-F} 43.1), -101.3 (1 F, d, ²*J*_{F-F} 43.1); [HRMS (NSI, [M + H]⁺) Found: 324.1022; calc. for C₁₄H₁₅F₅NO₂: 324.1023]; *m/z* (CI) 352 (25%, [M + C₂H₅]⁺), 324 (100%, [M + H]⁺), 304 (90), 100 (90); GC (XX%) *t*_R 10.71 mins (70 – 320 °C, 20 °C min⁻¹).

1-(*N,N*-diethylcarbamoyloxy)-2,2-difluoro-1-(3'-trifluoromethylphenyl) ethene 12bj

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11j** (248 mg, 1.1 mmol) to afford **12bj** (120 mg, 37%) as a pale yellow oil; *R*_f (40% diethyl ether in hexane) 0.33; ν_{max} (film)/cm⁻¹ 2982, 2939, 1728, 1424, 1345, 1252, 1144, 1127, 1073, 1000, 923, 808, 695; δ_{H} (400 MHz, CDCl₃) 1.21 (3 H, t, *J* 7.2, NCH₂CH₃), 1.30 (3 H, t, *J* 7.2, NCH₂CH₃), 3.39 (2 H, q, *J* 7.2, NCH₂CH₃), 3.49 (2 H, q, *J* 7.2, NCH₂CH₃), 7.53 (1 H, t, *J* 7.7, Ar*H*), 7.58 (1 H, br. d, *J* 7.8, Ar*H*), 7.63 (1 H, br. t, *J* 7.7, Ar*H*), 7.68 (1 H, br. s, Ar*H*); δ_{C} (100 MHz, CDCl₃) 12.7, 13.6, 41.6, 42.2, 111.1 (dd, ²*J*_{C-F} 37.3, 19.5), 121.5-121.8 (m), 123.2 (q, ¹*J*_{C-F} 271.2), 124.3 (d, ⁴*J*_{C-F} 3.14), 128.1 (dd, ⁴*J*_{C-F} 7.0, 3.0), 128.6, 130.6 (q, ²*J*_{C-F} 32.6) 130.8 (br. d, ³*J*_{C-F} 6.9), 152.1, 154.7 (app. t, ¹*J*_{C-F} 291.0); δ_{F} (376 MHz, CDCl₃) -63.0 (3 F, s), -91.8 (1 F, d, ²*J*_{F-F} 45.2), -102.1 (1 F, d, ²*J*_{F-F} 45.2); [HRMS (APCI, [M + H]⁺) Found: 324.1018; Calc. for C₁₄H₁₅F₅NO₂: 324.1023]; *m/z* (CI) 352 (25%, [M + C₂H₅]⁺), 324 (100%, [M + H]⁺), 304 (25), 253 (25), 100 (90); GC (98%) *t*_R 10.55 mins (70 – 320 °C, 20 °C min⁻¹).

1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-(4'-cyanophenyl) ethene 12bk

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11k** (200 mg, 1.1 mmol) to afford **12bj** (101 mg, 36%) as a pale yellow solid; *R*_f (40% diethyl ether in light petroleum ether) 0.23; mp 80-82 °C; (Found: C, 60.55; H, 4.99; N, 9.57; C₁₄H₁₄F₂N₂O₂ requires C, 60.00; H, 5.03; N, 9.57%); *v*_{max}(film)/cm⁻¹ 2967, 2932, 2229, 1720, 1415, 1269, 1146, 982, 846, 822; *δ*_H(400 MHz, CDCl₃) 1.20 (3 H, t, *J* 7.2, NCH₂CH₃), 1.29 (3 H, t, *J* 7.2, NCH₂CH₃), 3.38 (2 H, q, *J* 7.2, NCH₂CH₃), 3.48 (2 H, q, *J* 7.2, NCH₂CH₃), 7.53 (2 H, br. d, *J* 8.3 Ar*H*), 7.69 (2 H, br. d, *J* 8.3 Ar*H*); *δ*_C(100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.3, 111.1, 111.2 (dd, ²*J*_{C-F} 37.4, 20.3), 117.9, 125.2 (dd, ⁴*J*_{C-F} 7.4, 3.7), 131.8, 134.5 (br. d, ³*J*_{C-F} 7.4), 152.0, 154.9 (app. t, ¹*J*_{C-F} 294.0); *δ*_F(376 MHz, CDCl₃) -89.3 (1 F, d, ²*J*_{F-F} 39.1), -99.3 (1 F, d, ²*J*_{F-F} 39.1); [HRMS (APCI, [M + H]⁺) Found: 281.1089; Calc. for C₁₄H₁₅N₂O₂F₂: 281.1102]; *m/z* (CI) 321 (8), 309 (20%, [M + C₂H₅]⁺), 281 (100%, [M + H]⁺), 100 (20); GC (98%) *t*_R 12.62 mins (70 – 320 °C, 20 °C min⁻¹).

1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-(3'-cyanophenyl) ethene 12bl

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11l** (200 mg, 1.1 mmol) to afford **12bl** (82 mg, 29%) as a pale yellow oil; *R*_f (40% diethyl ether in light petroleum ether) 0.30; *v*_{max}(film)/cm⁻¹ 2980, 2939, 2235, 1728, 1420, 1267, 1179, 1144, 1012, 928, 799, 754, 684; *δ*_H(400 MHz, CDCl₃) 1.21 (3 H, t, *J* 7.1, NCH₂CH₃), 1.29 (3 H, t, *J* 7.1, NCH₂CH₃), 3.38 (2 H, q, *J* 7.1, NCH₂CH₃), 3.47 (2 H, q, *J* 7.1, NCH₂CH₃), 7.49-7.71 (4 H, envelope, Ar*H*); *δ*_C(100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.3, 110.7 (dd, ²*J*_{C-F} 37.8, 20.2), 112.6, 117.9, 128.4 (dd, ⁴*J*_{C-F} 6.2, 4.0), 129.4, 129.5 (dd, ⁴*J*_{C-F} 7.8, 3.3), 130.9, 131.4 (br. d, ³*J*_{C-F} 6.6), 152.1, 154.7 (app. t, ¹*J*_{C-F} 292.3); *δ*_F(376 MHz, CDCl₃) -89.3 (1 F, d, ²*J*_{F-F} 39.1), -99.3 (1 F, d, ²*J*_{F-F} 39.1); [HRMS (APCI, [M + H]⁺) Found: 281.1093; Calc. for C₁₄H₁₅N₂O₂F₂: 281.1102]; *m/z* (CI)

309 (25%, $[M + C_2H_5]^+$), 281 (100%, $[M + H]^+$), 100 (25); GC (97%) t_R 12.45 mins (70 – 320 °C, 20 °C min⁻¹).

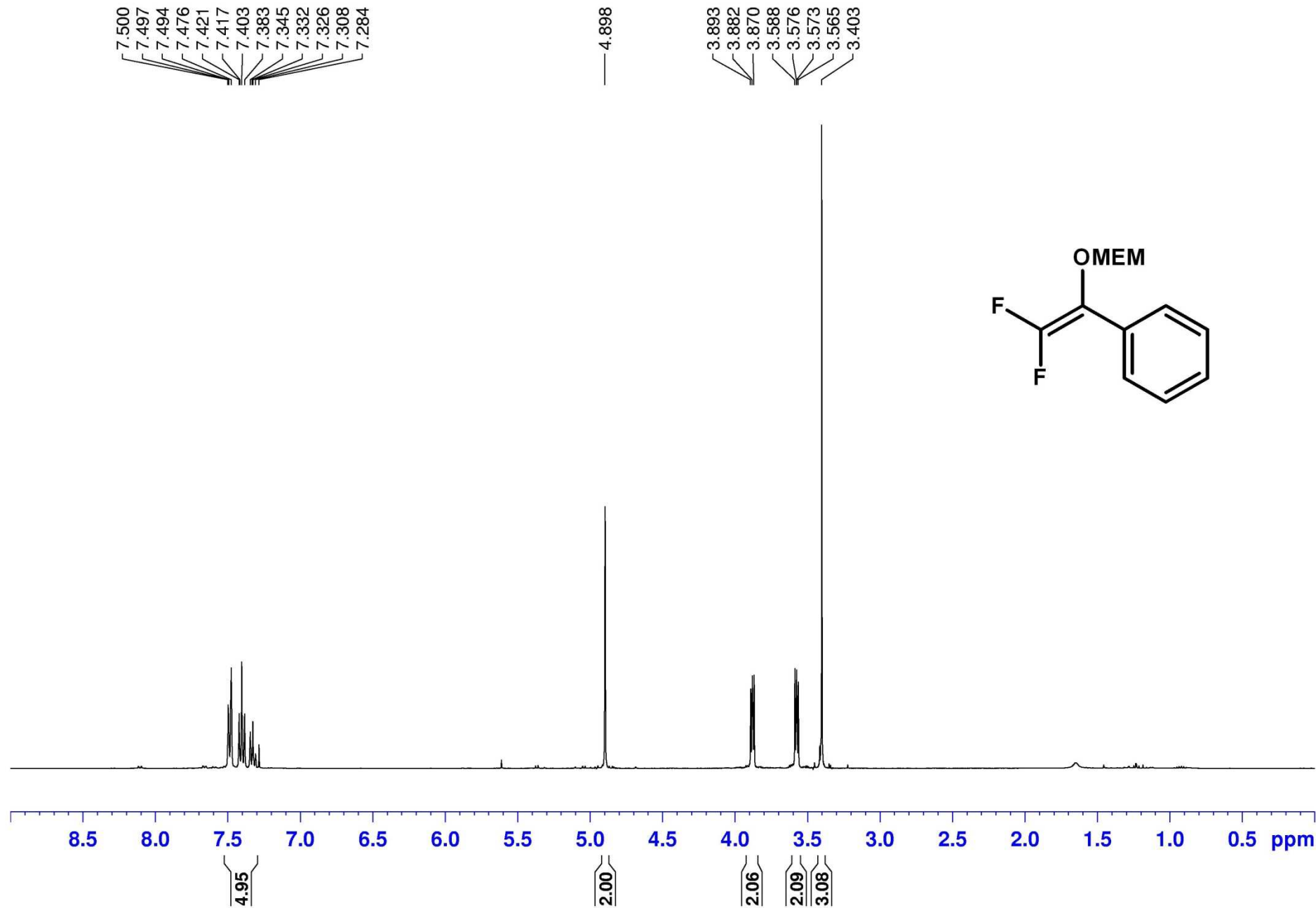
1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-(4'-nitrophenyl) ethene 12bm

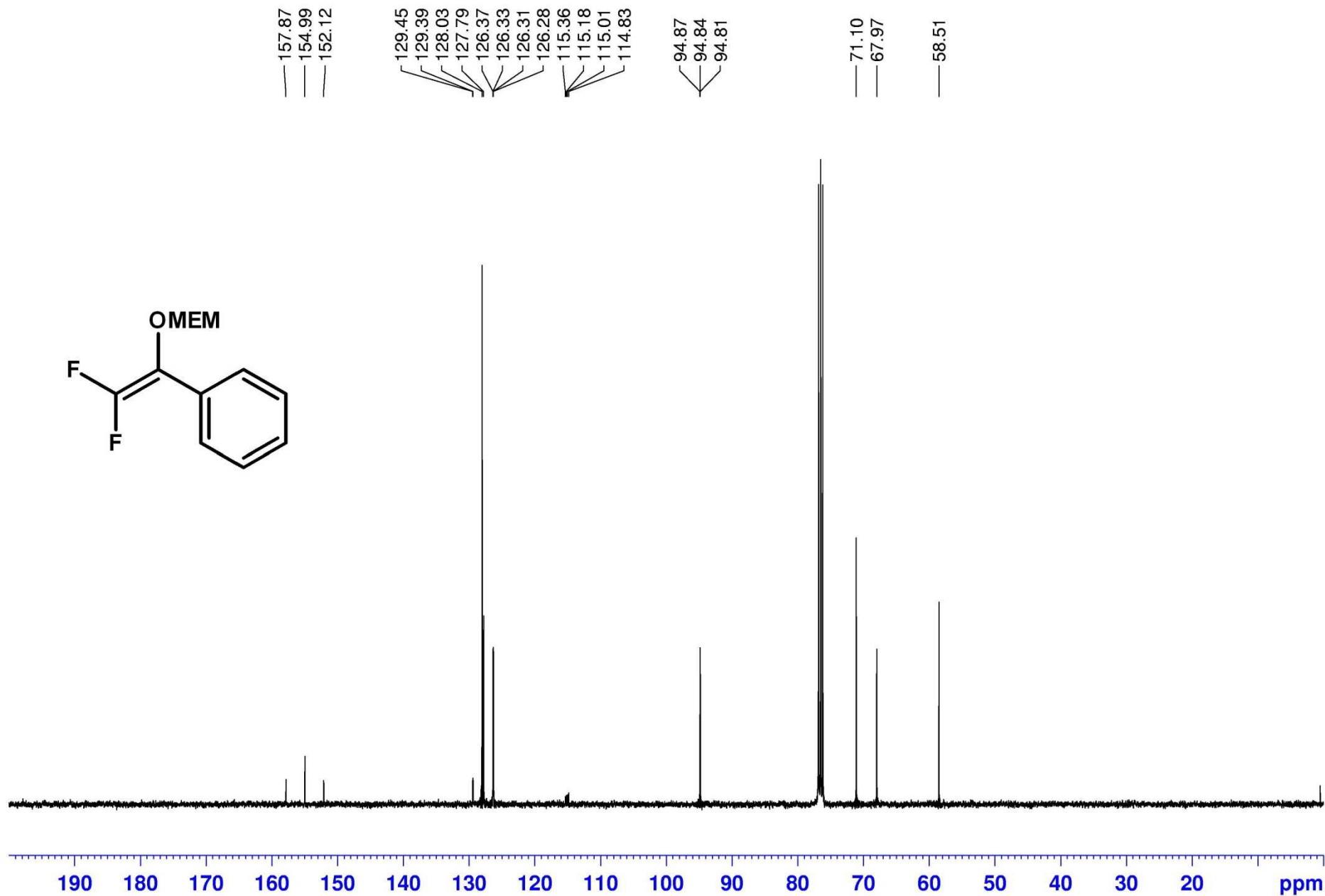
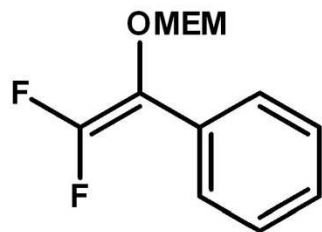
Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11m** (274 mg, 1.1 mmol) to afford **12bm** (125 mg, 42%) as a pale yellow oil; R_f (40% diethyl ether in light petroleum ether) 0.42; $\nu_{max}(\text{film})/\text{cm}^{-1}$ 1731, 1600, 1522, 1476, 1460, 1427, 1383, 1350, 1332, 1270, 1223, 1151, 988, 854, 753; δ_H (400 MHz, CDCl₃) 1.20 (3 H, t, J 7.0, NCH₂CH₃), 1.30 (3 H, t, J 7.0, NCH₂CH₃), 3.38 (2 H, q, J 7.1, NCH₂CH₃), 3.49 (2 H, q, J 7.1, NCH₂CH₃), 7.59 (2 H, d, J 8.8, ArH), 8.25 (2 H, d, J 8.8 ArH); δ_C (100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.3, 111.1 (dd, $^2J_{C-F}$ 36.9, 20.4), 123.4, 125.4 (dd, $^4J_{C-F}$ 7.6, 3.8), 136.4 (br. d, $^3J_{C-F}$ 7.3), 146.5, 152.0, 155.0 (app. t, $^1J_{C-F}$ 294.3); δ_F (376 MHz, CDCl₃) -88.7 (1 F, d, $^2J_{F-F}$ 36.7), -98.8 (1 F, d, $^2J_{F-F}$ 36.7); [HRMS (ES-TOF, $[M + Na]^+$) Found: 323.0830; Calc. for C₁₃H₁₄N₂O₄F₂Na: 323.0819]; m/z (CI) 341 (2), 329 (5%, $[M + C_2H_5]^+$), 301 (100%, $[M + H]^+$), 285 (5), 100 (20); GC (95%) t_R 13.22 mins (70 – 320 °C, 20 °C min⁻¹).

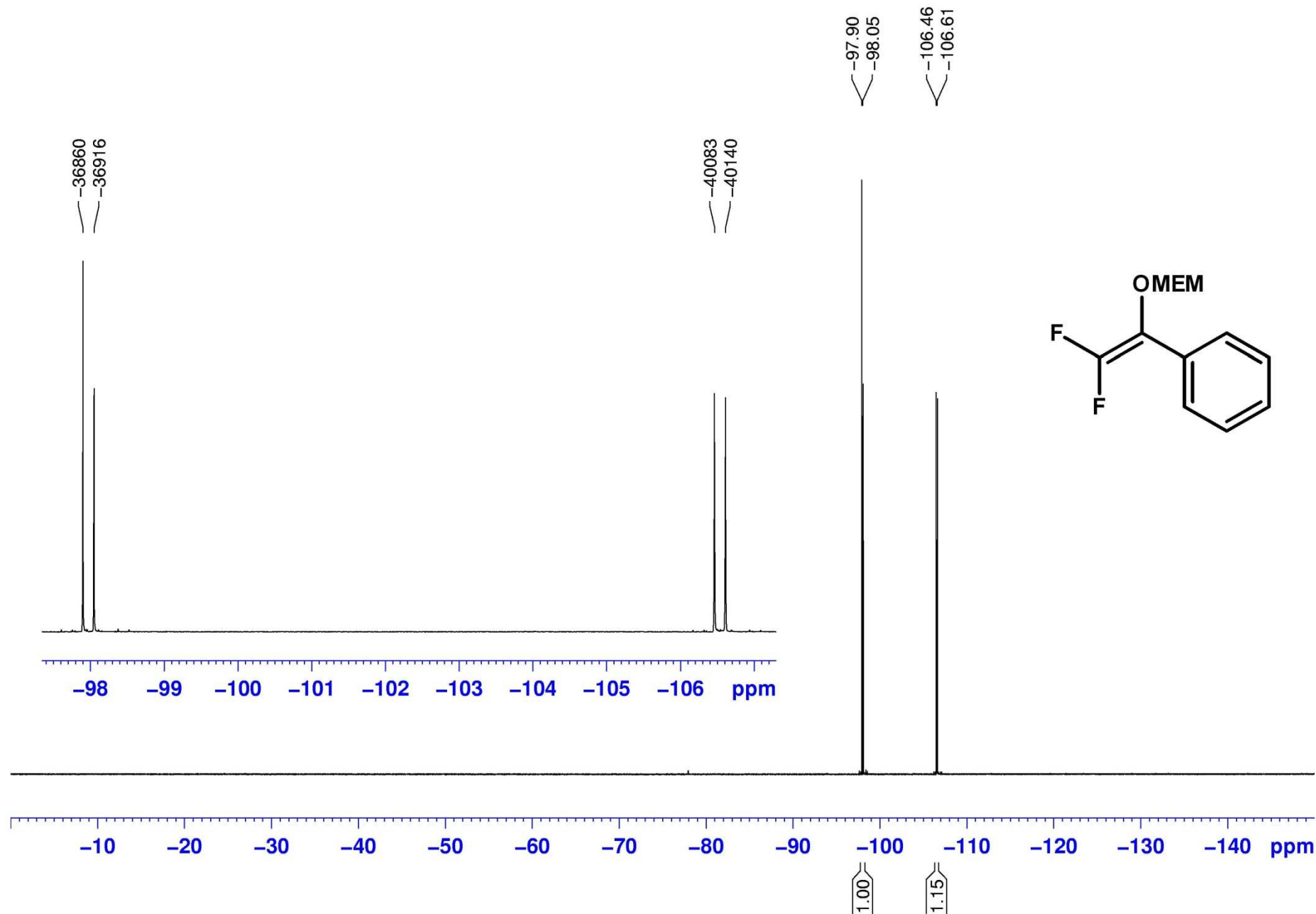
1-(*N,N*-Diethylcarbamoyloxy)-2,2-difluoro-1-(3'-nitrophenyl) ethene 12bn

Was prepared from **9b** (3.95 cm³ of a 0.25 M solution) and **11n** (222 mg, 1.1 mmol) to afford **12bn** (58 mg, 18%) as a pale yellow oil; R_f (25% diethyl ether in light petroleum ether) 0.42; $\nu_{max}(\text{film})/\text{cm}^{-1}$ 3012, 2943, 1729, 1620, 1424, 1343, 1254, 1168, 1148, 1096, 1075, 1002, 950, 801, 748; δ_H (400 MHz, CDCl₃) 1.21 (3 H, t, J 7.2, NCH₂CH₃), 1.32 (3 H, t, J 7.2, NCH₂CH₃), 3.39 (2 H, q, J 7.2, NCH₂CH₃), 3.51 (2 H, q, J 7.2, NCH₂CH₃), 7.59 (1 H, t, J 8.2, ArH), 7.76-7.80 (1H, m, ArH), 8.18 (1H, dd, J 8.2, $^4J_{H-H}$ 2.1, ArH), 8.28 (1 H, t, $^4J_{H-H}$ 2.1, ArH); δ_C (100 MHz, CDCl₃) 12.7, 13.7, 41.6, 42.3, 110.7 (dd, $^2J_{C-F}$ 37.5, 20.5), 119.8 (dd, $^4J_{C-F}$ 5.9, 4.4), 122.3, 129.2, 130.6 (dd, $^4J_{C-F}$ 8.1, 3.5), 131.9 (br. d, $^3J_{C-F}$ 7.3), 148.0, 152.0,

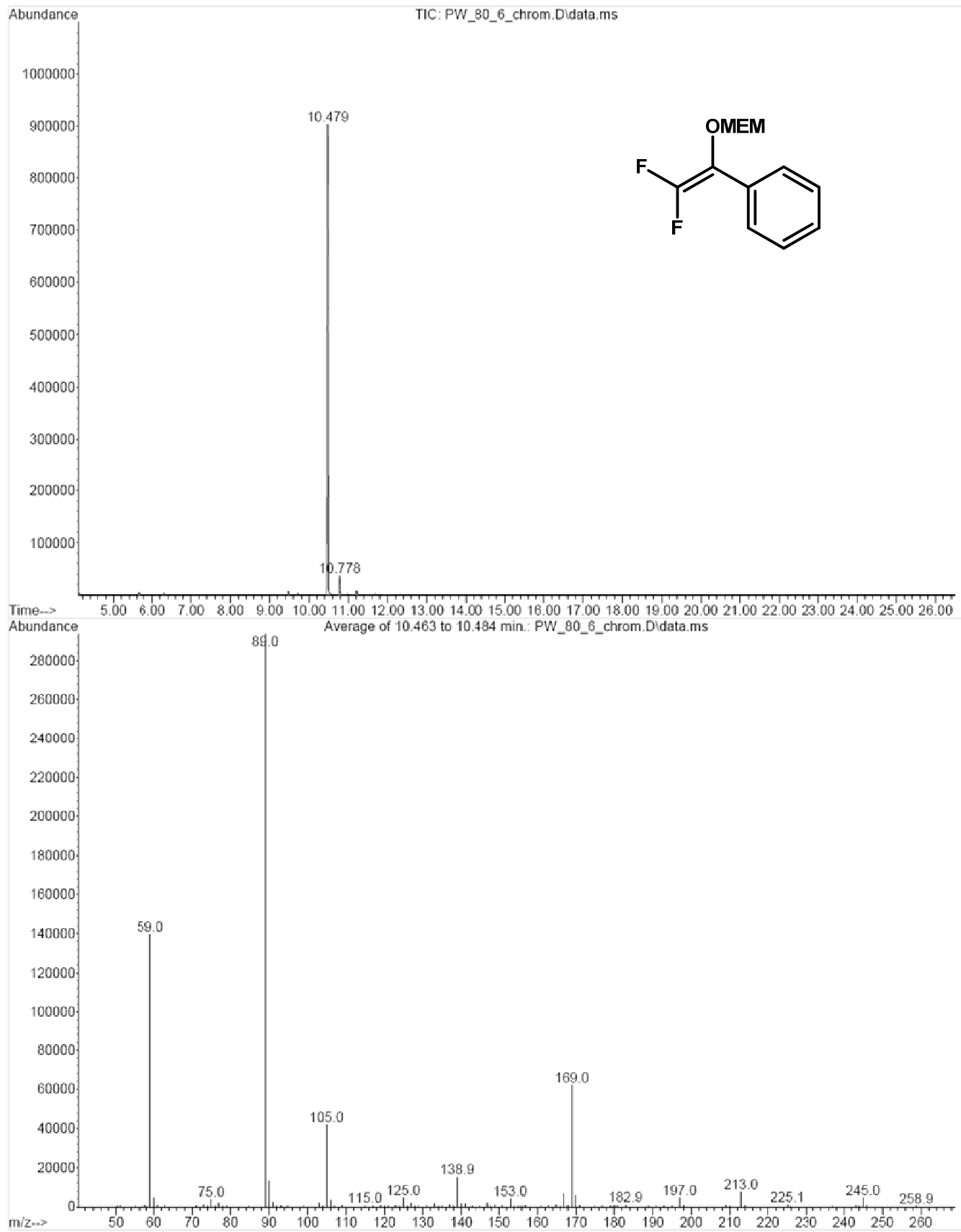
154.9 (app. t, $^1J_{\text{C-F}}$ 293.2); δ_{F} (376 MHz, CDCl_3) -90.3 (1 F, d, $^2J_{\text{F-F}}$ 42.3), -100.7 (1 F, d, $^2J_{\text{F-F}}$ 42.3); [HRMS (NSI, $[\text{M} + \text{H}]^+$) Found: 301.0991; calc. for $\text{C}_{13}\text{H}_{15}\text{F}_2\text{N}_2\text{O}_4$: 301.0999]; m/z (CI) 329 (15%, $[\text{M} + \text{C}_2\text{H}_5]^+$), 301 (100%, $[\text{M} + \text{H}]^+$), 100 (27); GC (98%) t_{R} 13.00 mins (70 – 320 °C, 20 °C min^{-1}).

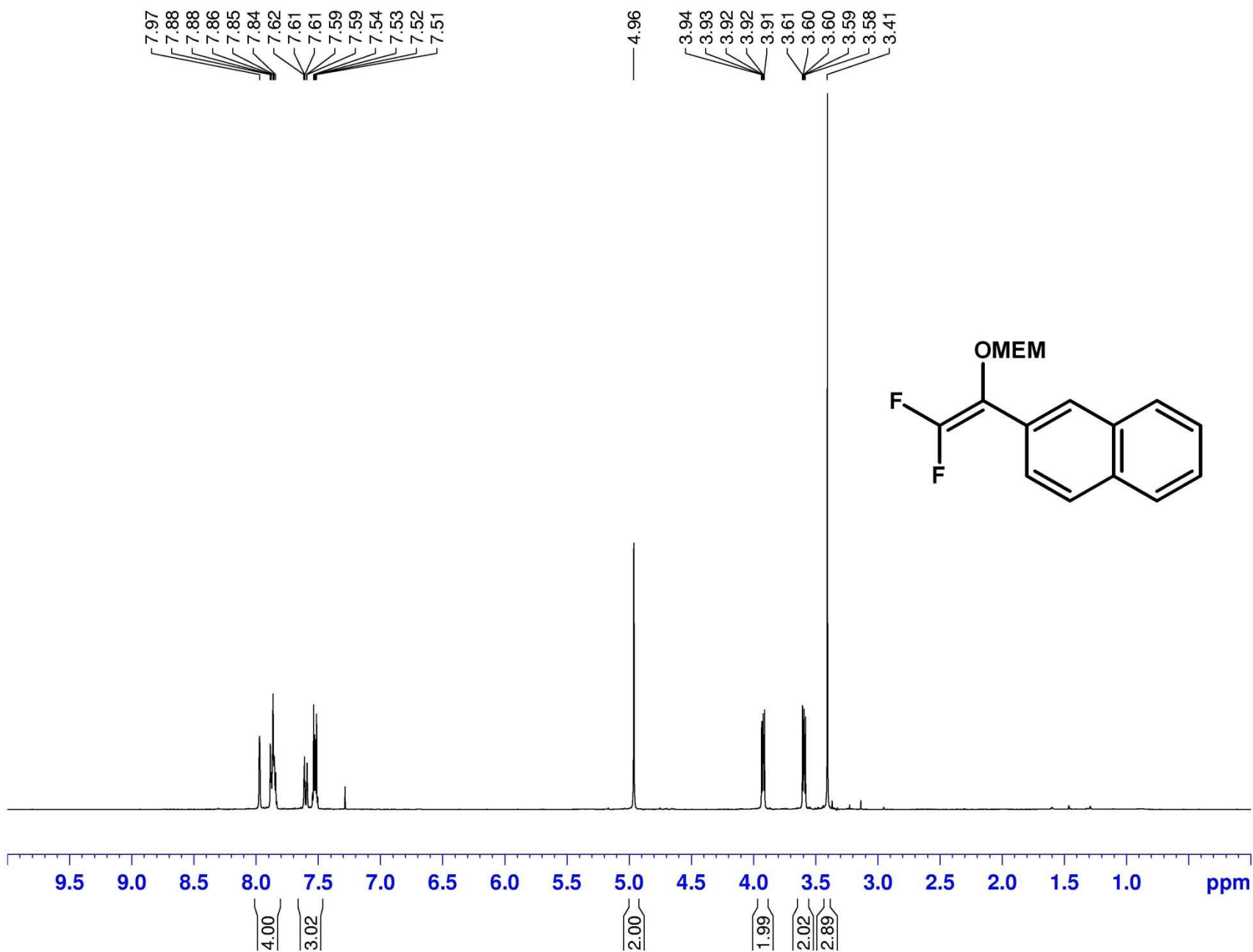


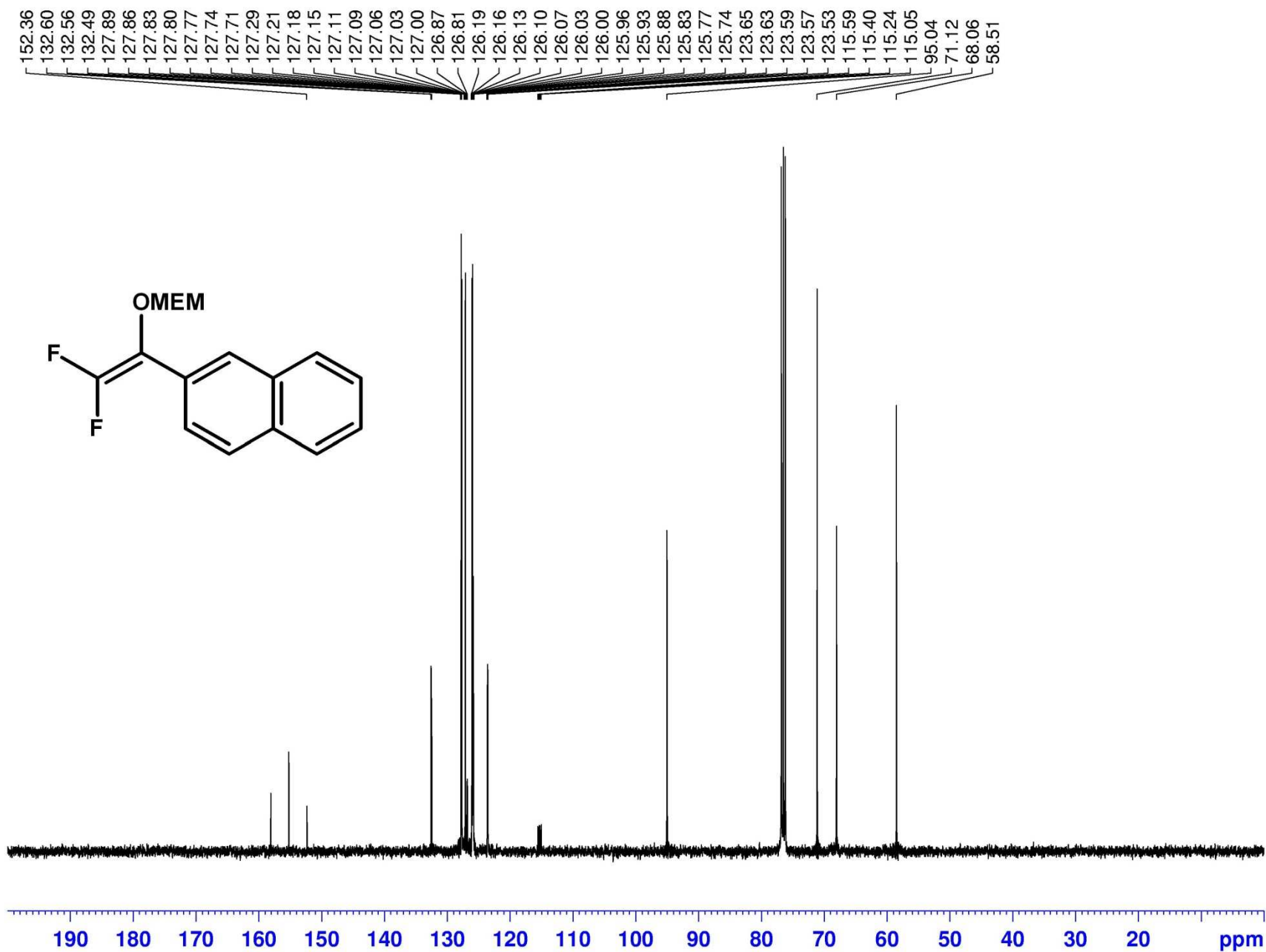


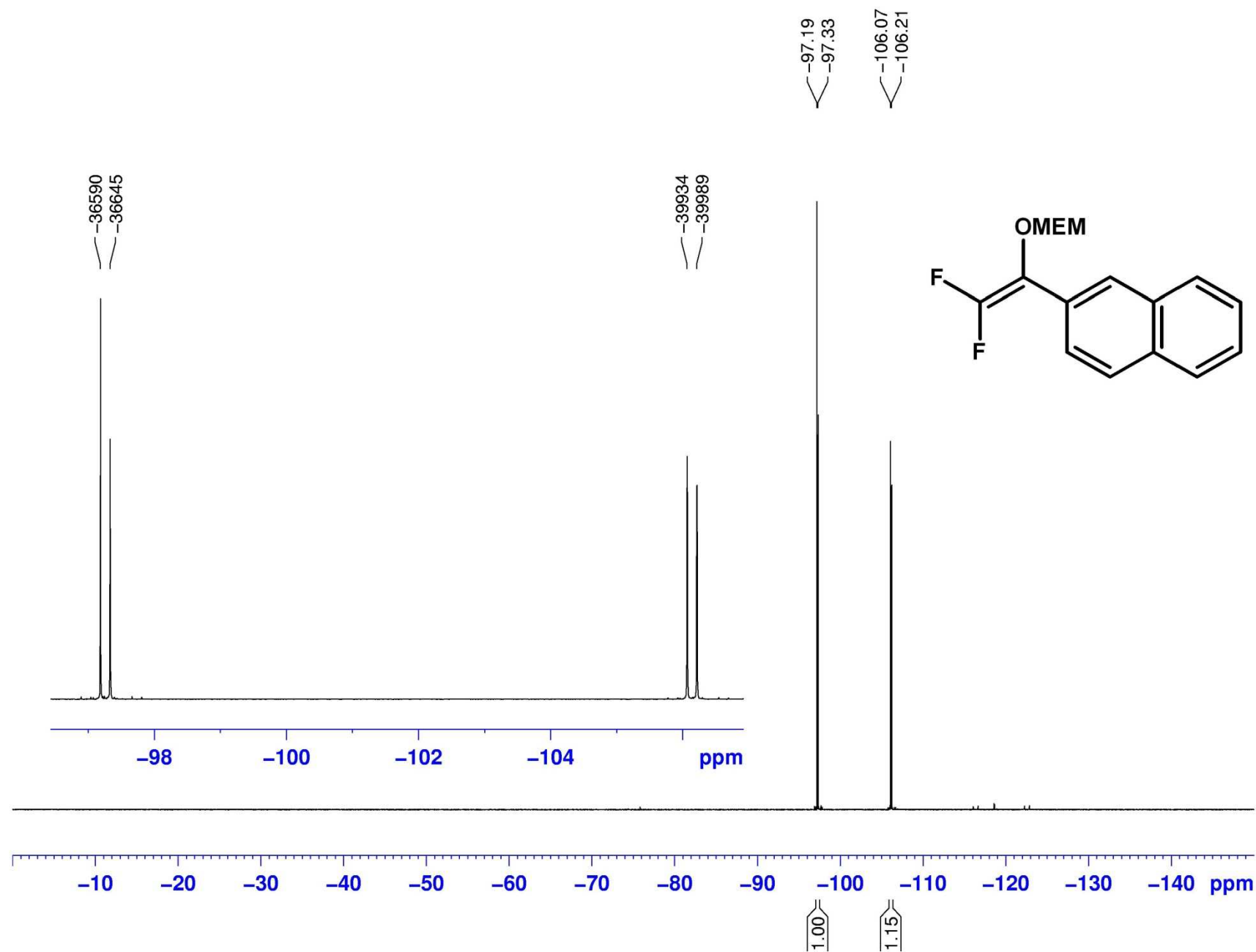


File :E:\PW\PW_80_6_chrom.D
Operator : PW
Acquired : 17 Jan 2011 12:56 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 21

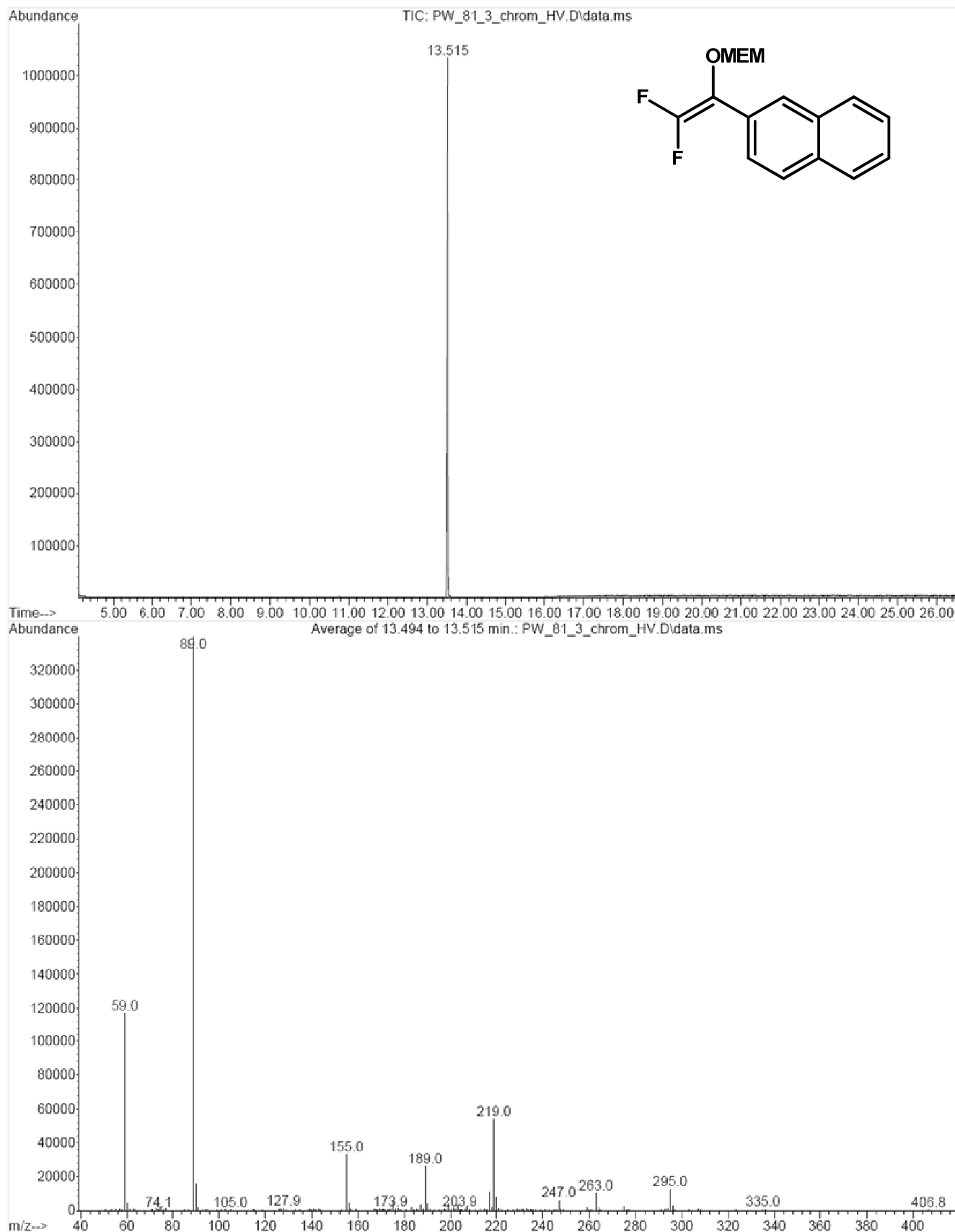


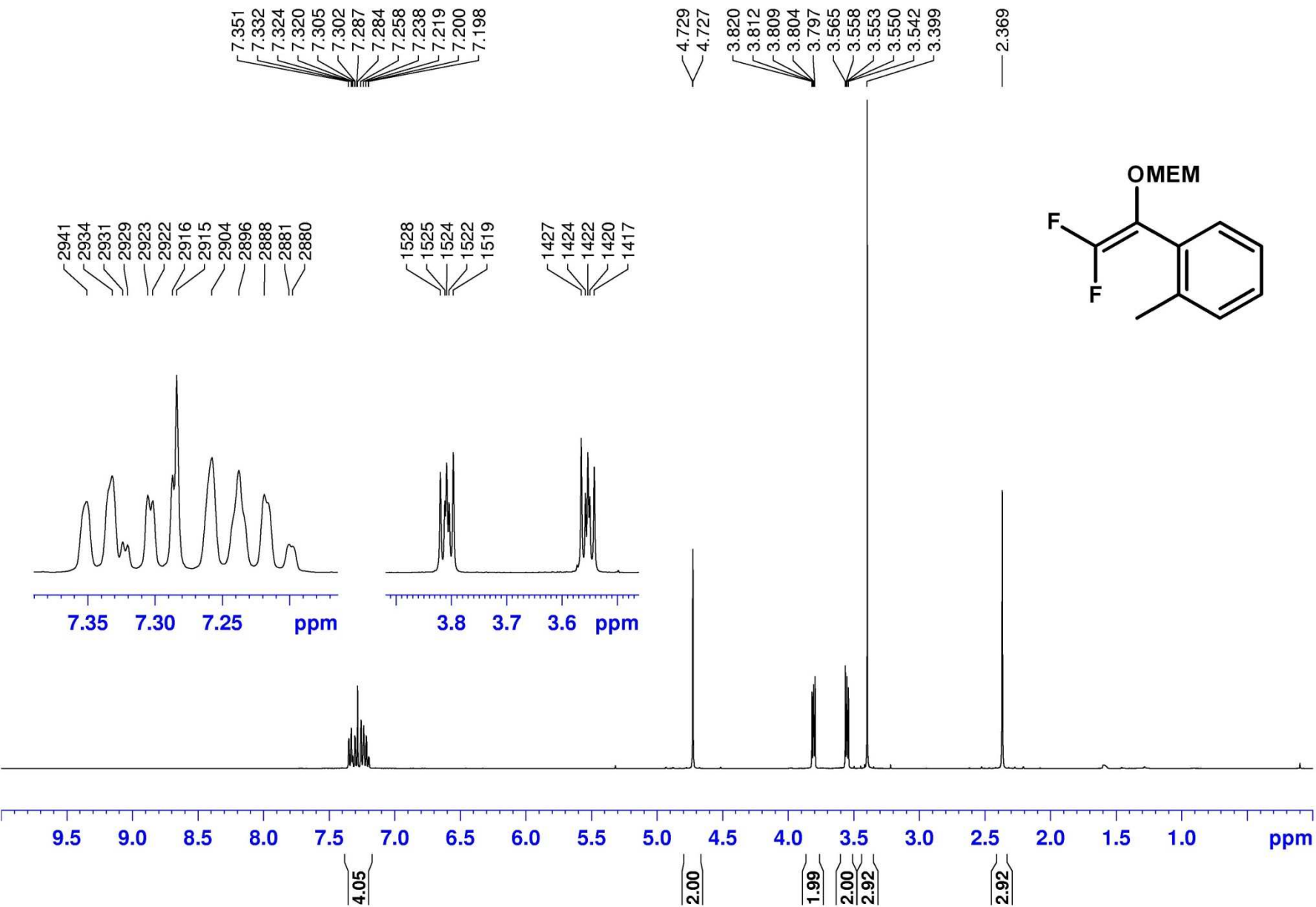


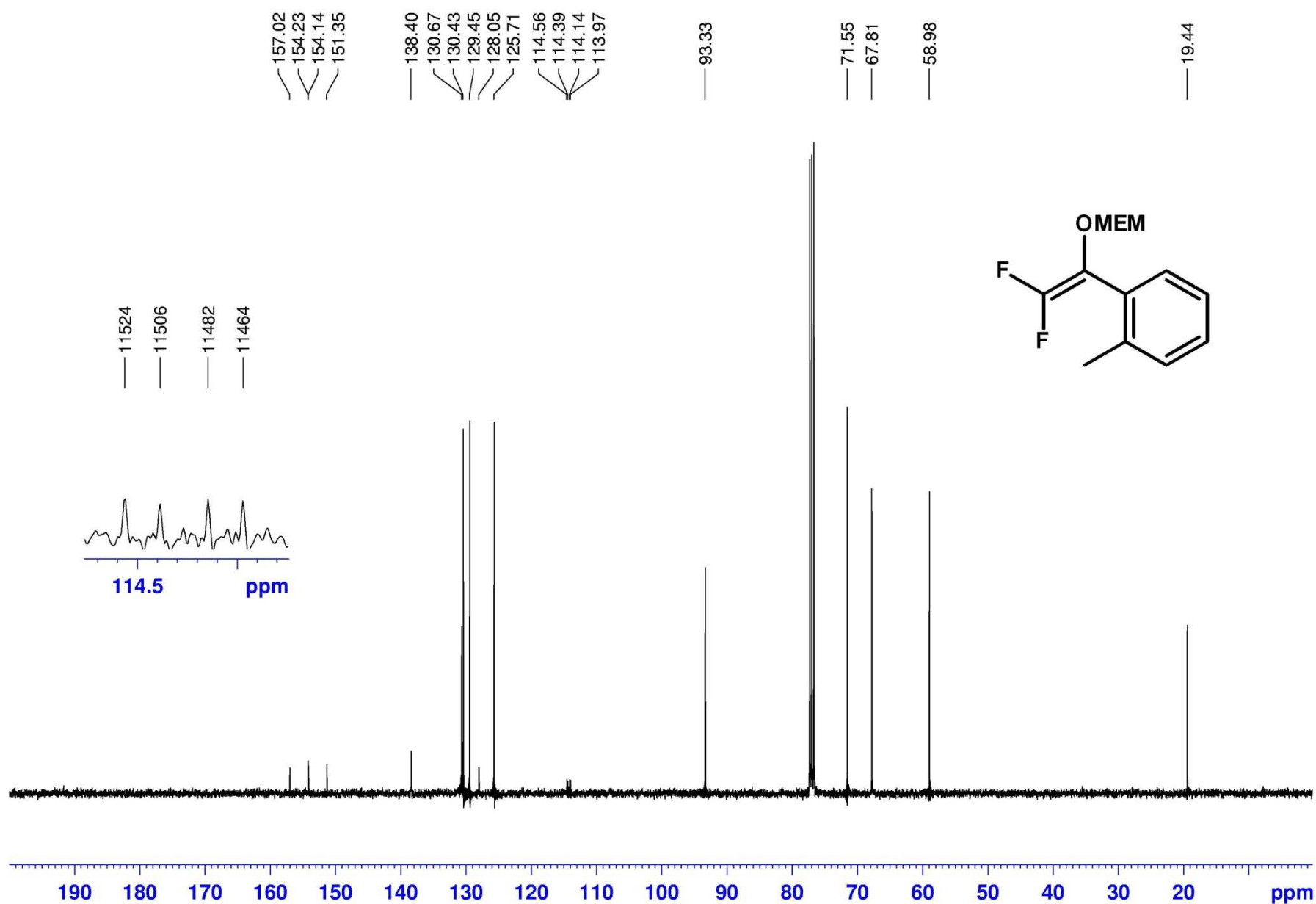


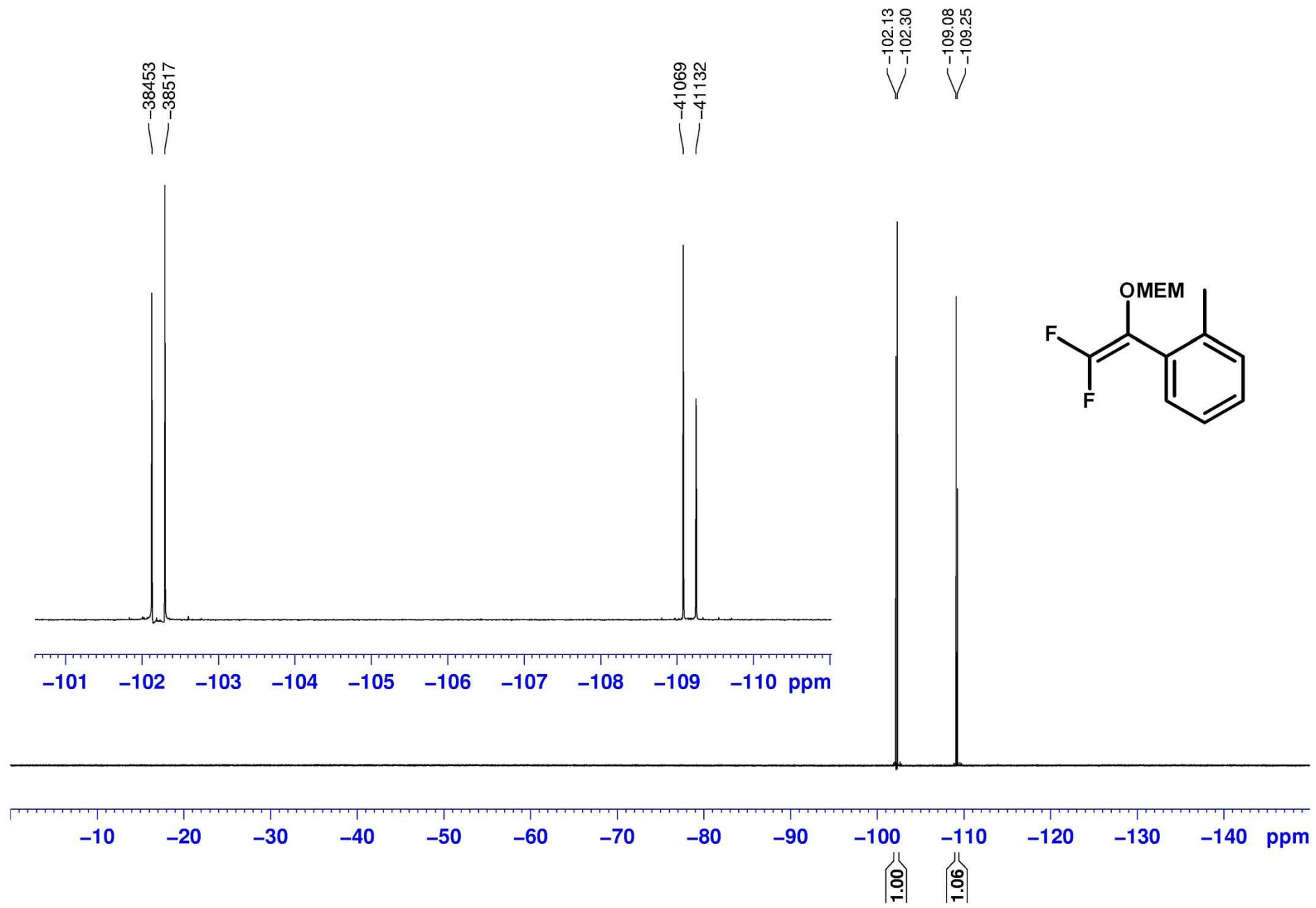


File :E:\PW\PW_81_3_chrom_HV.D
Operator : PW
Acquired : 1 Dec 2010 15:23 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name: Sample 1
Misc Info :
Vial Number: 13

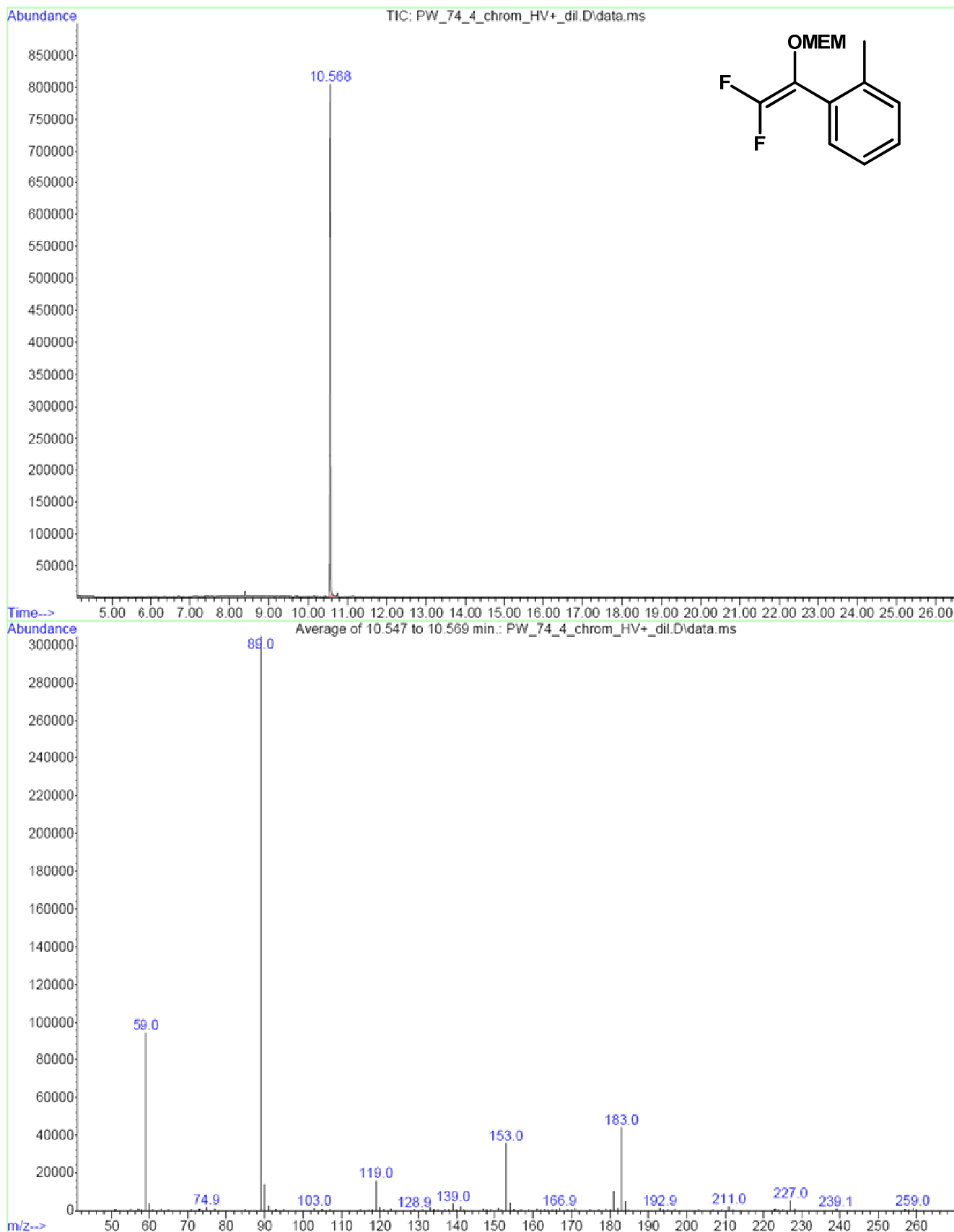


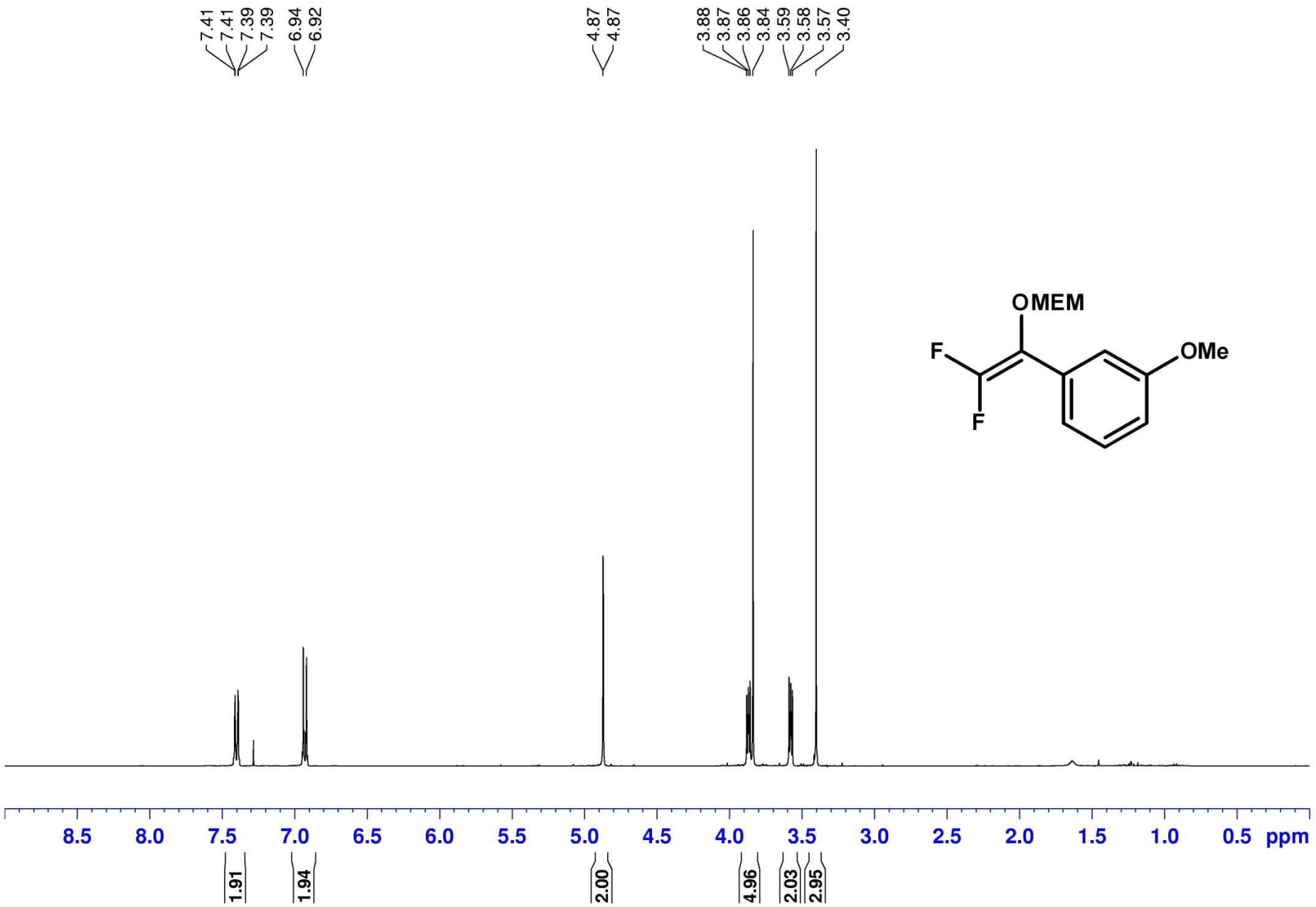


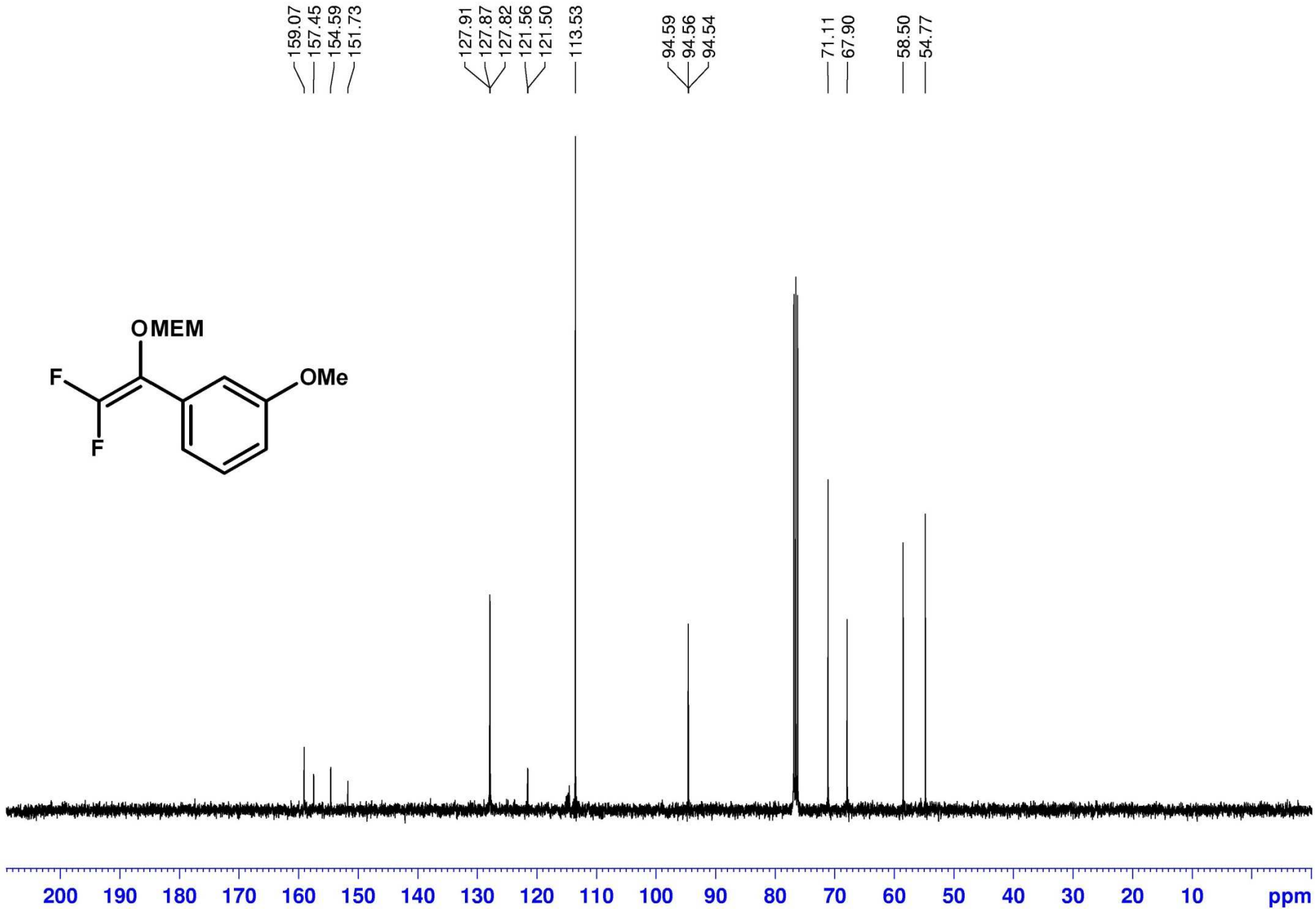


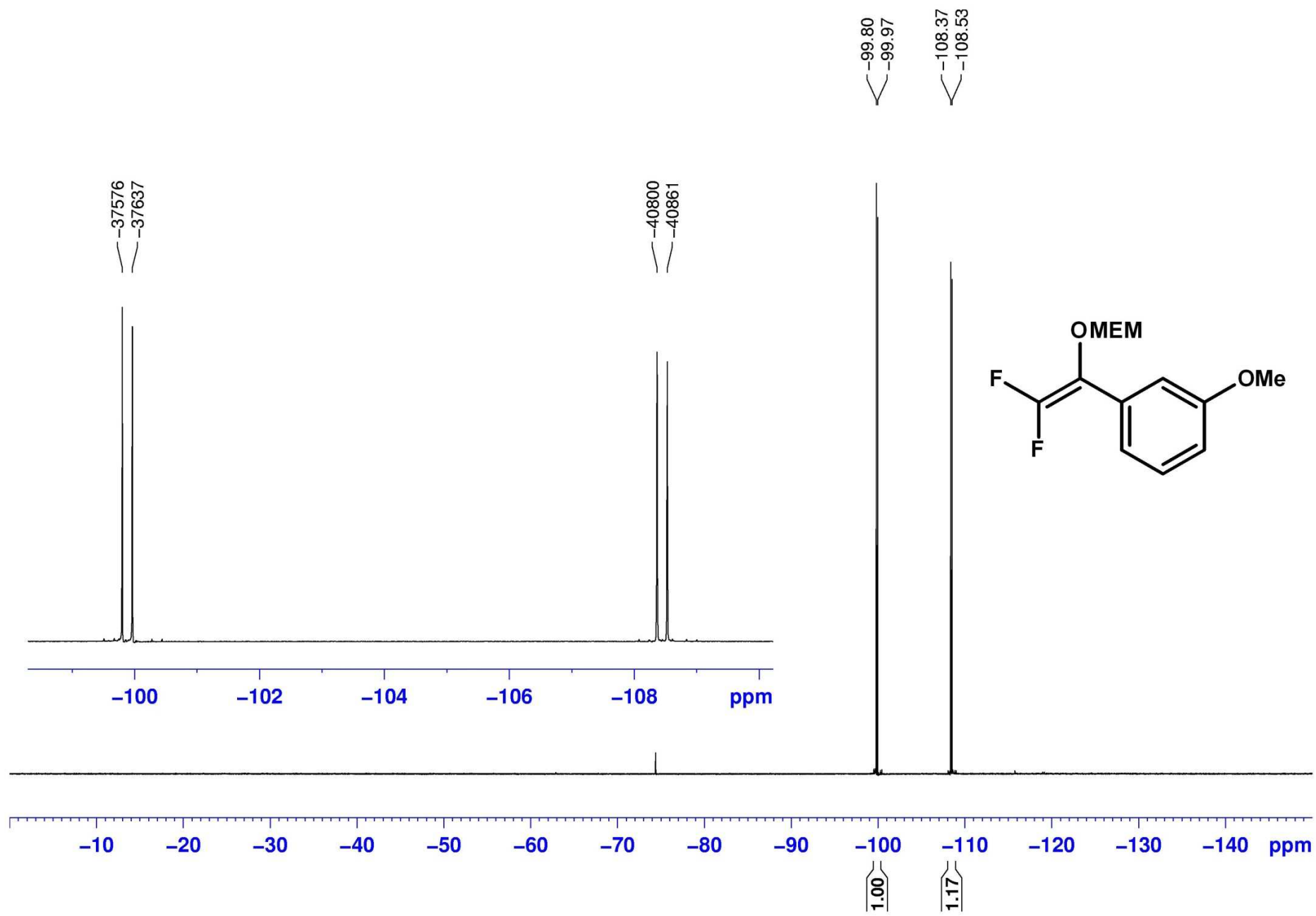


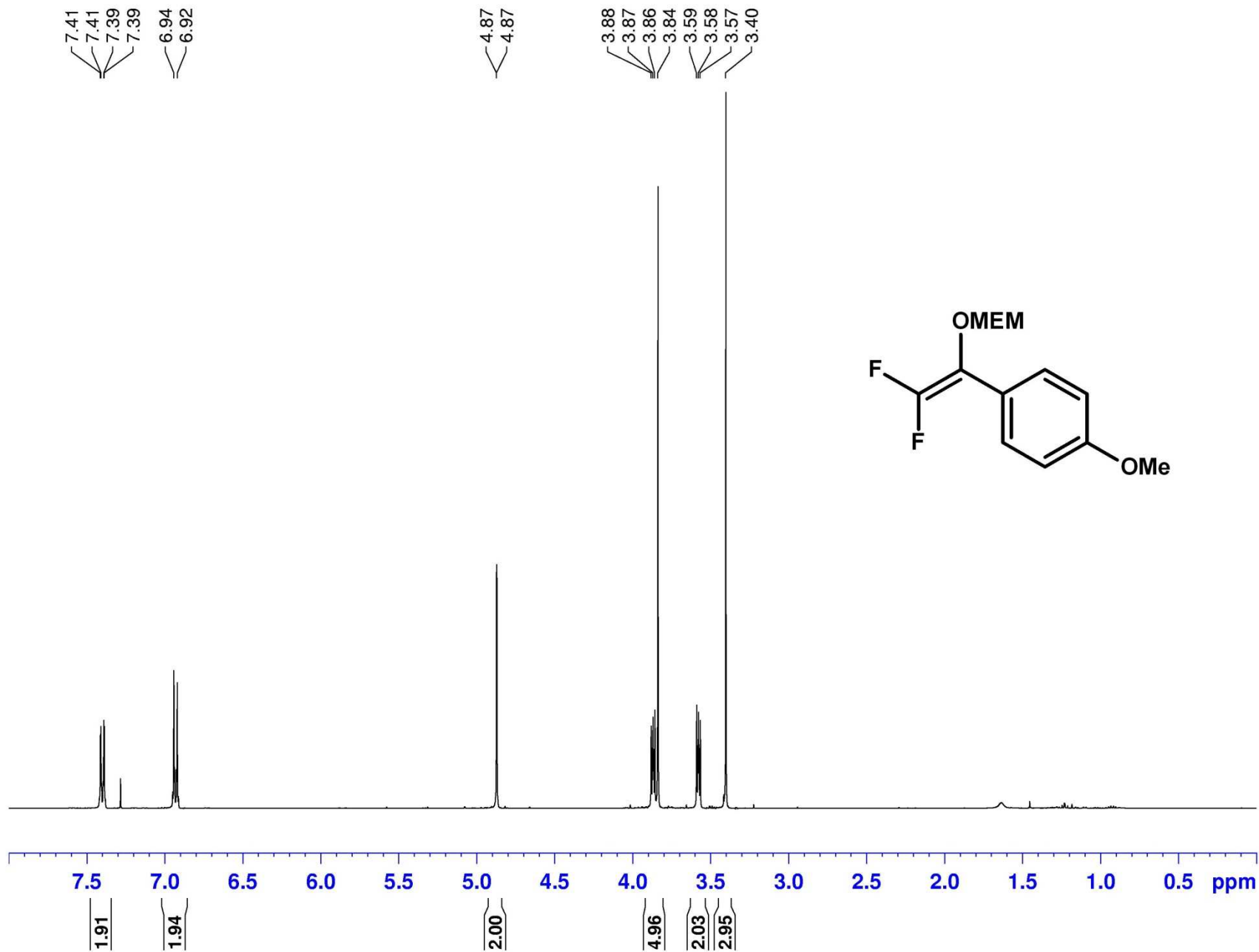
File : F:\PW\PW_74_4_chrom_HV+_dil.D
Operator : PW
Acquired : 24 Jan 2011 12:30 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 3

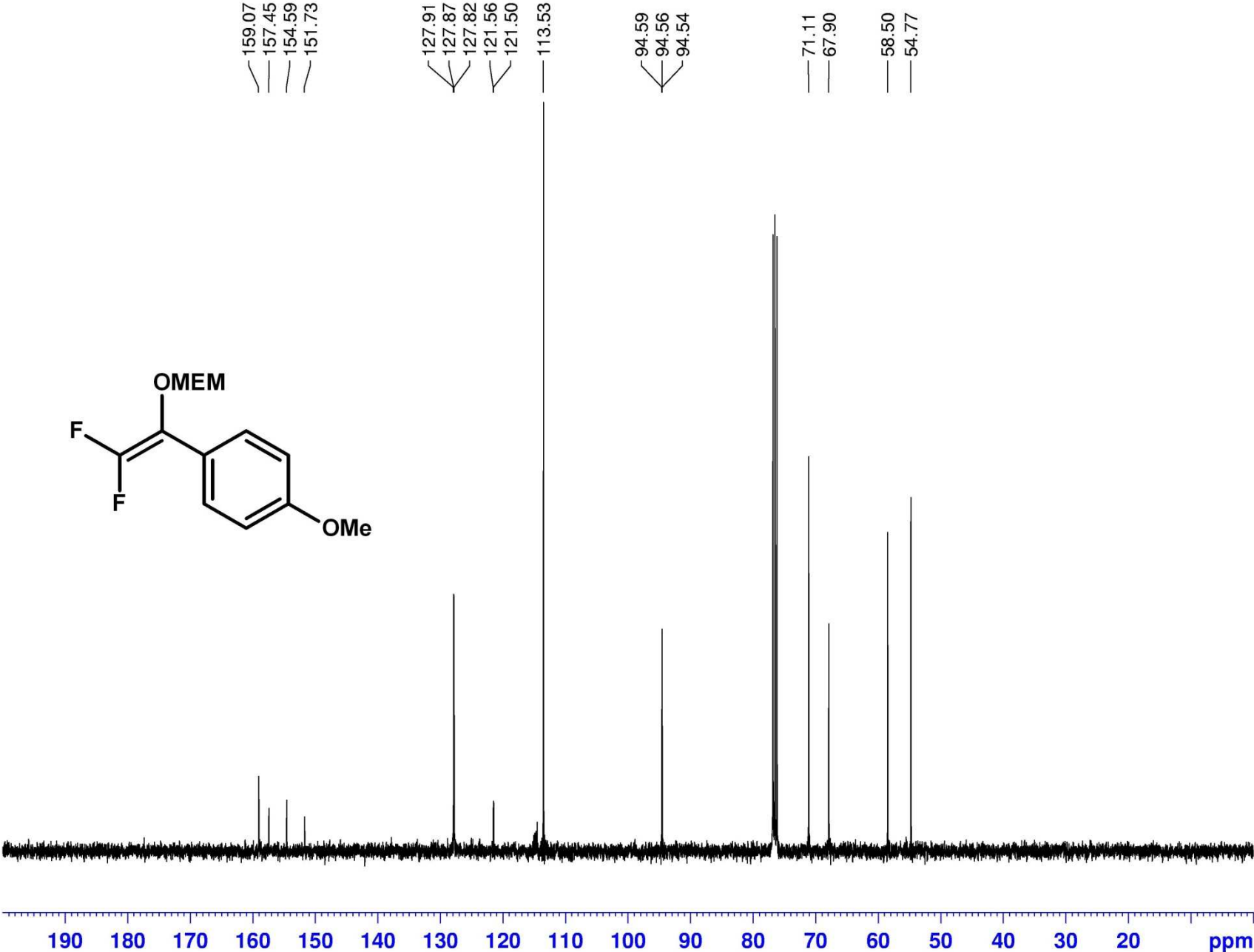


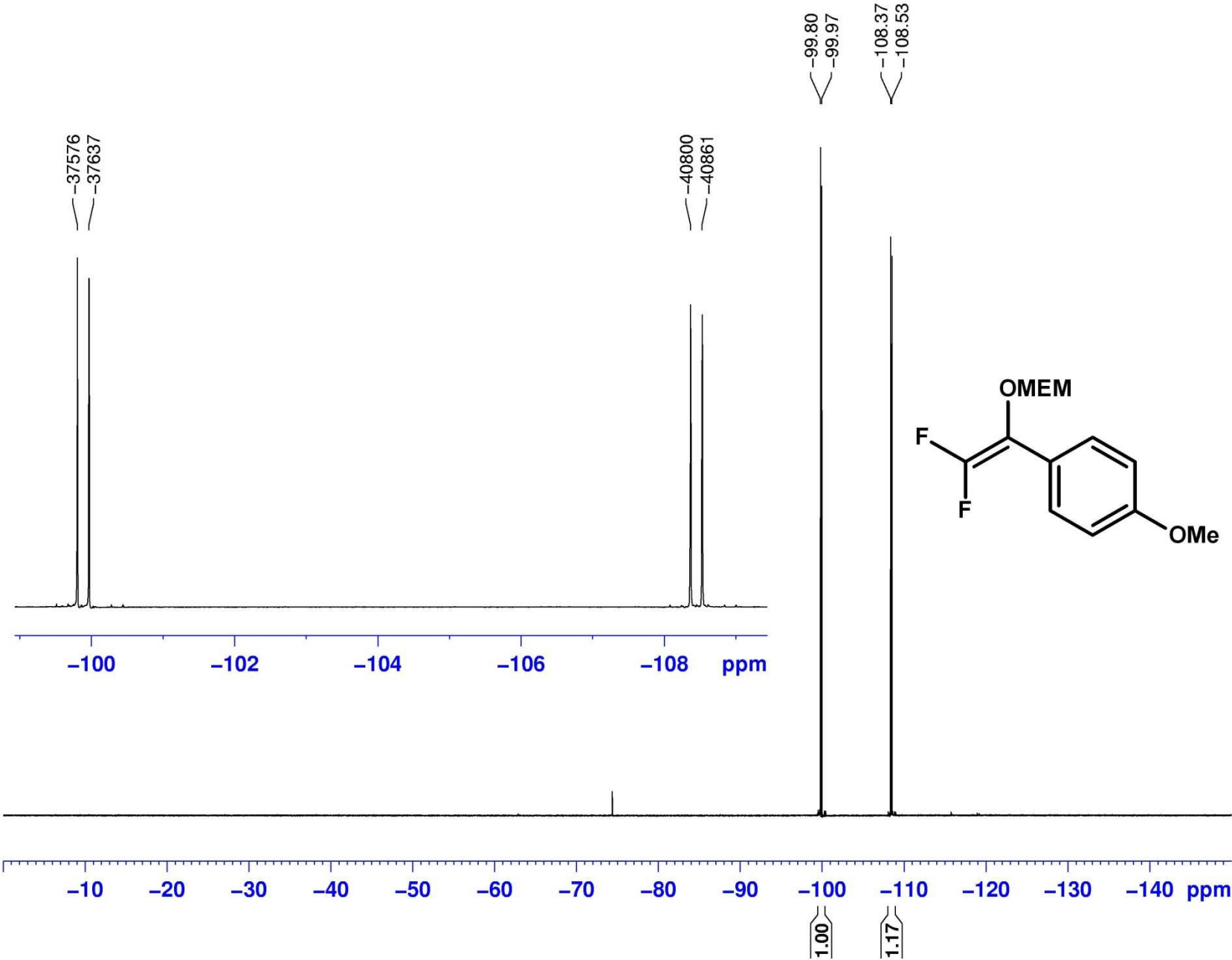


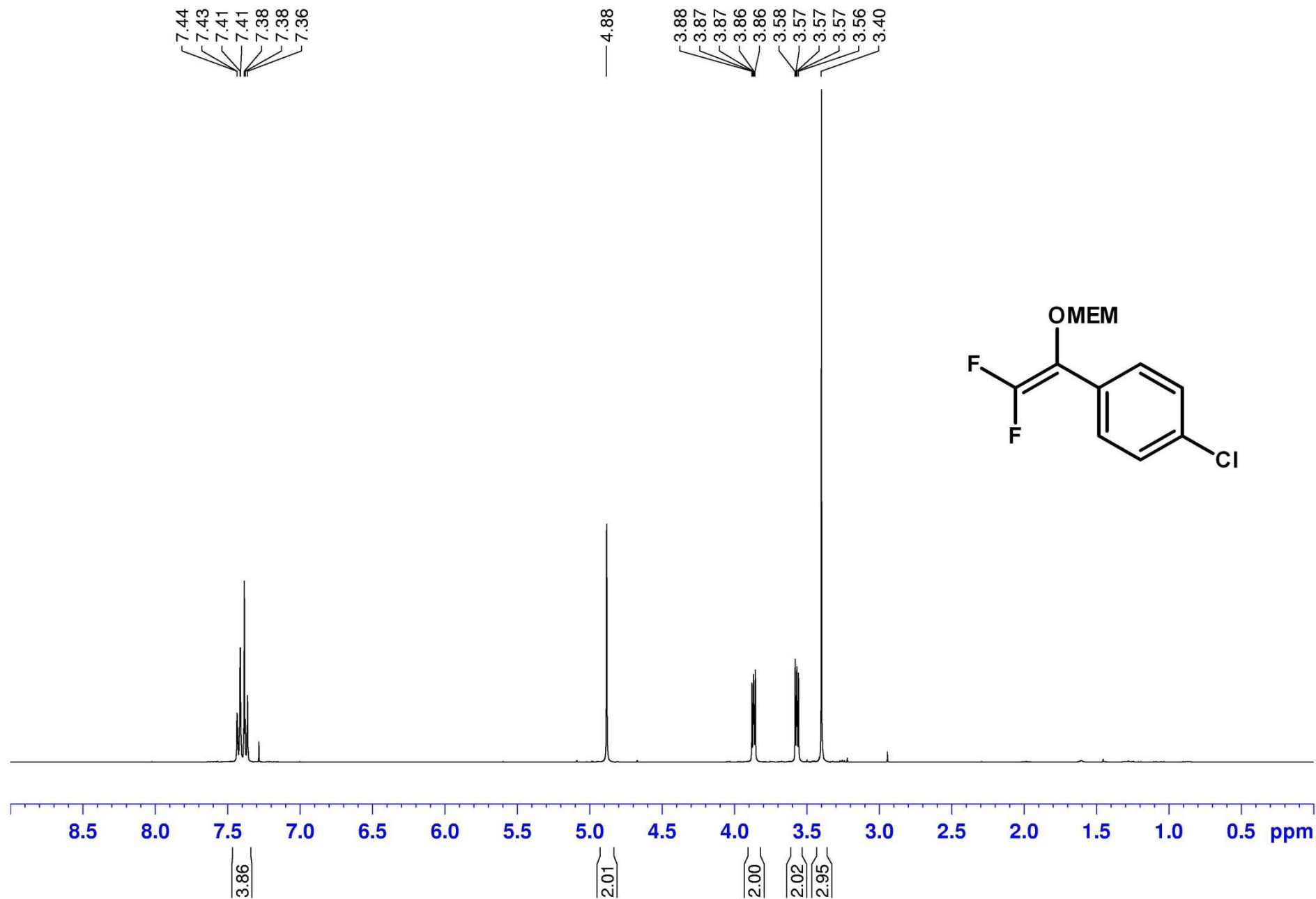


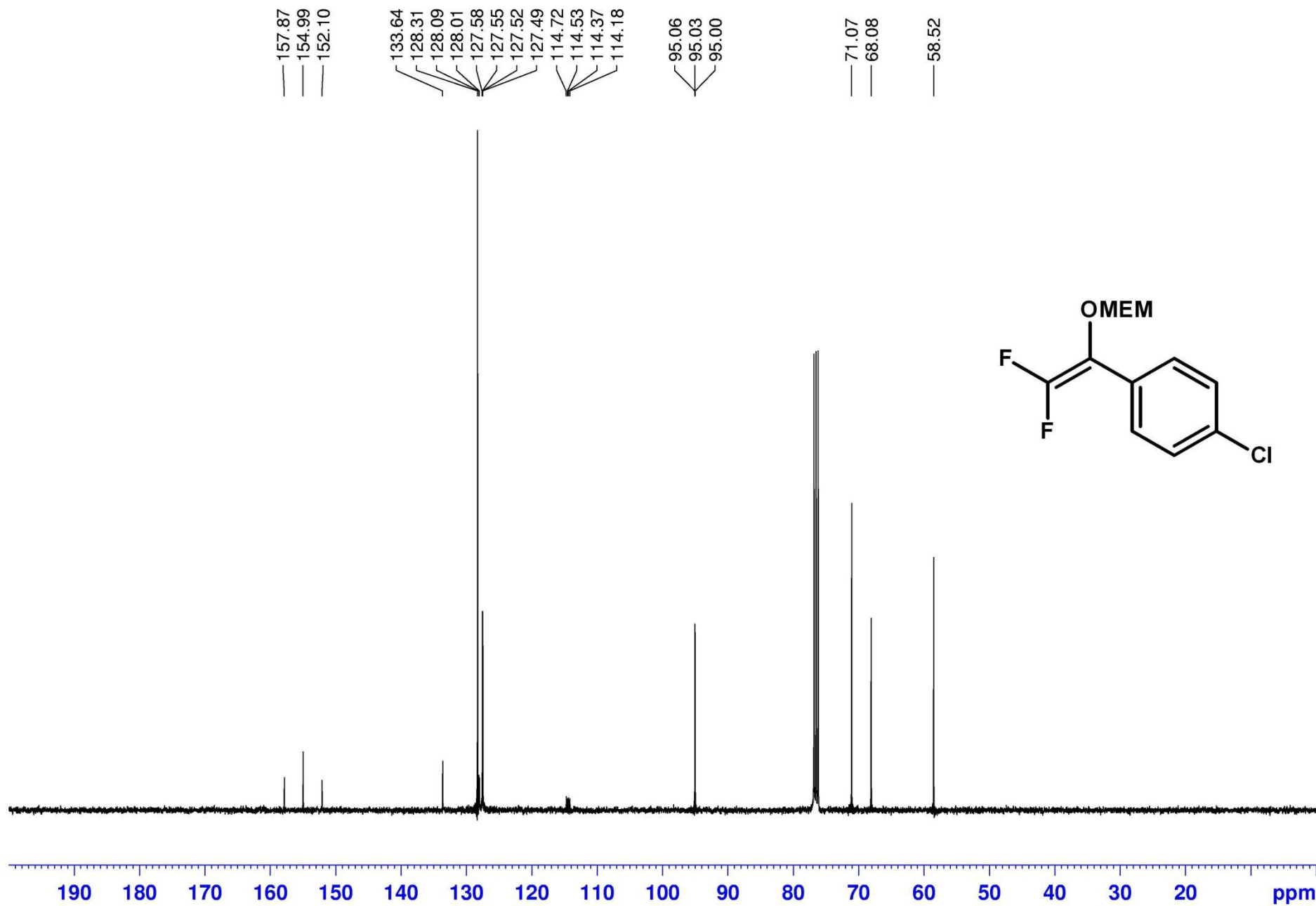


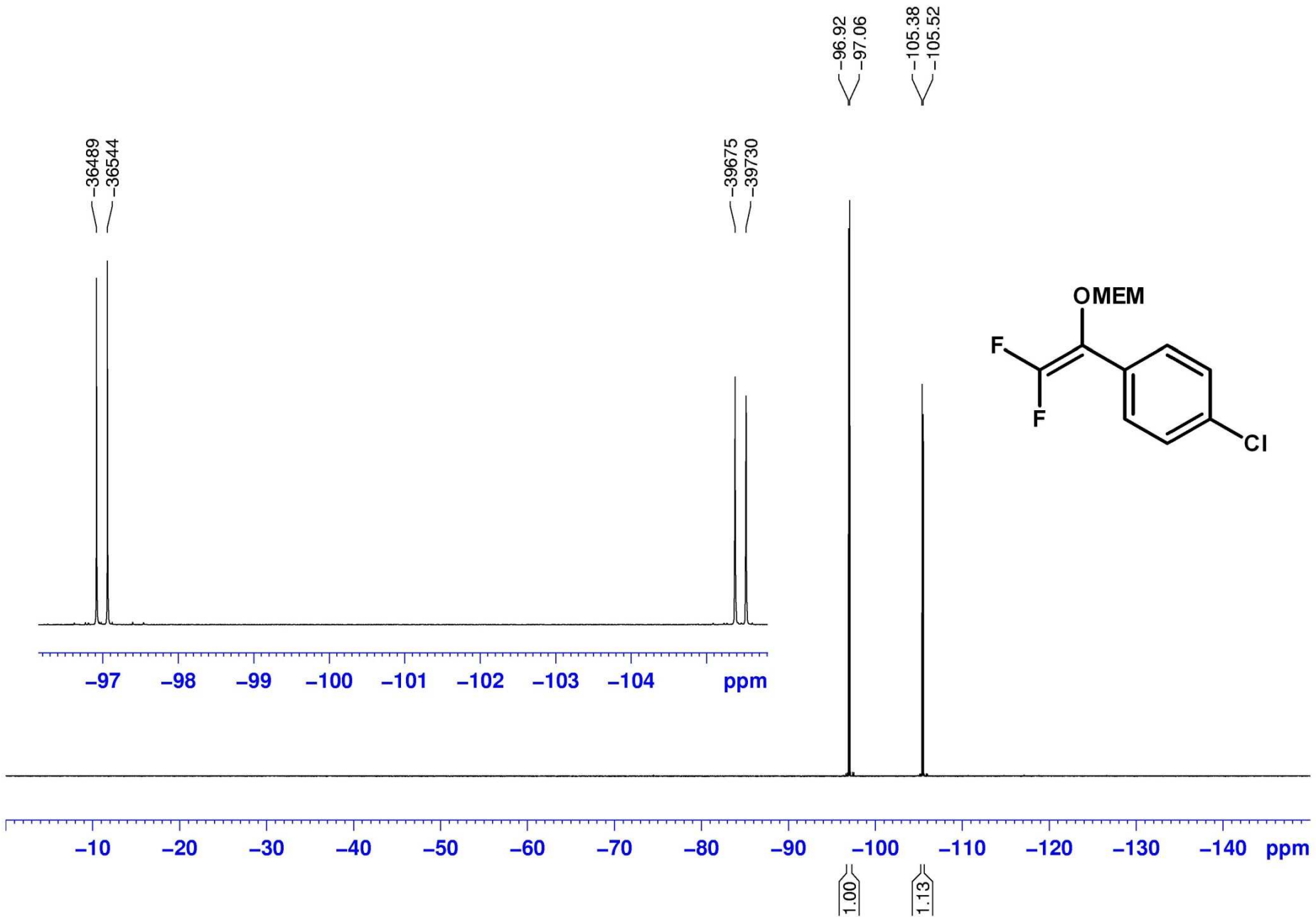




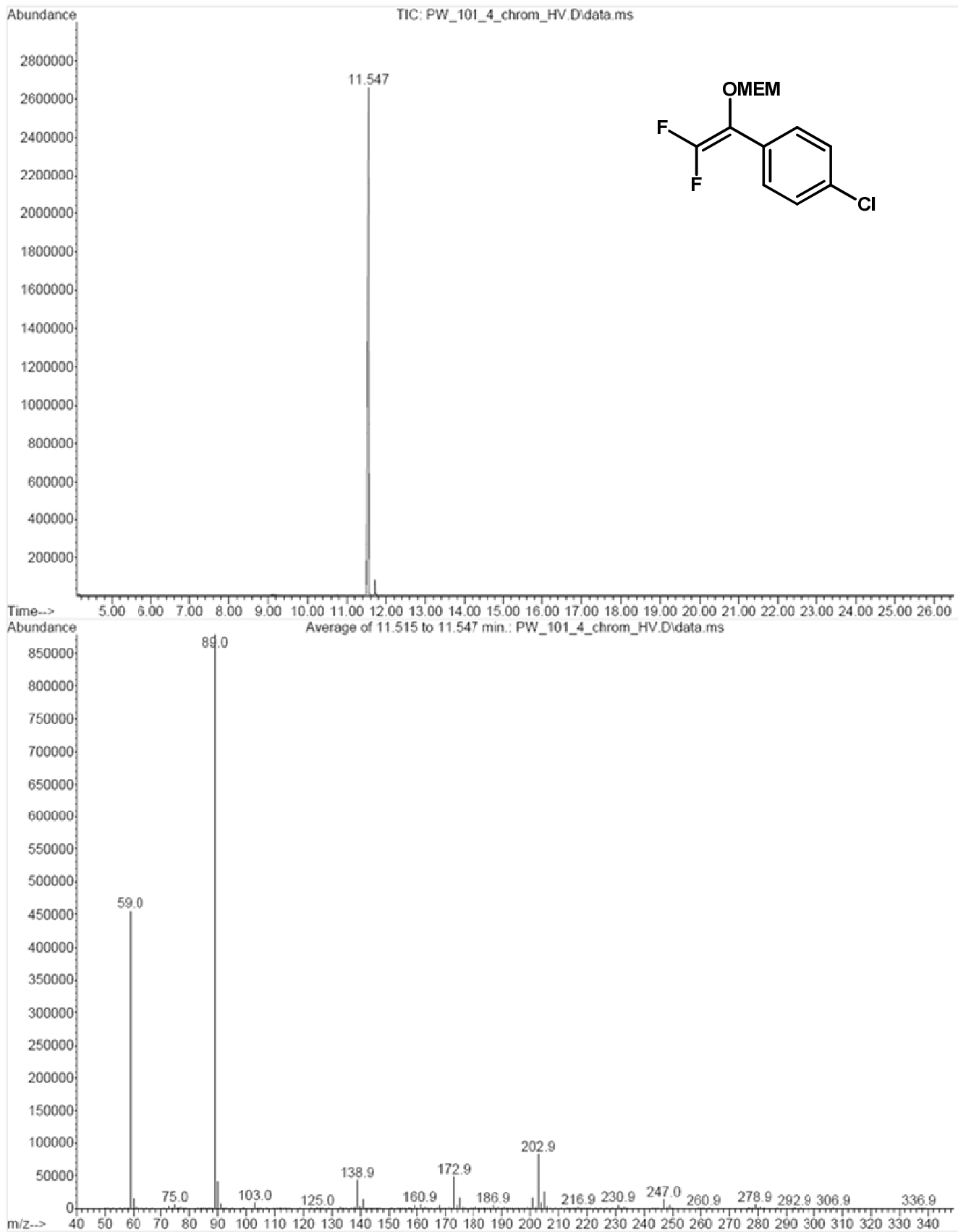


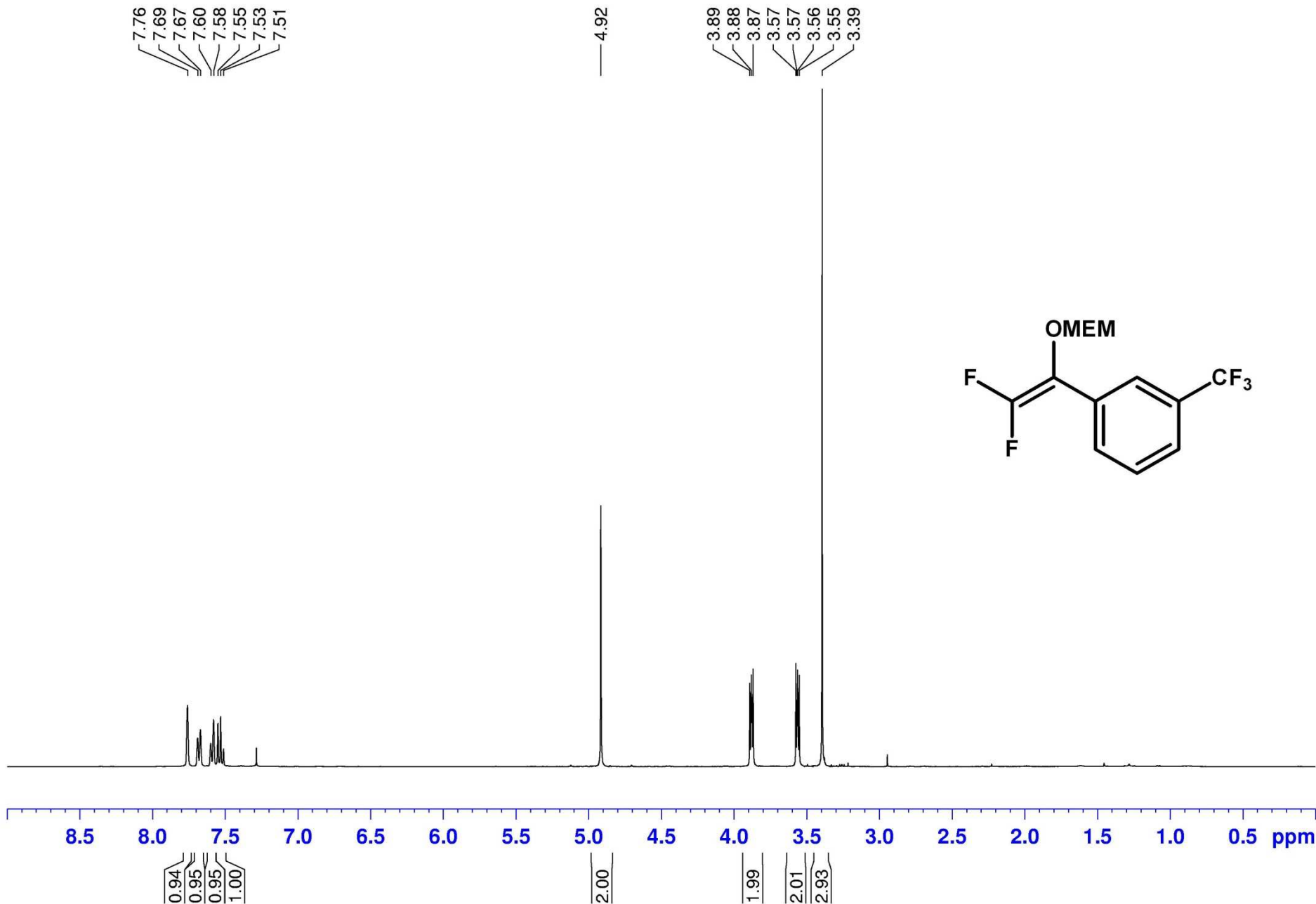


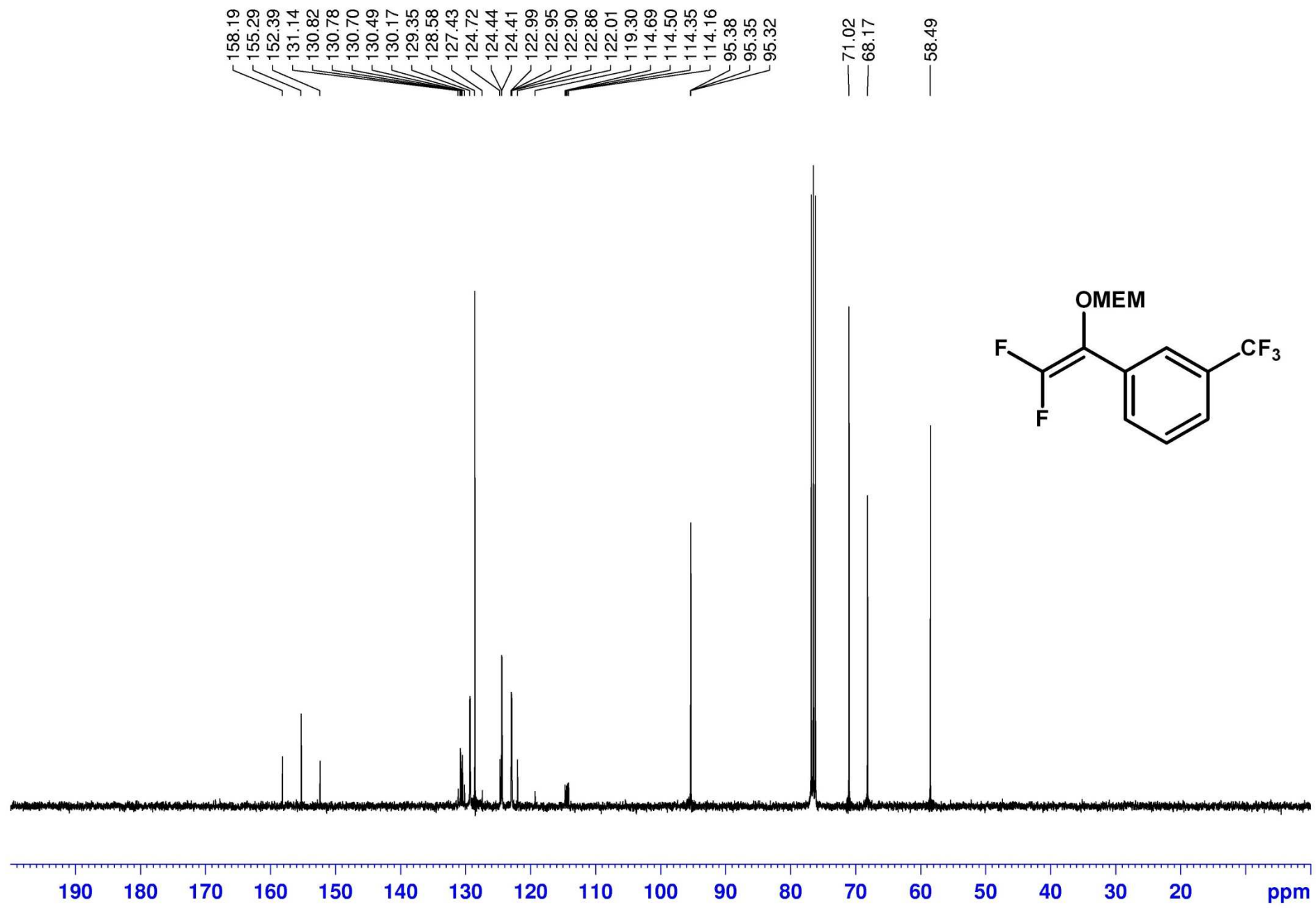


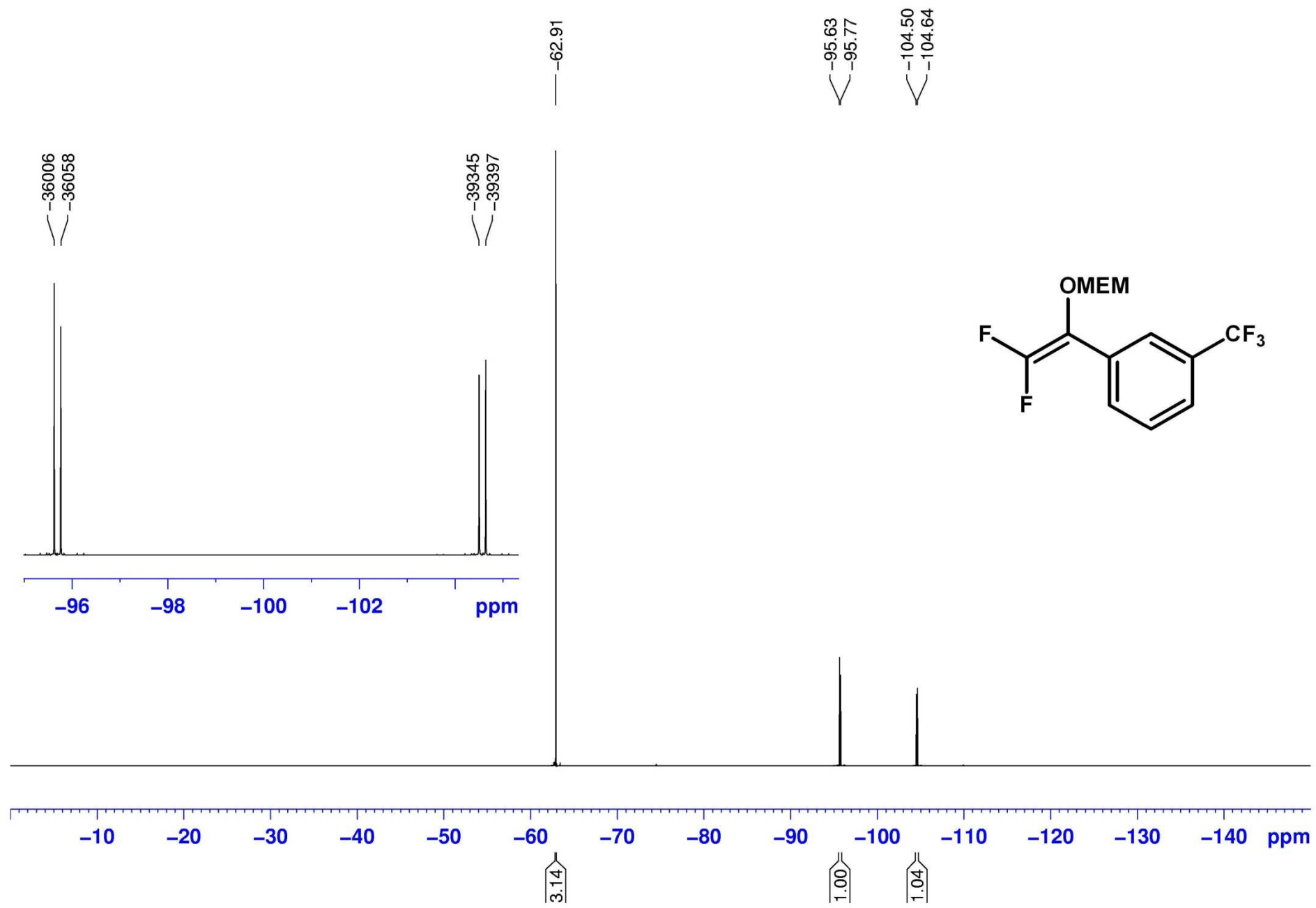


File :E:\PW\PW_101_4_chrom_HV.D
Operator : NS
Acquired : 18 Jan 2011 12:36 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 21

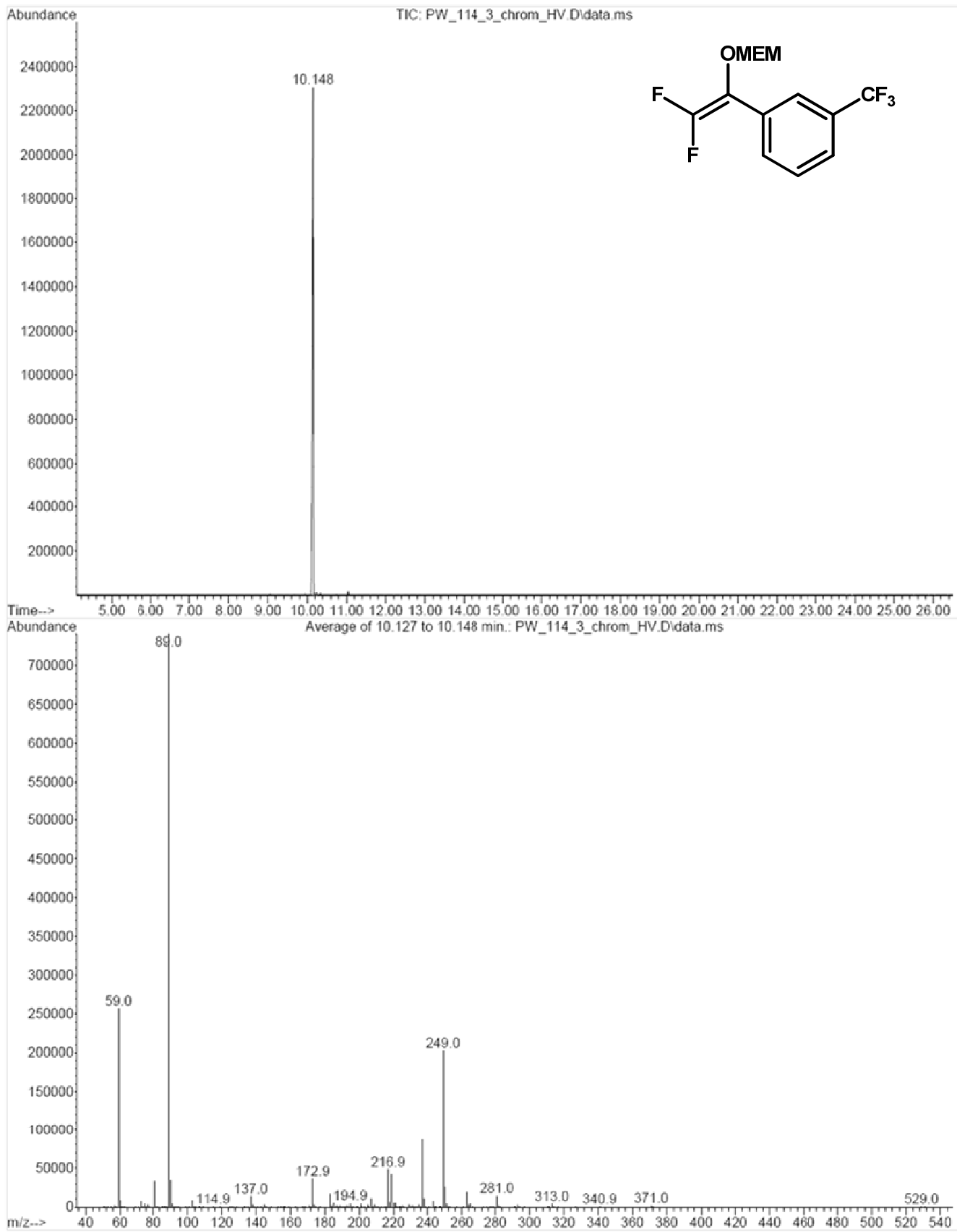


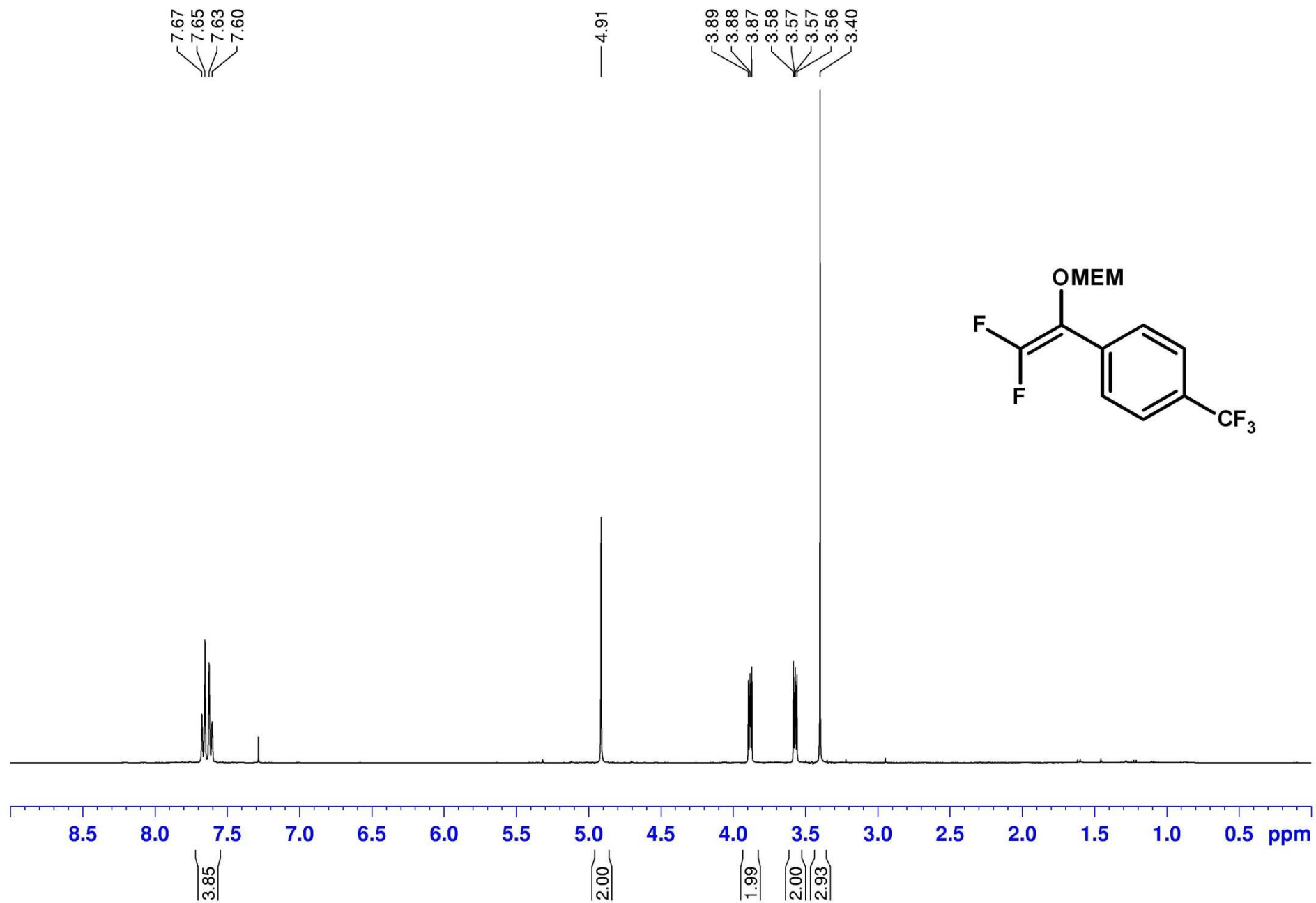


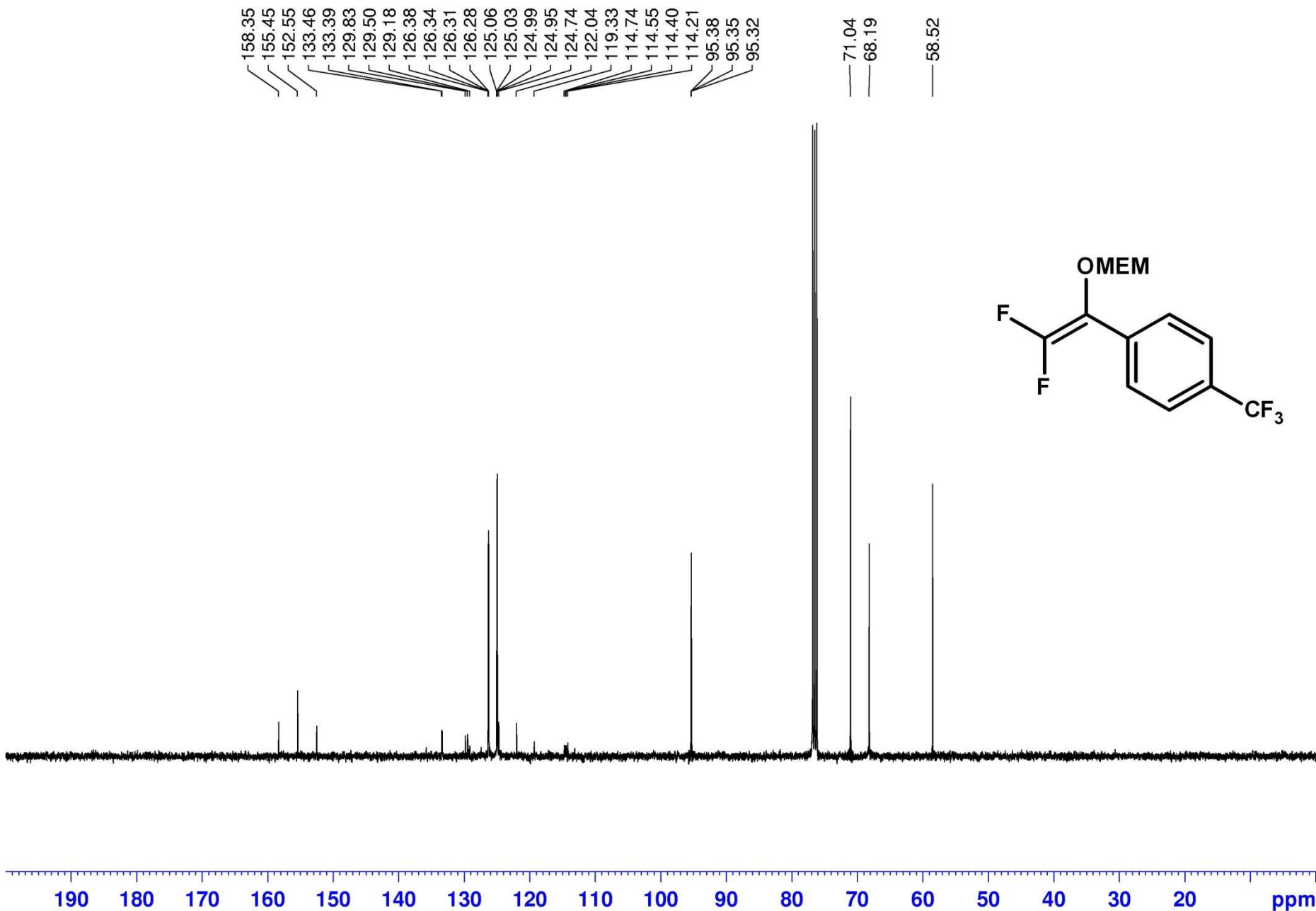


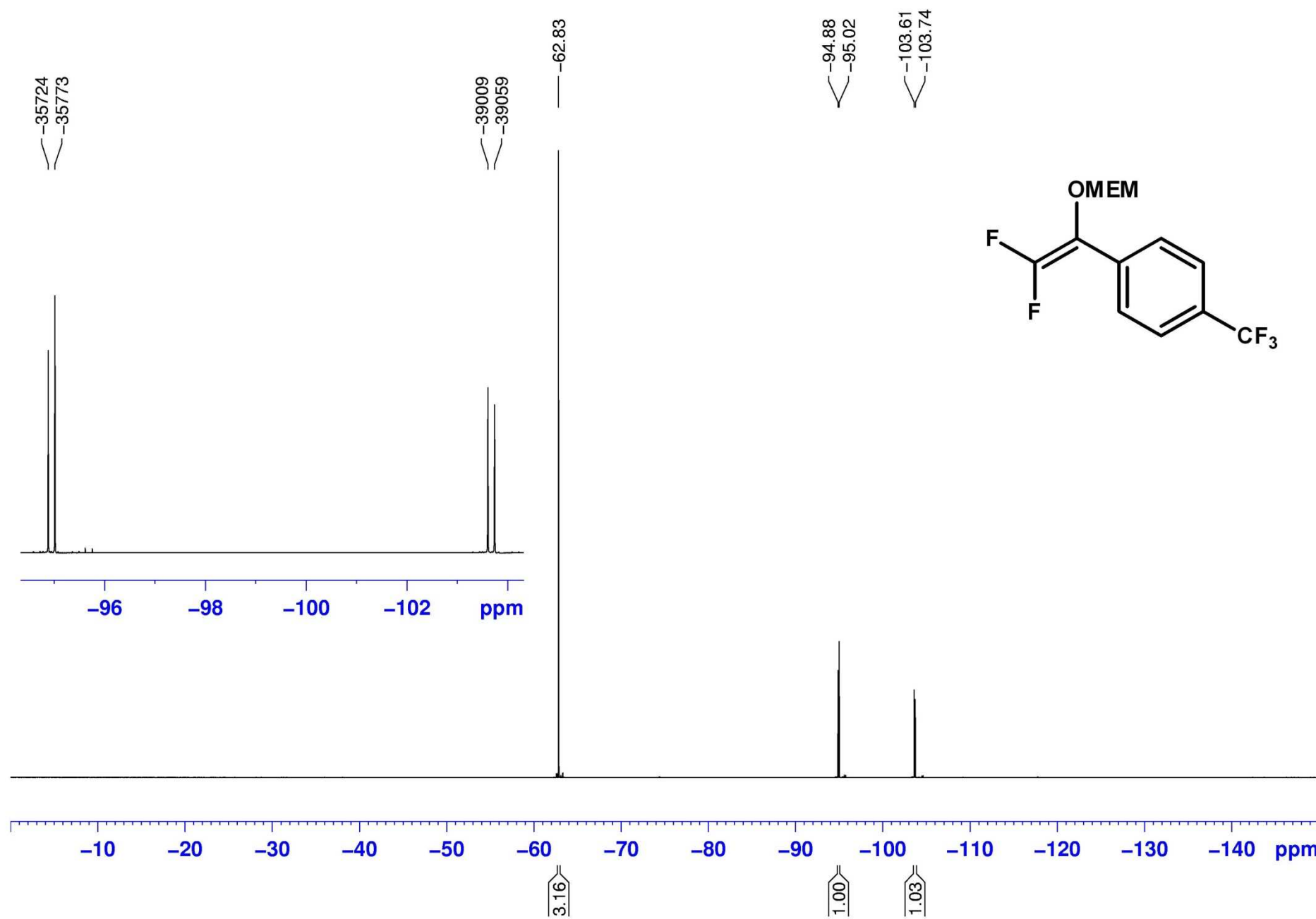


File :E:\PW\PW_114_3_chrom_HV.D
Operator : PW
Acquired : 20 Jan 2011 16:12 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 4

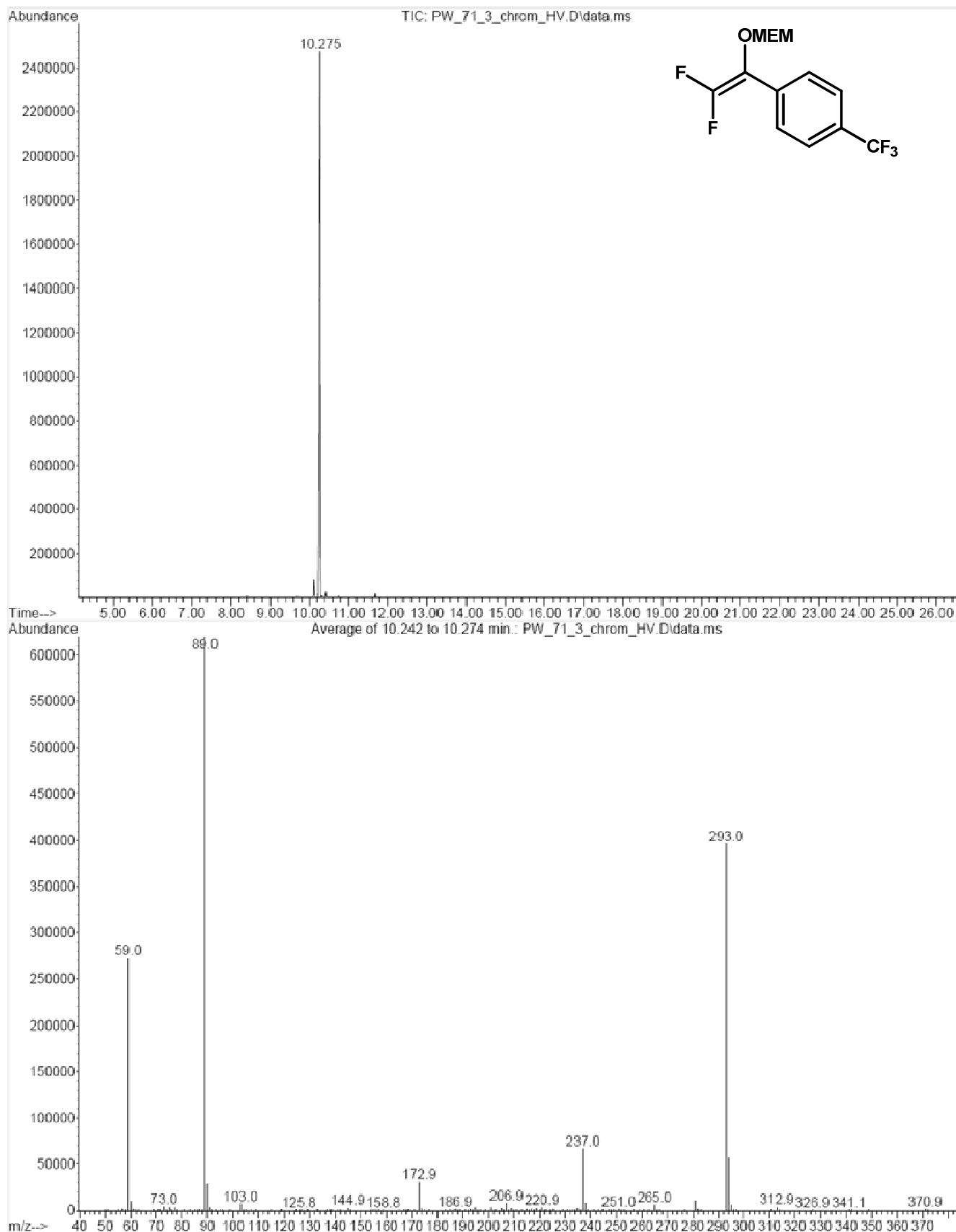


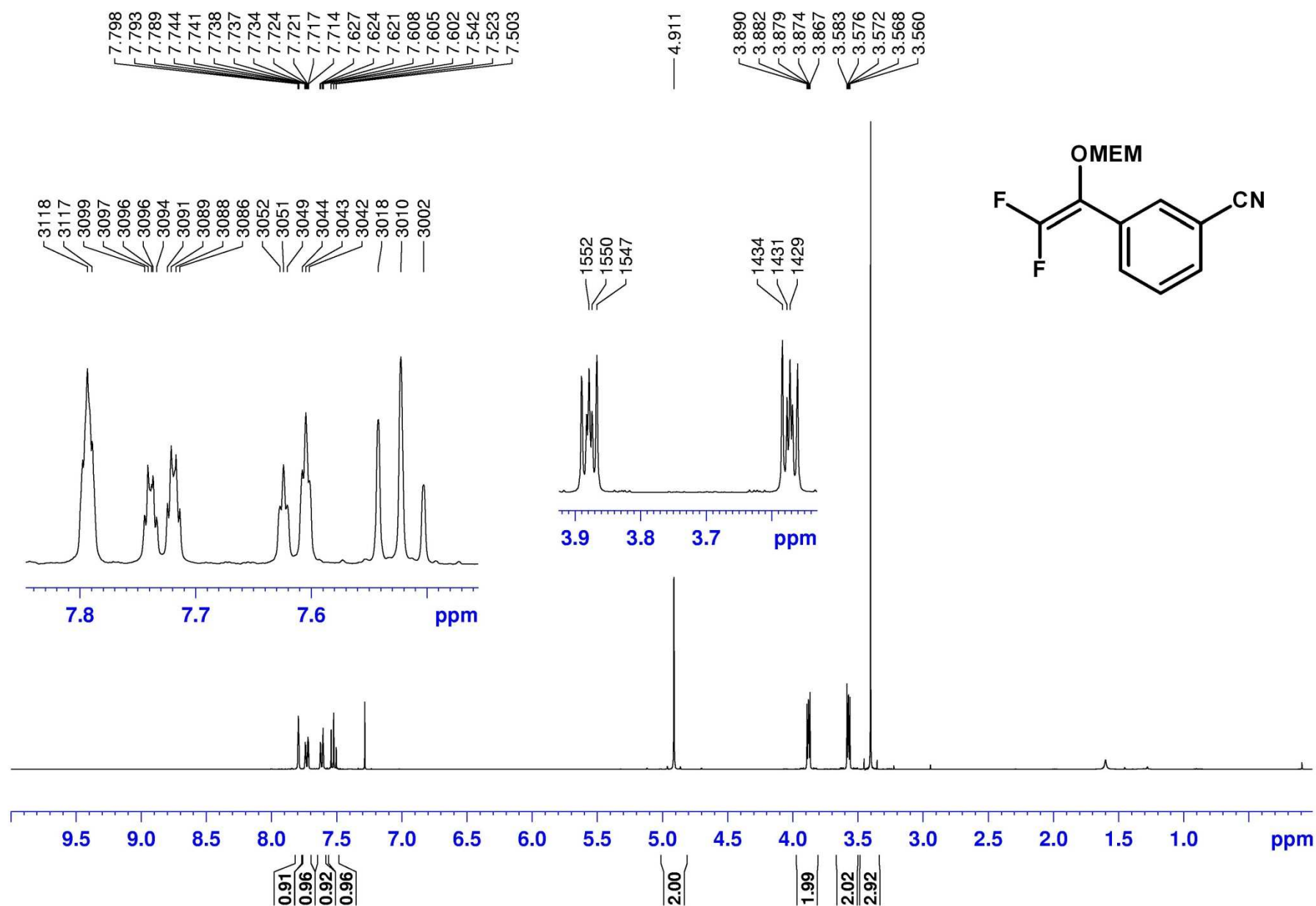


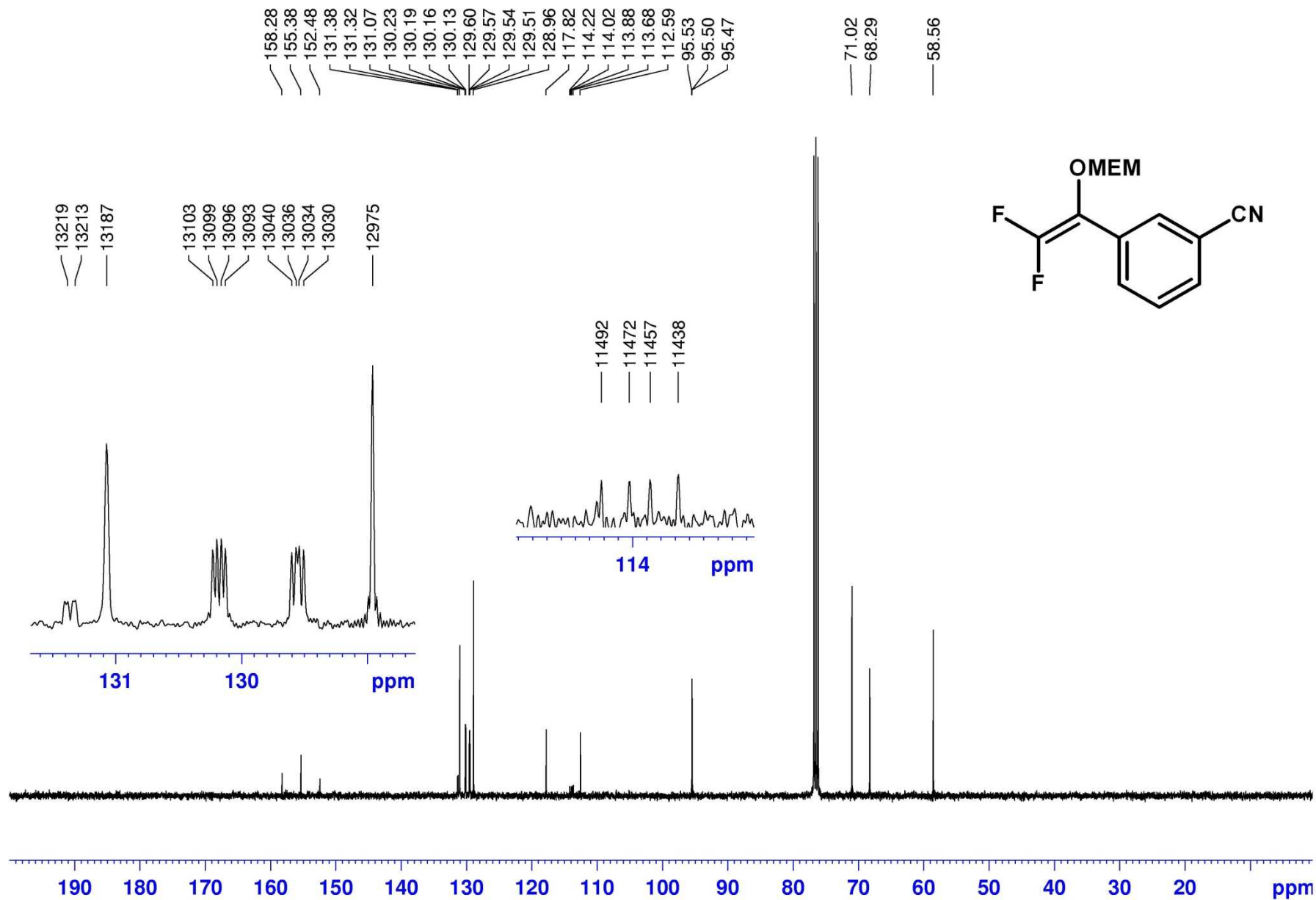


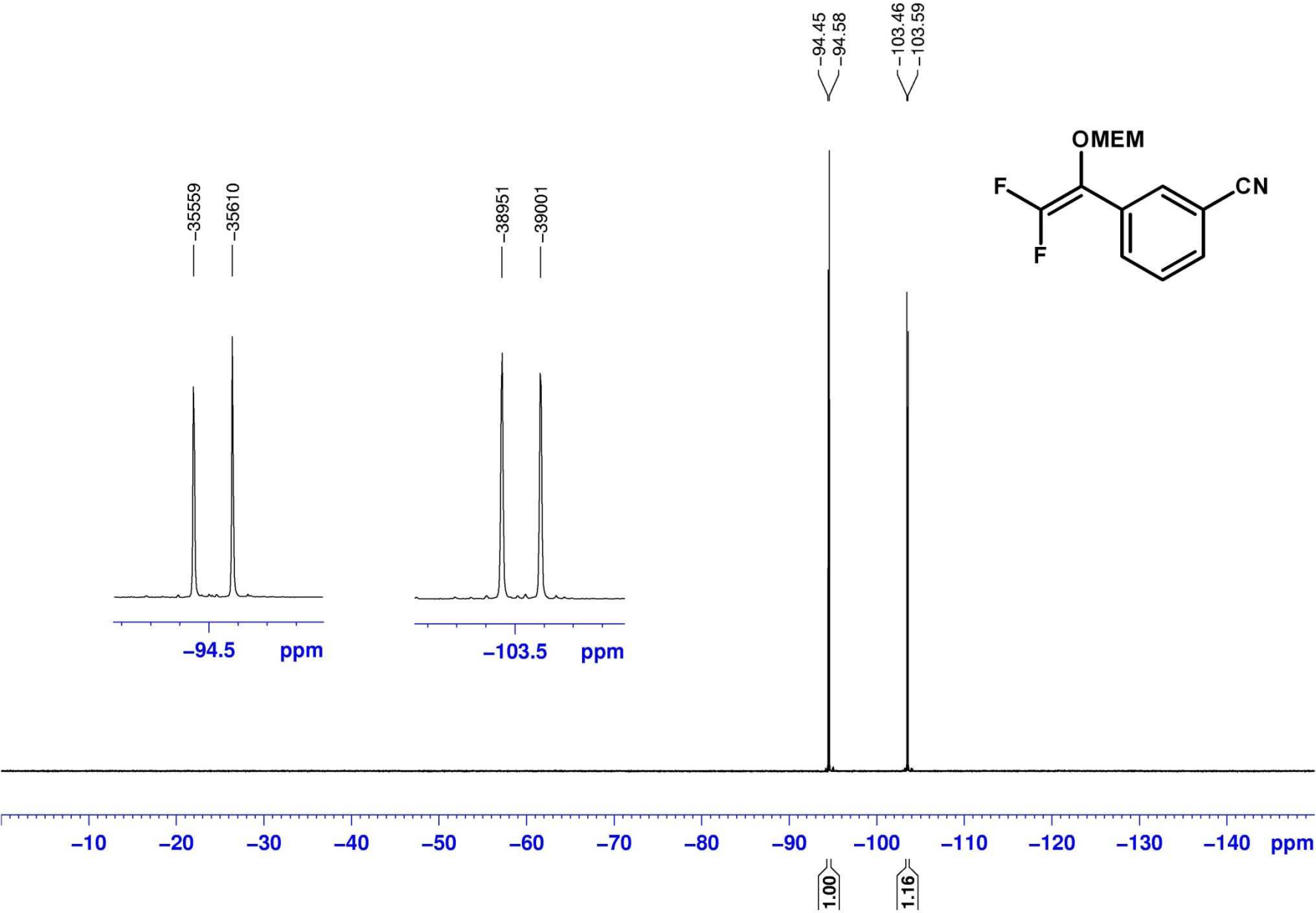


File : E:\PW\PW_71_3_chrom_HV.D
Operator : PW
Acquired : 20 Jan 2011 15:41 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 3

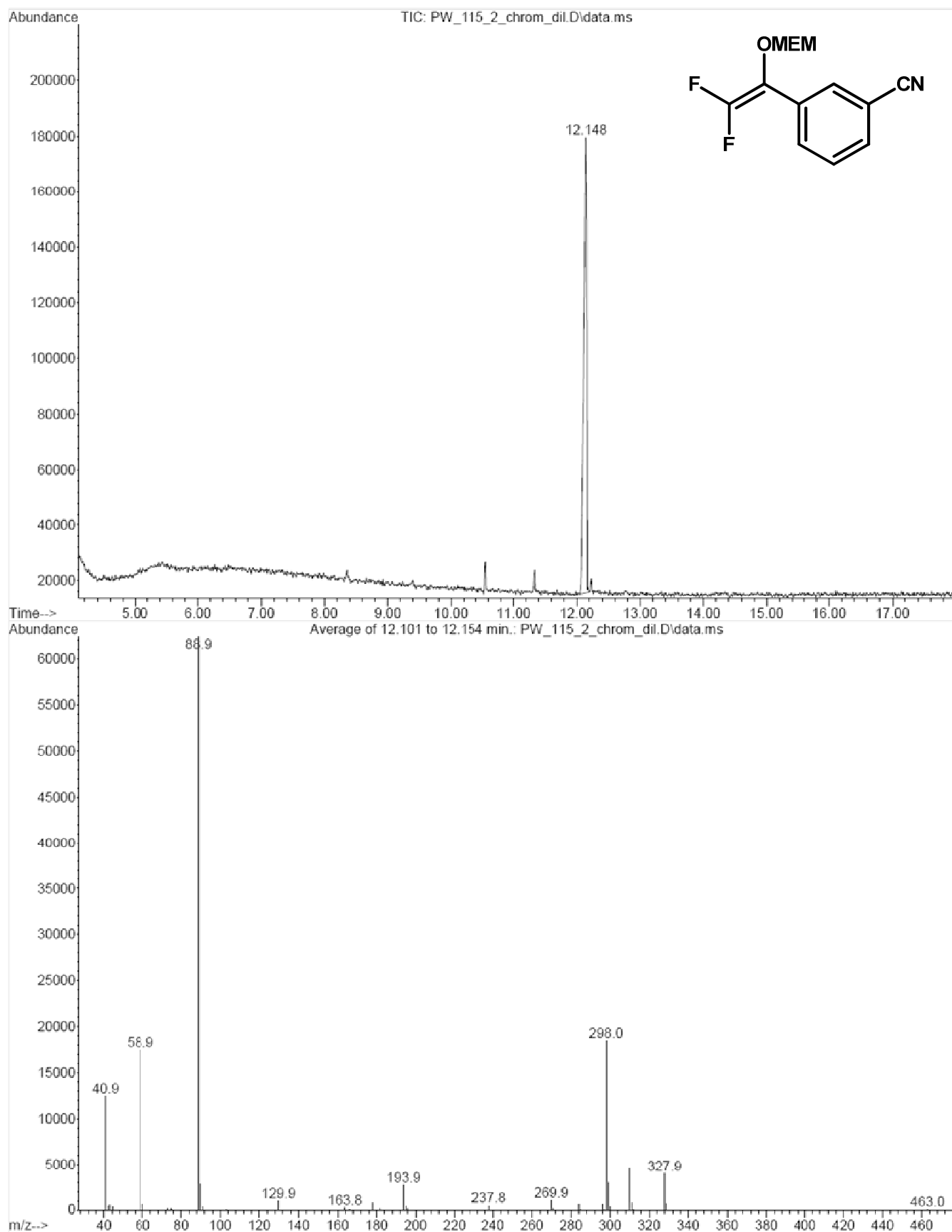


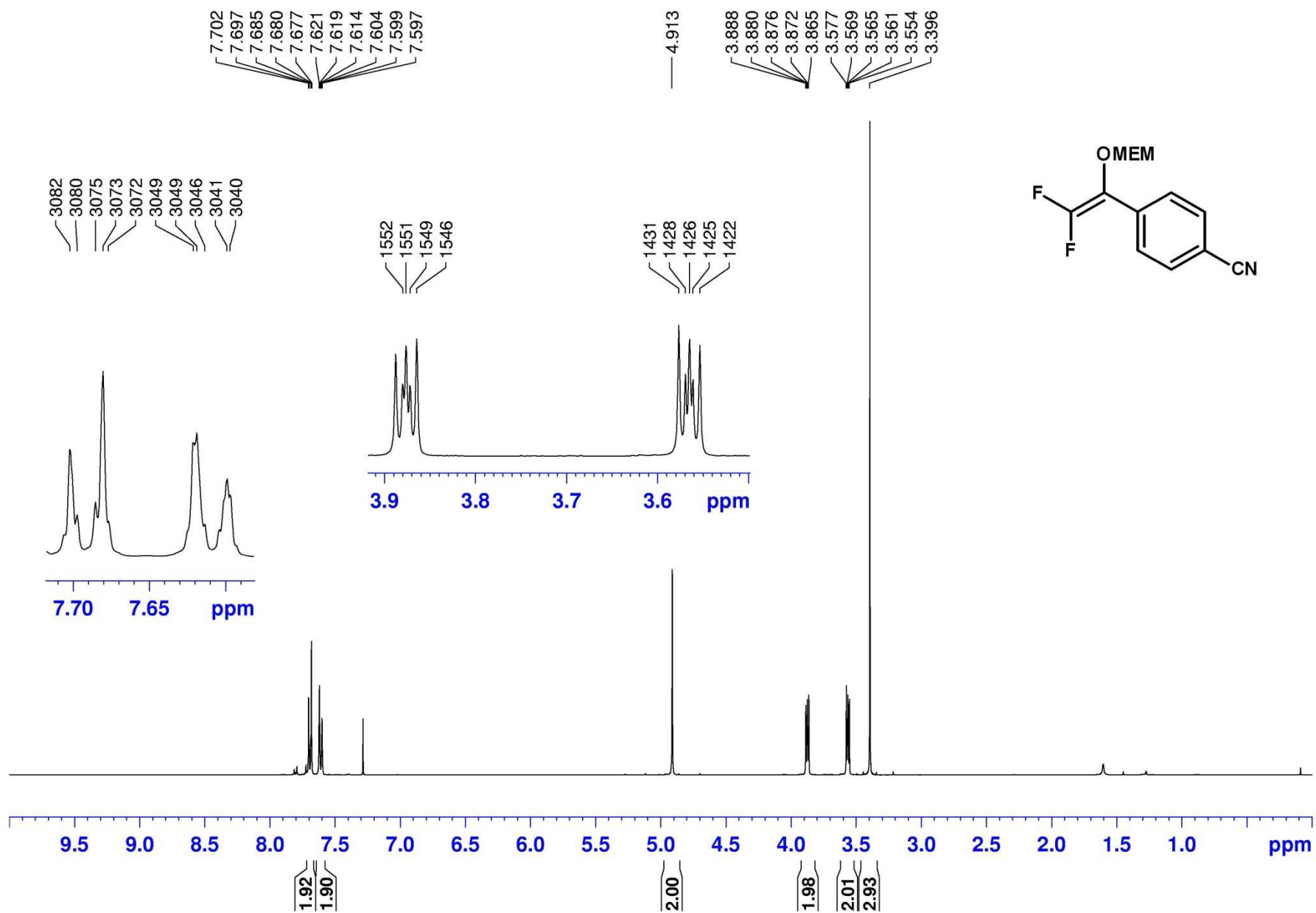


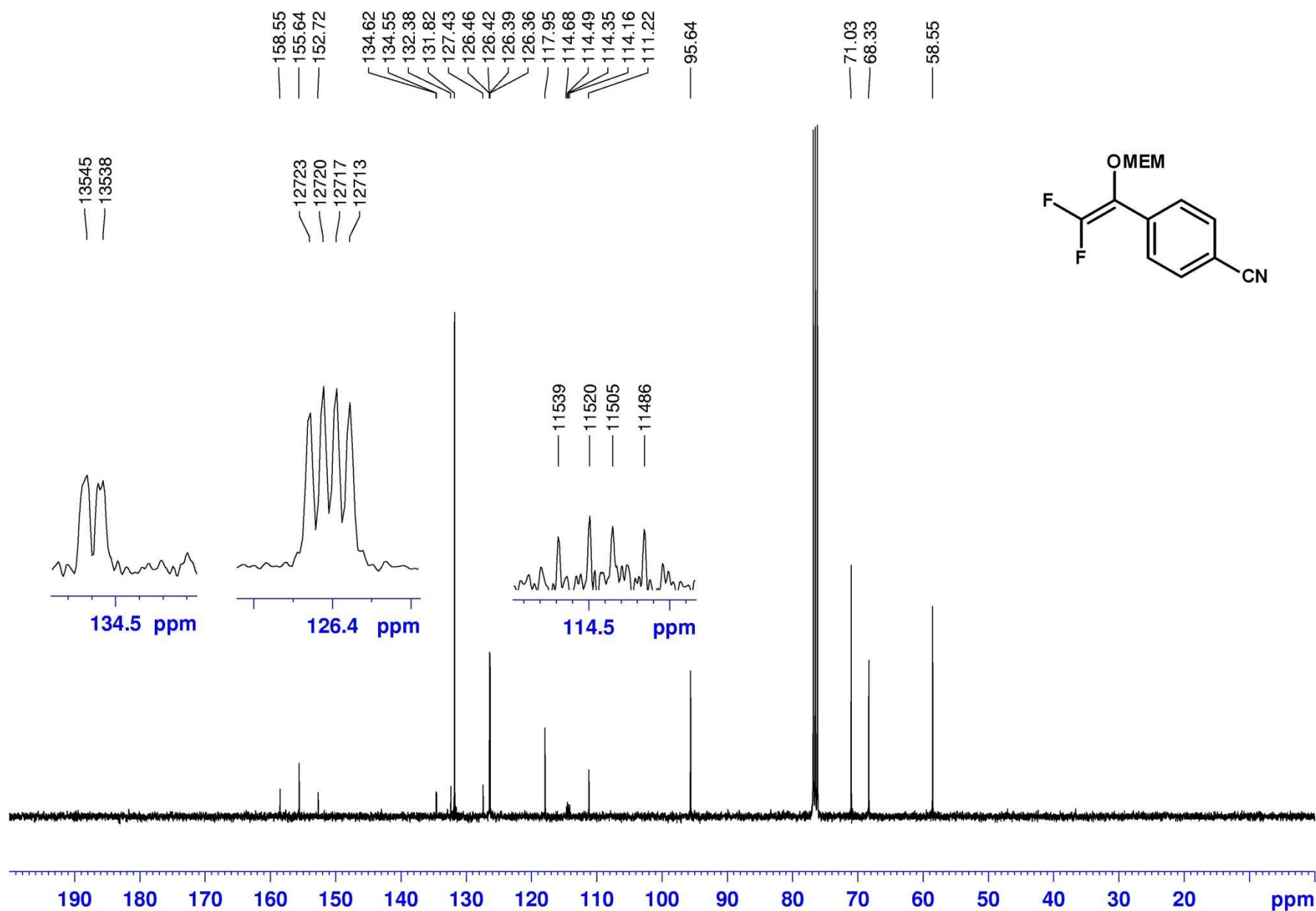


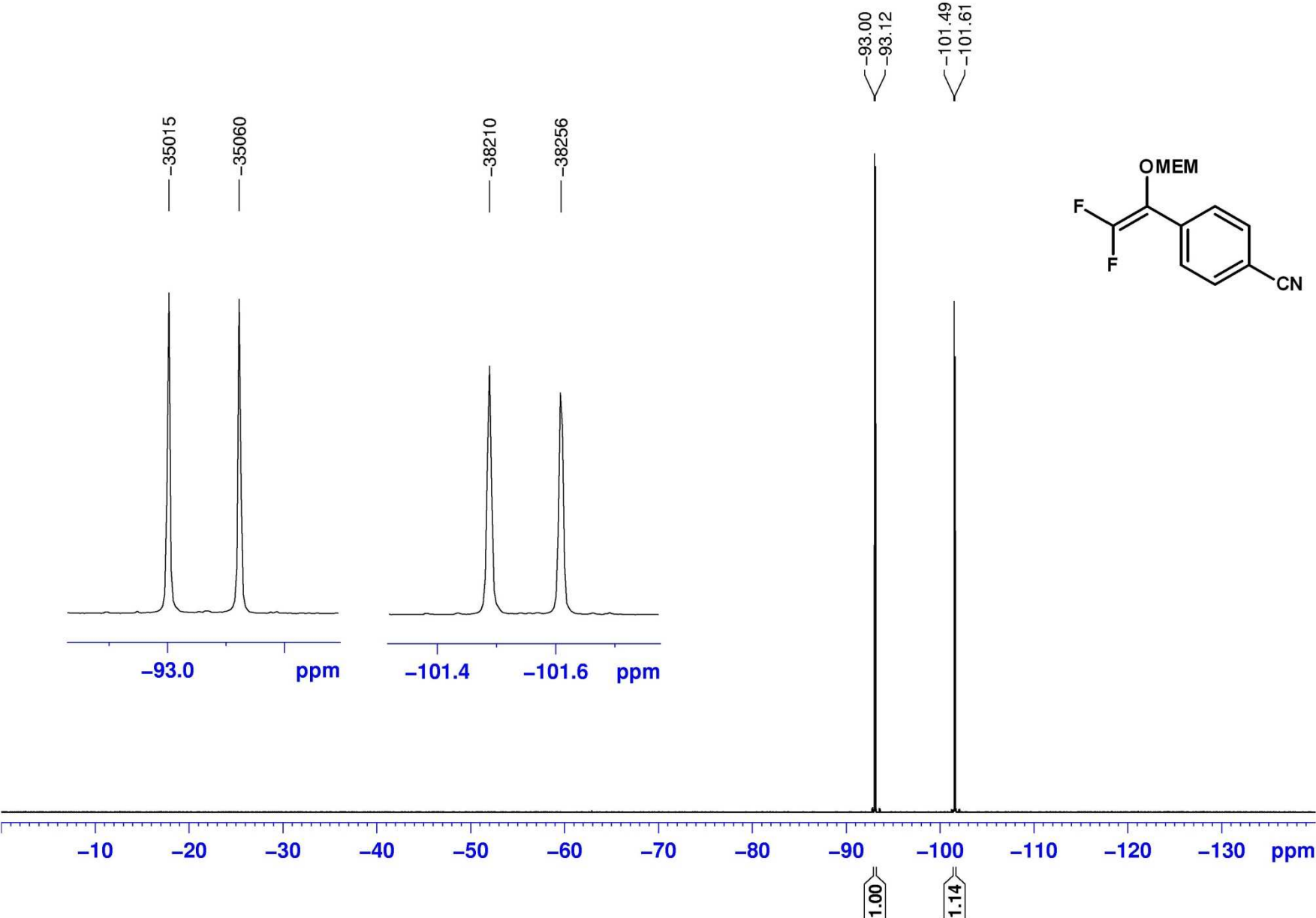


File :E:\PW\PW_115_2_chrom_dil.D
Operator : pk
Acquired : 10 Nov 2010 19:21 using AcqMethod BASIC_PCI_GC250_70C.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 3

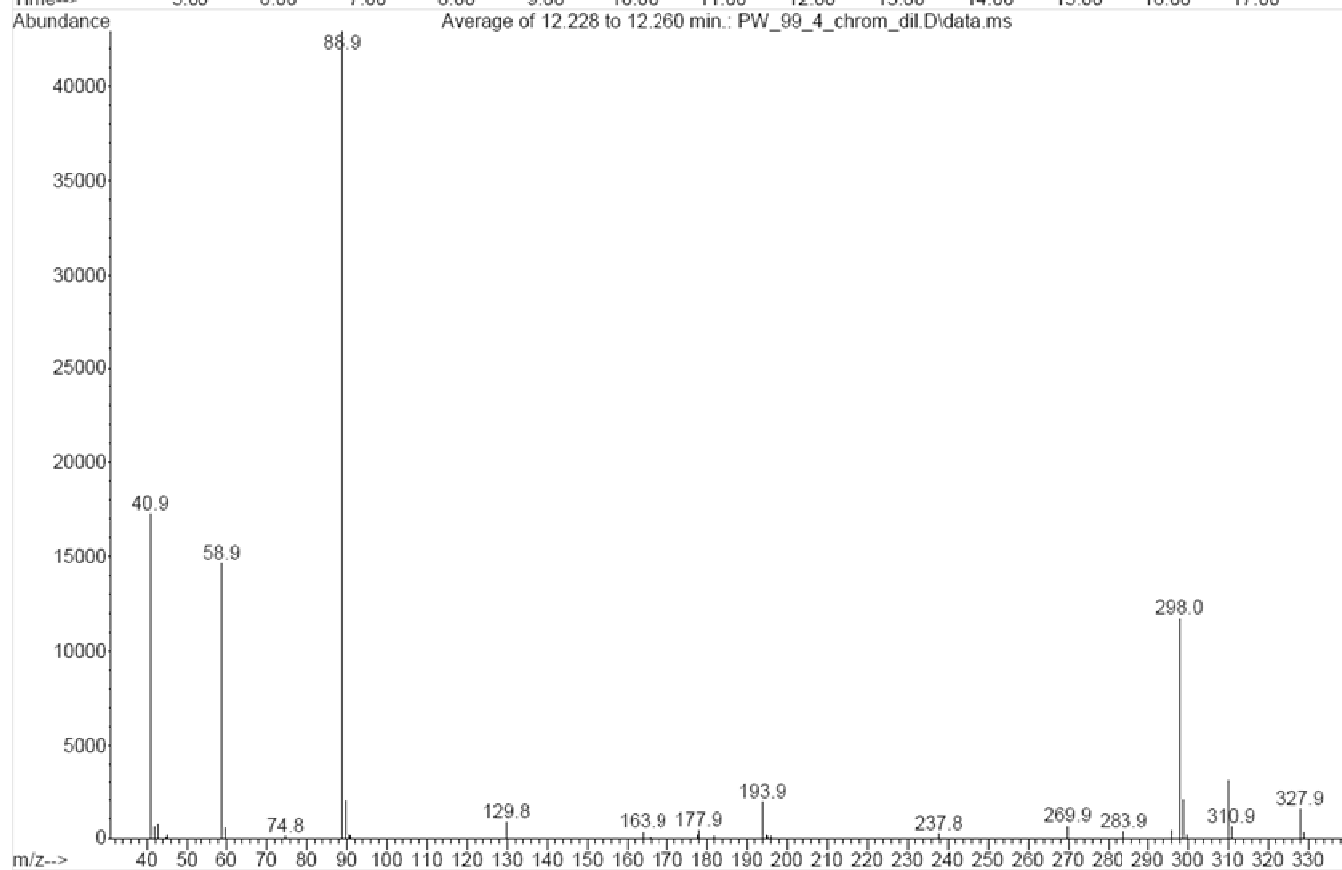
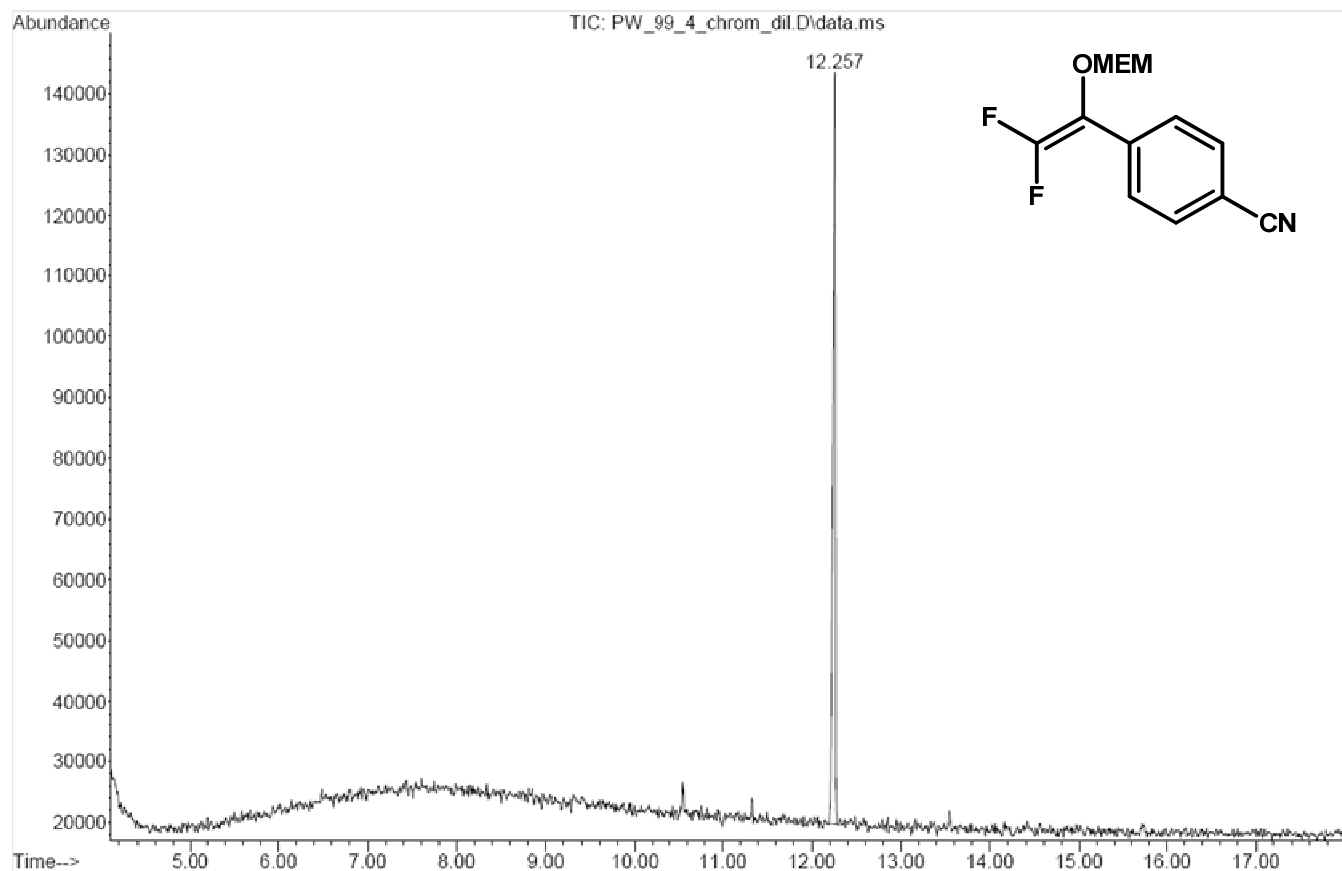


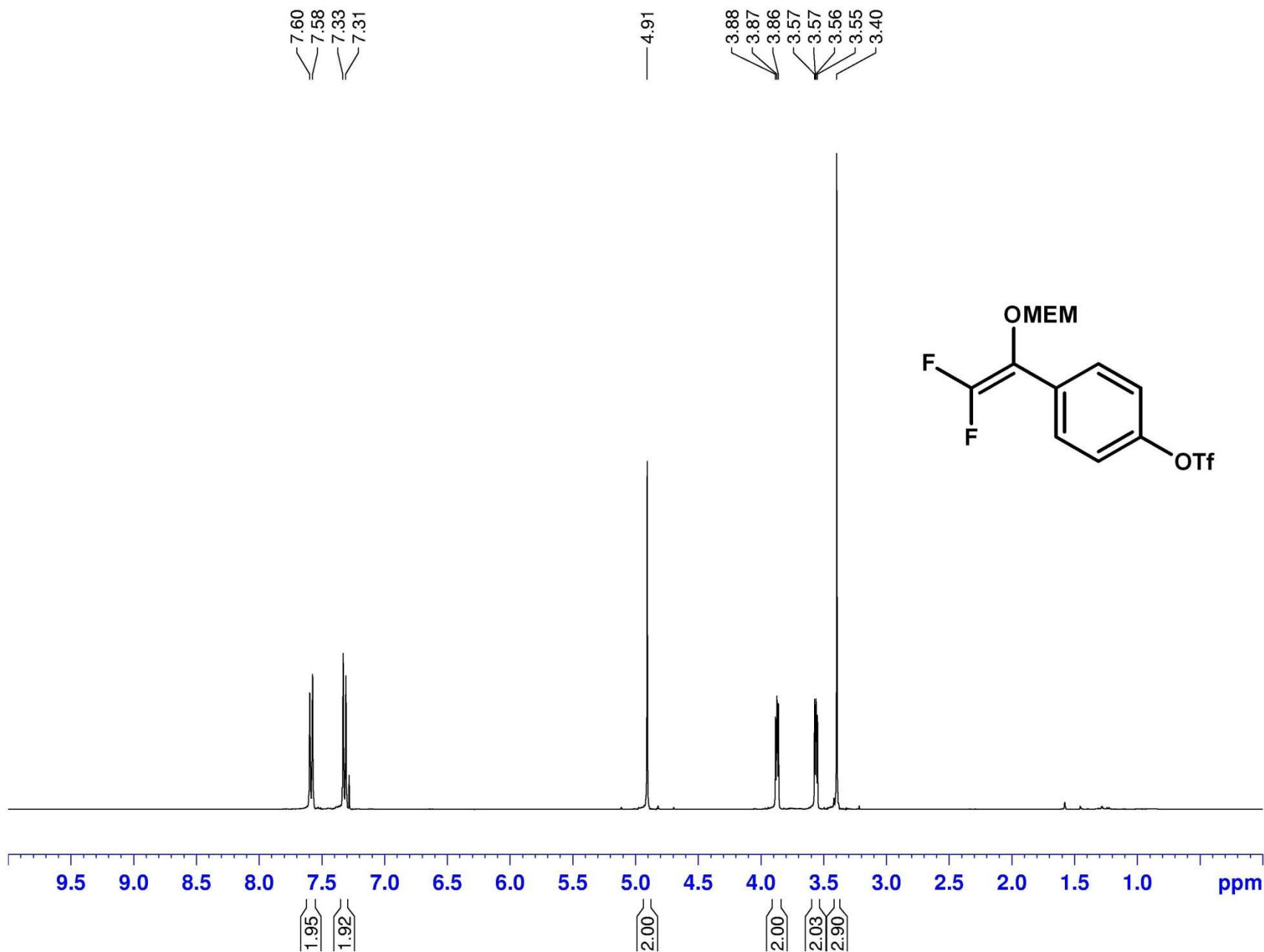


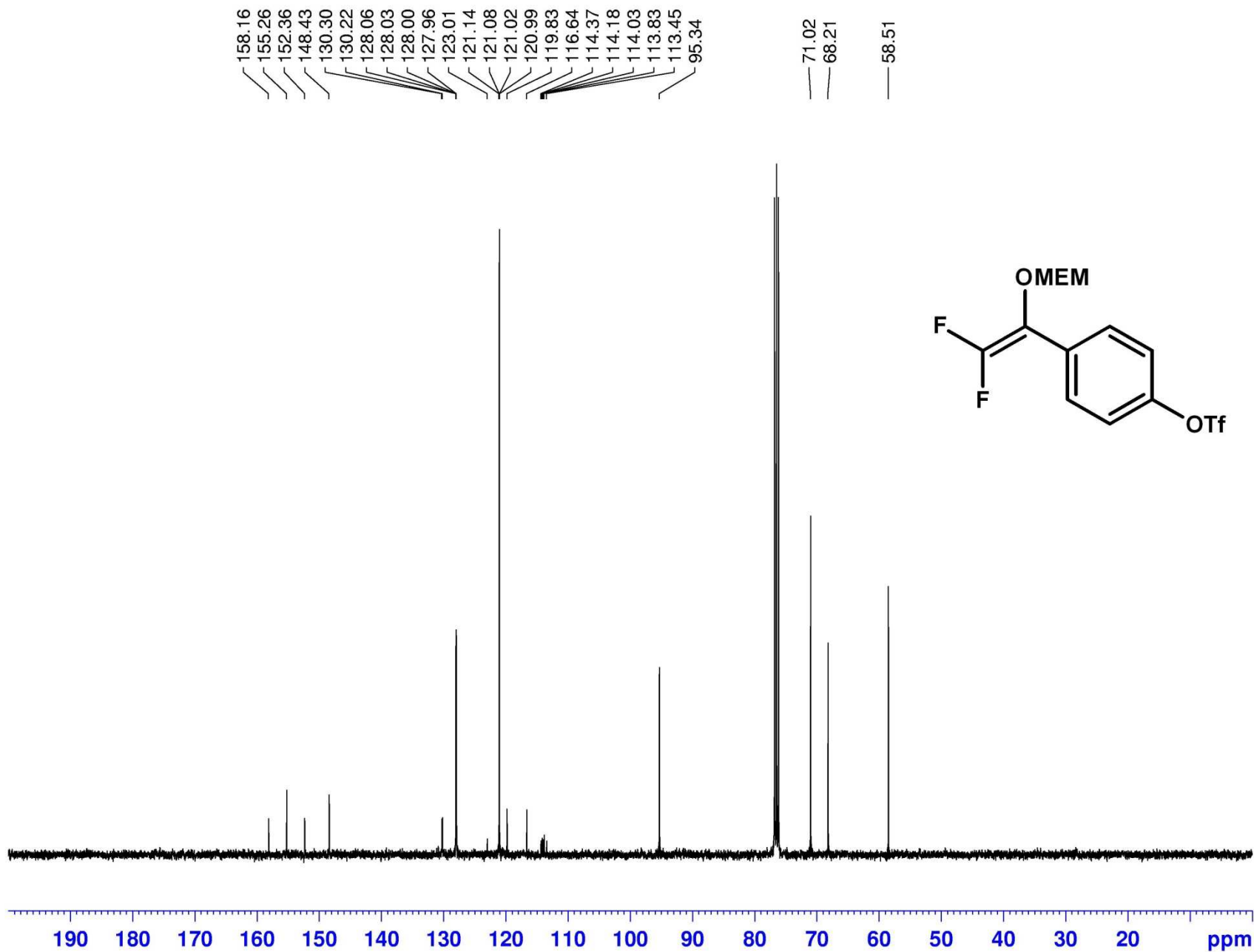


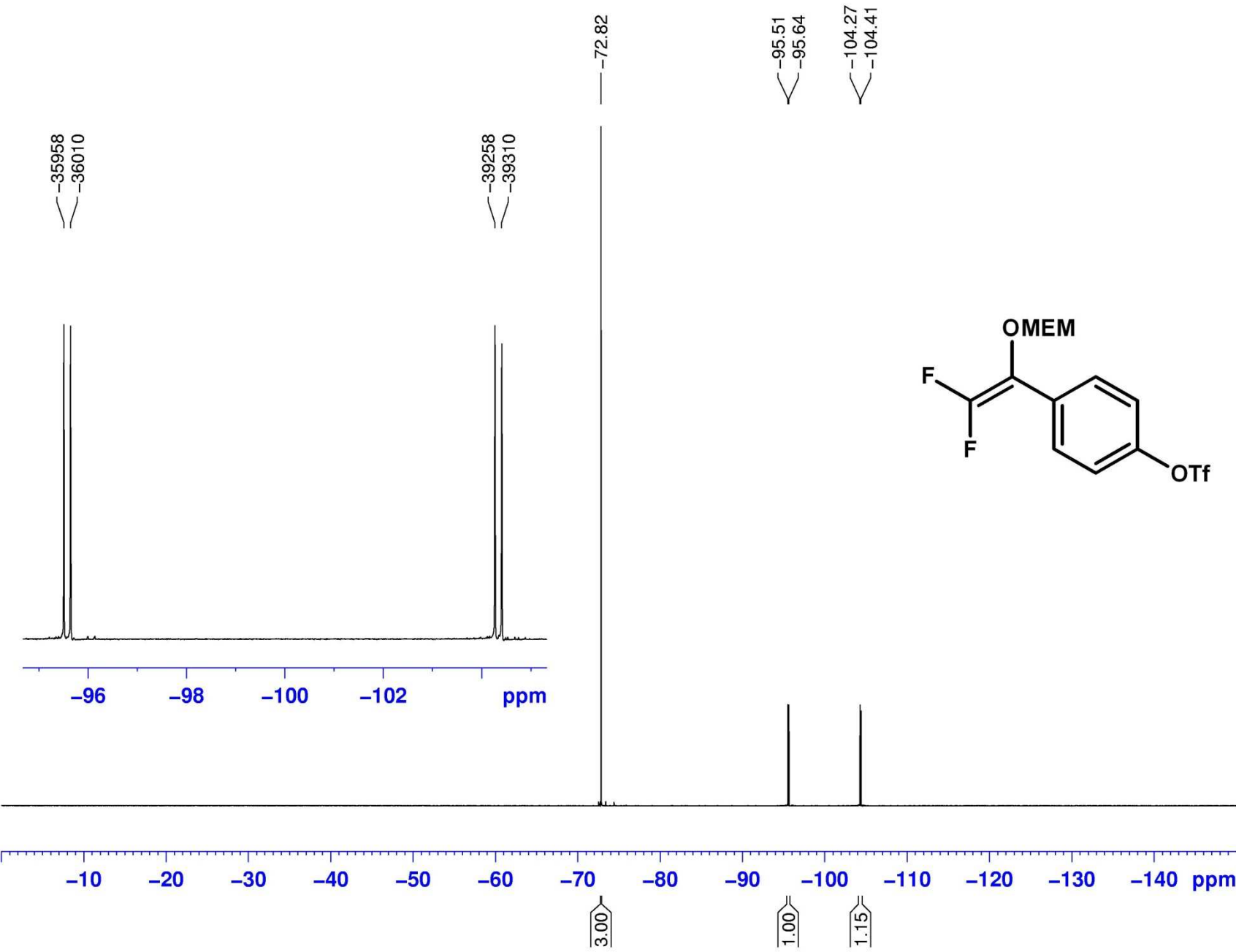


File :E:\FW\PW_99_4_chrom_dil.D
Operator : pk
Acquired : 10 Nov 2010 18:37 using AcqMethod BASIC_PCI_GC250_70C.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 1

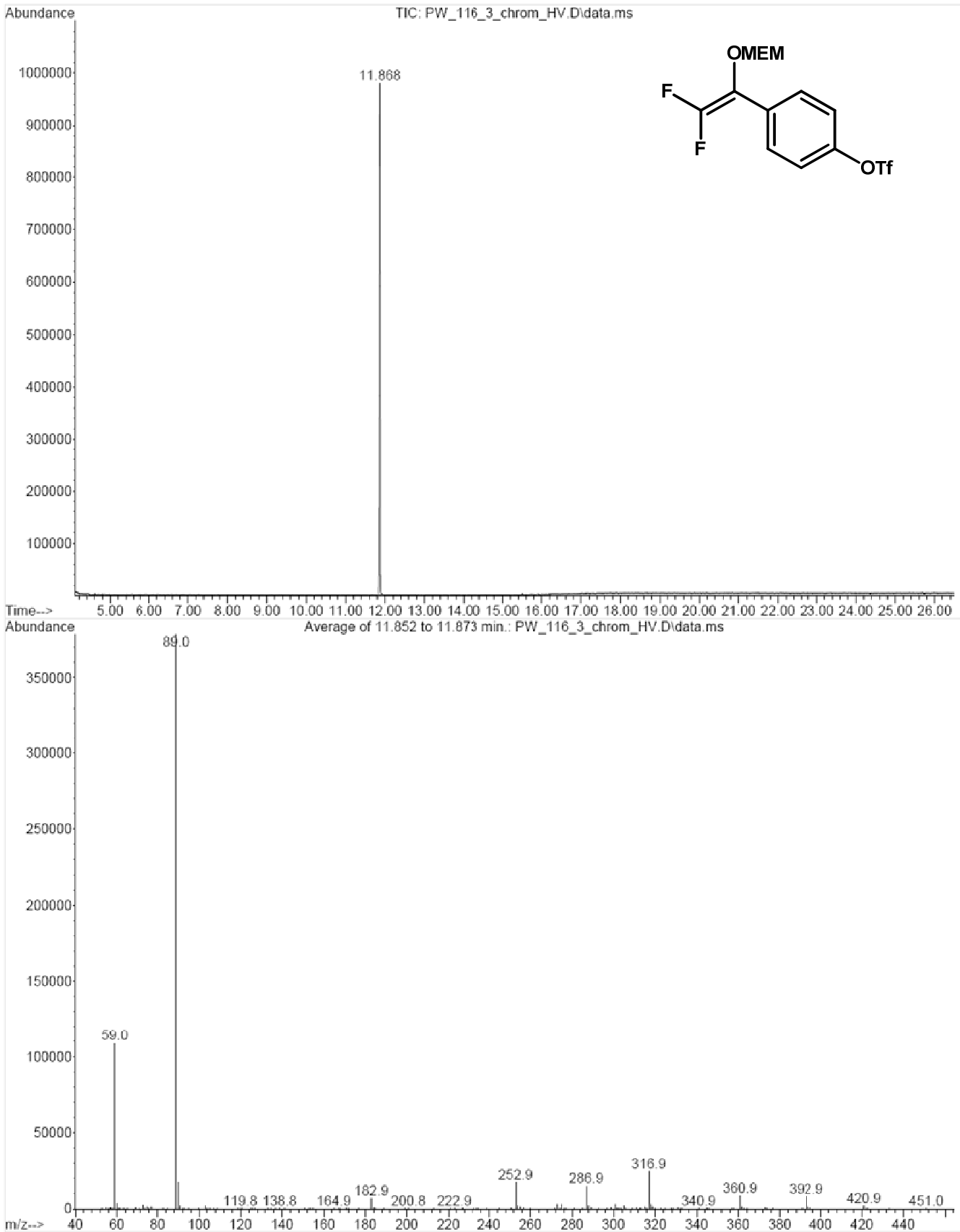


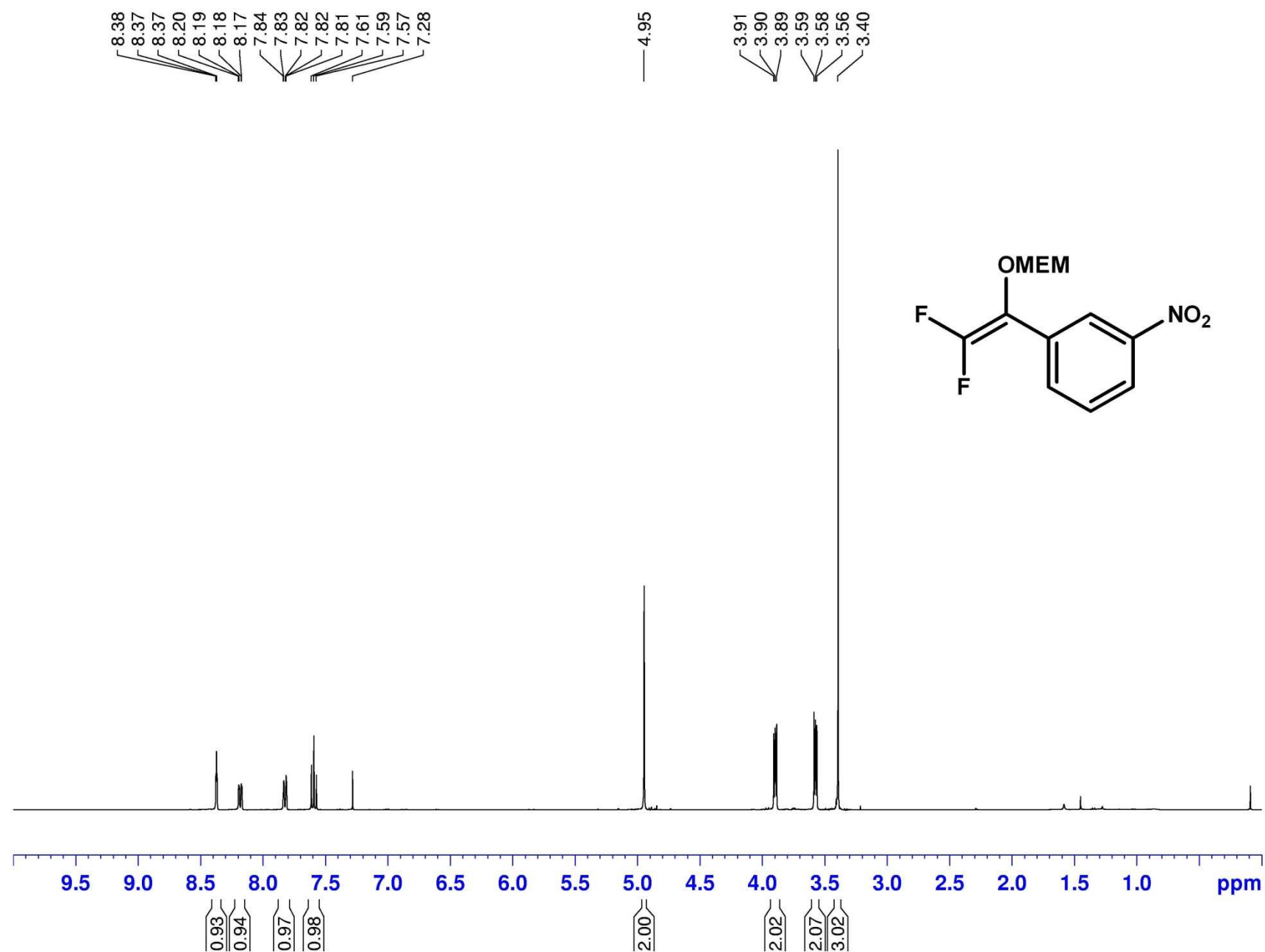


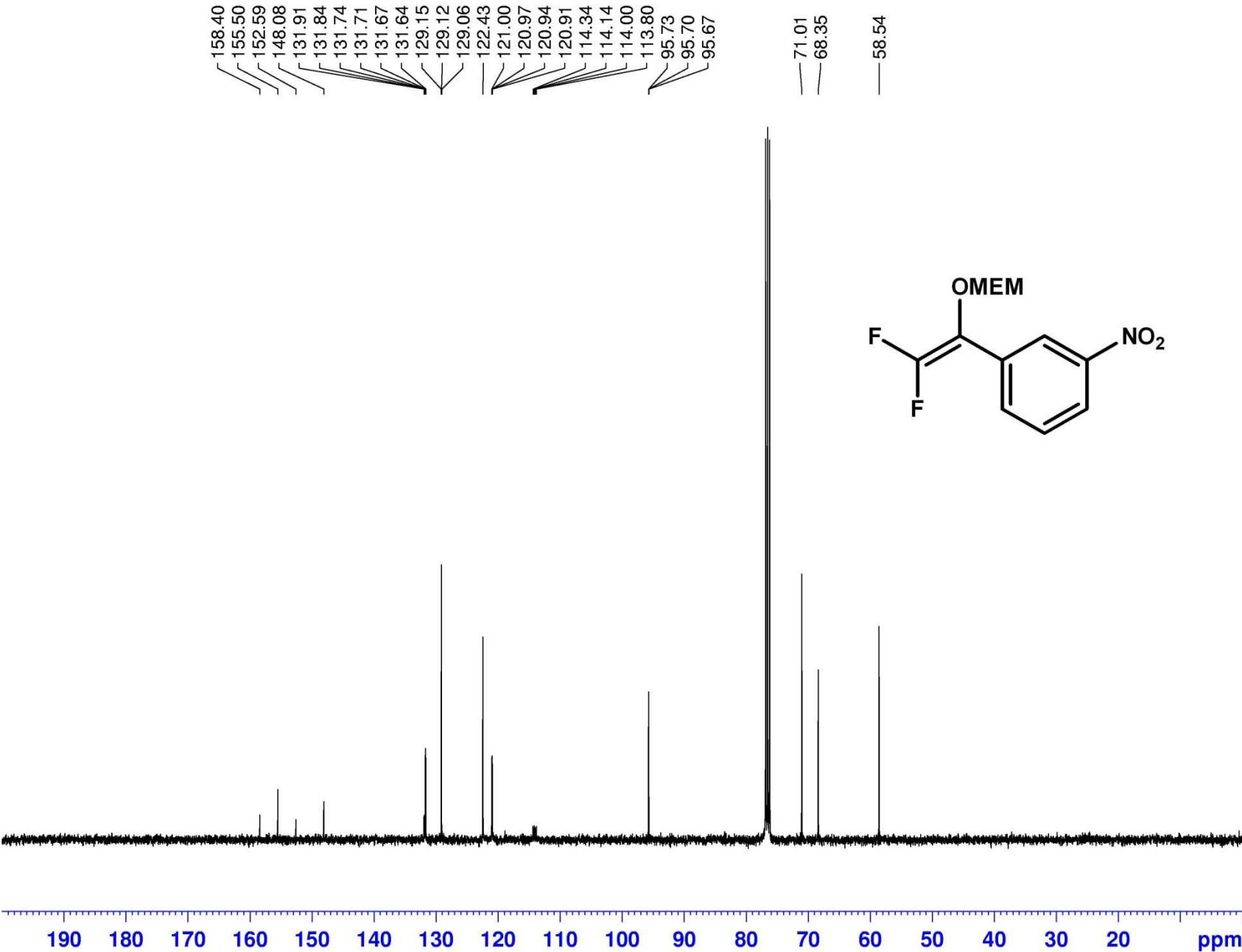


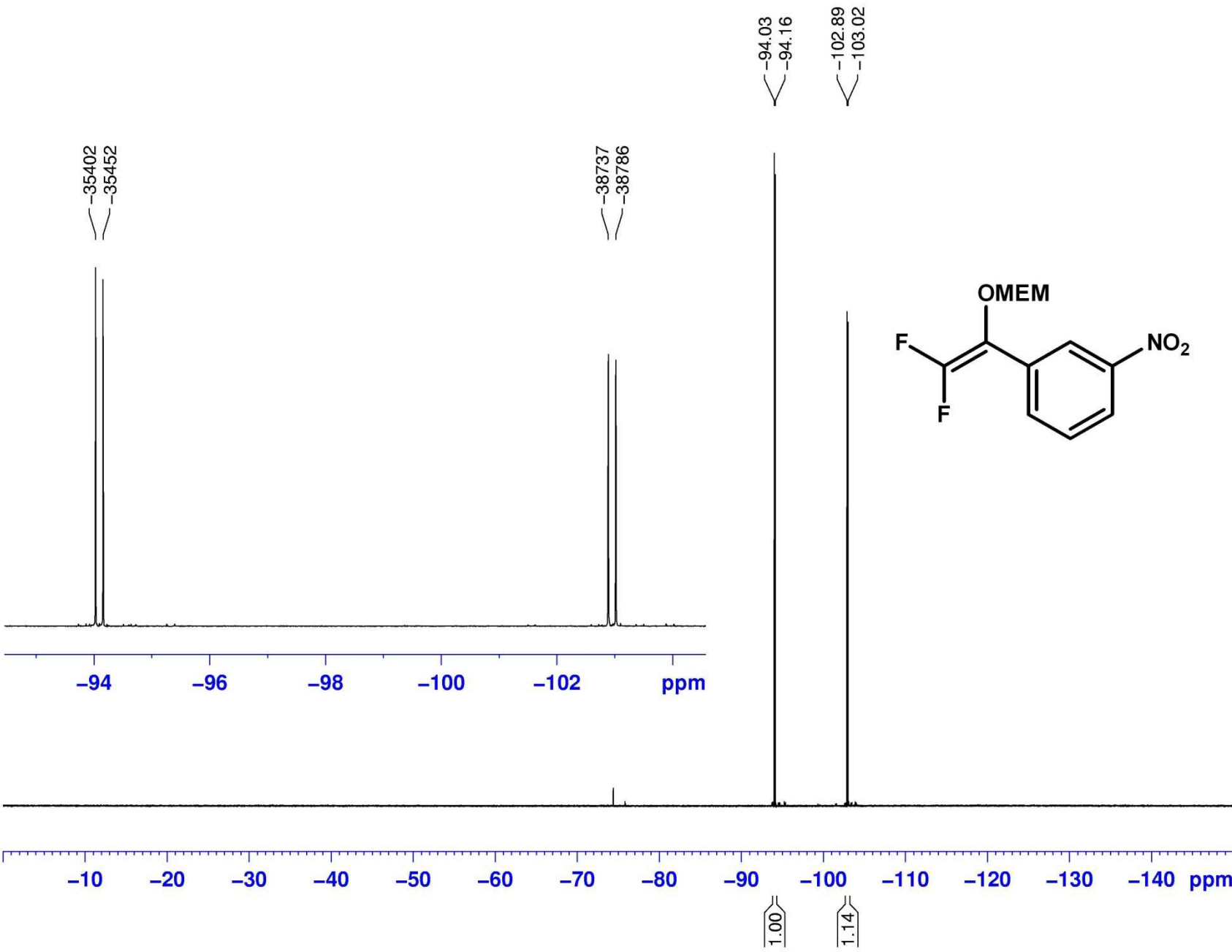


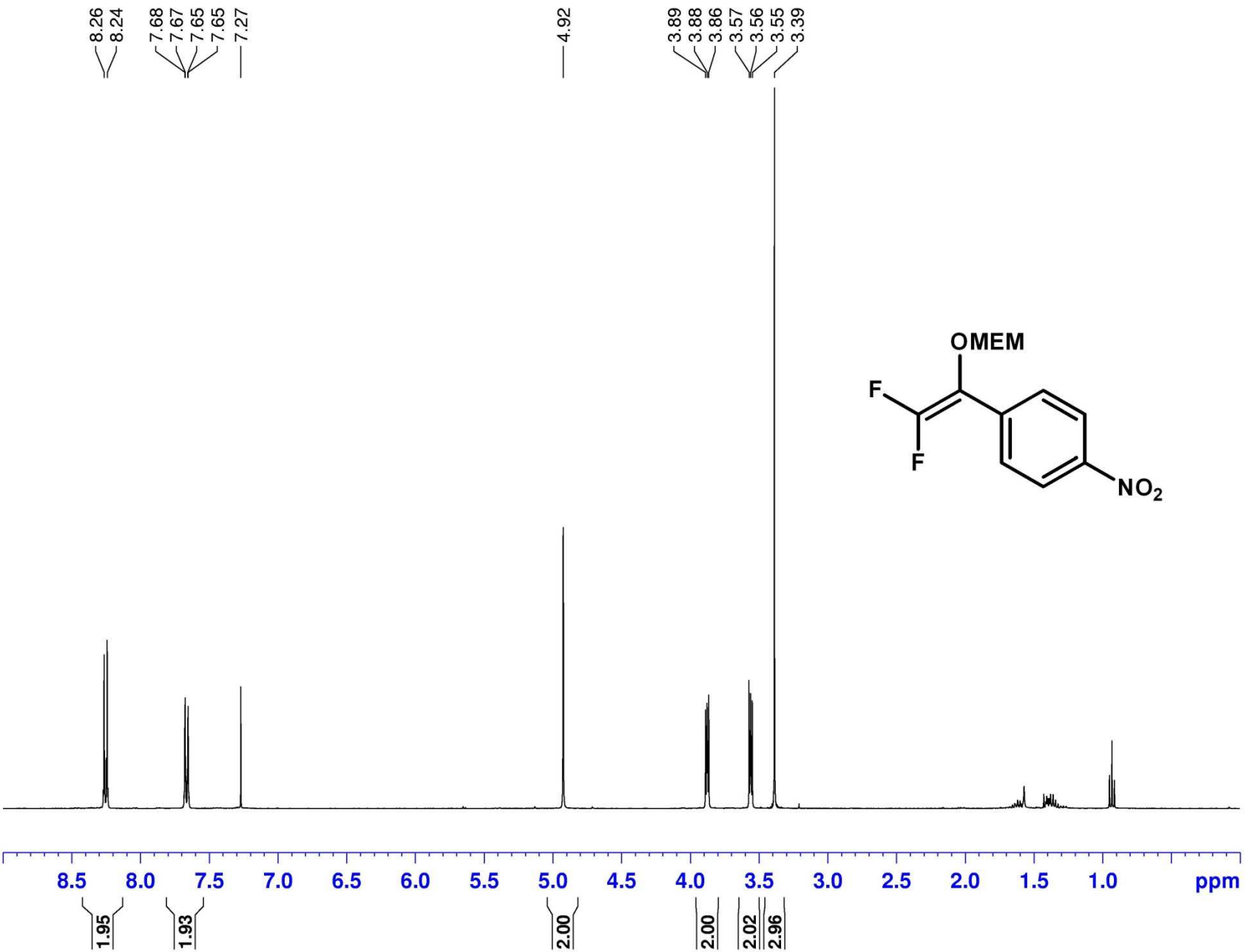
File :E:\PW\PW_116_3_chrom_HV.D
Operator : PW
Acquired : 1 Dec 2010 15:54 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 14

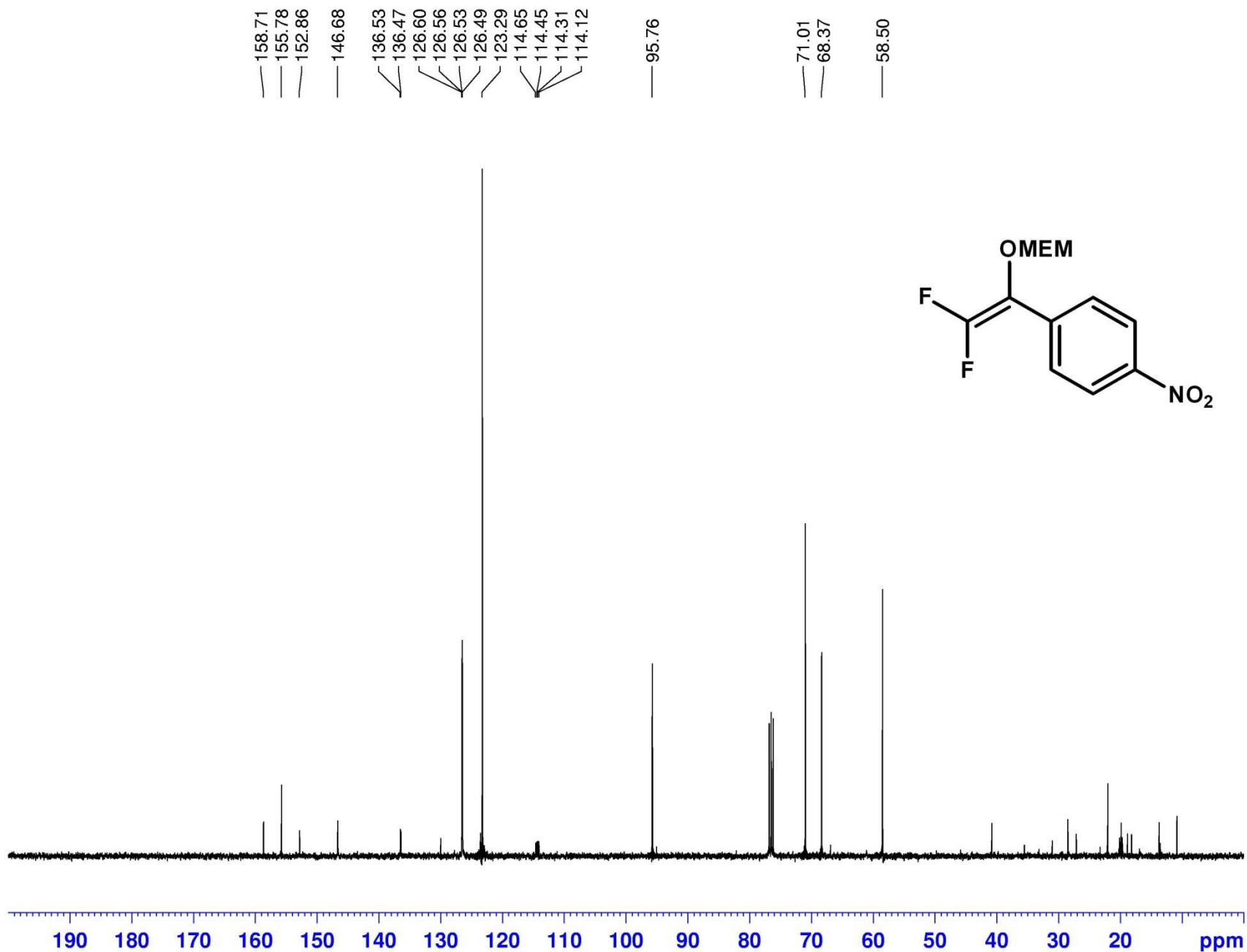


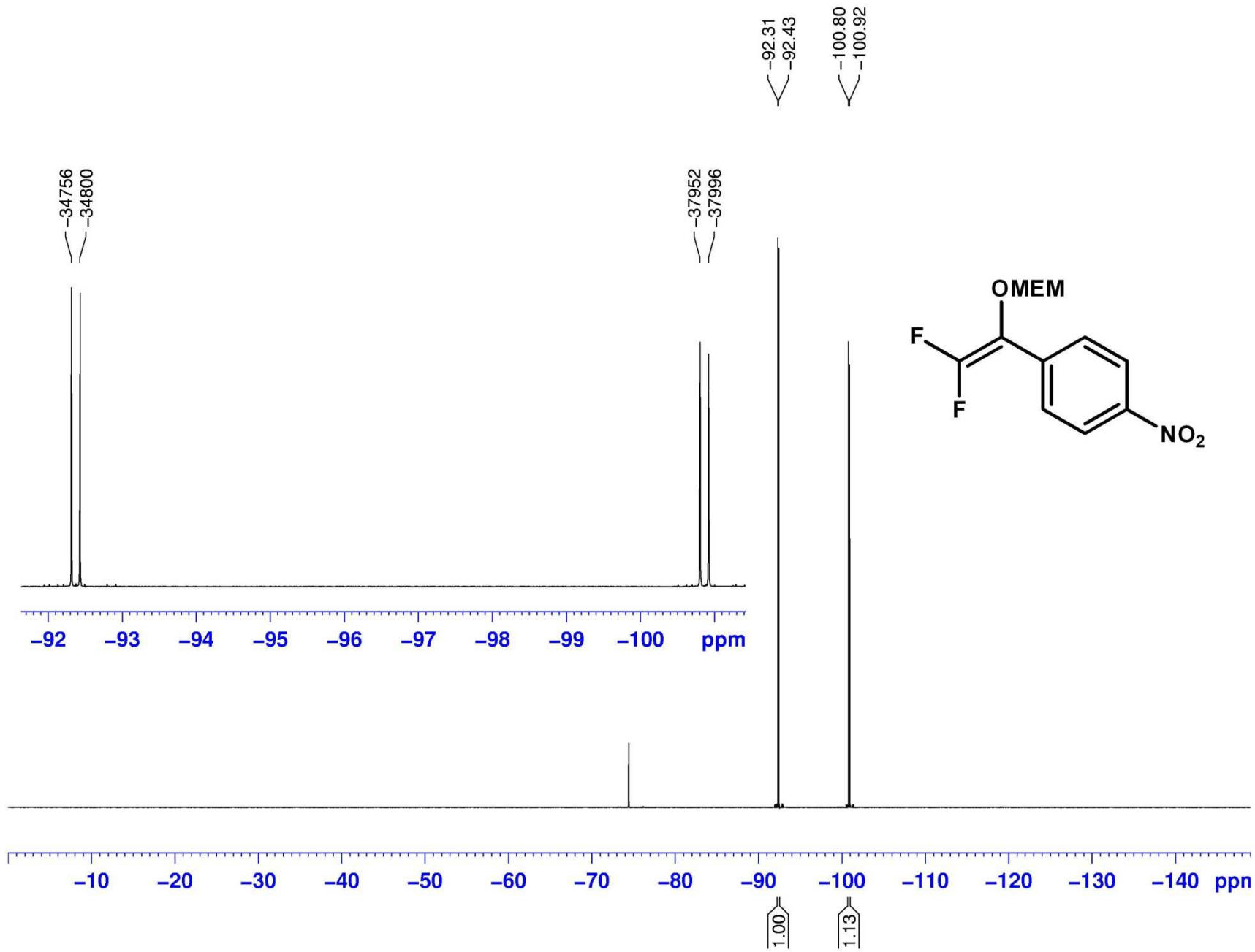


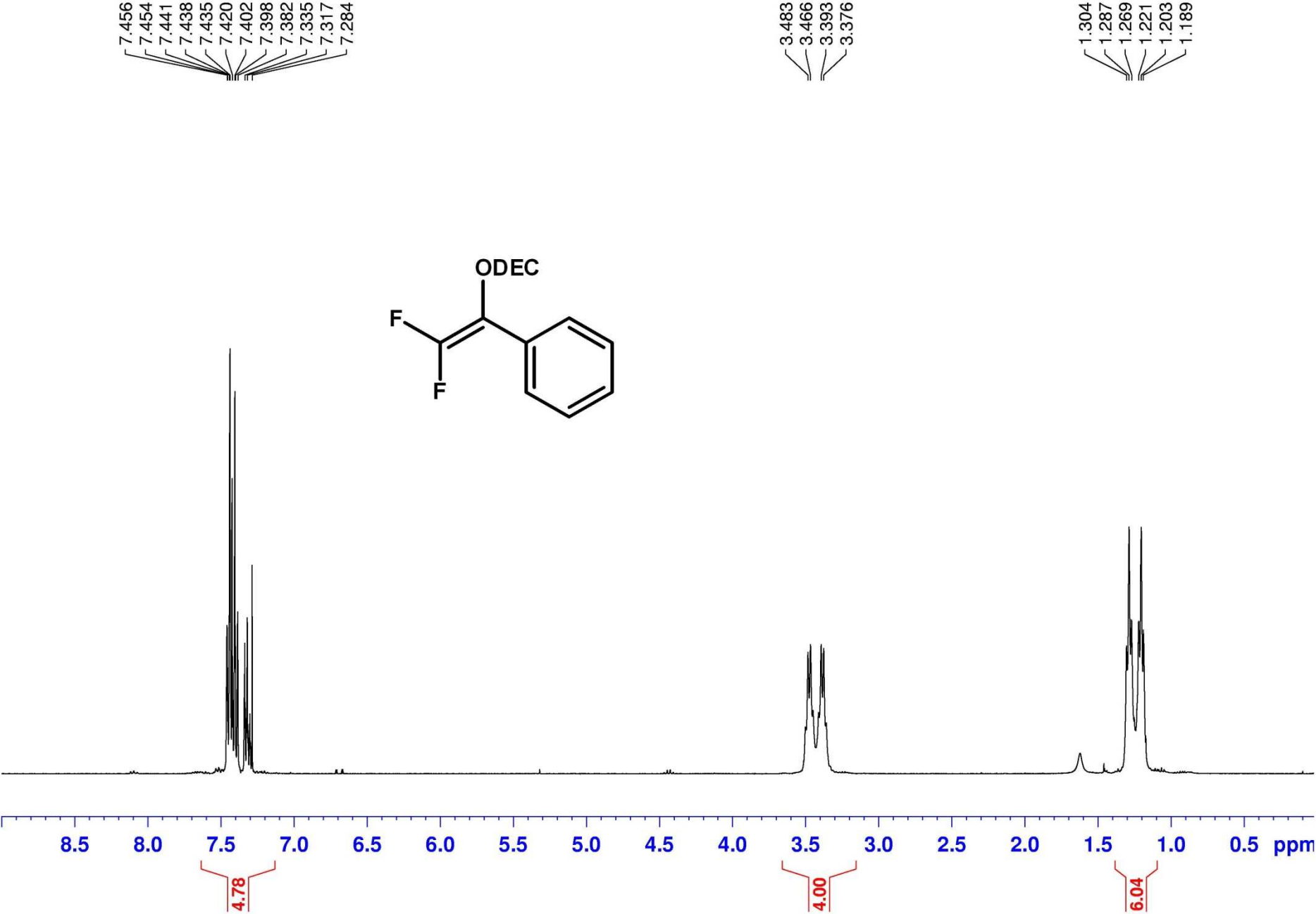


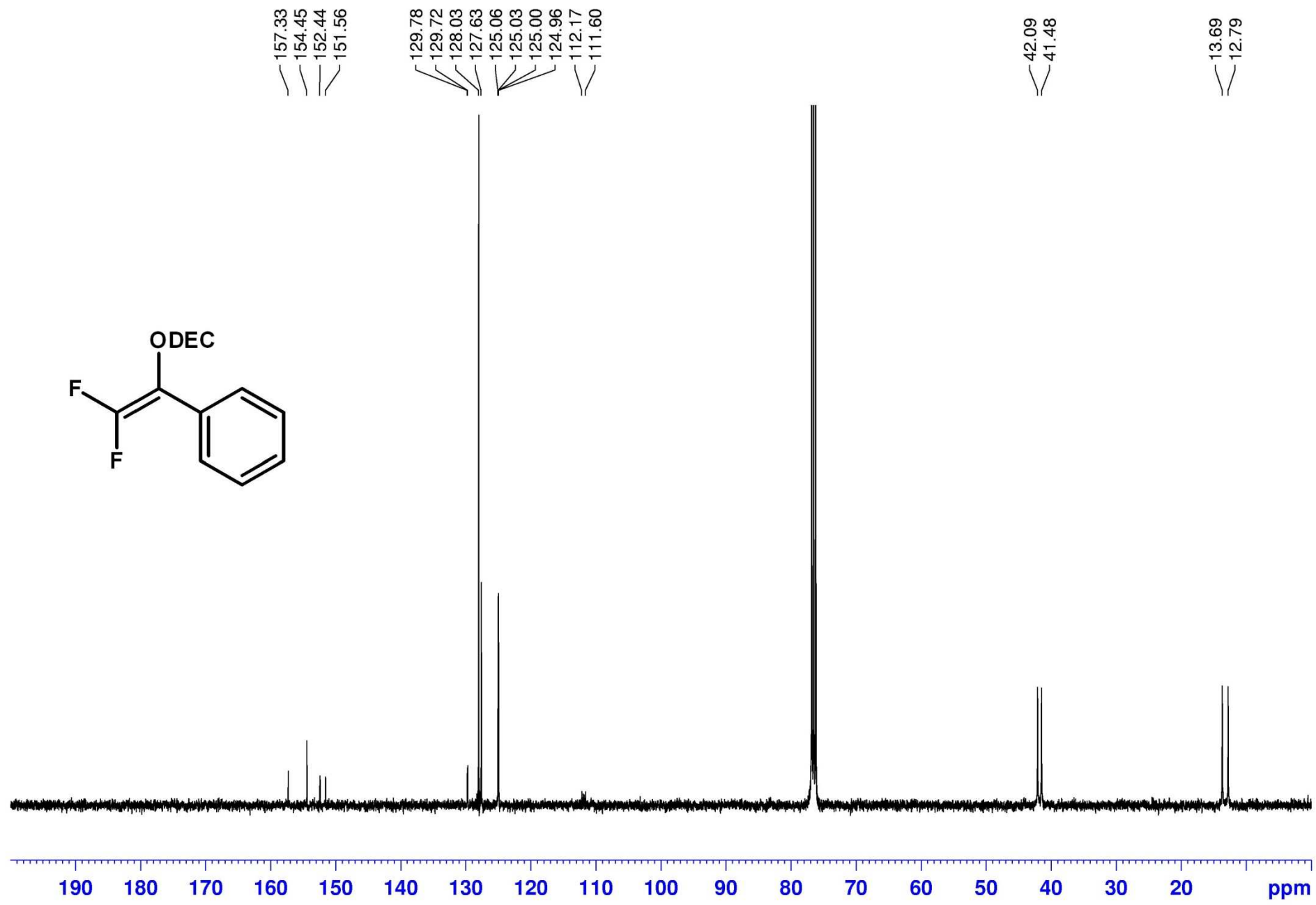


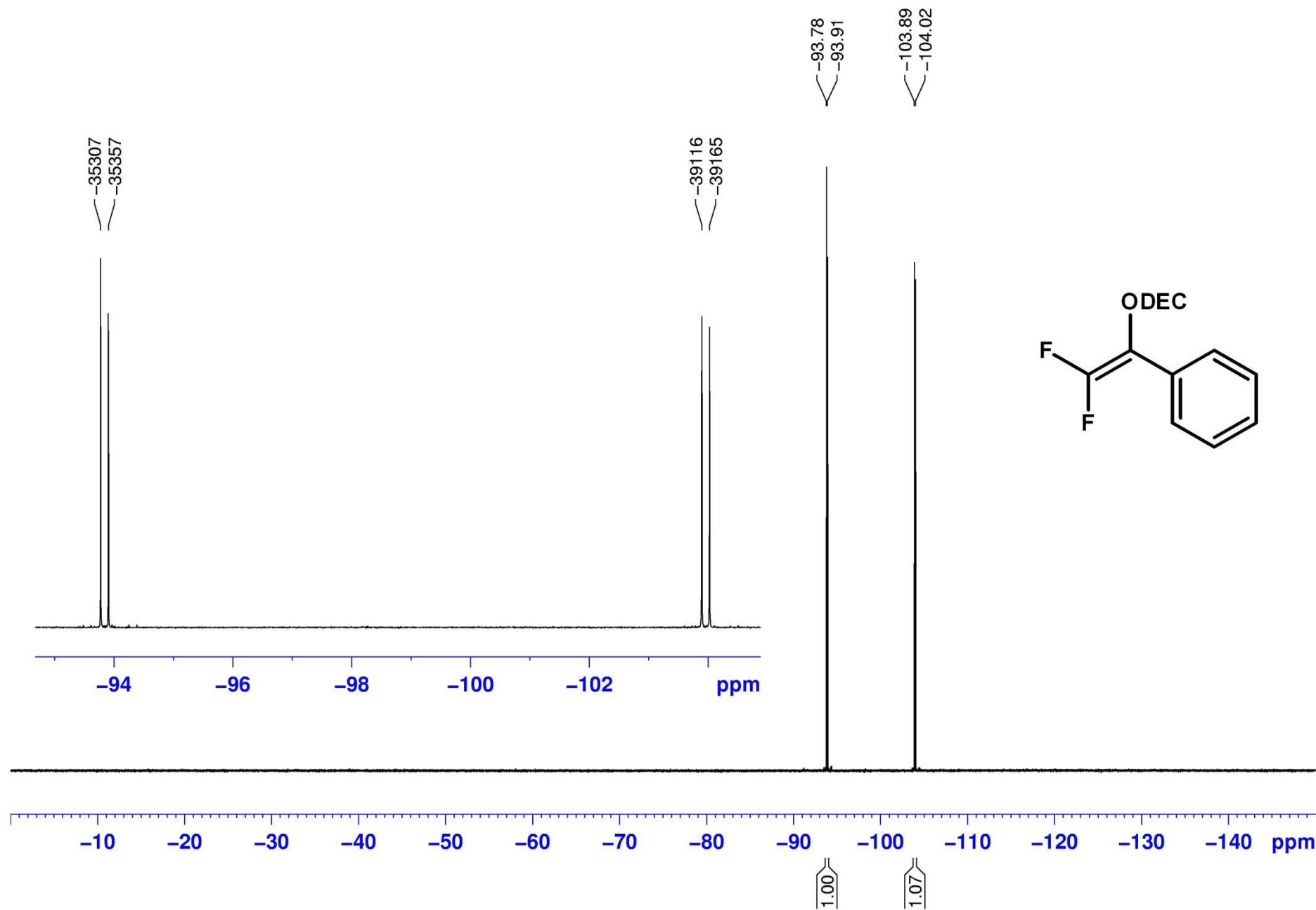




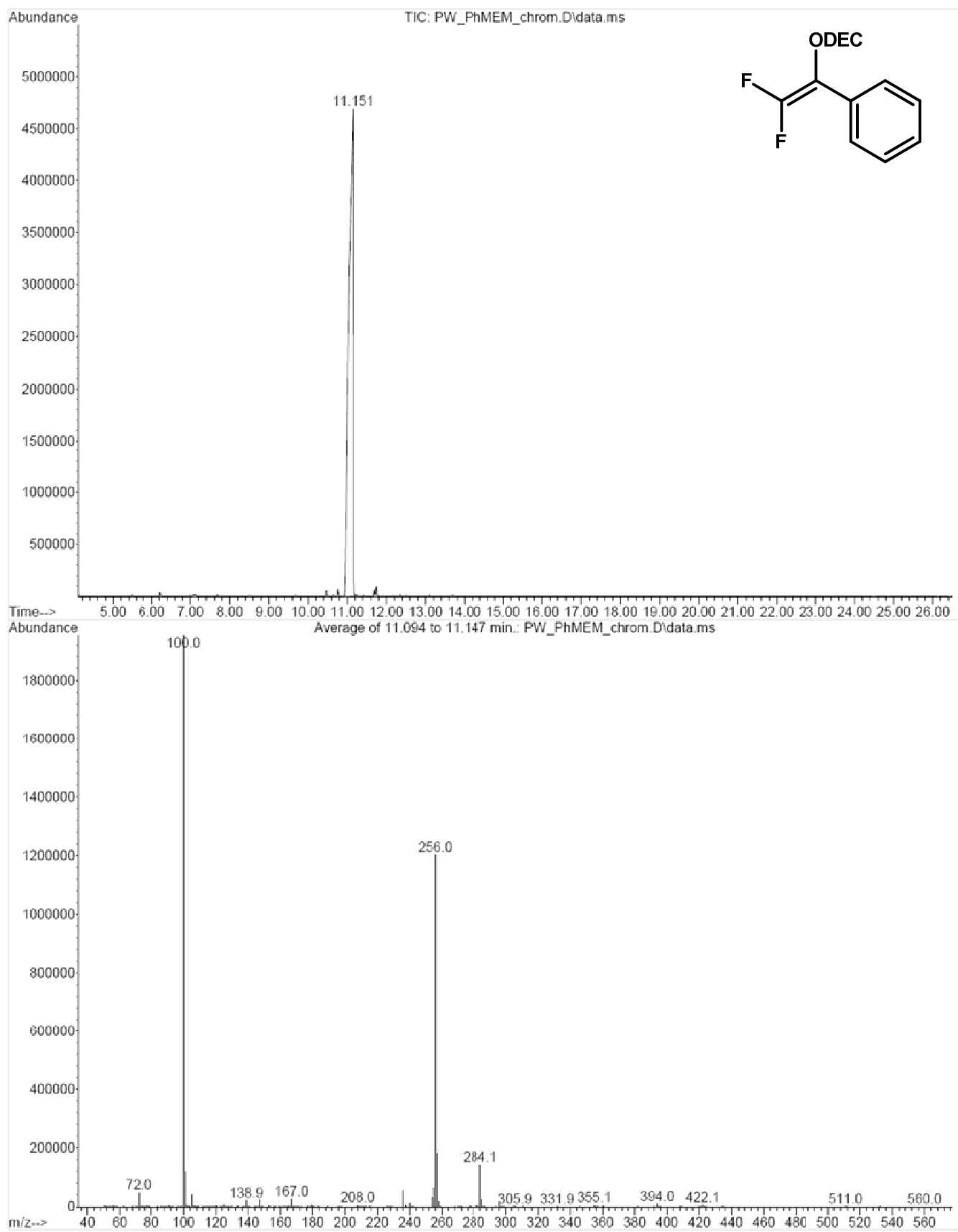


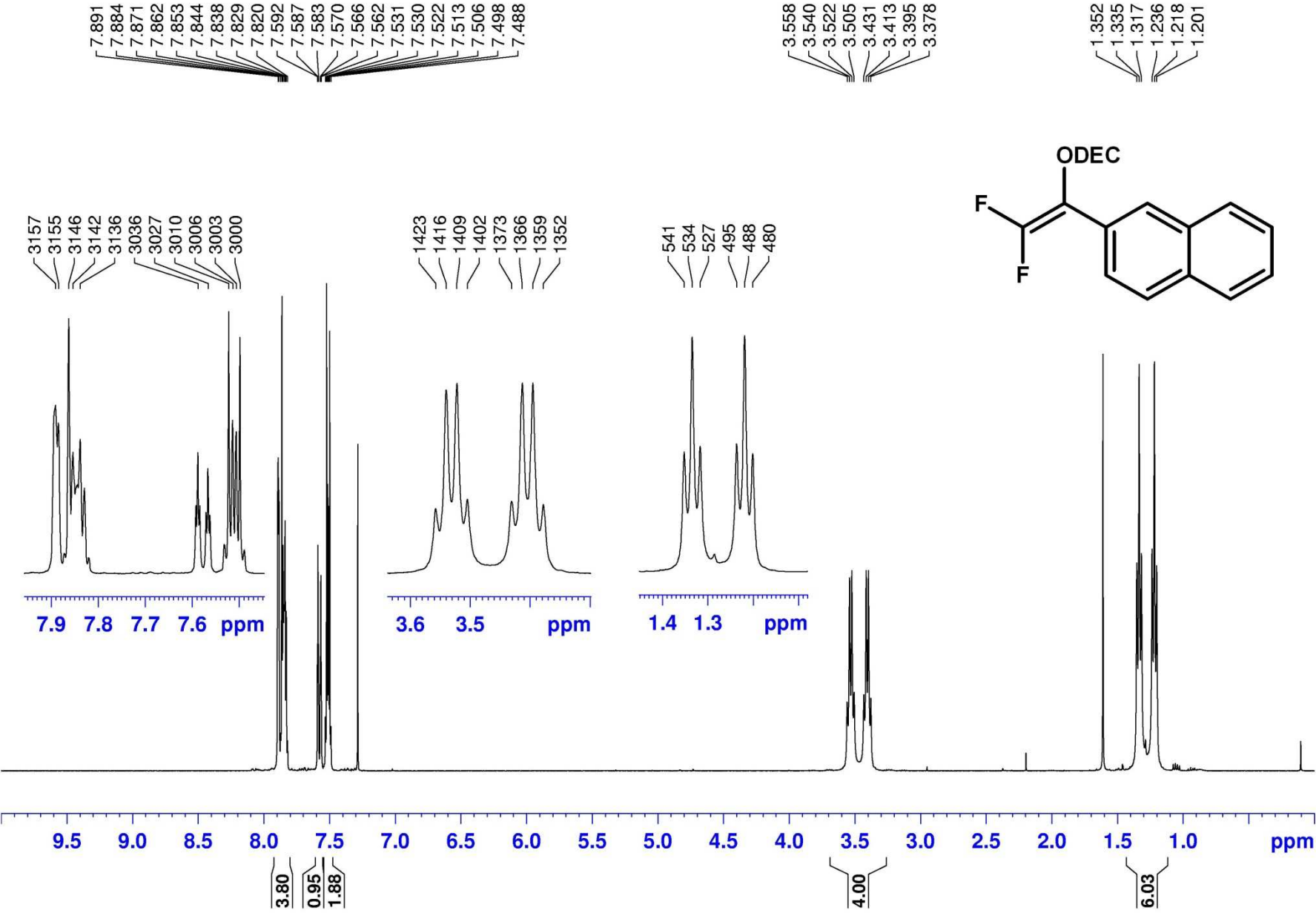


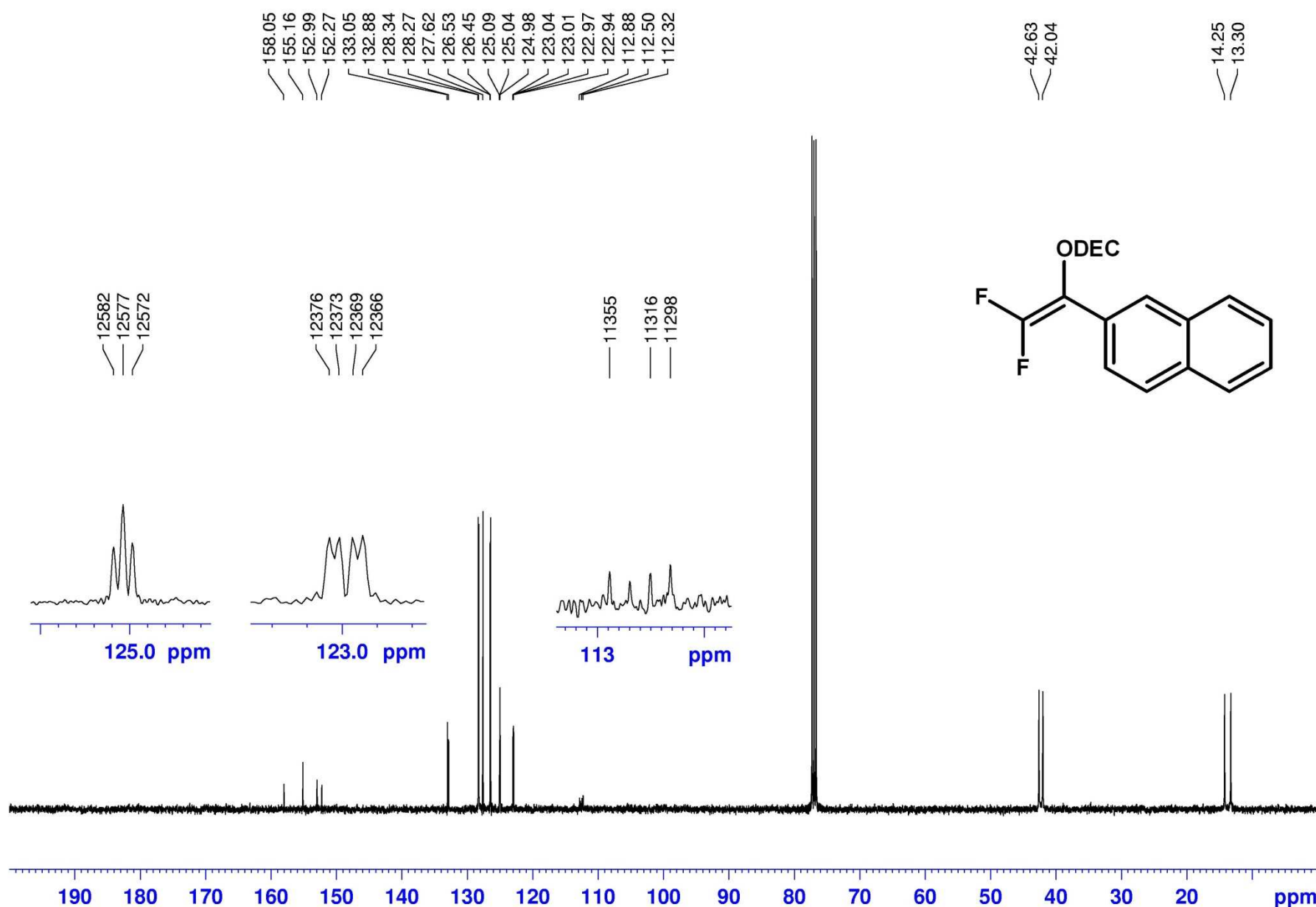


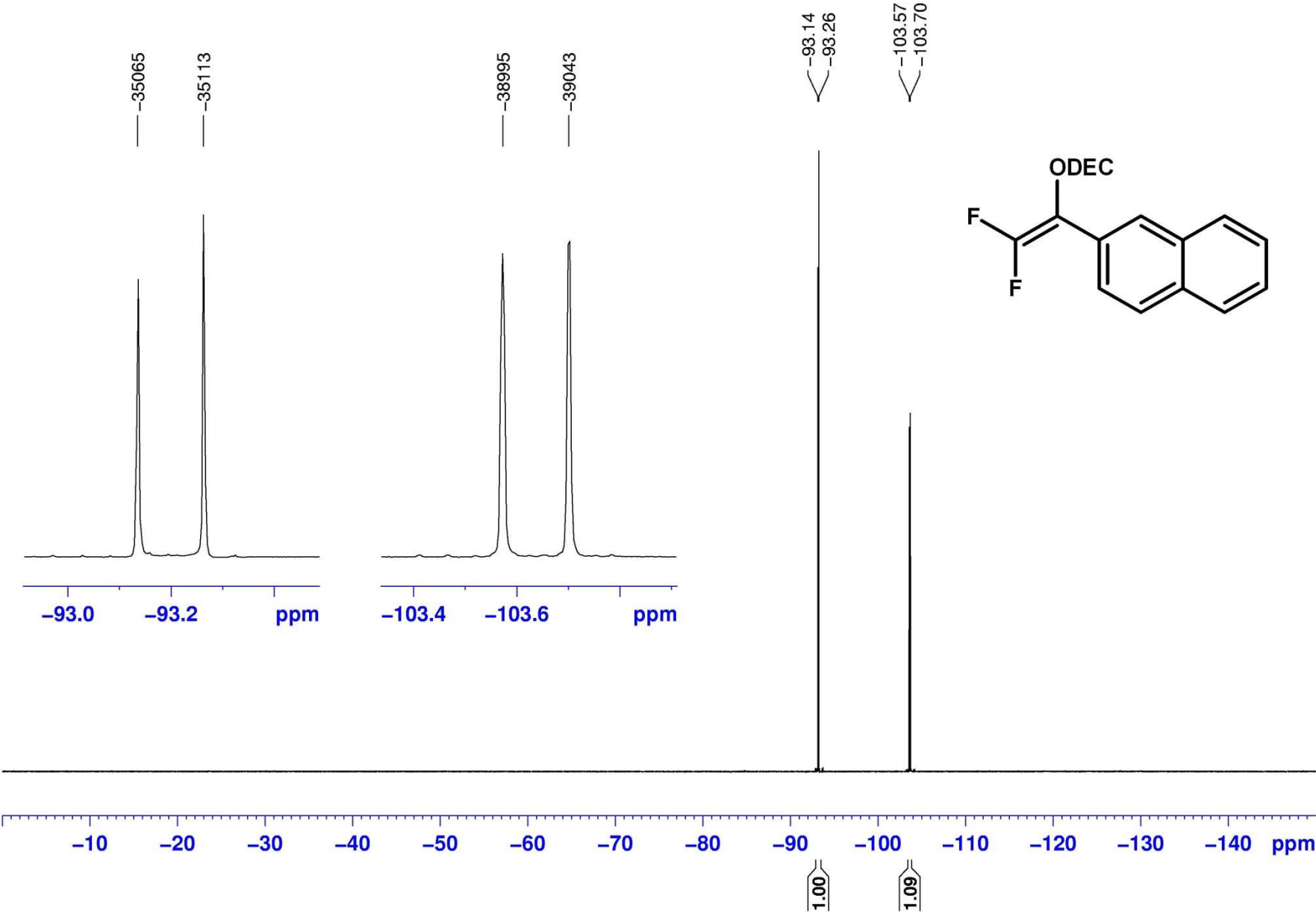


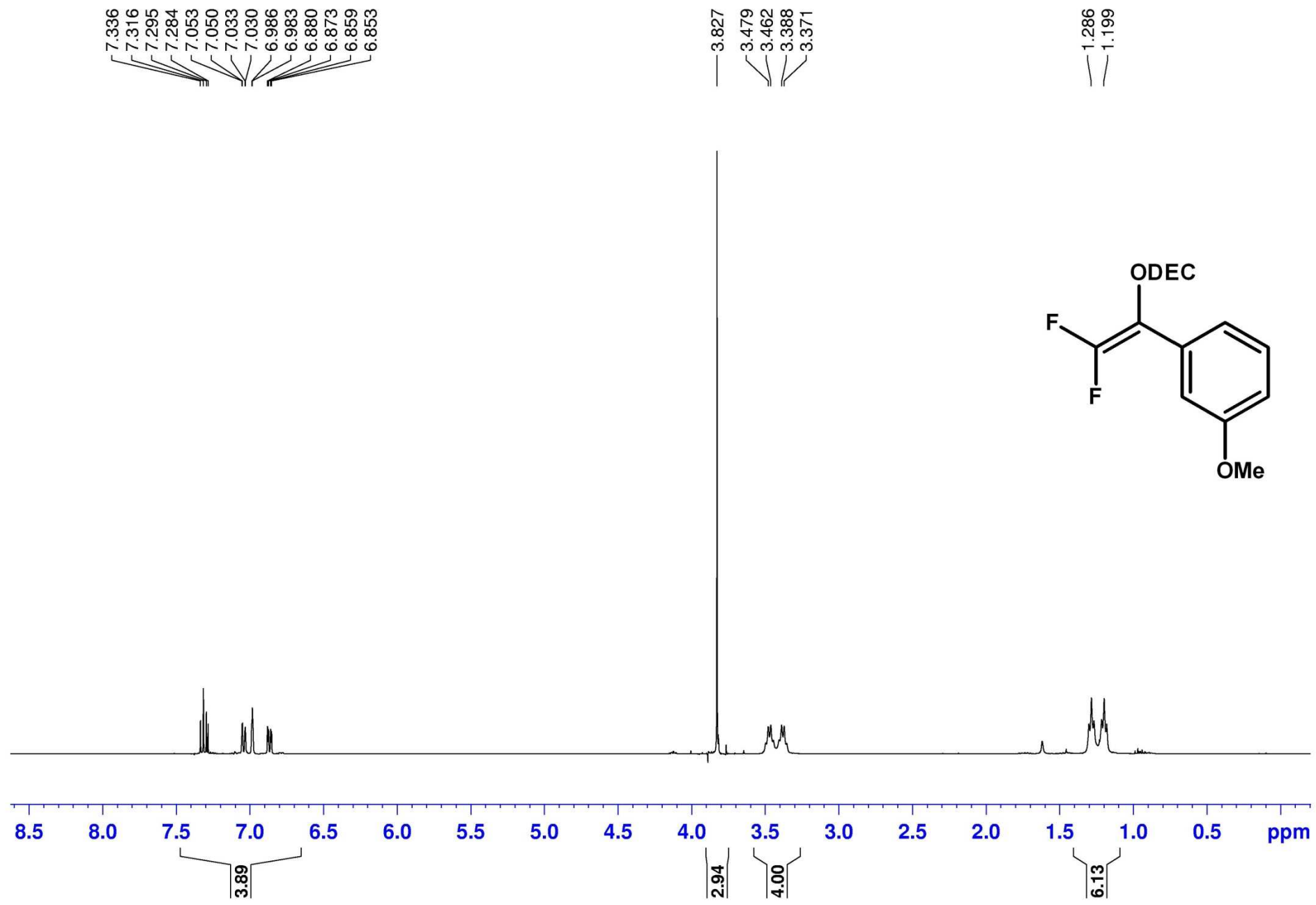
File :E:\PW\PhMEM_chrom.D
Operator : PW
Acquired : 14 Jan 2011 15:12 using AcqMethod BASIC_PCI_GC320_70.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 18

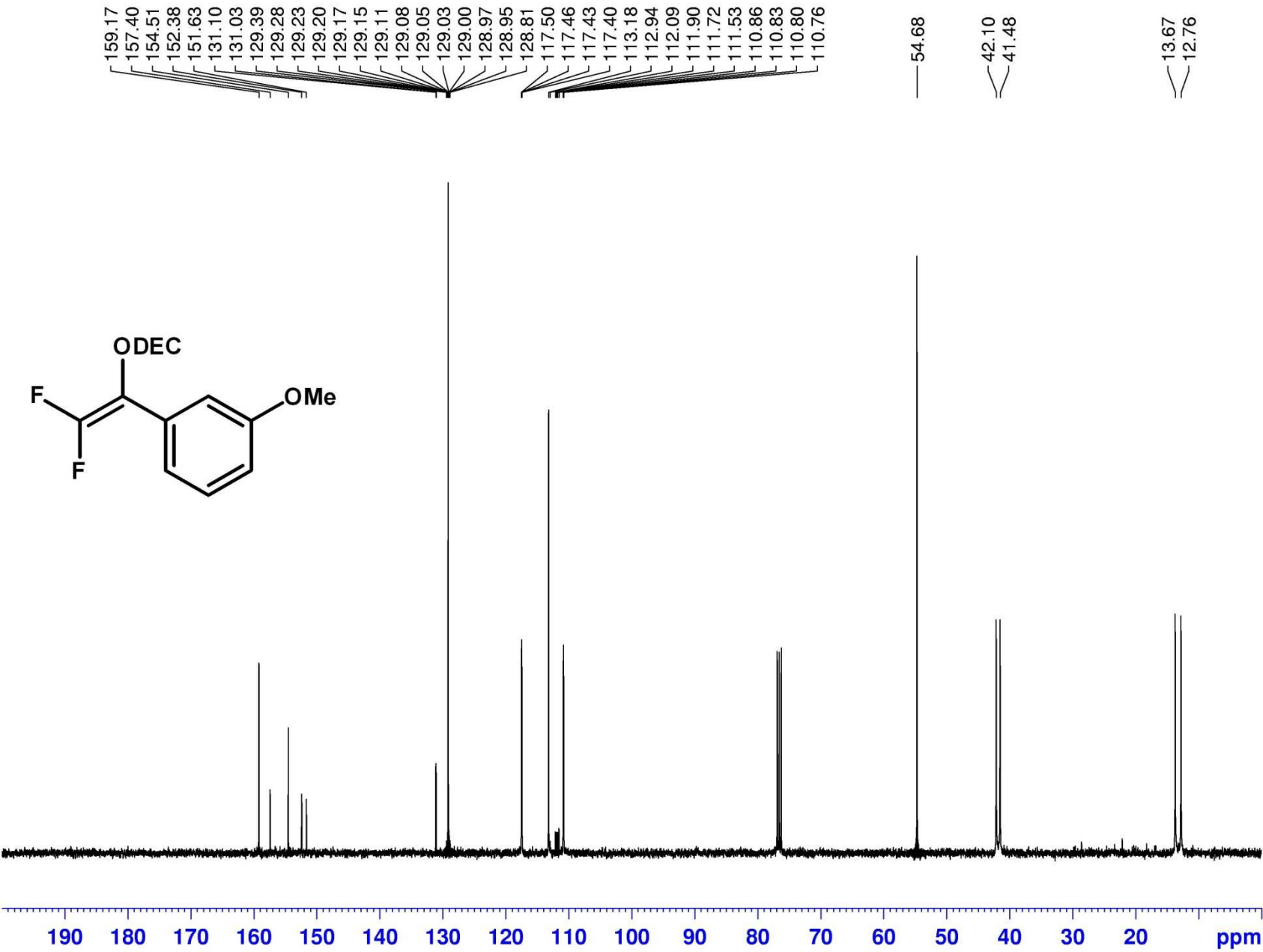


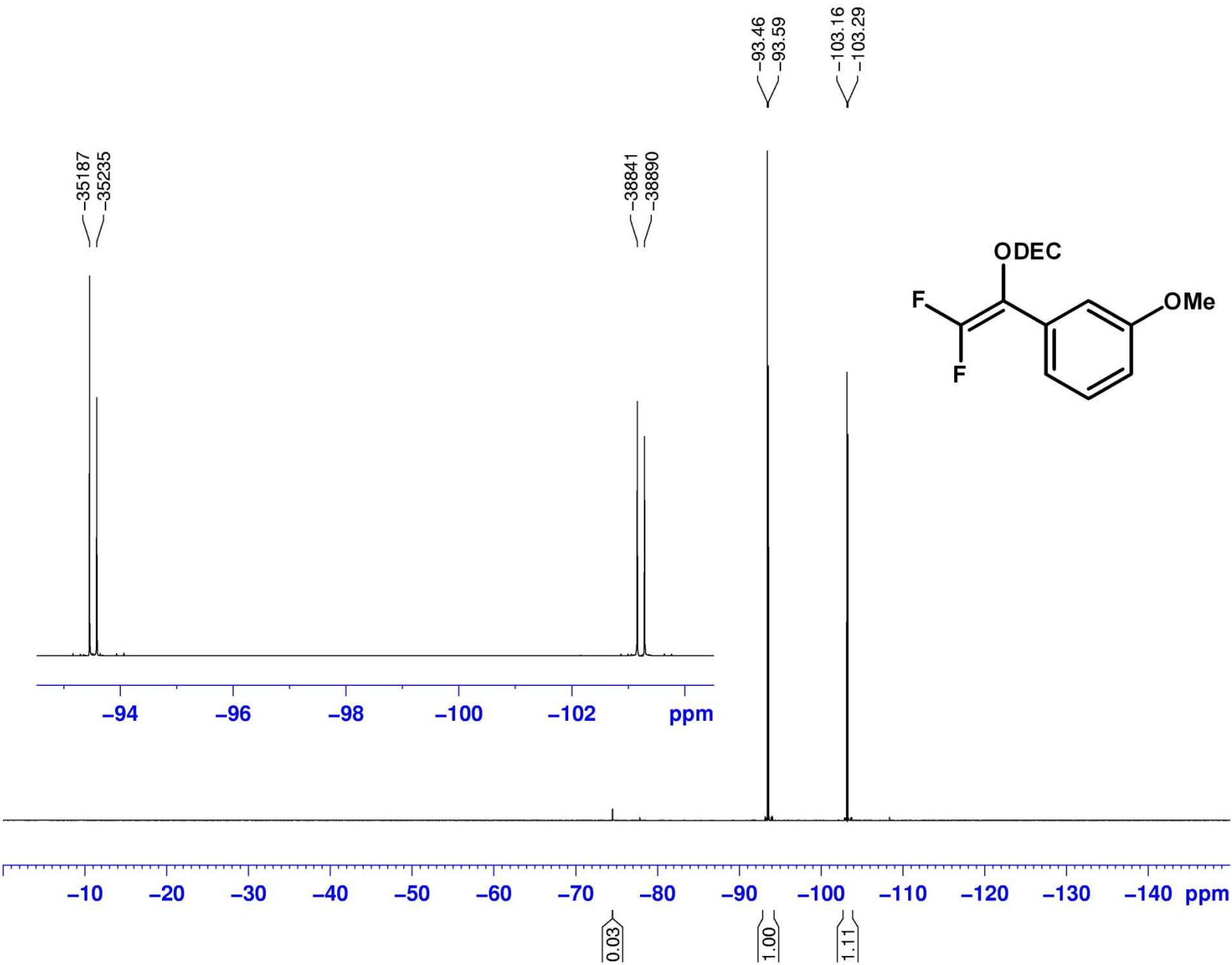


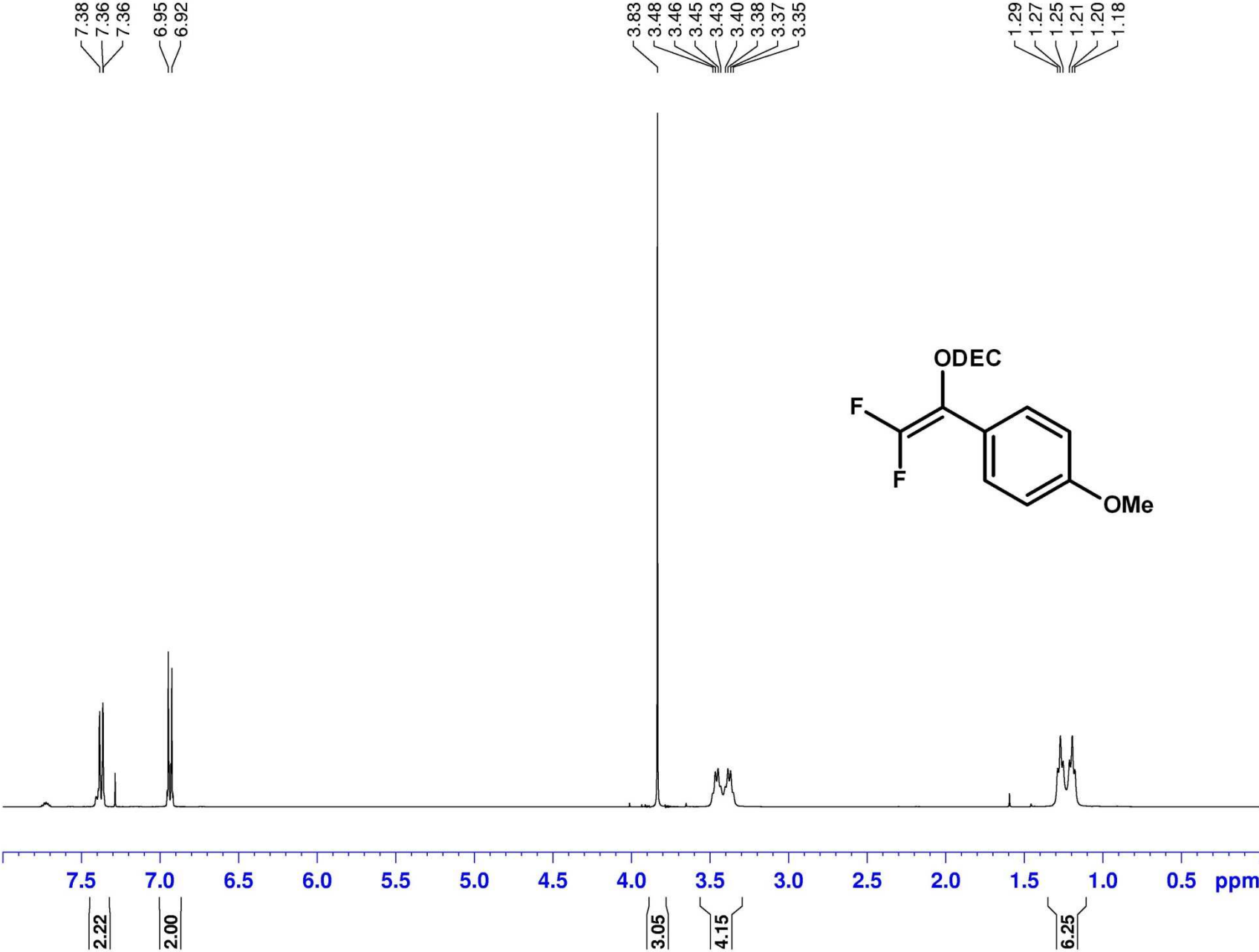


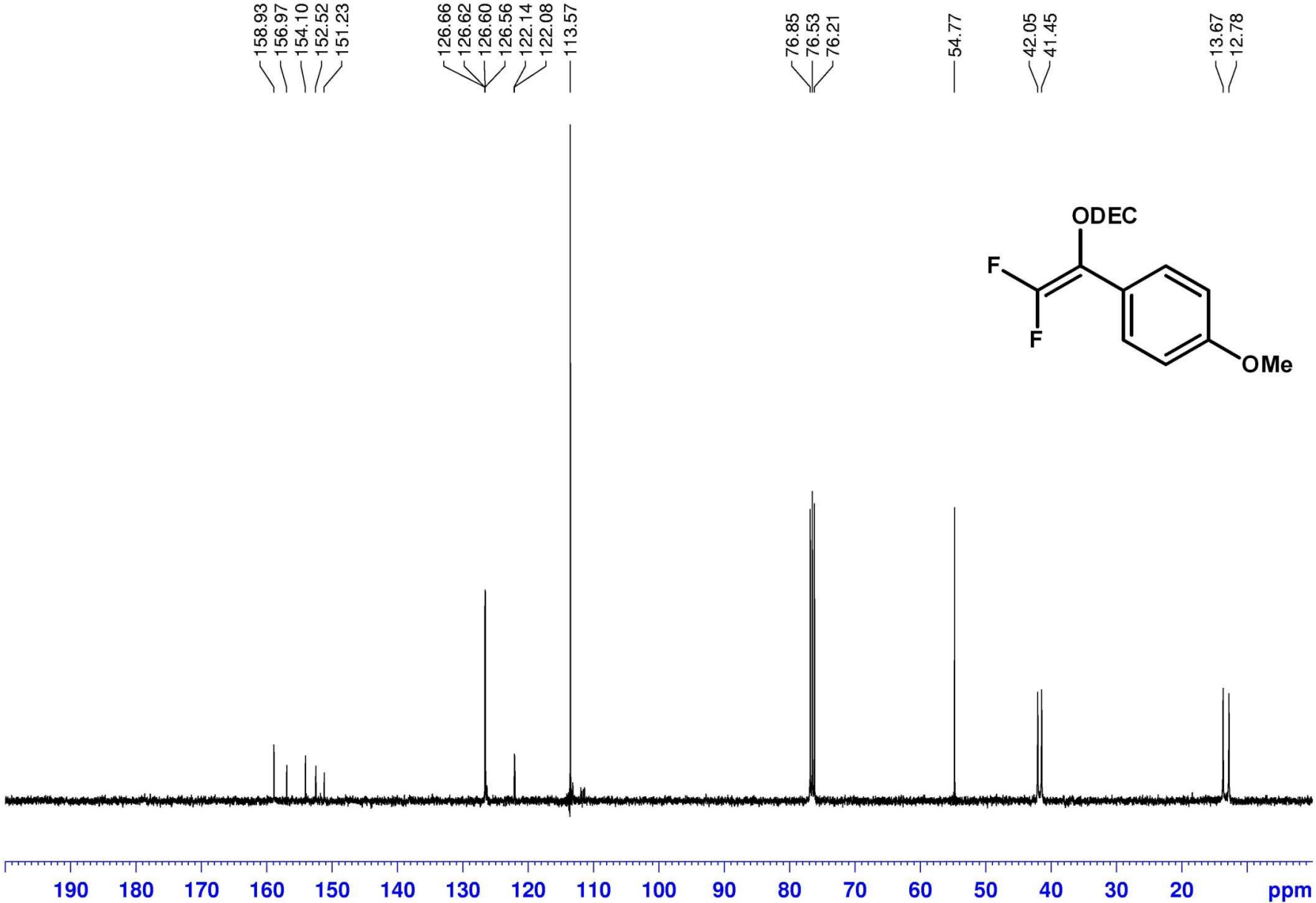


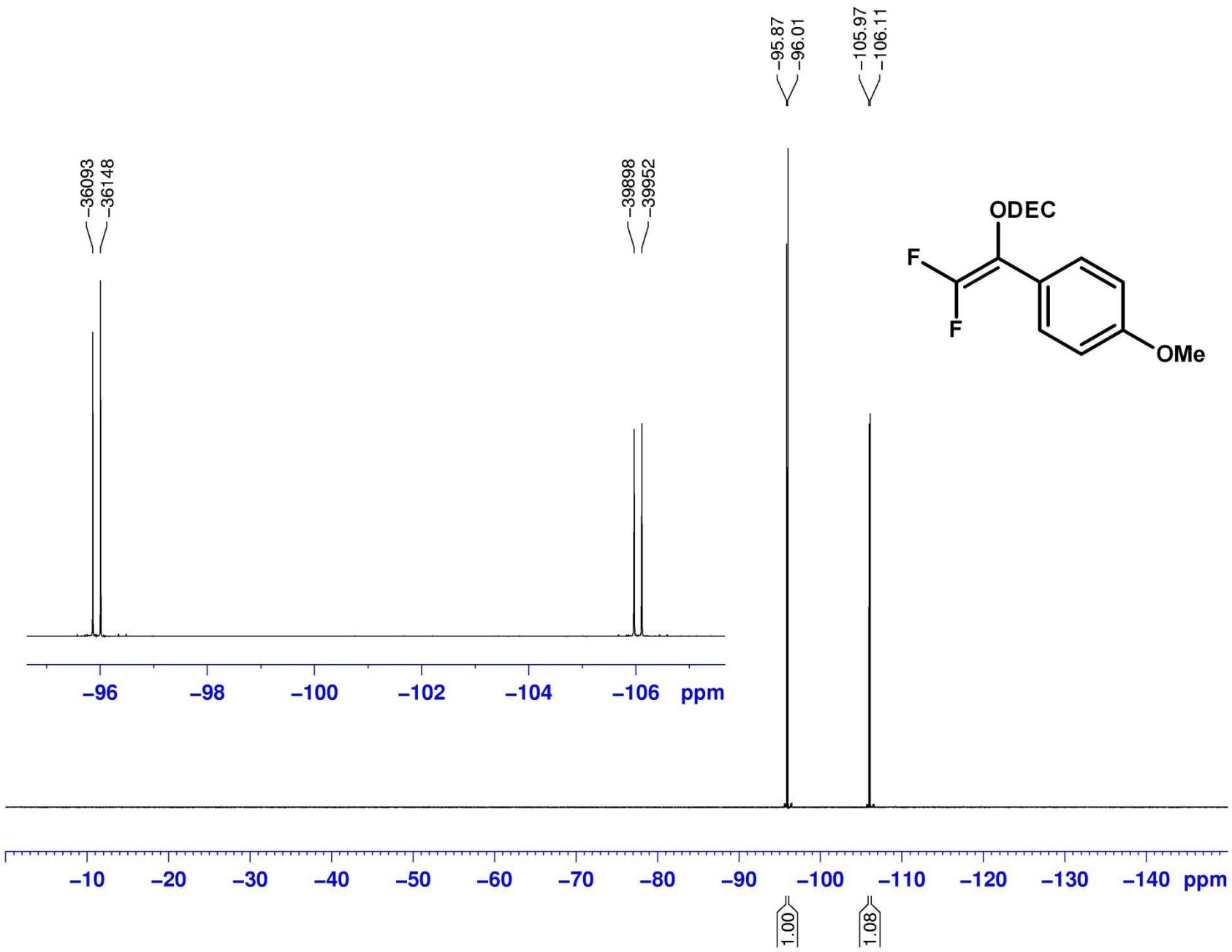




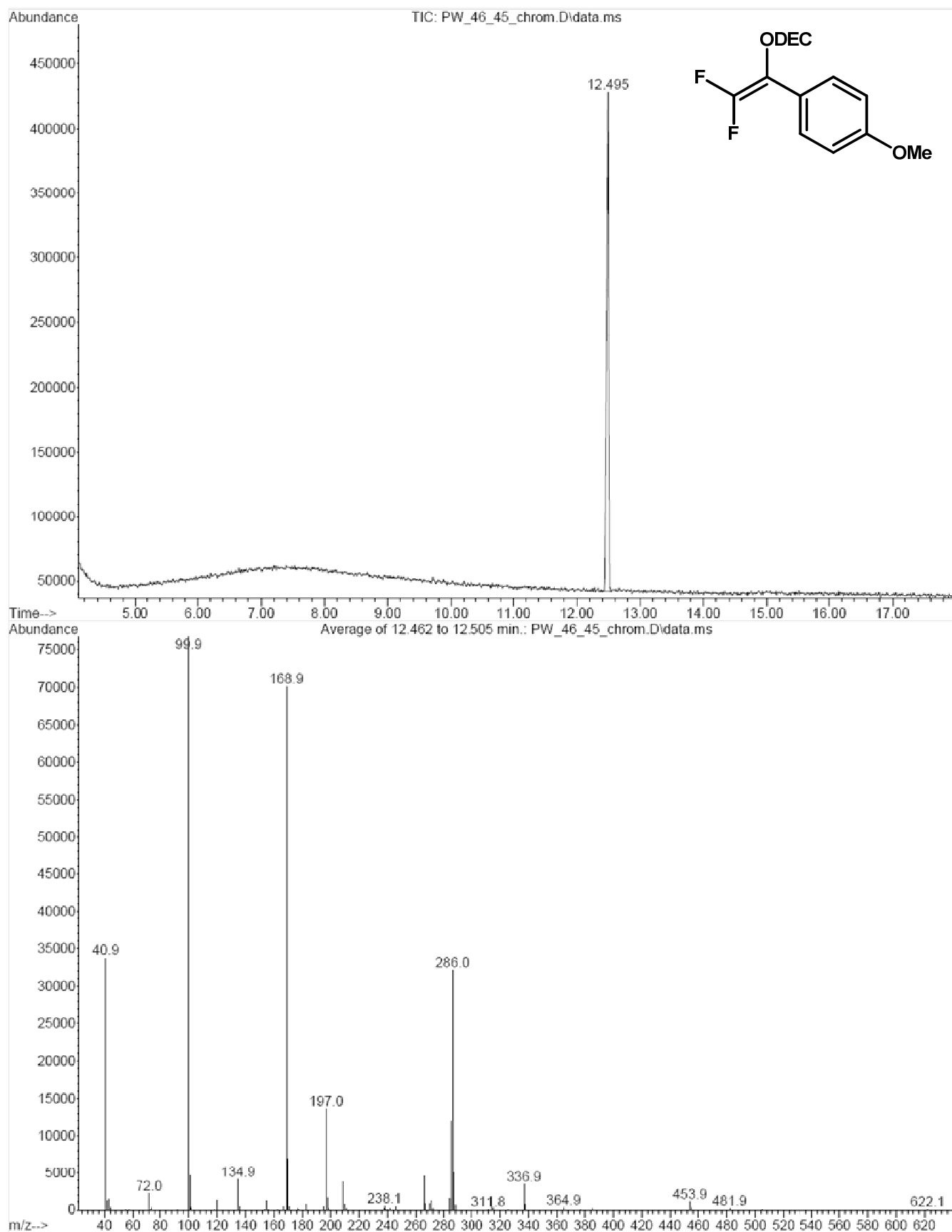


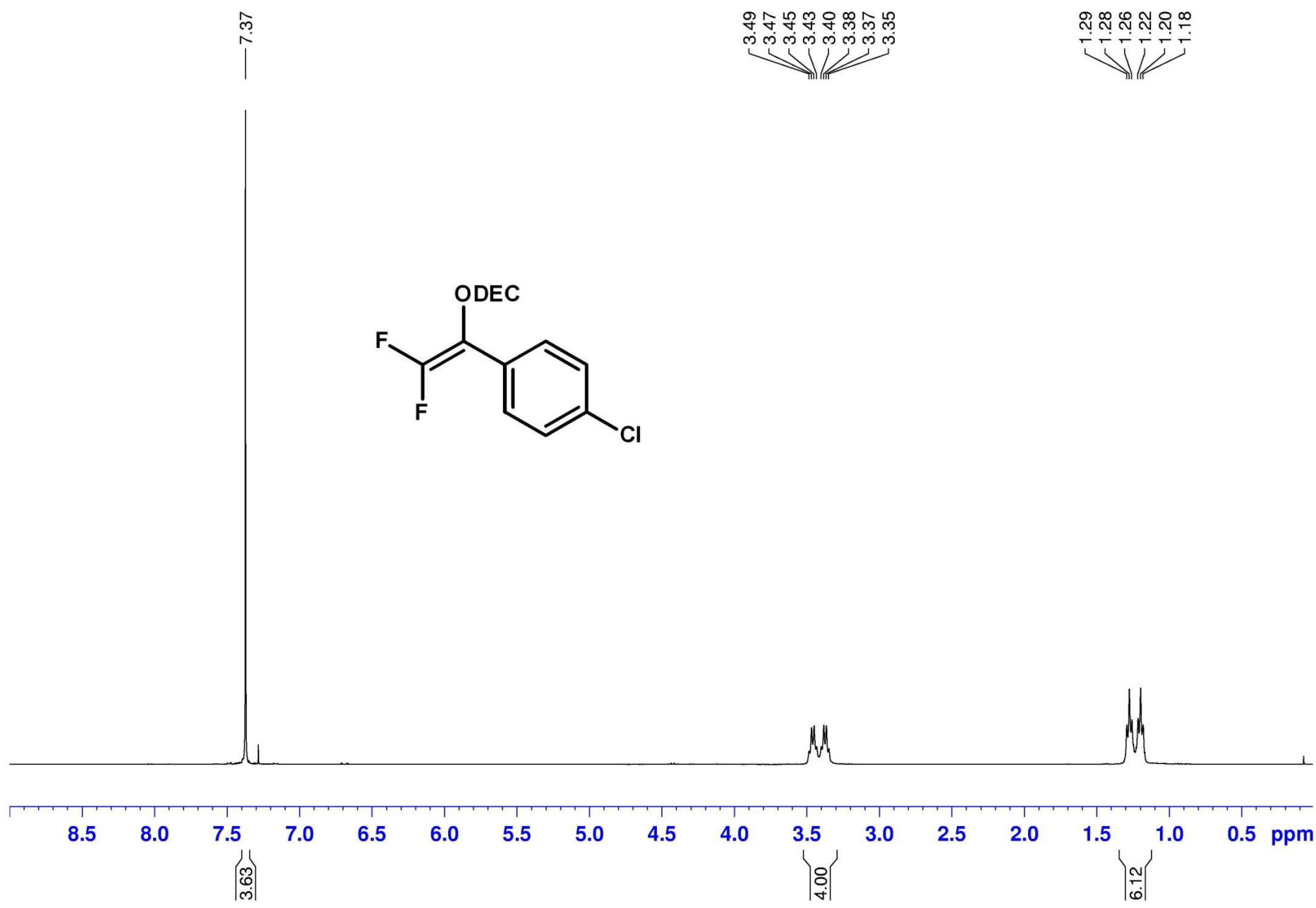


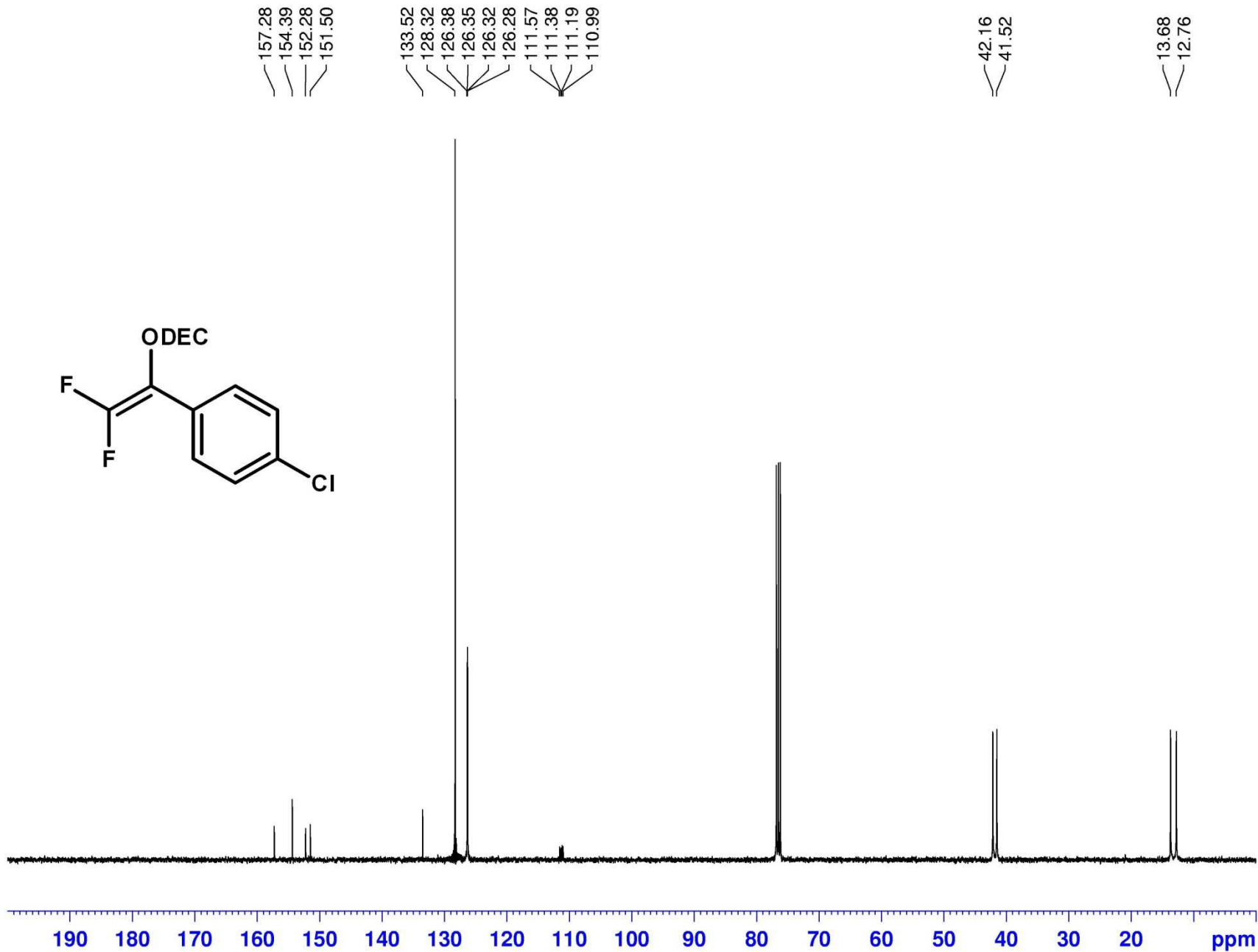


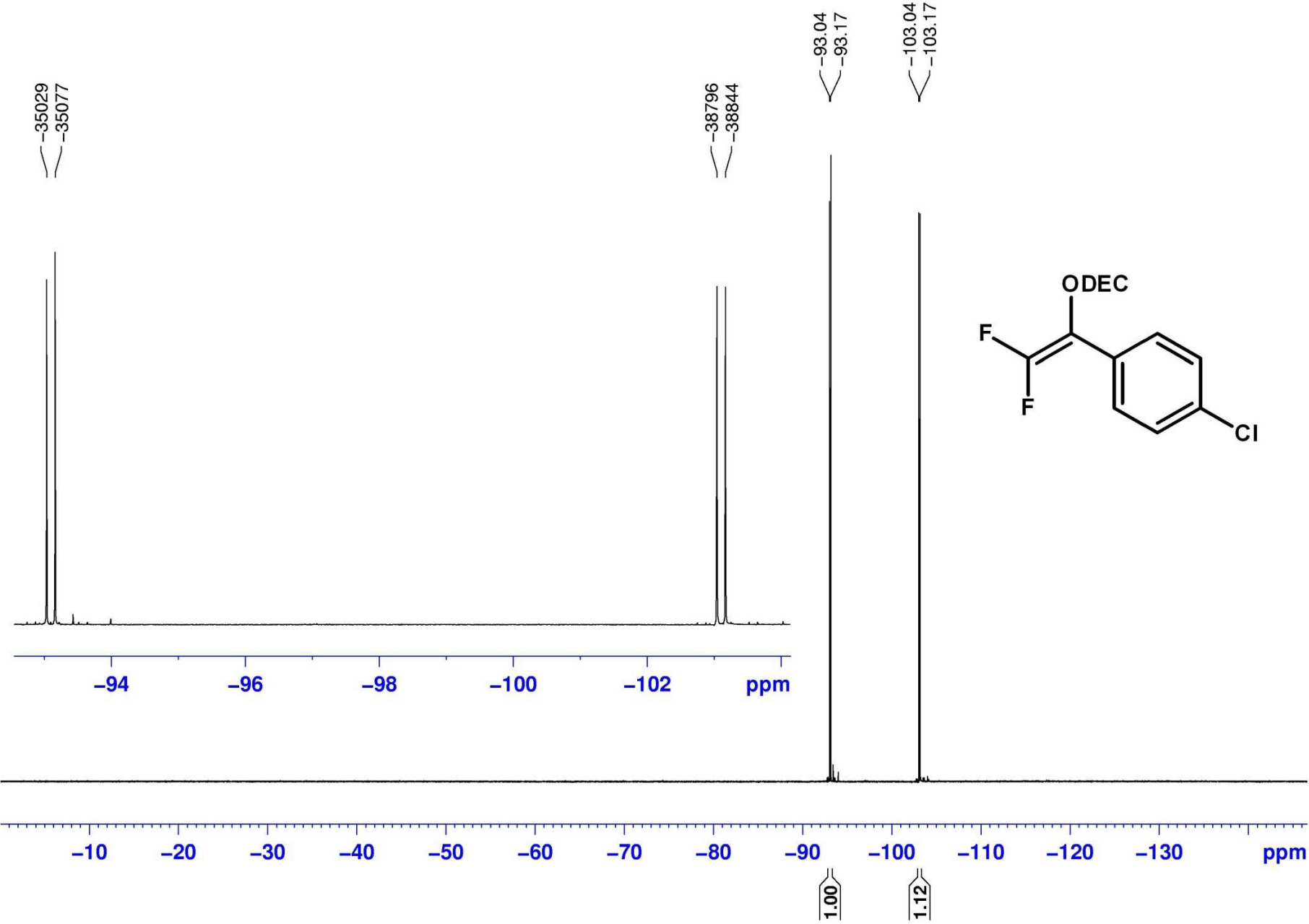


File : E:\PW\PW_46_45_chrom.D
Operator : NS
Acquired : 17 Nov 2010 16:26 using AcqMethod BASIC_PCI_GC250_70C.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 21

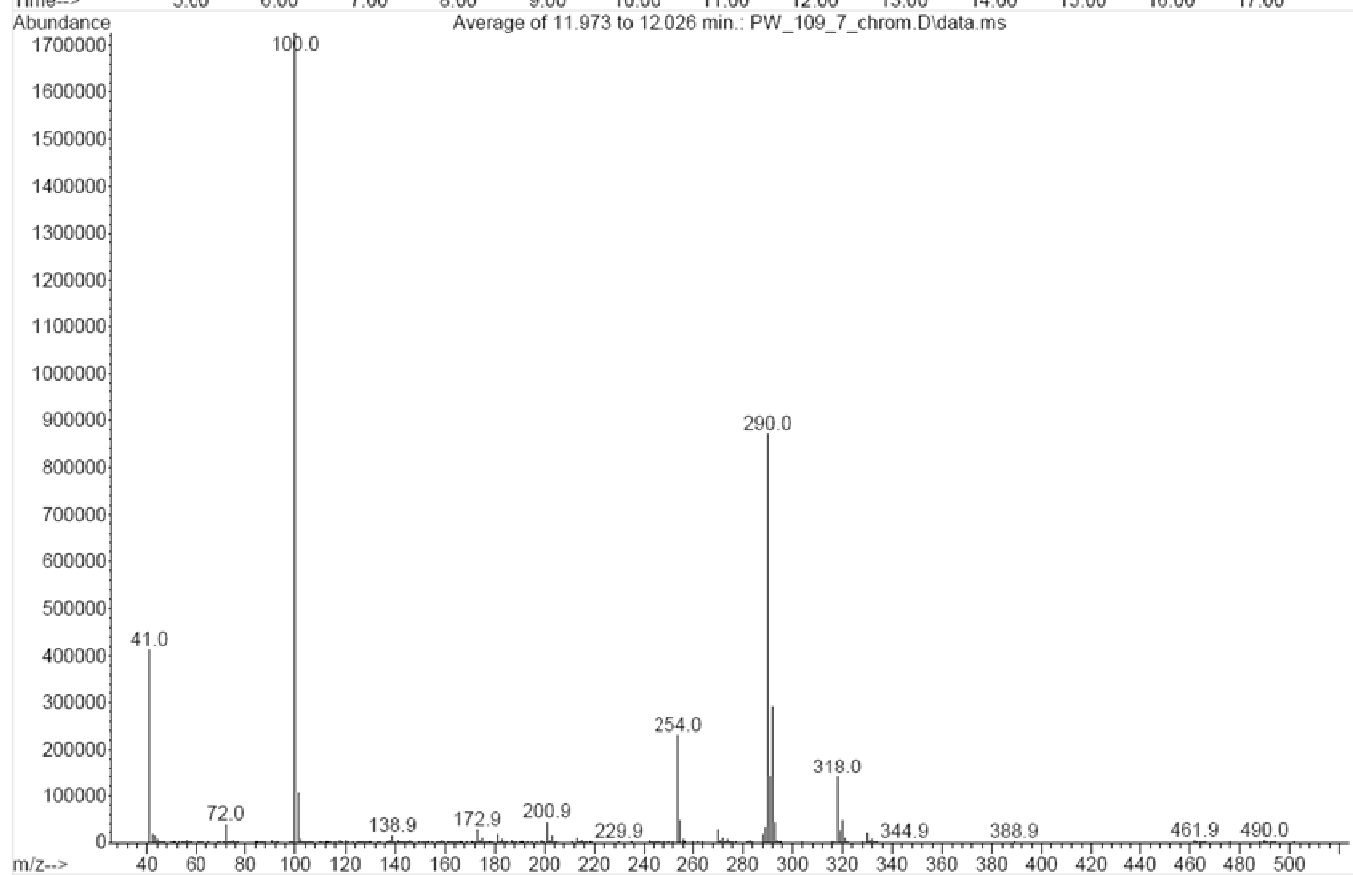
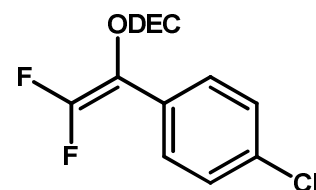
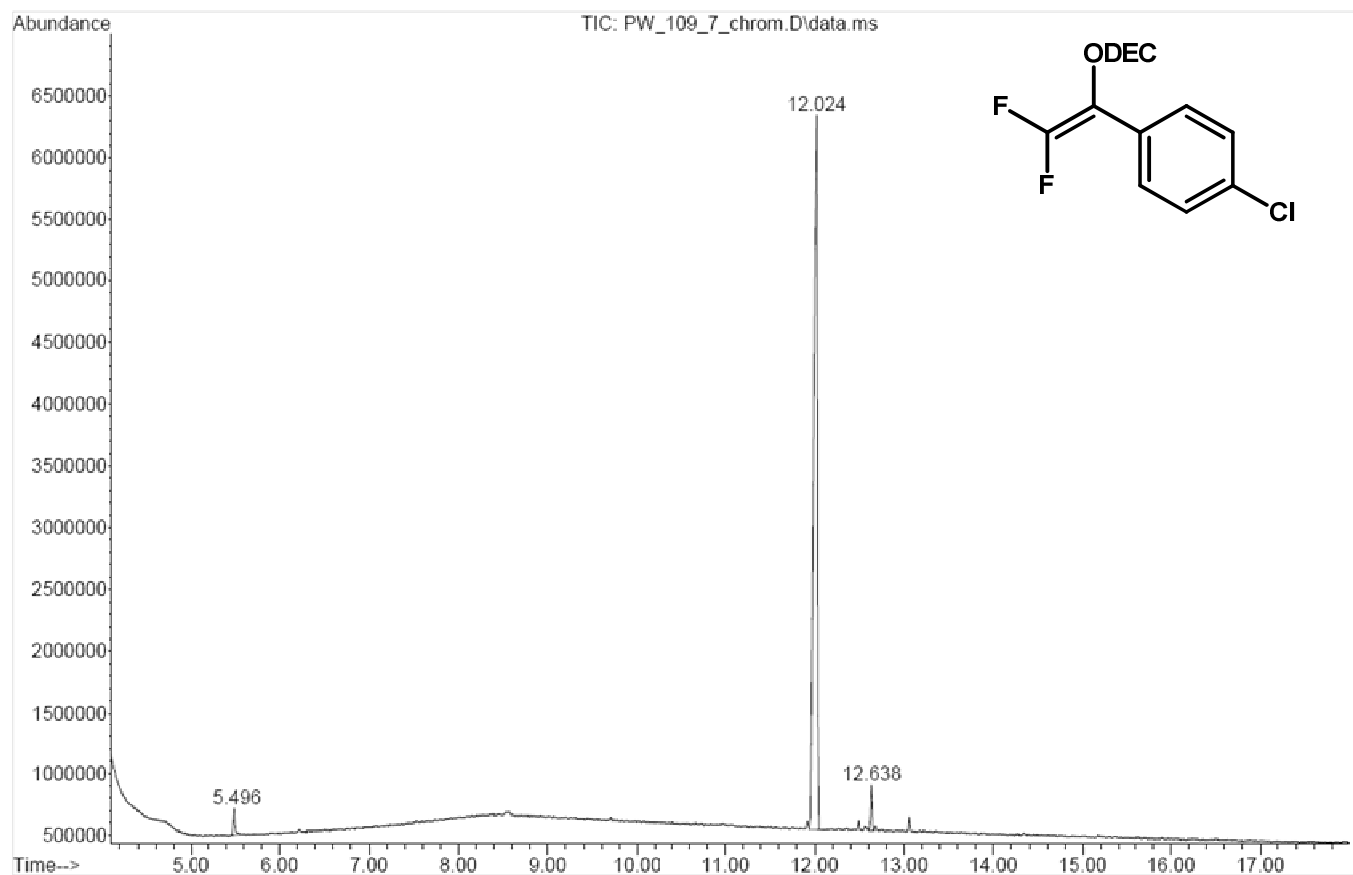


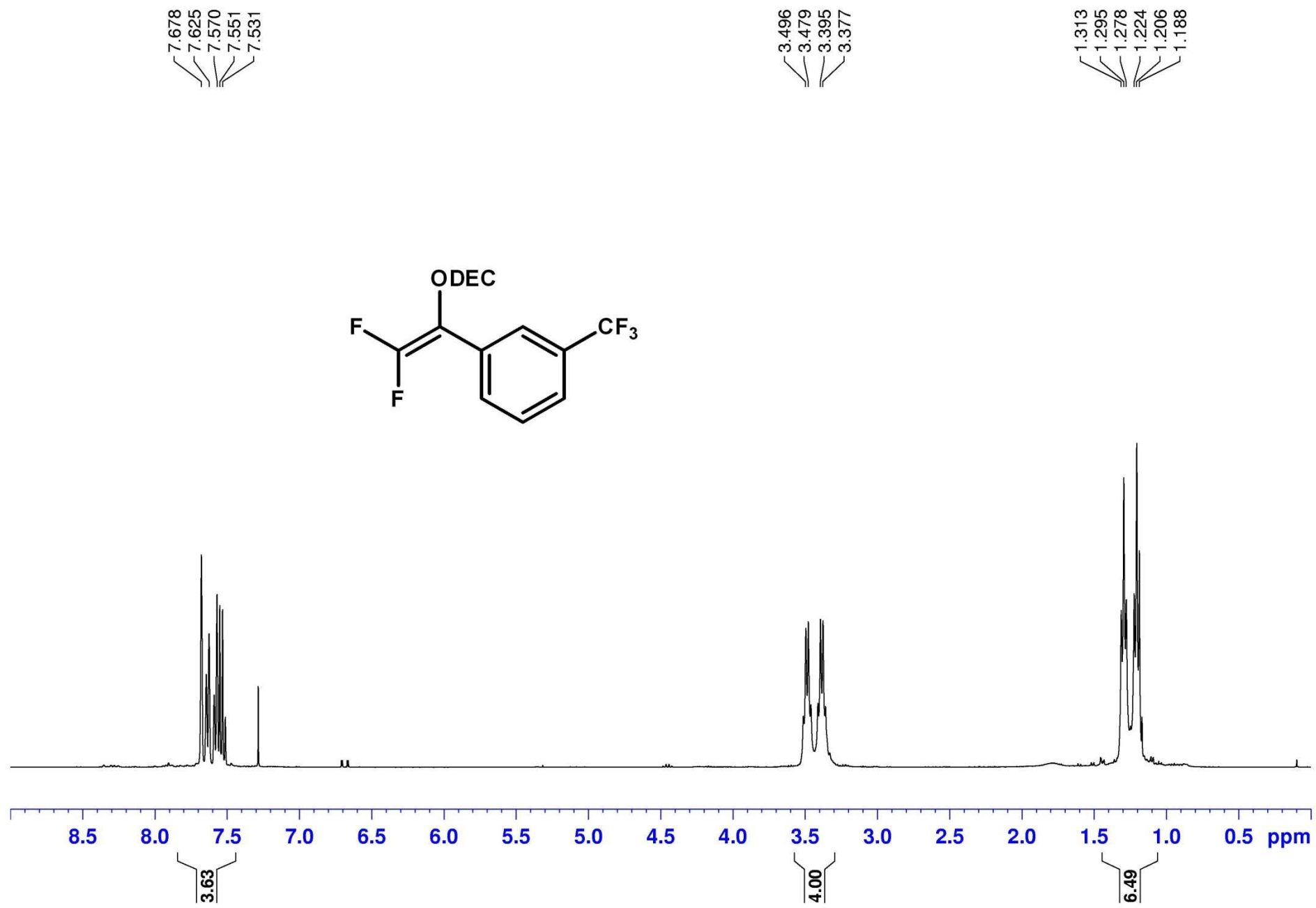


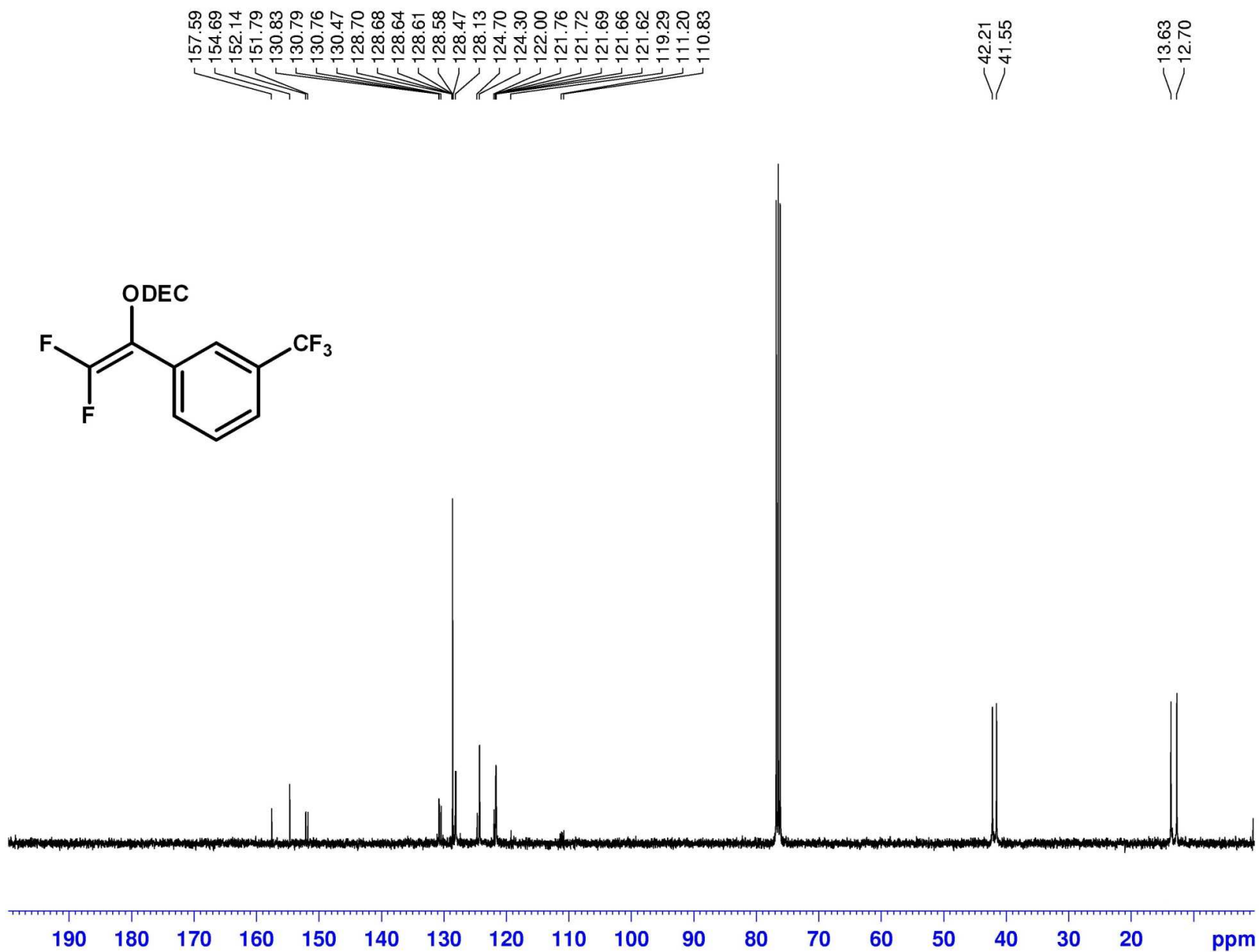


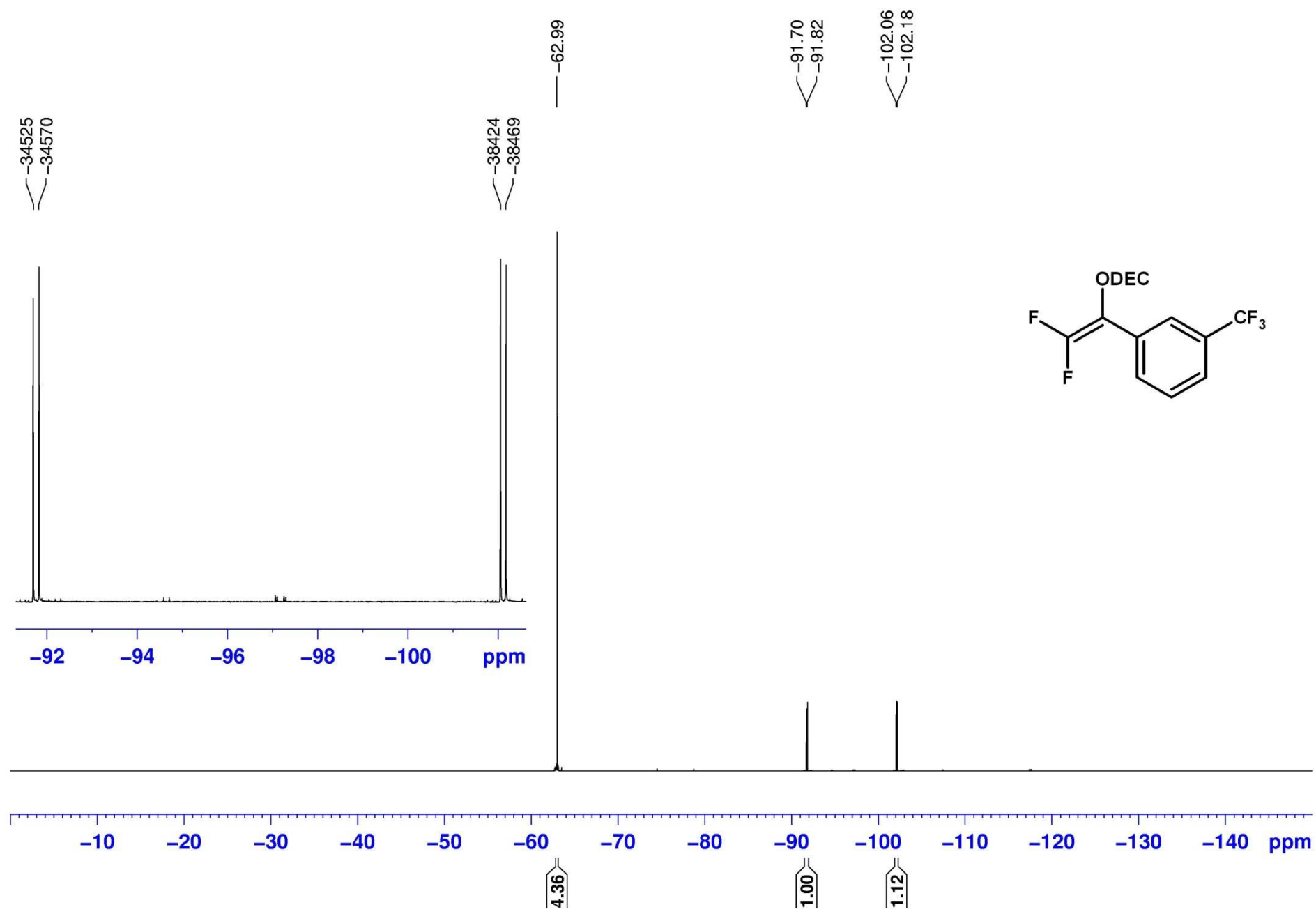


File :E:\FW\PW_109_7_chrom.D
Operator : SK
Acquired : 23 Nov 2010 18:59 using AcqMethod BASIC_PCI_GC250_70C.M
Instrument : GCMS AG
Sample Name: Sample 1
Misc Info :
Vial Number: 4

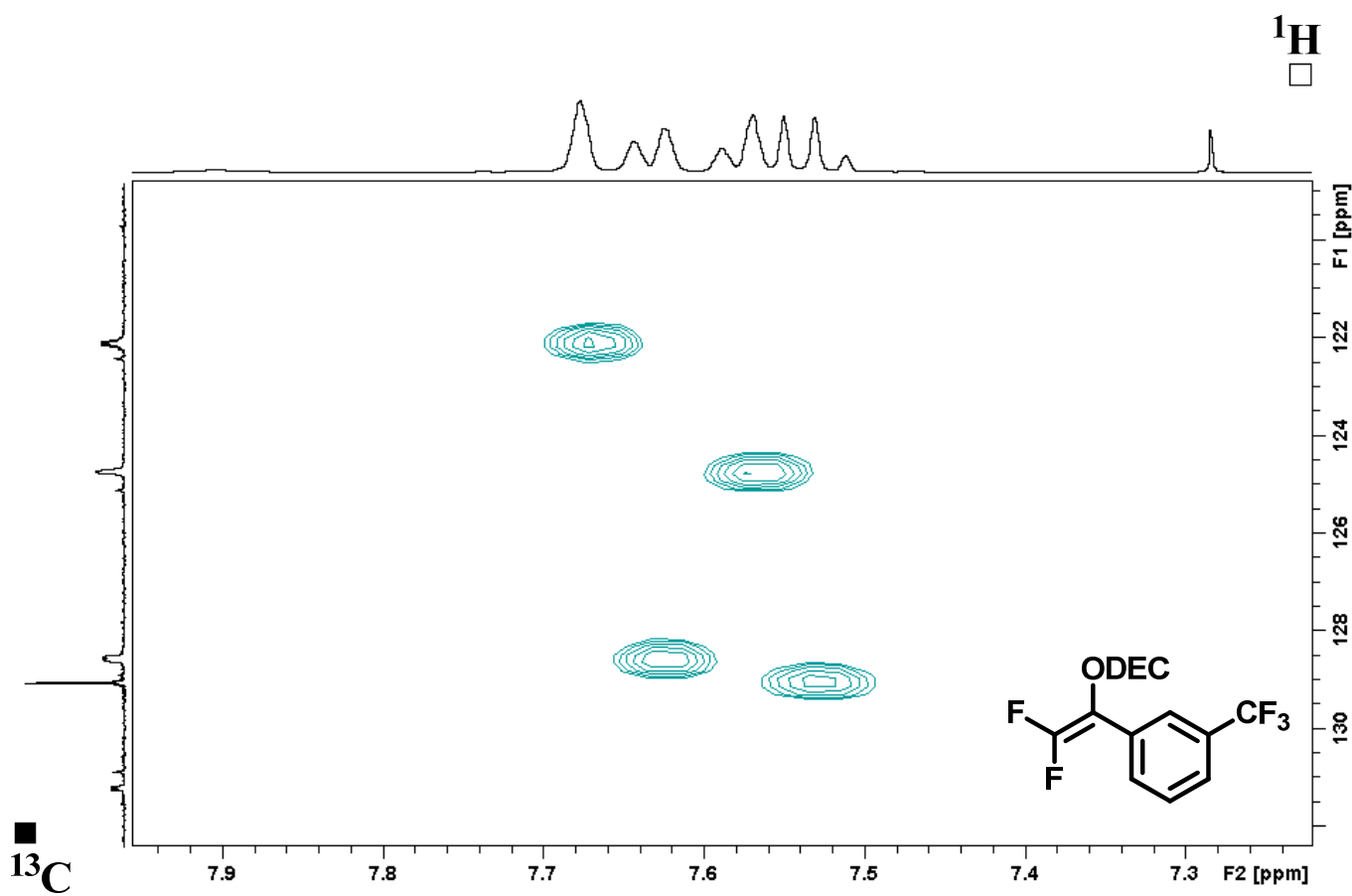
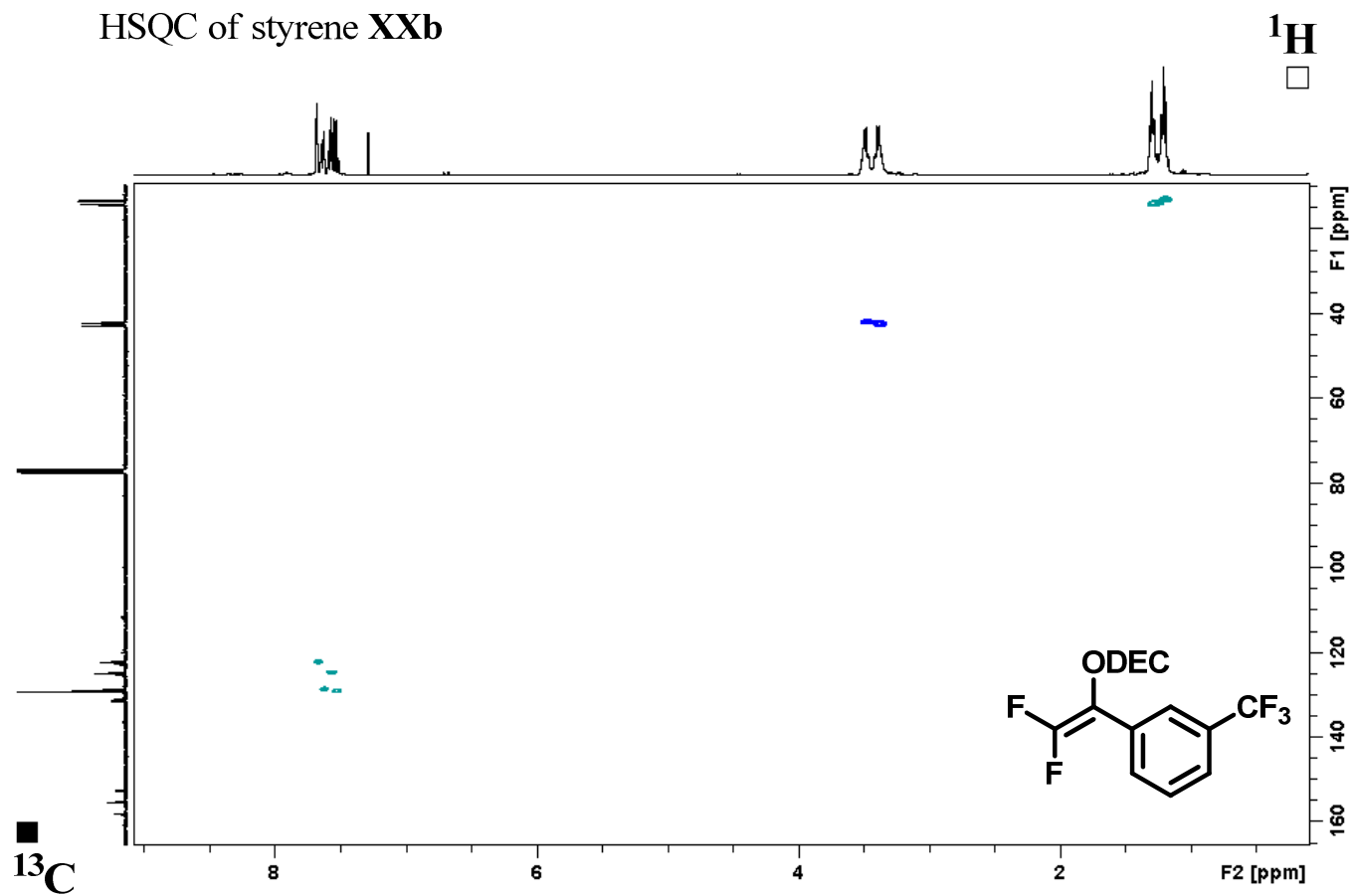




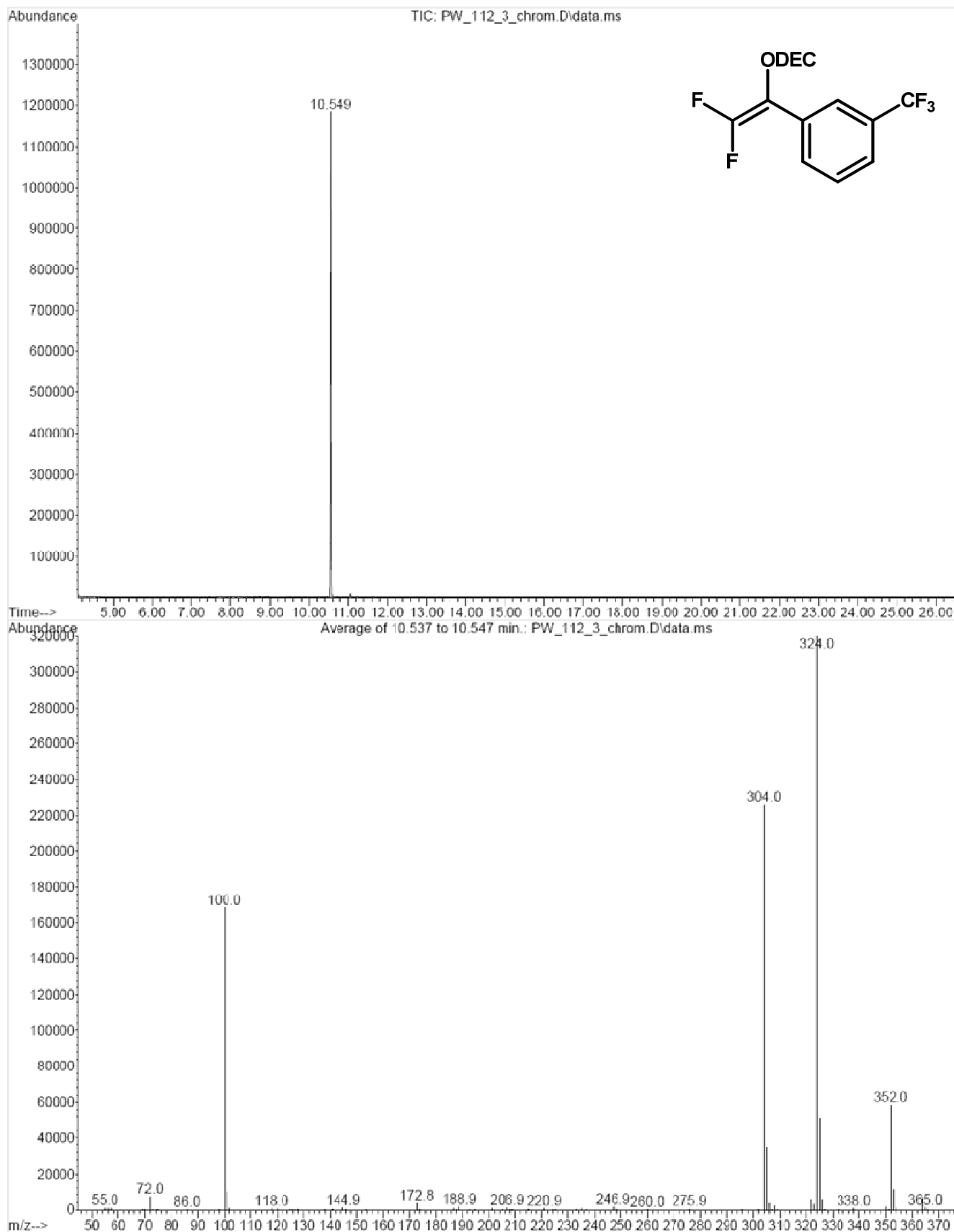


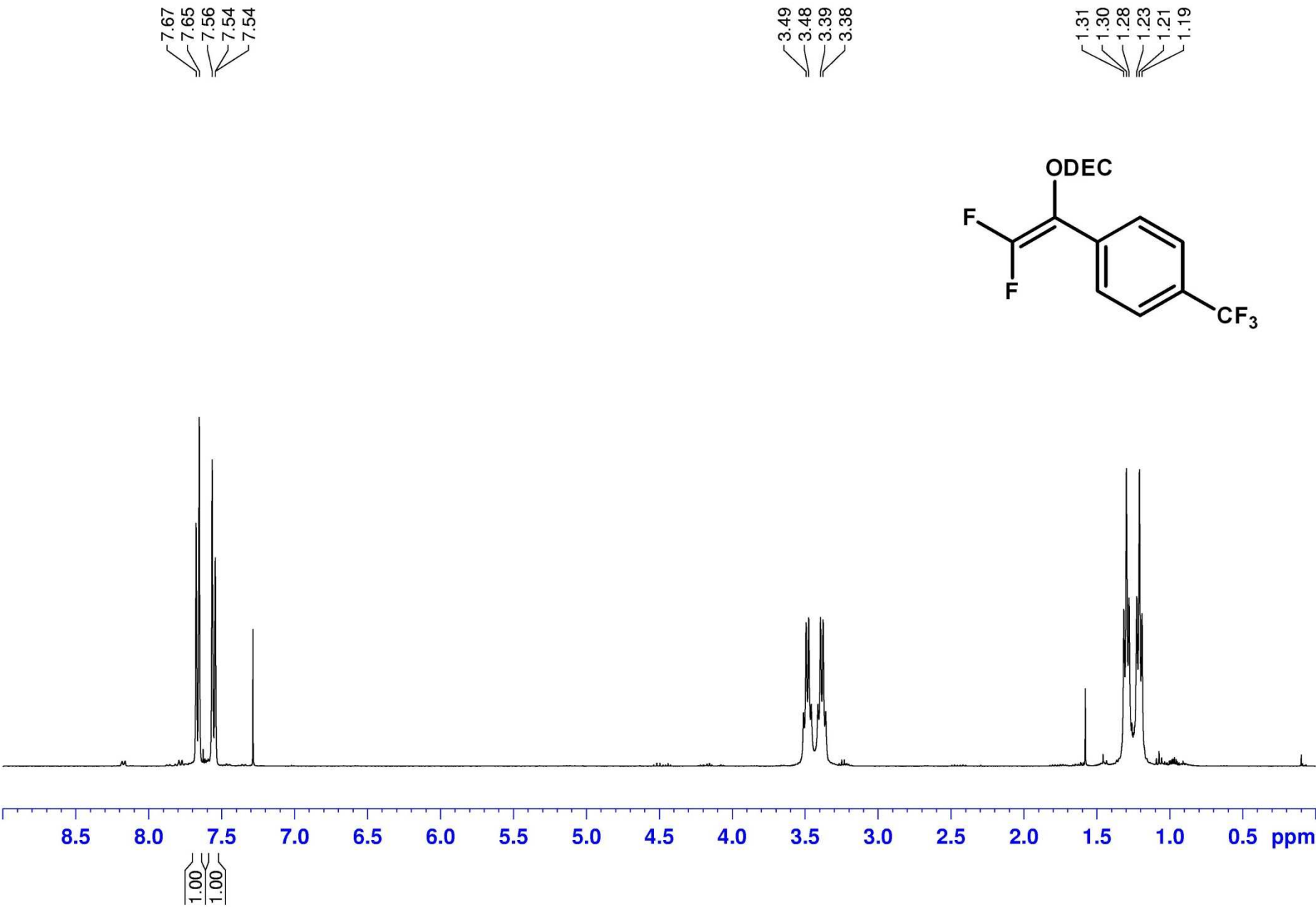


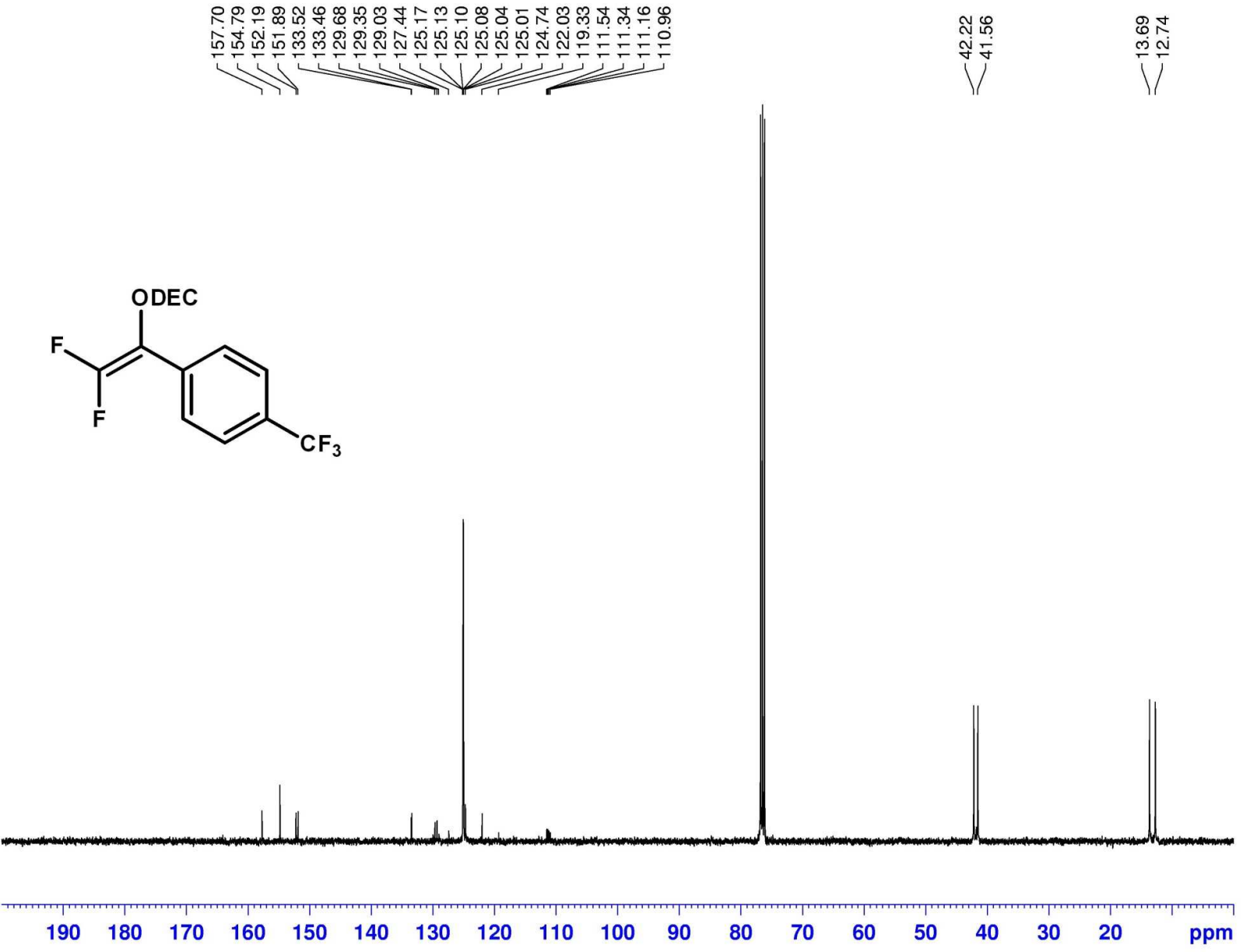
HSQC of styrene **XXb**

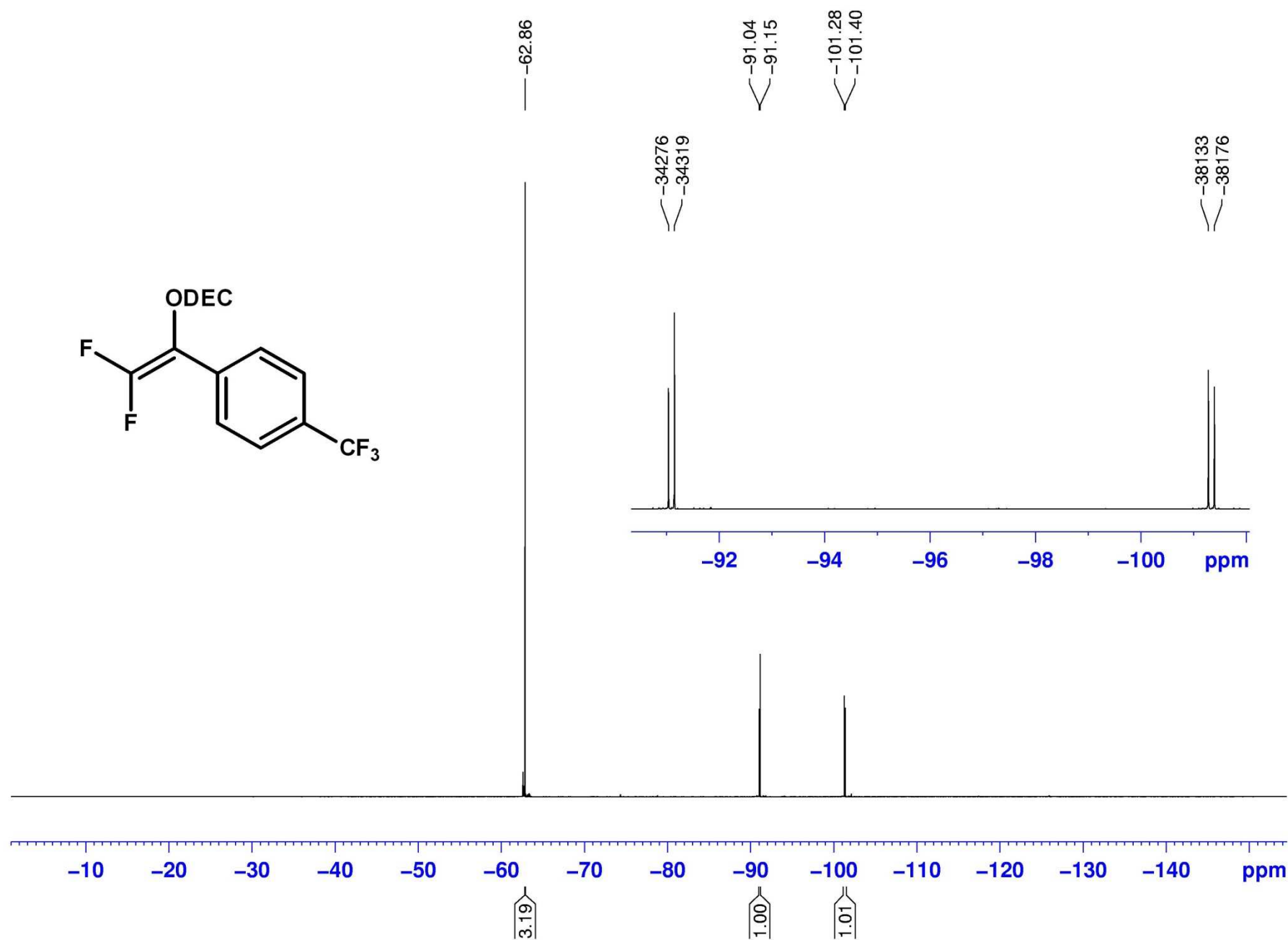


File : F:\PW\PW_112_3_chrom.D
Operator : NS
Acquired : 20 Jan 2011 11:29 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 3

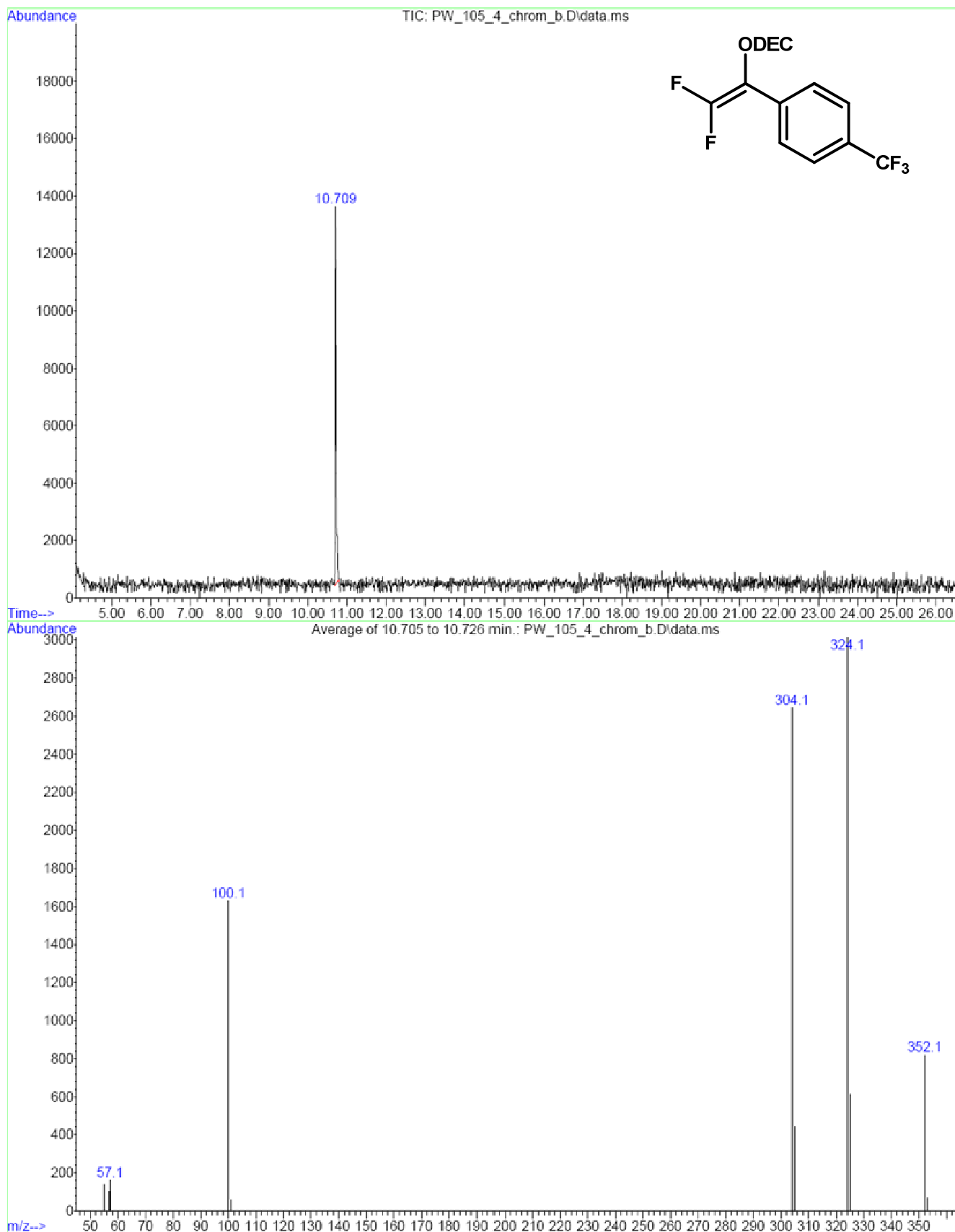


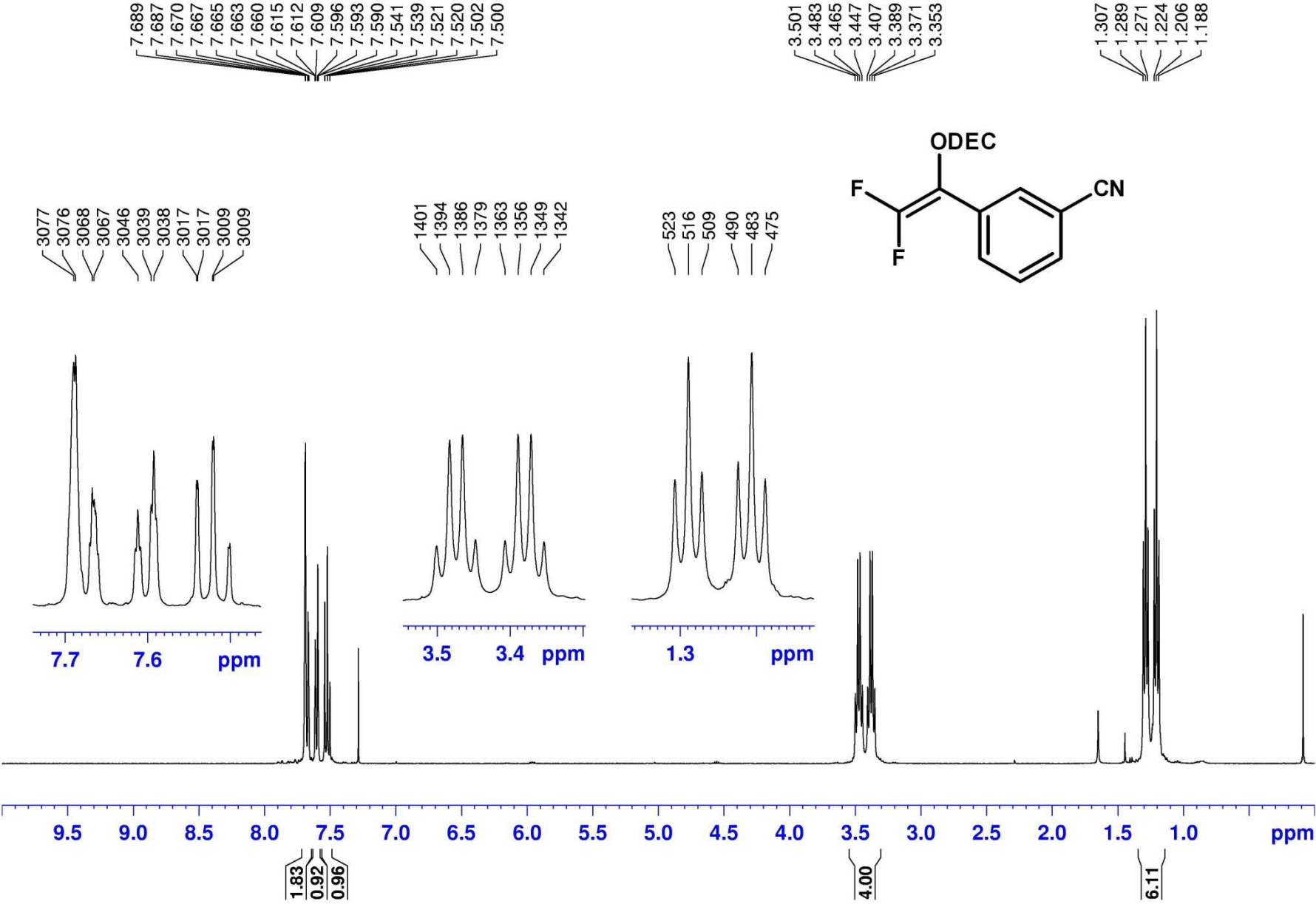


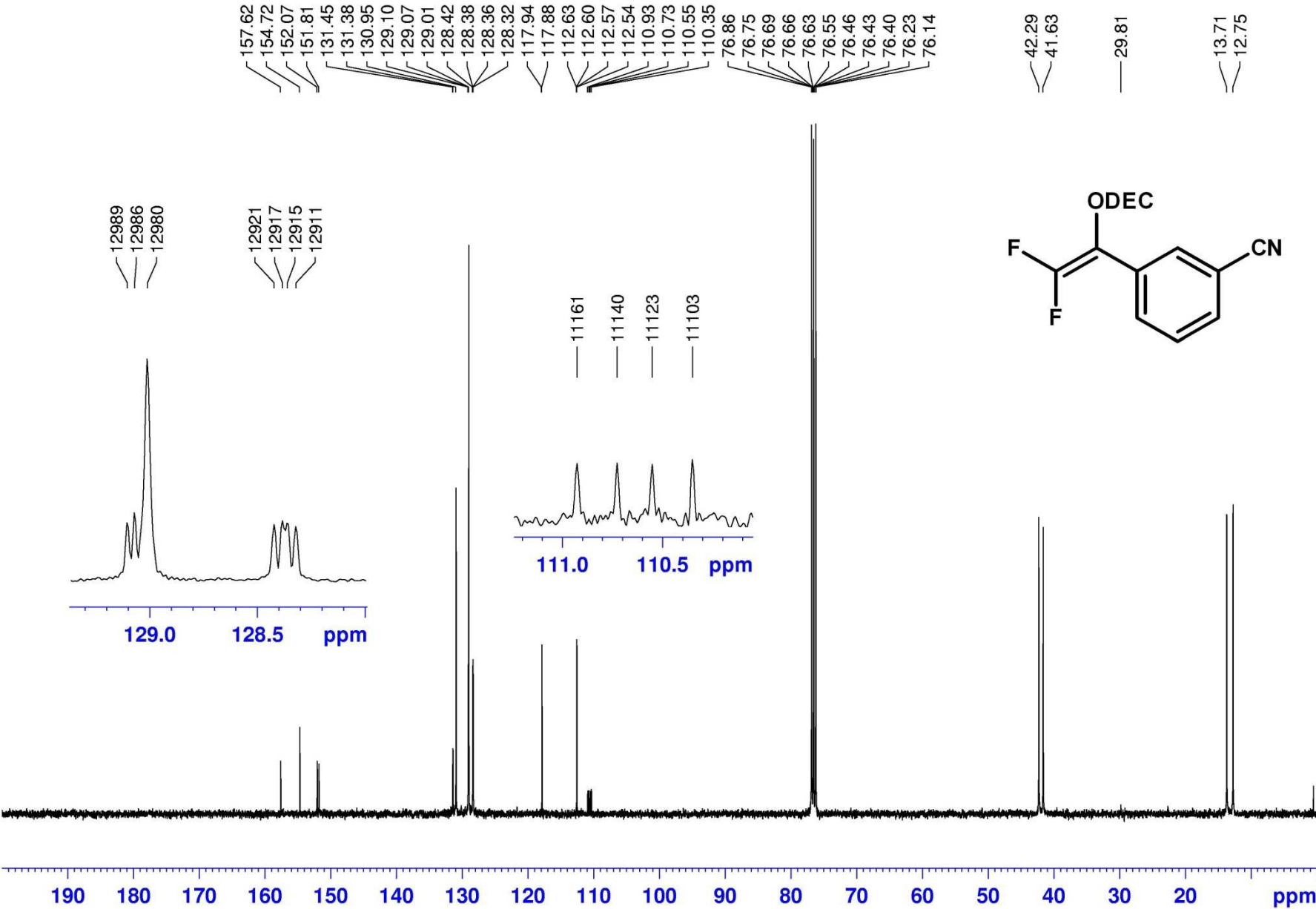


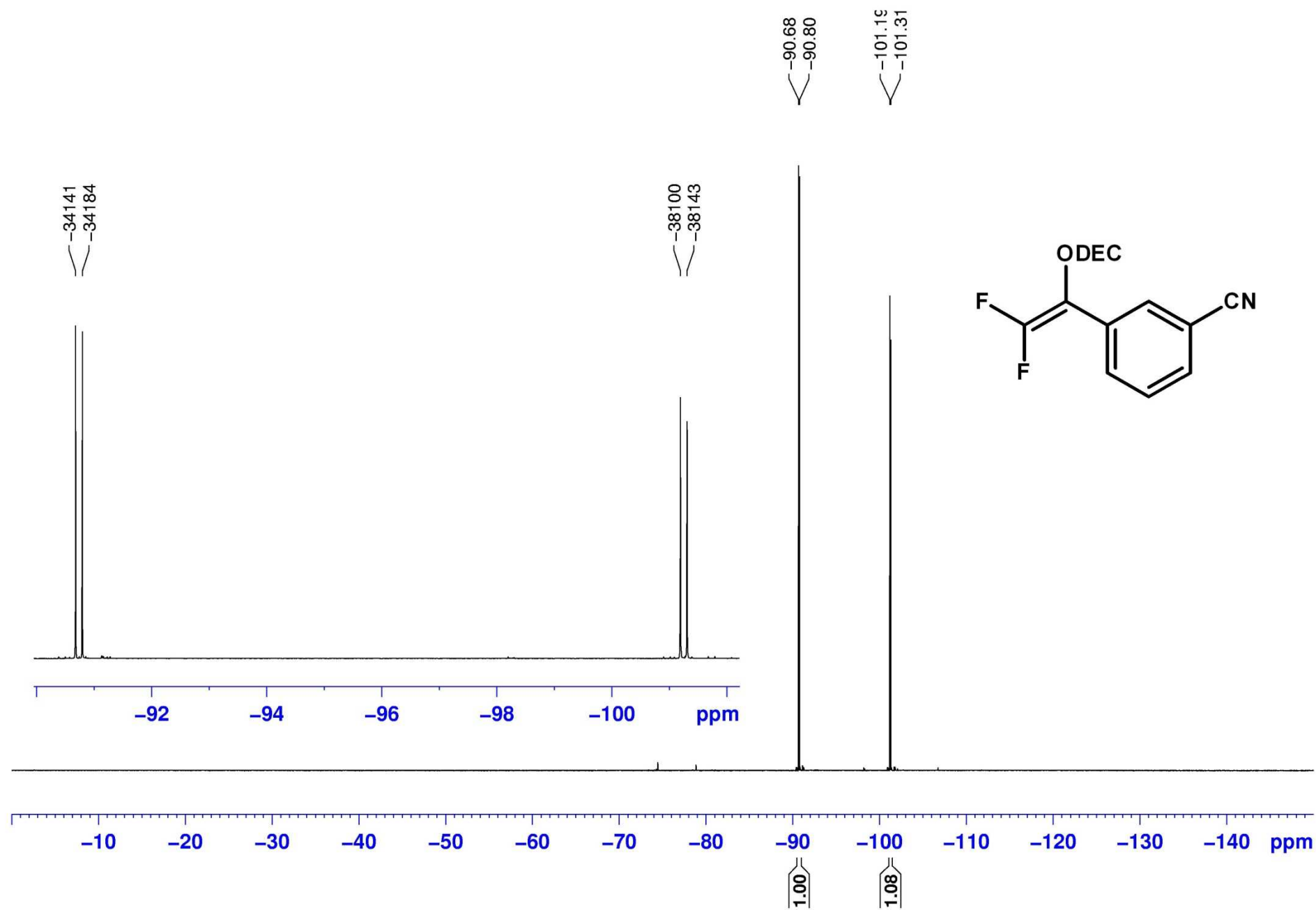


File : F:\PW\PW_105_4_chrom_b.D
Operator : PW
Acquired : 23 Feb 2011 14:15 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS_AG
Sample Name:
Misc Info :
Vial Number: 1

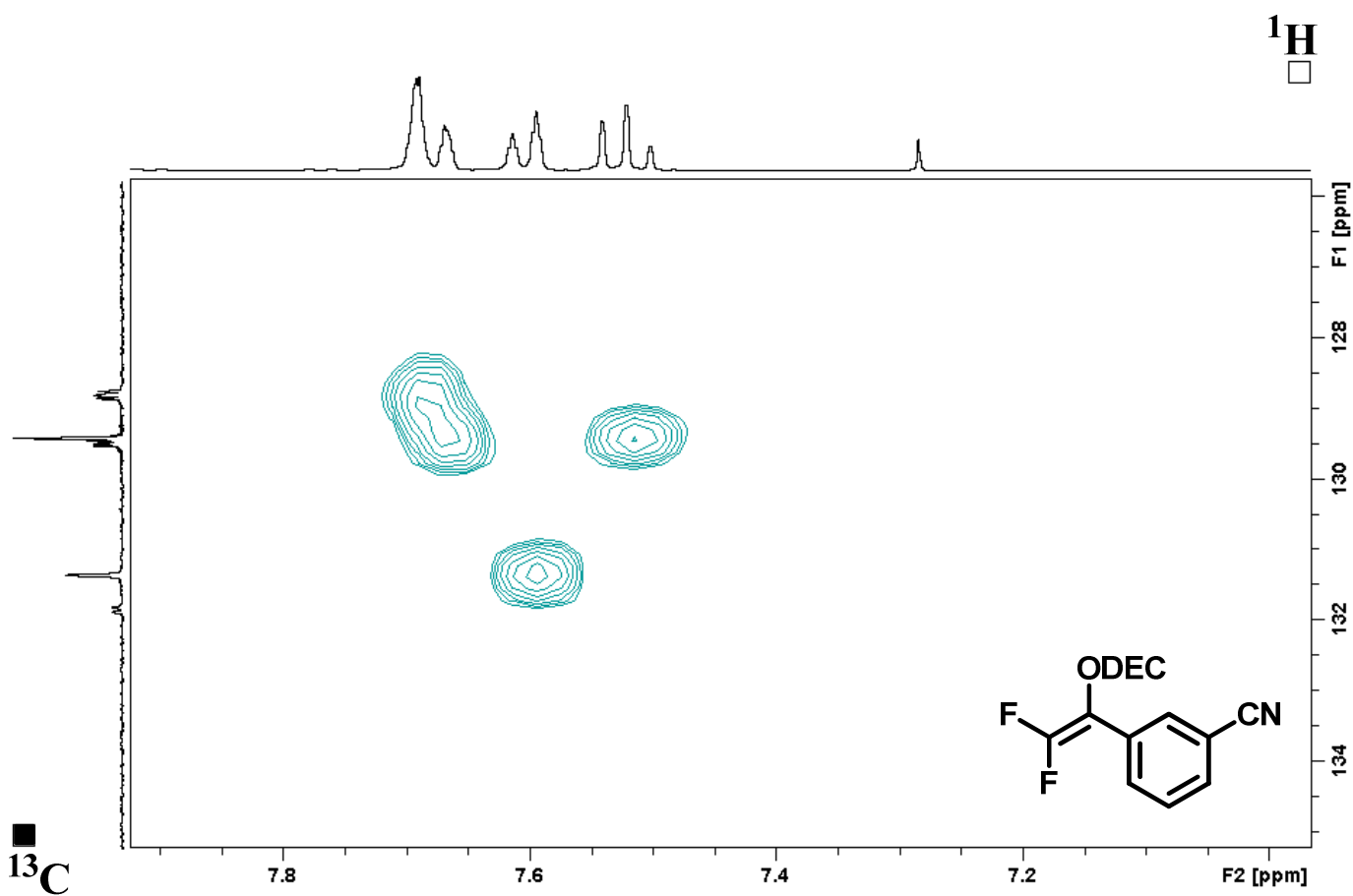
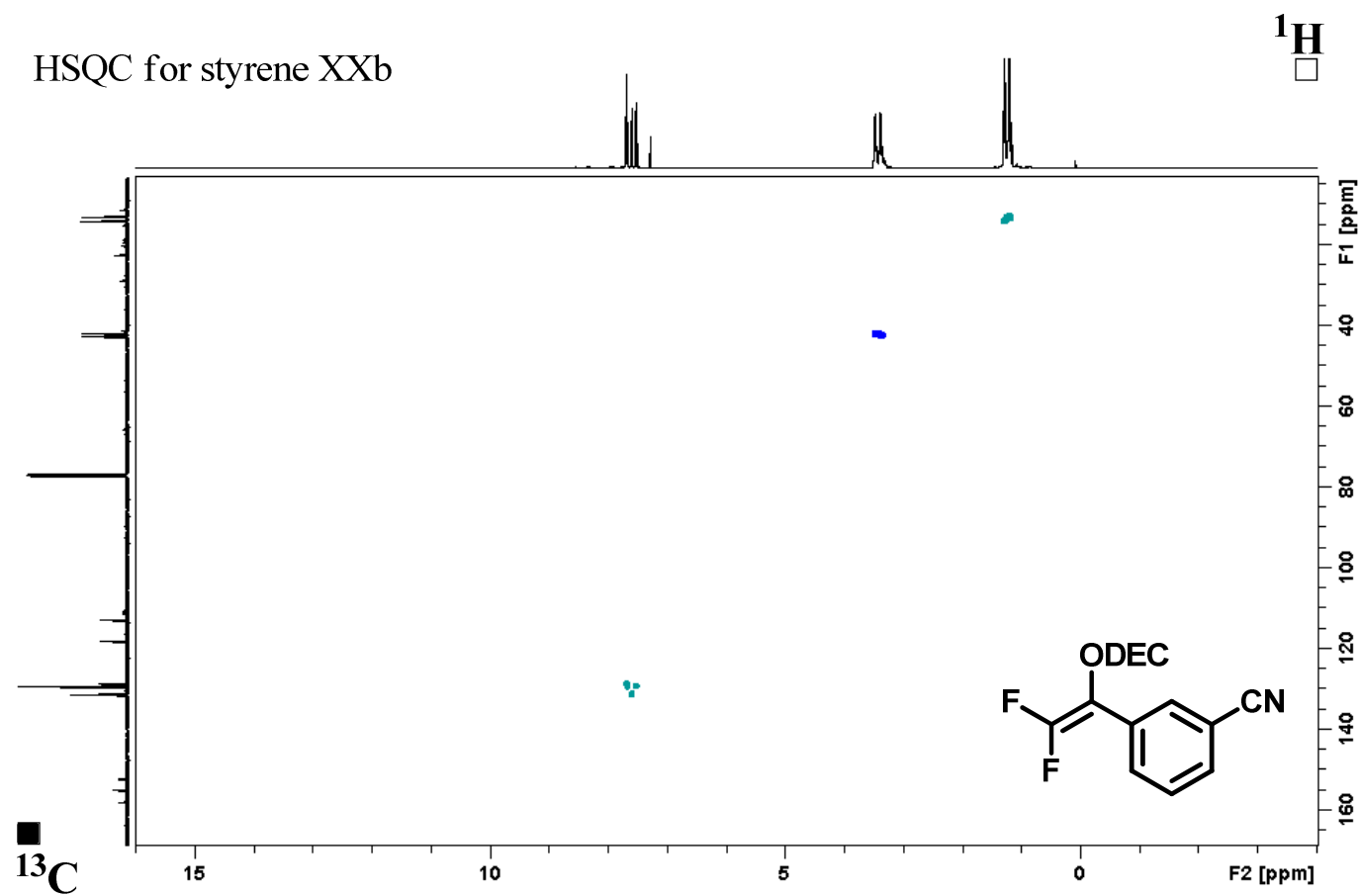




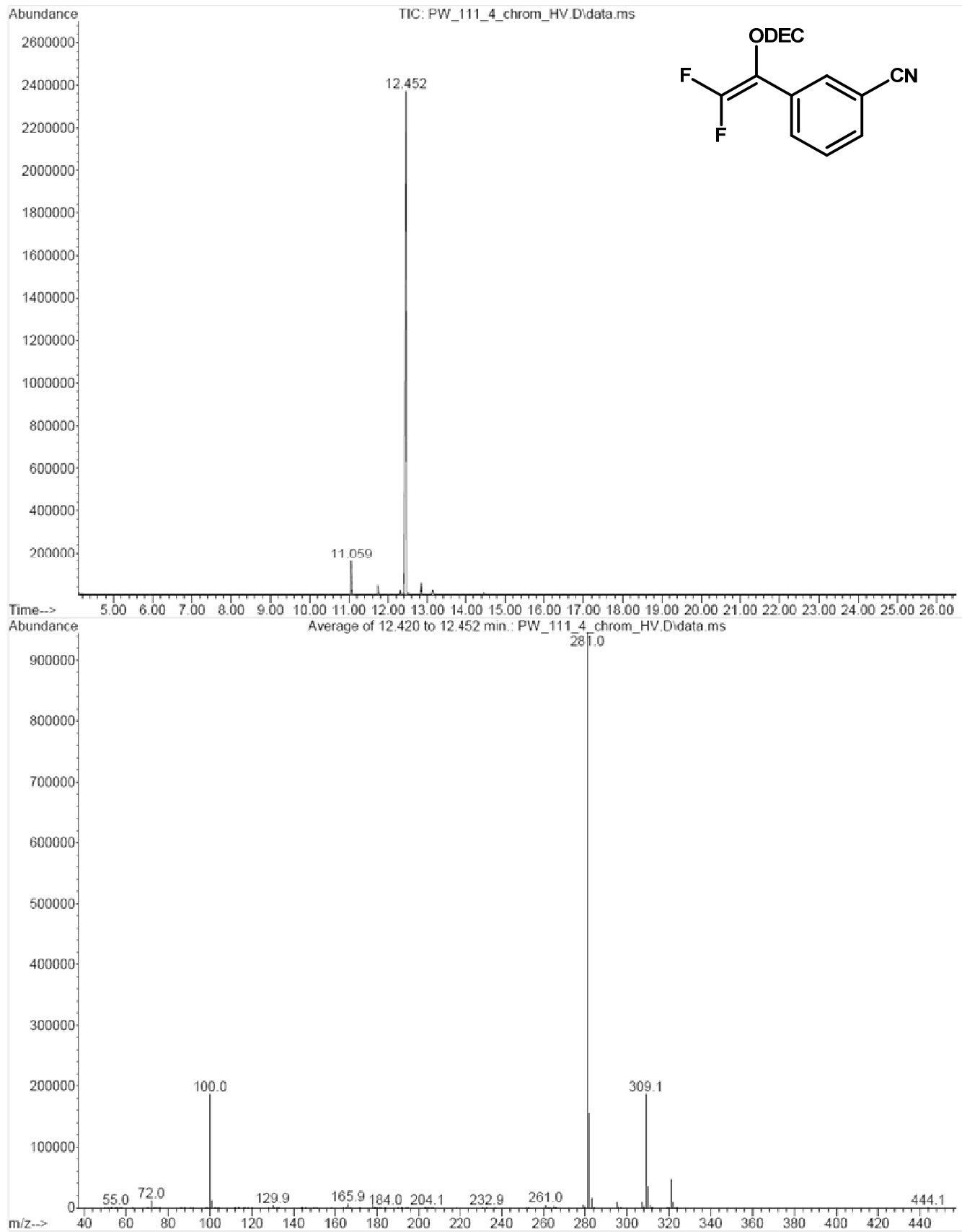


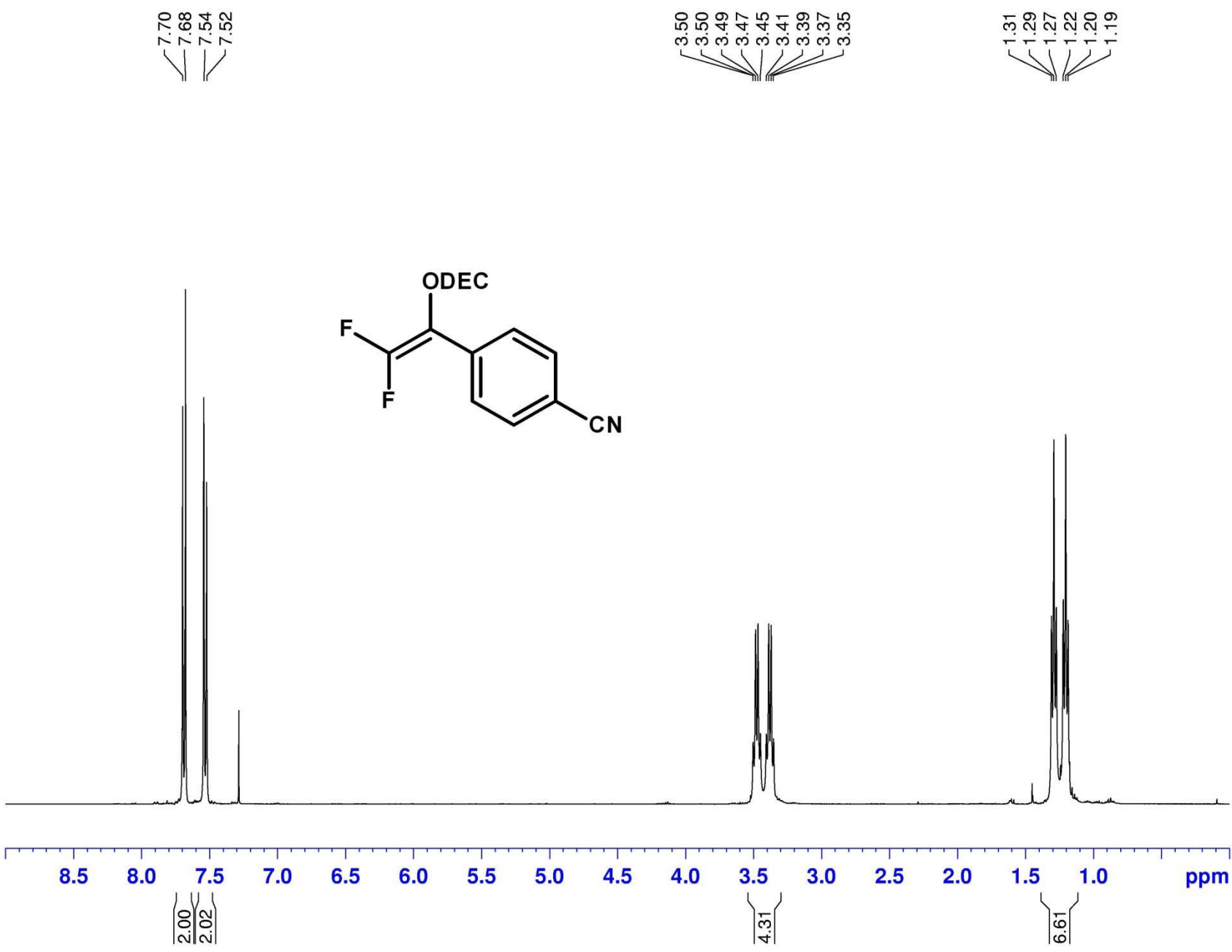


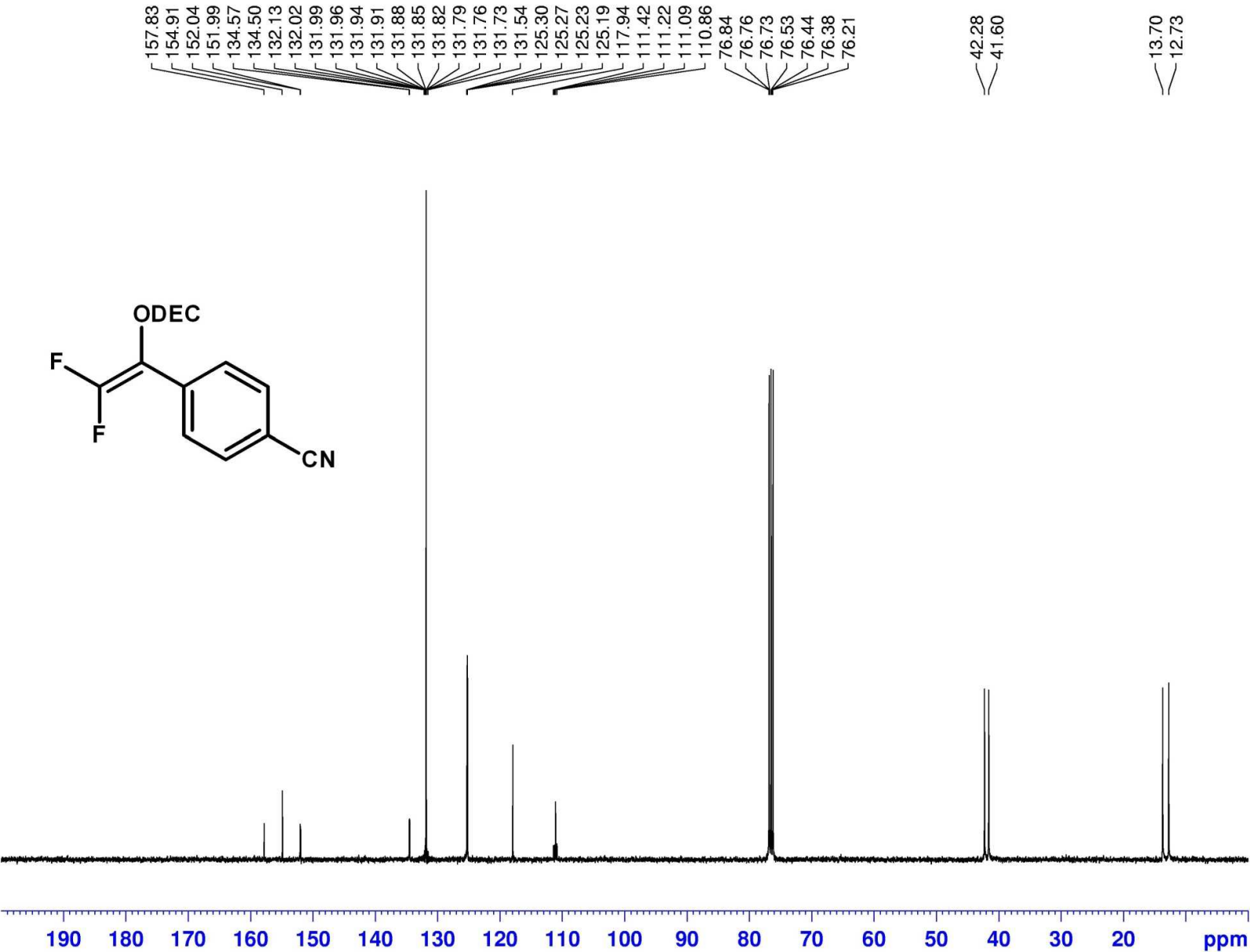
HSQC for styrene XXb

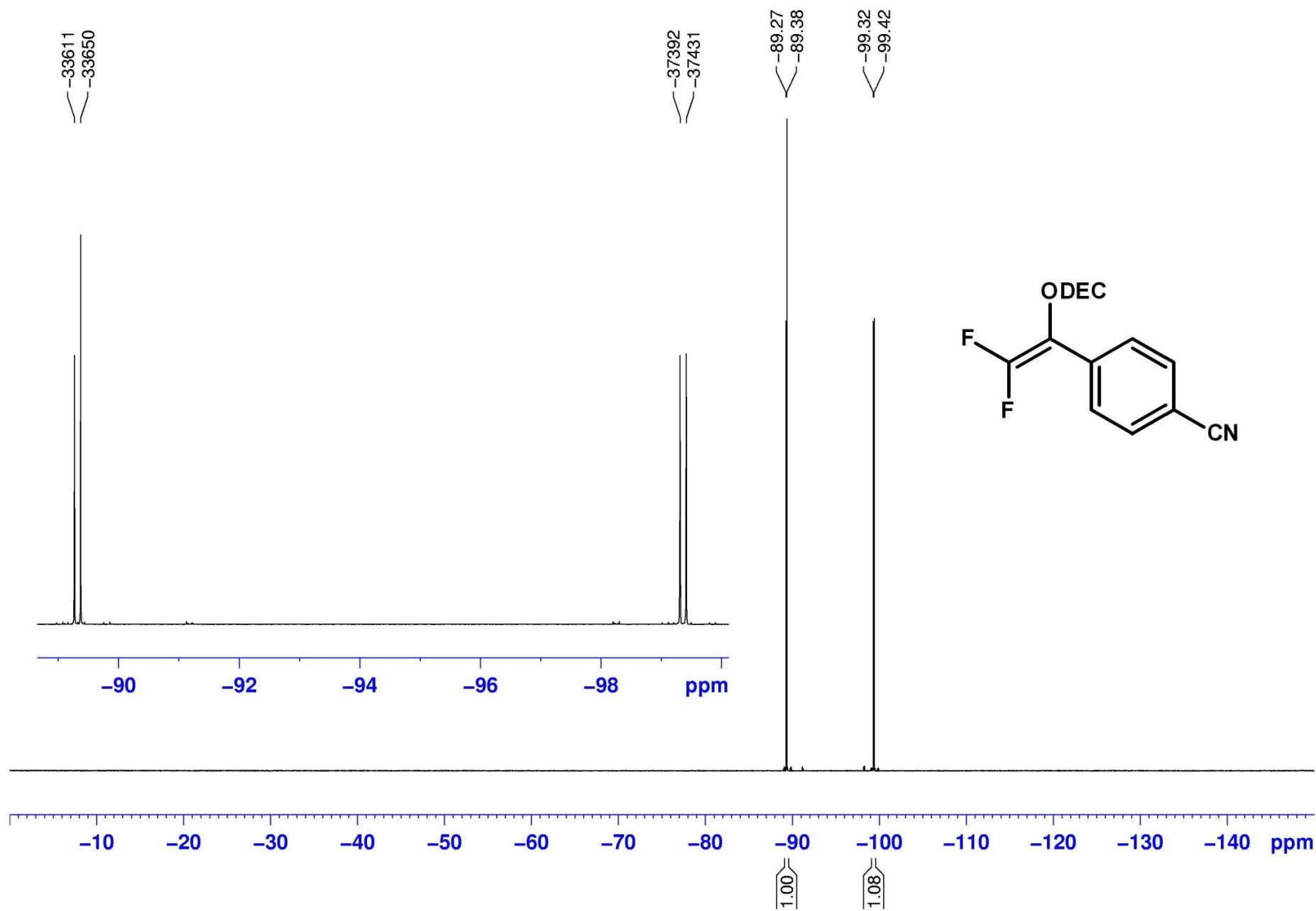


File :F:\PW\PW_111_4_chrom_HV.D
Operator : NS
Acquired : 20 Jan 2011 12:00 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 4

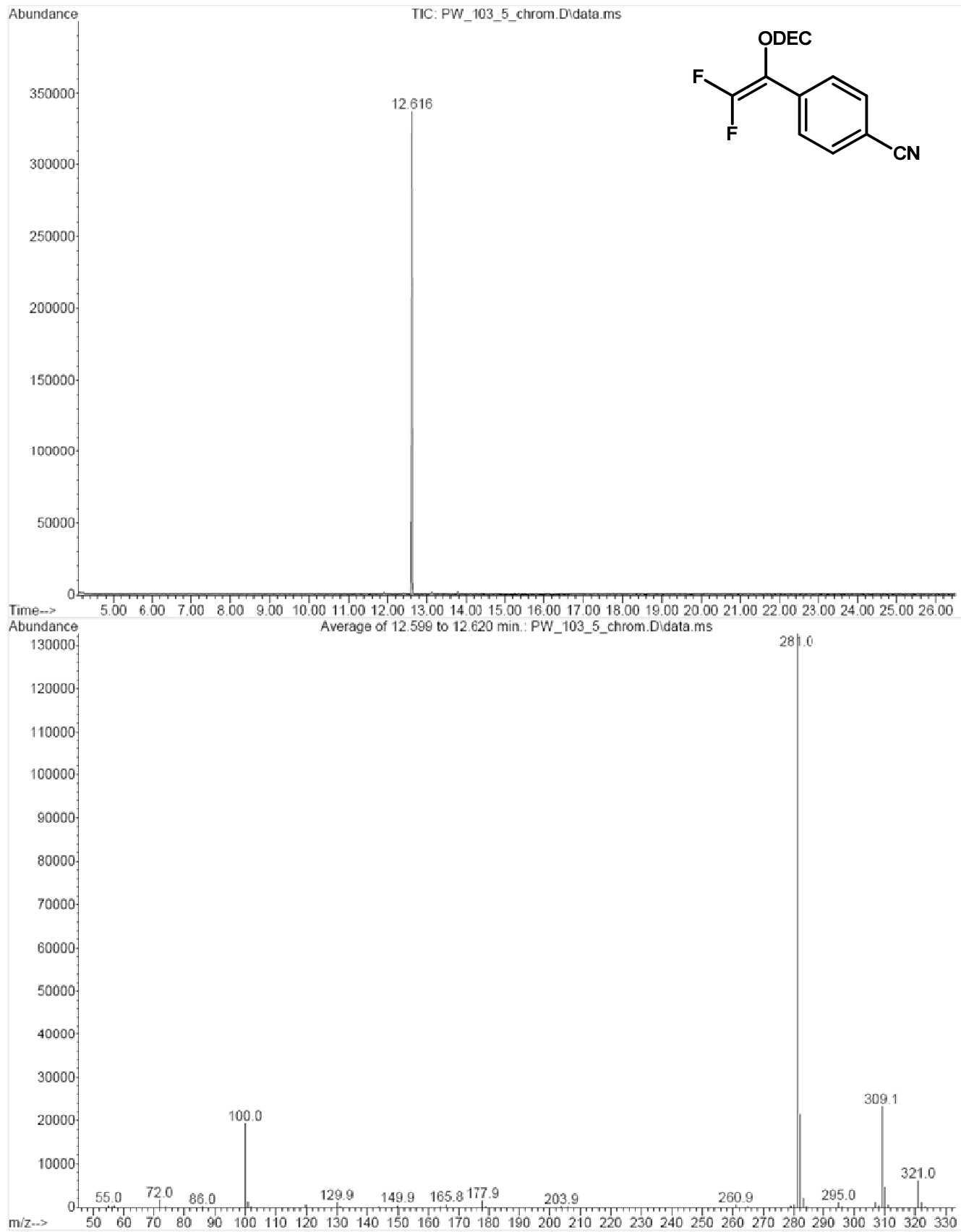


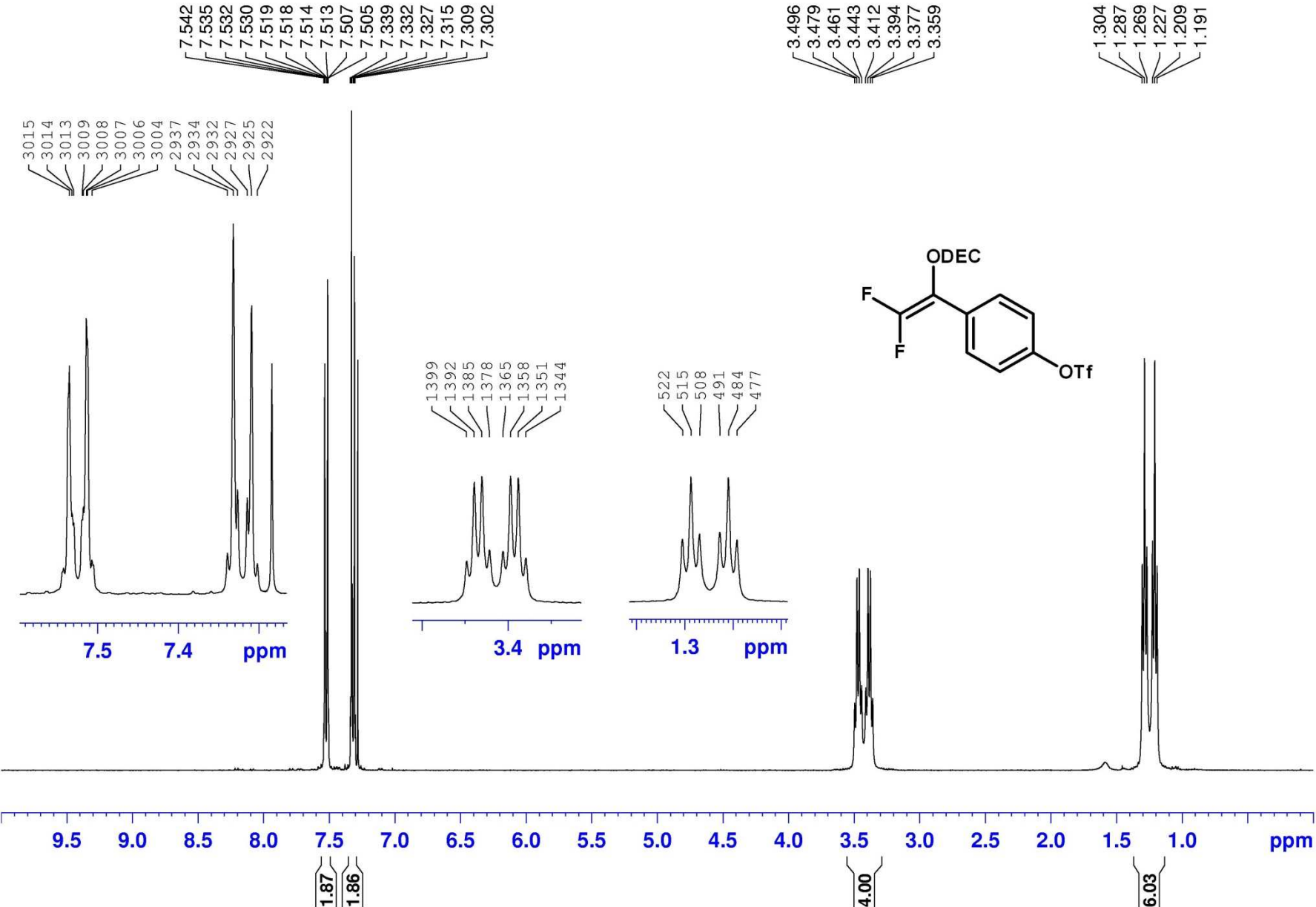


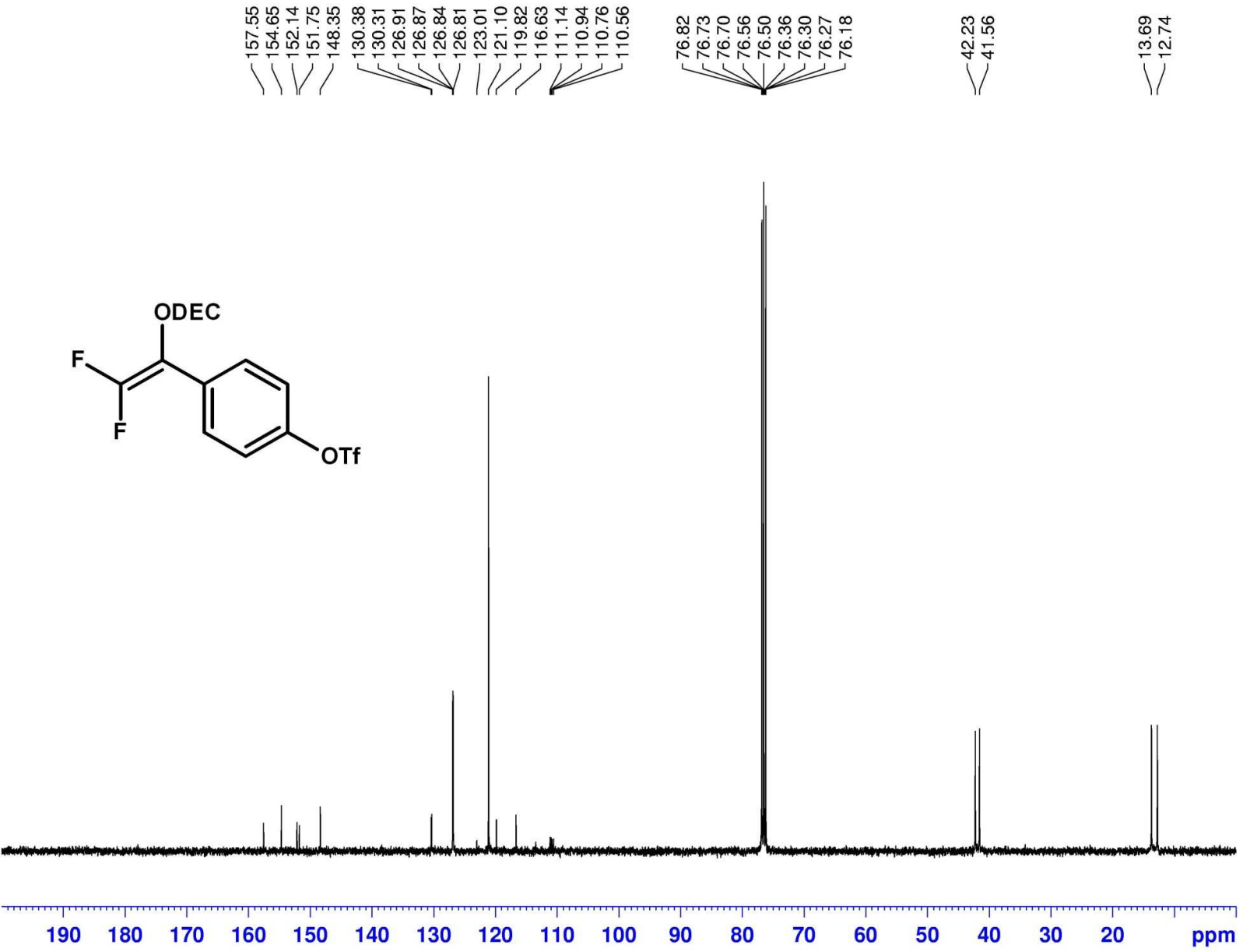


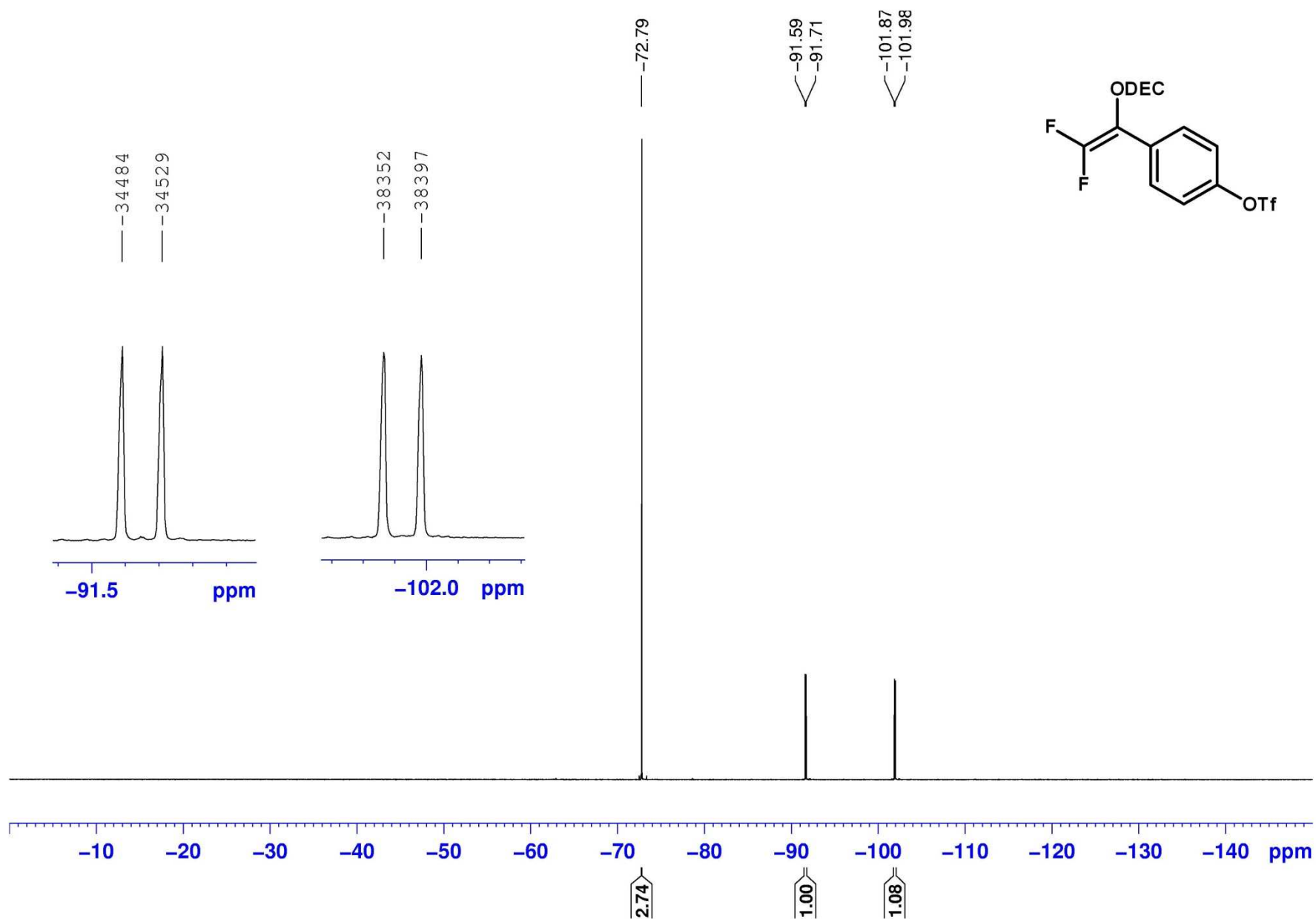


File :E:\PW\PW_103_5_chrom.D
Operator : PW
Acquired : 17 Jan 2011 9:45 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 20

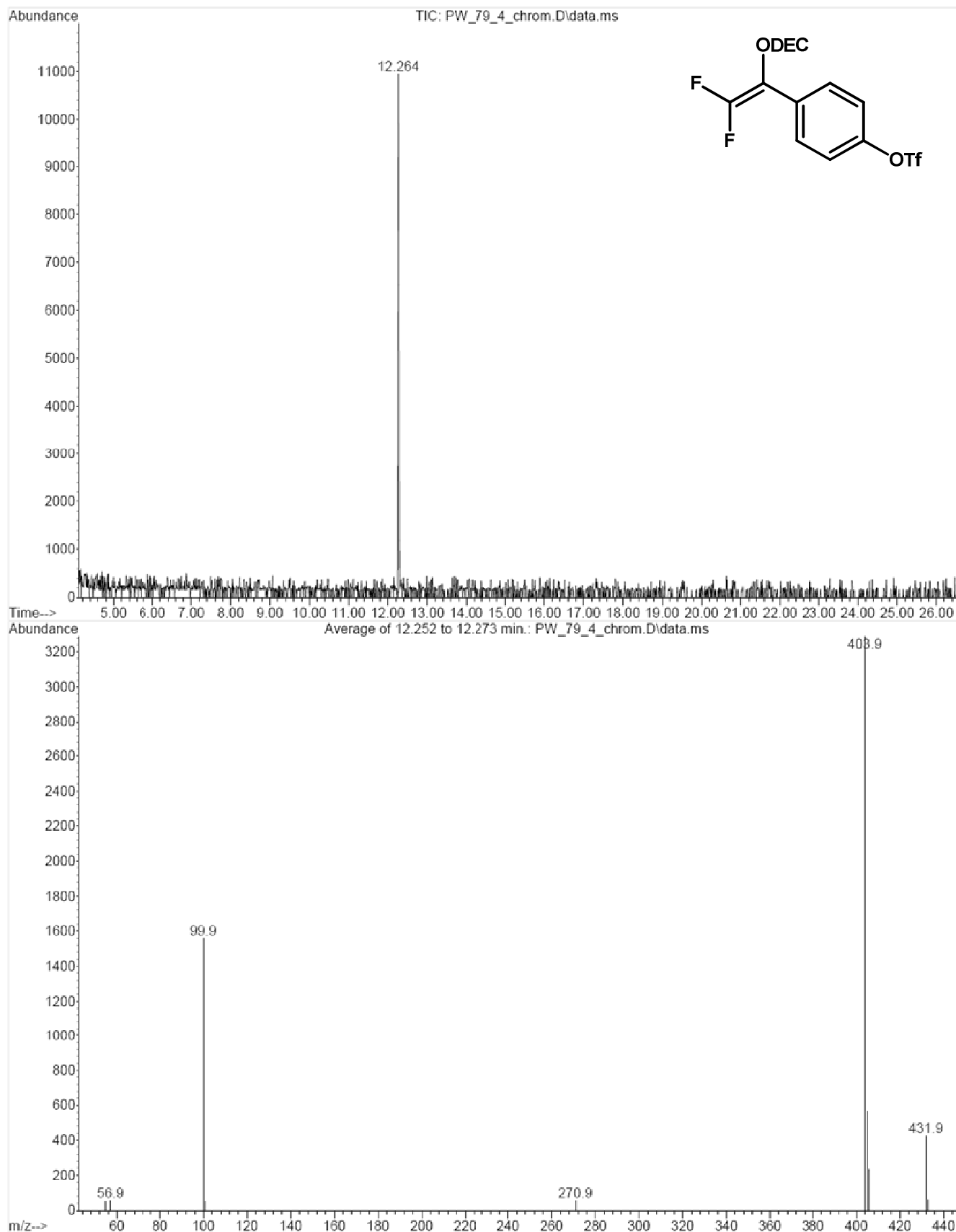


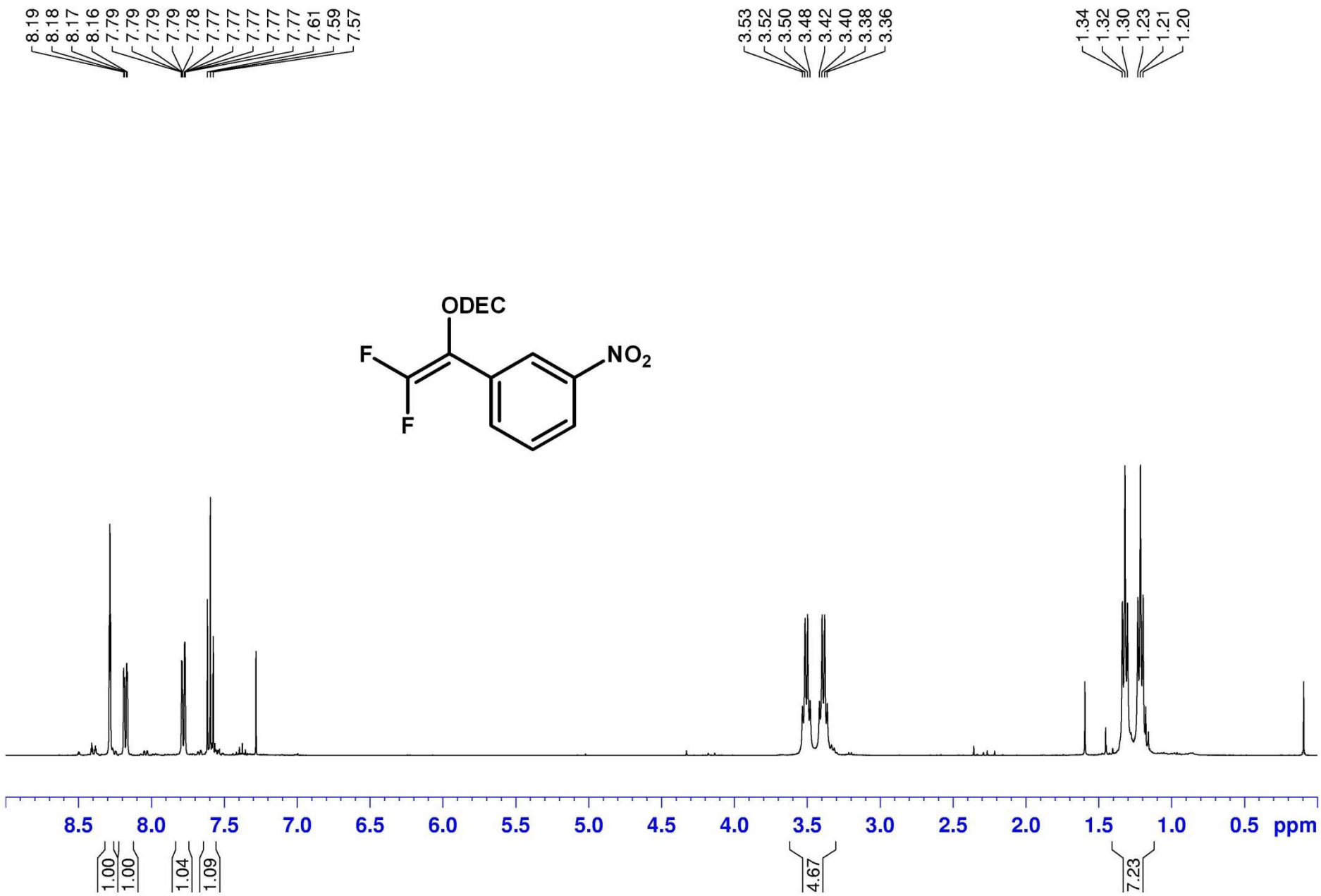


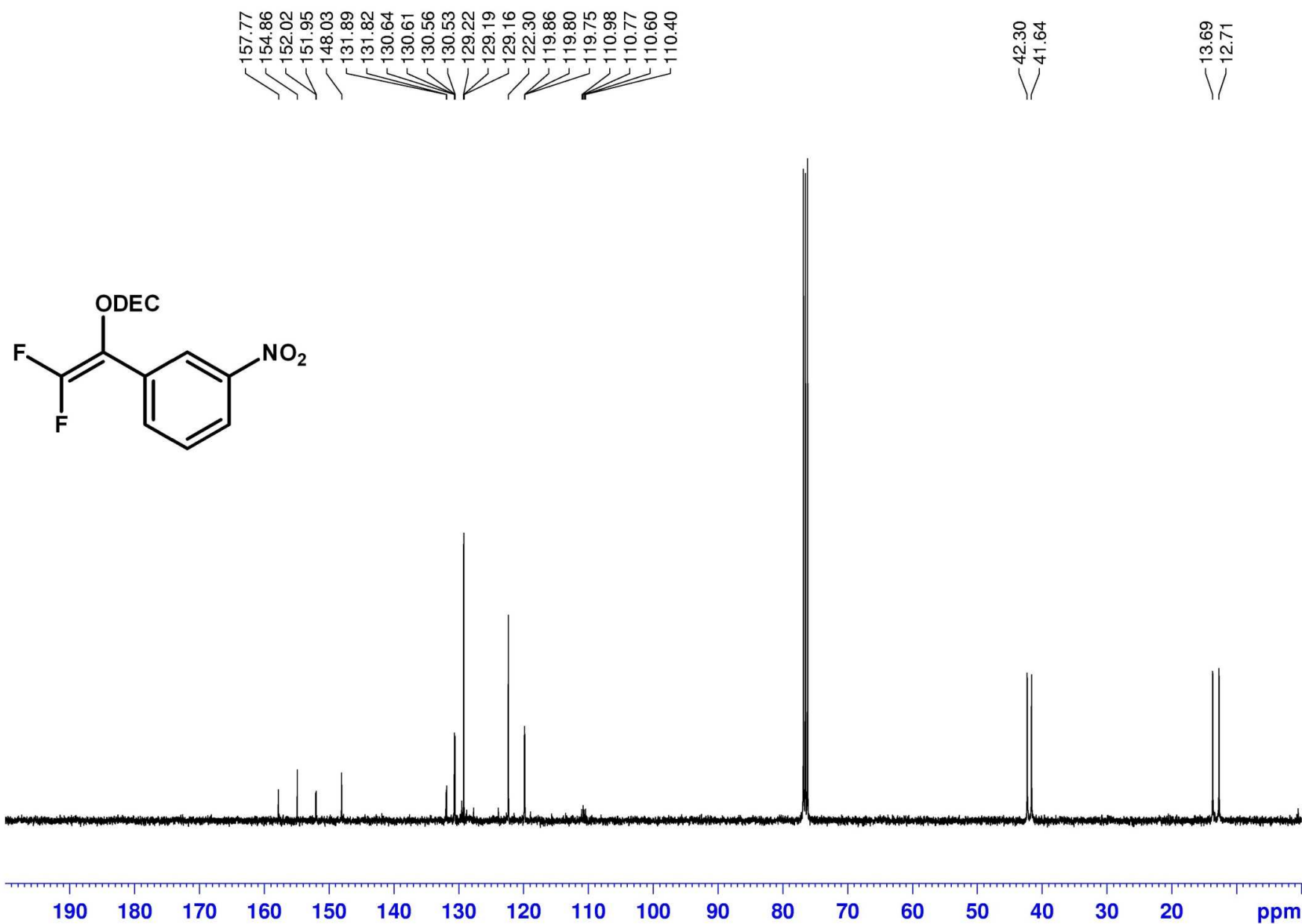


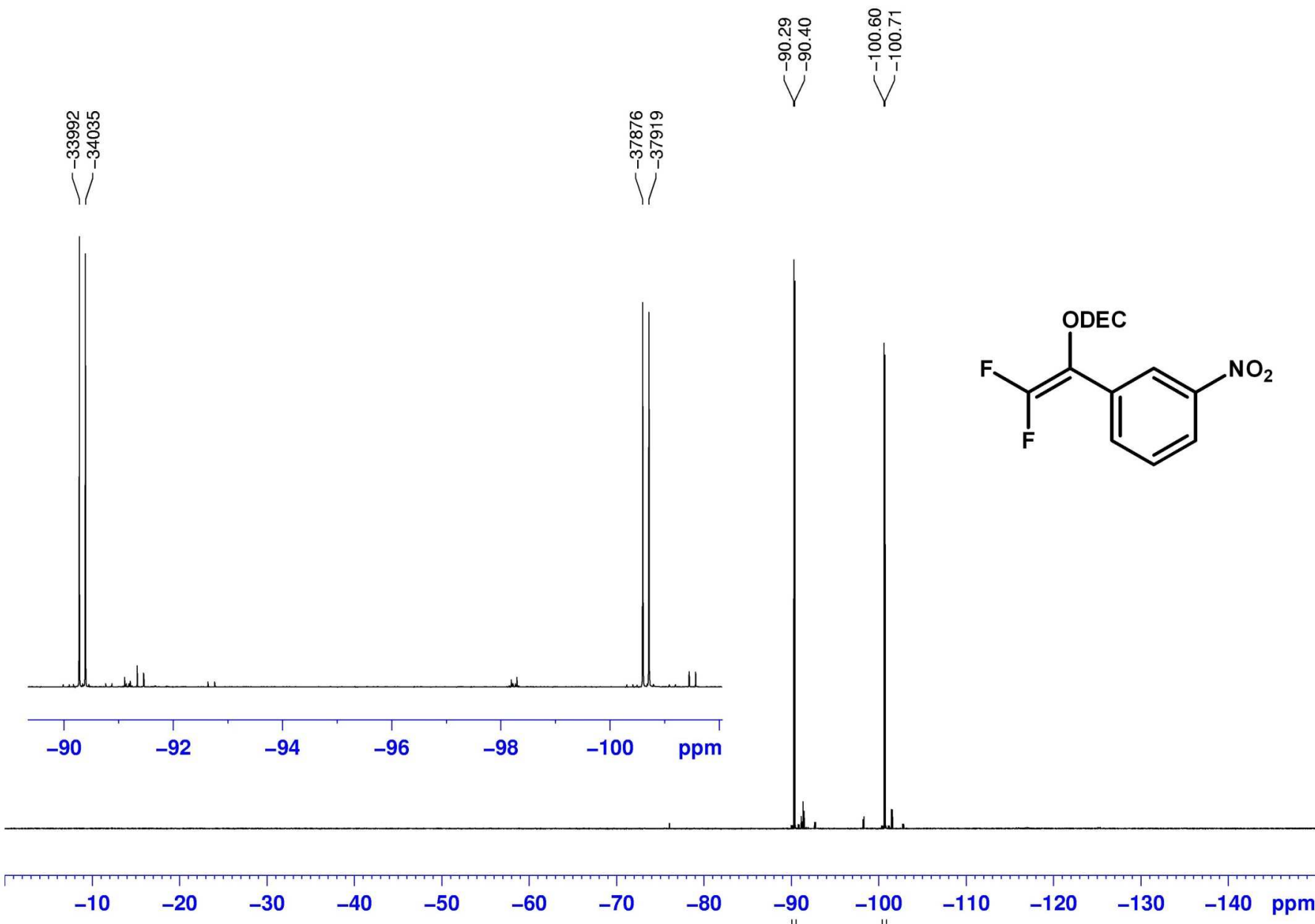


File :E:\PW\PW_79_4_chrom.D
Operator : pk
Acquired : 16 Nov 2010 19:33 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 19

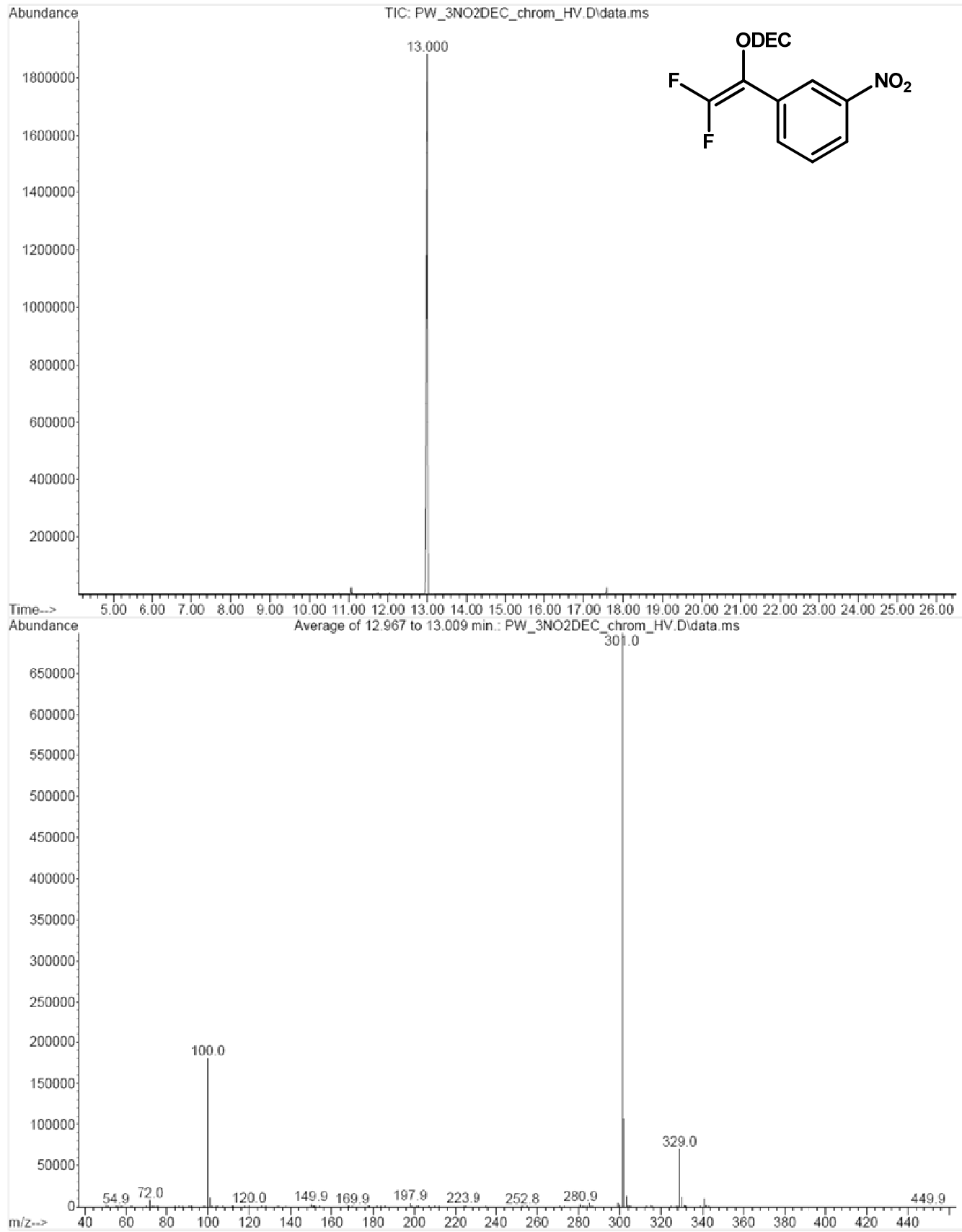


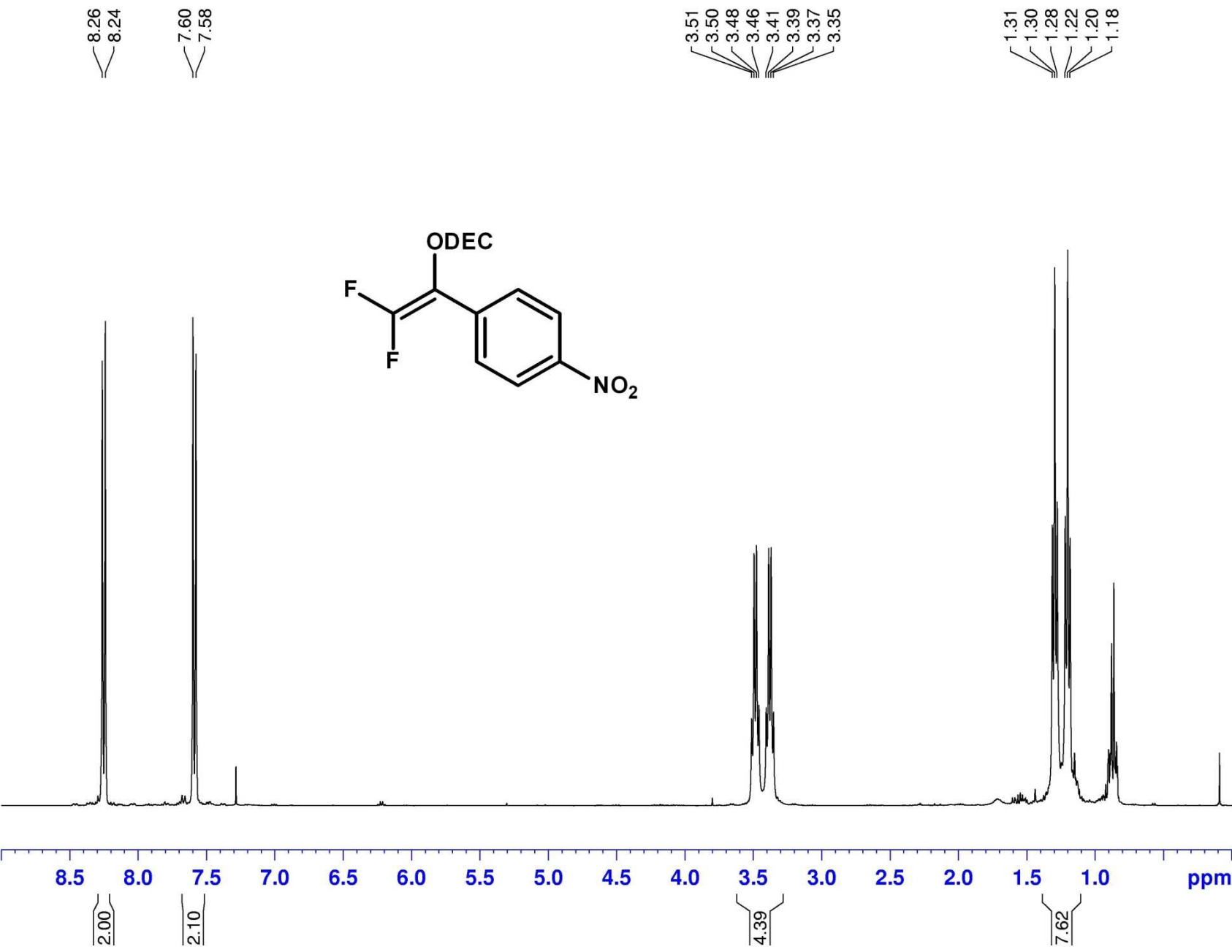


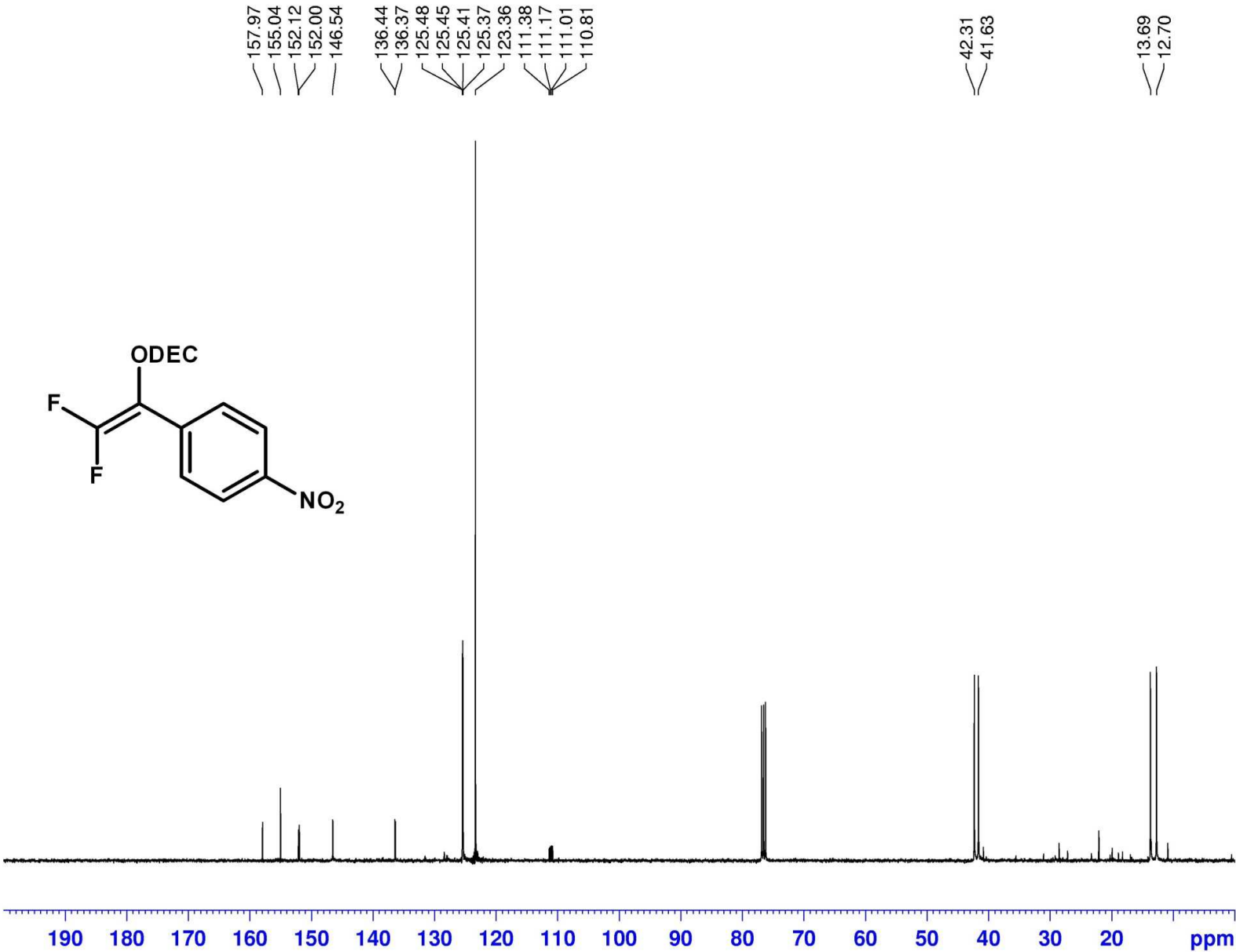


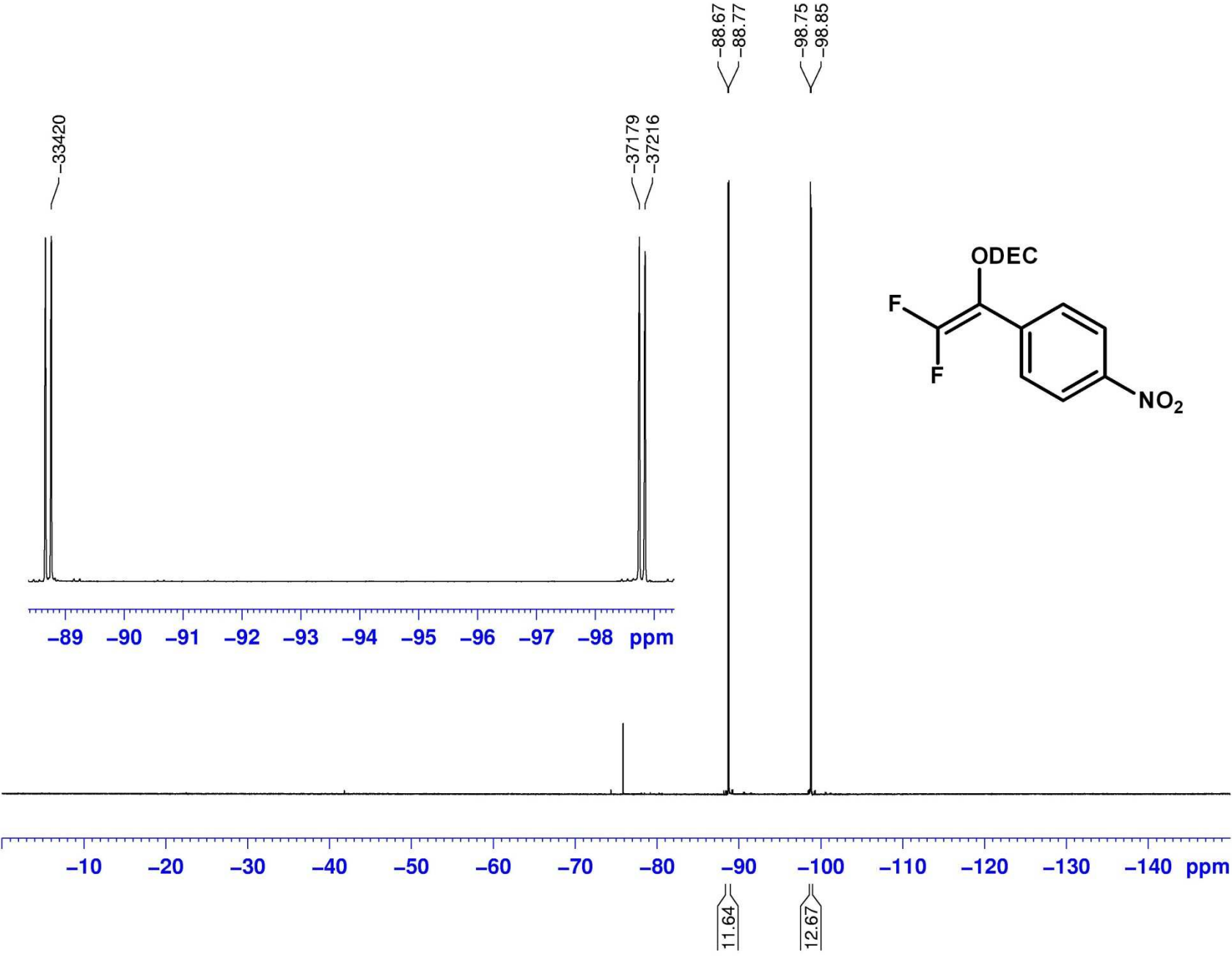


File :E:\PW\PW_3NO2DEC_chrom_HV.D
Operator : PW
Acquired : 11 Jan 2011 9:54 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name:
Misc Info :
Vial Number: 1

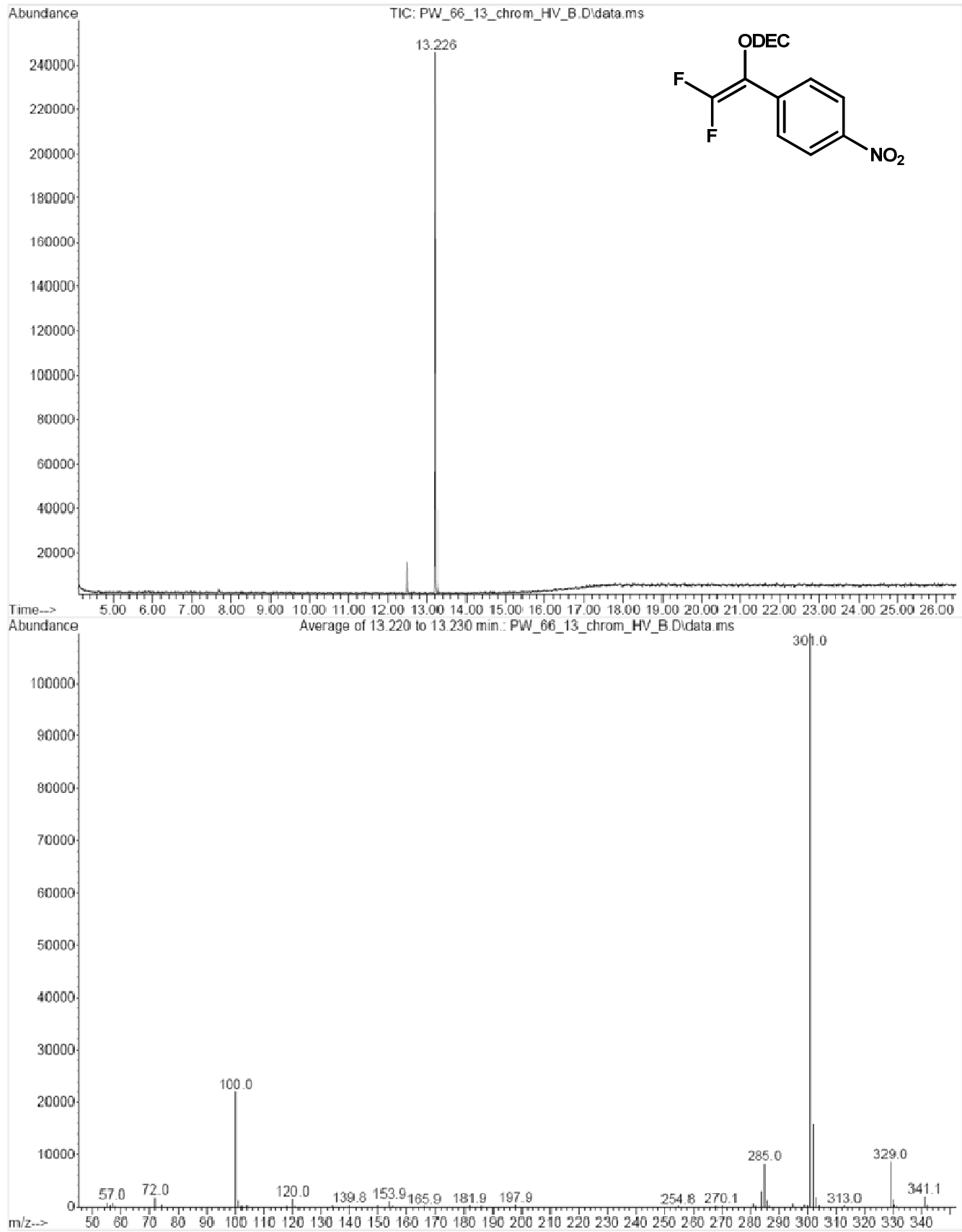






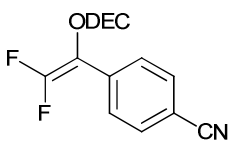
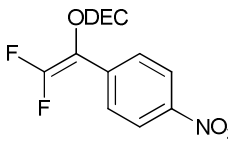
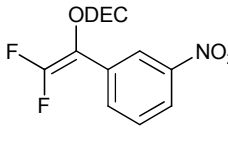
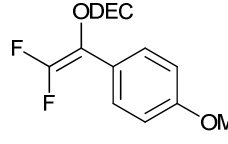


File :E:\PW\PW_66_13_chrom_HV_B.D
Operator : PW
Acquired : 2 Dec 2010 14:03 using AcqMethod BASIC_PCI_GC320_70_SPLIT10.M
Instrument : GCMS AG
Sample Name: Sample 1
Misc Info :
Vial Number: 16



General procedure for Negishi coupling in the presence of MgCl₂

Vinylzinc species **9b** (4 mL of a 0.2 M solution) was added to a suspension of MgCl₂ (95 mg, 1.0 mmol) (dried under vacuum until free flowing) in THF (1 cm³) at 0 °C. This mixture was stirred at 0 °C for 1 hour. A solution of aryl halide (1.1 mmol, 1.1 eq) and *tetrakis*(triphenylphosphino)palladium (23 mg, 2 mol%) in THF (3 cm³) was added in one portion and the reaction mixture stirred at 65 °C for the times indicated. The same work-up, isolation and purification as used for the Negishi coupling method was performed.

Halide (quantity)	Time (hours)	Product (overall isolated yield)
11k (200 mg)	16	 12bk (48%)
11m (274 mg)	0.3	 12bm (50%)
11n (222 mg)	0.5	 12bn (10%)
16a (257 mg)	16	 12ba (39%)

1. J. D. Katz, B. T. Lapointe and C. J. Dinsmore, *J. Org. Chem.*, **2009**, 74, 8866-8869.

Electronic structure calculations

Density functional theory (DFT) was employed to calculate the relative energies for each of the zinc complexes included in this study. All structures were initially optimized in Spartan '08 at the B3LYP/LACVP*(6-31G*) level of theory (gas phase). Subsequent optimization calculations were then performed in Gaussian '09 at the B3LYP/SDD (6-31G*) level of theory (gas phase). Calculations were carried out on a Dell Precision T1500 (Intel i7 Quad Core, 2.93 GHz) with 8GB RAM, Microsoft Windows 7 OS 64-bit, or a Dell Precision T7500 (2 x Intel E5530 processors, four cores each, 2.40 GHz) with 24 GB RAM Debian GNU/Linux 5.

Full Gaussian reference:

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Gaussian Archive Entries

All energies in hartrees

Phenyl ate complex 17

-2969.580826

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Cation 18

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Phenyl monomer 19

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H, 0, -3.0229403264, -2.4003390881, -1.2776175457
C, 0, -0.7198932441, 1.7539996149, -0.2729597295
C, 0, -2.0185216783, 4.2301559396, 0.2327842239
C, 0, -1.5428262292, 2.367039414, -1.2388730023
C, 0, -0.5696533969, 2.4308704632, 0.9541623292
C, 0, -1.2070804425, 3.6494737363, 1.2093134406
C, 0, -2.1839792902, 3.5855306413, -0.9948799863
H, 0, -1.6858321777, 1.8915216786, -2.2078428752
H, 0, 0.0616141258, 2.0021047997, 1.7318135822
H, 0, -1.068720779, 4.1460625062, 2.1676822296
H, 0, -2.8105486464, 4.0327170597, -1.7638031512
H, 0, -2.5151545399, 5.1781985115, 0.425510448

Phenyl anion

-231.5705821

C, 0, 0., 0., 1.5771647
C, 0, 0., 0., -1.3584244
C, 0, -1.1709671, 0., 0.7665471
C, 0, 1.1709671, 0., 0.7665471
C, 0, 1.1997107, 0., -0.6374292
C, 0, -1.1997107, 0., -0.6374292
H, 0, -2.1589033, 0., 1.2581169
H, 0, 2.1589033, 0., 1.2581169
H, 0, 2.1534457, 0., -1.1795099
H, 0, -2.1534457, 0., -1.1795099
H, 0, 0., 0., -2.4504199

ZnCl(THF)2

-1152.110253

Zn, 0, -0.0848139781, -0.8052839792, 0.9247161264
Cl, 0, -0.2218563778, -2.7597747448, 1.72468709
O, 0, -1.6048065861, 0.2968674716, 0.315553845
O, 0, 1.5740653778, 0.2198698345, 0.6465279222
C, 0, -1.8349980563, 1.7215429655, 0.6442043991
H, 0, -1.7397222319, 1.833483071, 1.7284518027
H, 0, -1.0590968427, 2.2987466087, 0.1379413565
C, 0, -2.8925895441, -0.3646425715, -0.0392653132
H, 0, -2.8599473941, -0.5471860373, -1.1163824286
H, 0, -2.9320776959, -1.311530496, 0.5019645017
C, 0, 2.8376559293, -0.2407824495, 1.2881767573
H, 0, 2.6902060574, -0.1698458695, 2.366887421
H, 0, 2.9852398396, -1.2840177935, 0.9983592903
C, 0, 1.8711427369, 1.1641503527, -0.4530466313
H, 0, 1.5943093785, 2.1624635013, -0.1016792131
H, 0, 1.2537776064, 0.8830817815, -1.308774759
C, 0, 3.9007486739, 0.6934750184, 0.7257111746
H, 0, 3.9768364015, 1.6019276146, 1.3321714066
H, 0, 4.8827544217, 0.2142445482, 0.7045789363

C, 0, 3.3701919952, 1.0182926704, -0.6812937748
H, 0, 3.8043875004, 1.9312243936, -1.0967295302
H, 0, 3.5749200709, 0.195407958, -1.3741652328
C, 0, -3.2503724488, 1.9970459816, 0.1516692549
H, 0, -3.7180552174, 2.811301685, 0.7110364222
H, 0, -3.2413419663, 2.2707138883, -0.9085458552
C, 0, -3.9570726393, 0.6467793475, 0.3624627228
H, 0, -4.2384059838, 0.514161625, 1.412379445
H, 0, -4.8579961269, 0.5438783239, -0.2476192364

Vinyl monomer 20a

-1230.309377

Zn, 0, -0.3551192138, 0.4476736371, -0.4285239531
Cl, 0, -0.7625131256, 1.3303359444, 1.5786938208
C, 0, -0.4176675503, 0.8481725317, -2.3444873081
H, 0, -0.3016360733, 0.0307014435, -3.0660048307
C, 0, -0.596323673, 2.0681206857, -2.8738951962
H, 0, -0.6254851666, 2.2496350046, -3.9516502272
H, 0, -0.7261610756, 2.9574245632, -2.2573123985
O, 0, 1.613618139, -0.5143614854, -0.005158015
O, 0, -1.4260278176, -1.509037107, -0.2023049461
C, 0, 2.5205800458, -0.7191172781, -1.1231799447
H, 0, 2.3335311403, -1.7125640591, -1.5438106248
H, 0, 2.2816401018, 0.0339659821, -1.8795379506
C, 0, 2.3720041421, -0.3090248862, 1.2121854846
H, 0, 2.4911666317, -1.2758638381, 1.721130382
H, 0, 1.791138283, 0.3644425442, 1.8434144524
C, 0, -2.6828504502, -1.6255533125, -0.9068488421
H, 0, -2.759959351, -0.7701305355, -1.5813760126
H, 0, -2.6759916167, -2.5509571348, -1.5002086922
C, 0, -1.5468023654, -2.1394566871, 1.104666393
H, 0, -1.2231630475, -1.4029738889, 1.8433127622
H, 0, -0.8762072519, -3.0048588387, 1.1311298844
C, 0, -3.7350529247, -1.6722539636, 0.1960135804
H, 0, -3.9256233409, -0.6615806244, 0.5727378803
H, 0, -4.6825401687, -2.1035436975, -0.141202126
C, 0, -3.0288599327, -2.5265525773, 1.2642635136
H, 0, -3.3952076545, -2.3283441097, 2.2754768923
H, 0, -3.1759696941, -3.5925493364, 1.0561343468
C, 0, 3.9409912434, -0.5623833943, -0.5558289651
H, 0, 4.3722811898, -1.542065763, -0.3200890355
H, 0, 4.6113371801, -0.0624371509, -1.2610523835
C, 0, 3.7120267158, 0.2413174968, 0.7359390859
H, 0, 4.509569662, 0.1060584064, 1.472693249
H, 0, 3.6217188194, 1.3115749289, 0.5176911246

Vinyl anion

-77.89115858

C, 0, 0.5237106, 0.0400243, 0.

H, 0, 1.0084745, 1.0494245, 0.
H, 0, 1.3073325, -0.7477893, 0.
C, 0, -0.7942815, -0.2834456, 0.
H, 0, -1.3638647, 0.6994079, 0.

Vinyl DMC monomer 20b

-1552.868676

Zn, 0, 0.3111967688, 0.2723777667, -0.207864001
C, 0, -0.7153889395, 1.3571405555, 1.1030795478
C, 0, -0.3291130704, 2.025225729, 2.1941552985
O, 0, 0.5317807993, -1.8027966205, 0.4721067542
O, 0, -2.1183273507, 1.4480666182, 0.8528814515
O, 0, 2.4639882528, 0.6726716594, 0.7544832955
Cl, 0, 1.16790391, 0.1745026362, -2.2620282987
C, 0, 3.0252759748, 1.9529631388, 0.373022989
H, 0, 2.3074761278, 2.4641908383, -0.2730354134
H, 0, 3.1734028973, 2.5484834257, 1.2839674901
C, 0, 3.45863629, -0.3673863677, 0.5979659633
H, 0, 3.198872683, -0.9651857923, -0.2822631103
H, 0, 3.4237421638, -1.0028574064, 1.4879293914
C, 0, 4.3493037402, 1.6368283672, -0.3227430709
H, 0, 4.1702134627, 1.4284683689, -1.3826670535
H, 0, 5.0706823868, 2.455888711, -0.2422553905
C, 0, 4.7919014097, 0.3581820051, 0.4048842736
H, 0, 5.5099501378, -0.238525206, -0.166093539
H, 0, 5.2447350644, 0.6031194935, 1.3735134173
C, 0, -0.2057189053, -2.2064235562, 1.6485811754
H, 0, -0.6039583095, -1.3004668886, 2.1091770092
H, 0, 0.4858611455, -2.694143446, 2.3502229699
C, 0, 0.4774930367, -2.8679190677, -0.5242413254
H, 0, 1.4955798202, -3.2368700592, -0.6835631506
H, 0, 0.1170810922, -2.4231398094, -1.4530976498
C, 0, -0.4680301129, -3.9396724648, 0.0459247576
H, 0, -1.1109546504, -4.3680050765, -0.7284499497
H, 0, 0.1027483294, -4.7588909485, 0.4984426283
C, 0, -1.2573410445, -3.178427761, 1.1258522706
H, 0, -2.0813567541, -2.6169956438, 0.6750290113
H, 0, -1.6559260211, -3.8321047755, 1.907961683
O, 0, -1.9693552, -0.251147666, -0.658630387
C, 0, -2.6291560342, 0.6220660753, -0.0800473263
N, 0, -3.9530319852, 0.836673765, -0.3112639256
C, 0, -4.7284621936, 1.8863165471, 0.333885533
H, 0, -5.0484449511, 2.6354336281, -0.403047777
H, 0, -4.1305815721, 2.3739663839, 1.0999447306
H, 0, -5.6257794371, 1.4554820713, 0.7964919838
C, 0, -4.6379999361, 0.0517609936, -1.3261552046
H, 0, -5.0069264677, 0.703916489, -2.1288301617
H, 0, -5.4960810592, -0.4736018327, -0.8867611104
H, 0, -3.9416006064, -0.672587012, -1.7448734928

H, 0, 0.7197987066, 2.0313101353, 2.4693373607
H, 0, -1.0225500986, 2.5724153983, 2.8325339526

Vinyl DMC anion

-400.4800483

O, 0, -0.2511105479, -1.805609743, -0.0607599135
C, 0, -0.1458066811, -0.5857405562, 0.0093819737
O, 0, 0.9324362272, 0.162234179, -0.0223250386
C, 0, 2.3016319033, -0.4726612442, -0.3872973347
C, 0, 3.1902654897, 0.4828609398, -0.0280570737
H, 0, 4.2497787985, 0.2906235138, -0.2154789591
H, 0, 2.9630658988, 1.4522549624, 0.4404220666
N, 0, -1.3094276634, 0.2141174927, 0.1997191579
C, 0, -1.2874414573, 1.6467282894, 0.0139452857
H, 0, -1.9819480038, 2.1320979655, 0.7183856668
H, 0, -1.5931323553, 1.9474066738, -1.0068582482
H, 0, -0.2764897312, 2.0088267566, 0.1932227255
C, 0, -2.5942763534, -0.4224396936, 0.0504692749
H, 0, -3.309060991, -0.0348950021, 0.7938212253
H, 0, -2.4569312942, -1.4944475951, 0.19343376
H, 0, -3.0379984391, -0.2558310388, -0.9504501686

F2 Vinyl DMC Monomer 20c

-1751.33321

Zn, 0, -0.384450545, -0.0175577405, -0.3645284122
C, 0, 0.7670713035, -1.4474006979, 0.410700765
C, 0, 0.4688430605, -2.4922752136, 1.1783642049
O, 0, -0.5533292492, 1.7611630737, 0.8665544261
O, 0, 2.1471081501, -1.4177968022, 0.0854643838
O, 0, -2.4806815519, -0.5260819274, 0.3980069331
Cl, 0, -1.1092683883, 0.6618013193, -2.3648678369
C, 0, -3.0447023621, -1.7505608859, -0.1419804676
H, 0, -2.3111154075, -2.1929875581, -0.8200274182
H, 0, -3.2198671014, -2.4412578234, 0.6906610836
C, 0, -3.4719768228, 0.5338485724, 0.3559661827
H, 0, -3.1866817932, 1.2350997814, -0.4345753933
H, 0, -3.4548438443, 1.0454383708, 1.322198503
C, 0, -4.3432088485, -1.3365756573, -0.8310854562
H, 0, -4.1351914993, -0.9988802166, -1.8518060133
H, 0, -5.0709515613, -2.1528232859, -0.873182212
C, 0, -4.8002798287, -0.1554249059, 0.0389058945
H, 0, -5.5000345979, 0.512725528, -0.4722393777
H, 0, -5.2804180914, -0.5167899708, 0.9564425794
C, 0, 0.1029070677, 1.7490752097, 2.1606711746
H, 0, 0.5569692903, 0.7649305403, 2.29388413
H, 0, -0.6614841575, 1.9006421061, 2.9339941947
C, 0, -0.3287923021, 3.0419266346, 0.2012118371
H, 0, -1.2994050119, 3.4159383702, -0.1333634851
H, 0, 0.3026731777, 2.8596147017, -0.6706700288

C, 0, 0.3564968527, 3.9281205414, 1.2443832009
H, 0, 1.0211422806, 4.6632900442, 0.7810783993
H, 0, -0.3843787347, 4.4714064419, 1.8433440948
C, 0, 1.1014238171, 2.9023206558, 2.1135429052
H, 0, 2.0194607656, 2.5769869355, 1.6138677111
H, 0, 1.3538802474, 3.2788313416, 3.1095193294
O, 0, 1.9296651306, 0.7586349134, -0.5427523001
F, 0, -0.7681673638, -2.7700454599, 1.6010693163
F, 0, 1.3207159138, -3.4134897509, 1.6382931026
C, 0, 2.6202097465, -0.2568324178, -0.4131689847
N, 0, 3.9380517381, -0.3305925741, -0.741309916
C, 0, 4.7257103415, -1.5521705484, -0.6412108642
H, 0, 4.9252239699, -1.9704770093, -1.6374652529
H, 0, 4.195506866, -2.2916186055, -0.0454188738
H, 0, 5.6871208088, -1.3272212251, -0.1638261962
C, 0, 4.5755884188, 0.8076551997, -1.3846595621
H, 0, 4.860670868, 0.5584347407, -2.4156787268
H, 0, 5.4811892964, 1.0933214746, -0.8347670626
H, 0, 3.8782169514, 1.6434317796, -1.4000862119

F2 Vinyl DMC anion

-598.9597458

O, 0, 1.312875499, -1.8666029682, 0.0039578706
C, 0, 1.0328951304, -0.6766792434, -0.0455815048
O, 0, -0.1540710381, -0.0973189682, -0.0540549428
C, 0, -1.3842893324, -0.9304565709, -0.0185367168
C, 0, -2.3813699555, -0.0433705758, -0.0743712031
N, 0, 2.0460156664, 0.3060202732, -0.1315933905
C, 0, 1.7708217908, 1.7190528075, 0.0121356155
H, 0, 0.7142224912, 1.897613802, -0.1794681942
H, 0, 2.0131476982, 2.0884167451, 1.0261938205
H, 0, 2.377726601, 2.2994861711, -0.7009224471
C, 0, 3.4126905603, -0.1053516035, 0.0686690758
H, 0, 4.077129536, 0.375803798, -0.6663856197
H, 0, 3.4597569448, -1.188249907, -0.048209981
H, 0, 3.7874782999, 0.1603411571, 1.0751365351
F, 0, -3.6976768787, -0.4047137995, -0.0615656131
F, 0, -2.3681312236, 1.3411570226, -0.1522757746

Vinyl MEM monomer 20d

-1613.188264

Zn, 0, 0.7828398387, 0.3614028182, 0.0051146836
C, 0, 0.3557153046, 1.7318635448, 1.3698576806
C, 0, 1.1046315648, 1.9853904453, 2.4537819925
H, 0, 0.7790188294, 2.6667676298, 3.2400545037
O, 0, 0.1493239278, -1.5955351503, 0.785627102
H, 0, 2.0671946628, 1.4998979787, 2.5738575871

O, 0, -0.8906828005, 2.3734597118, 1.3404711611
O, 0, 2.9189380154, -0.1822154263, 0.4685302454
Cl, 0, 0.9347077943, -0.0544434355, -2.1915106313
C, 0, 3.9089096906, 0.7810935071, 0.0150295316
H, 0, 3.3928566529, 1.569491934, -0.538262144
H, 0, 4.3834340398, 1.2186305432, 0.9017167586
C, 0, 3.3624583335, -1.5308559817, 0.1632904197
H, 0, 2.7817892817, -1.8988227226, -0.6891666341
H, 0, 3.1576232764, -2.1527787098, 1.0383300939
C, 0, 4.8991849528, -0.0133981807, -0.836622596
H, 0, 4.5452648054, -0.0680693958, -1.8716172909
H, 0, 5.8993322458, 0.4304082757, -0.8339056674
C, 0, 4.8460499869, -1.4024718777, -0.1814367267
H, 0, 5.1872021001, -2.2046633126, -0.8427850261
H, 0, 5.4591890963, -1.4241928233, 0.7275466042
C, 0, -0.5030980779, -1.6515111953, 2.0749212226
H, 0, -0.3022093009, -0.7044655986, 2.5779799751
H, 0, -0.0607879867, -2.4763514799, 2.6529219262
C, 0, -0.4592486032, -2.6168427283, -0.044453467
H, 0, 0.1309519774, -3.5363427692, 0.0618179714
H, 0, -0.3888502983, -2.2662640921, -1.0746336457
C, 0, -1.902834825, -2.8010935211, 0.4777717028
H, 0, -2.6458628819, -2.4798021063, -0.2559483053
H, 0, -2.0906792317, -3.8537851546, 0.7137186007
C, 0, -1.9717867539, -1.9079805064, 1.7420758701
H, 0, -2.4685397094, -0.9655606222, 1.5007119007
H, 0, -2.5044908019, -2.3856249791, 2.5704985523
O, 0, -1.8752196228, 0.9919311743, -0.2056421381
C, 0, -1.5589904458, 2.3409675015, 0.1286185923
H, 0, -2.4726525216, 2.9347358364, 0.2633602554
H, 0, -0.9510059076, 2.7716139284, -0.6861071617
C, 0, -2.5669485327, 0.8462695858, -1.4432906024
H, 0, -2.1915907322, -0.066705383, -1.9129398376
H, 0, -2.334784314, 1.6824302427, -2.1181524085
C, 0, -4.0721511067, 0.7456112124, -1.2502917831
H, 0, -4.5673655553, 0.7956003183, -2.236458121
H, 0, -4.4433431507, 1.5941772569, -0.6506837989
O, 0, -4.371043797, -0.4790513732, -0.6091795024
C, 0, -5.7491060664, -0.6427762996, -0.3522546235
H, 0, -5.8735838646, -1.6105467525, 0.1403021126
H, 0, -6.3408212027, -0.6358826337, -1.2822018932
H, 0, -6.136164686, 0.1481875662, 0.3099502587

Vinyl MEM anion

-460.7968386

C, 0, 4.1217511192, 0.2792636733, -0.3465491936
H, 0, 5.1264018648, 0.6894971922, -0.4916733955
H, 0, 3.9821408746, -0.6967273966, -0.839591646
C, 0, 3.2567244988, 1.015619635, 0.4092321975
O, 0, 1.9253800152, 0.4008986132, 0.5629940531

C, 0, 1.5889458414, -0.7425008379, -0.1304010691
H, 0, 1.7845124105, -0.632710912, -1.2166103804
H, 0, 2.1161567689, -1.6431908222, 0.2277761355
O, 0, 0.2025124932, -1.052000276, 0.0659205345
C, 0, -0.6562659818, -0.0219297715, -0.3731931819
H, 0, -0.336789744, 0.9492948027, 0.0192714508
H, 0, -0.671452151, 0.0459262597, -1.4767753482
C, 0, -2.0473718715, -0.3729575537, 0.1317354734
H, 0, -2.0499854717, -0.3797161757, 1.2339714391
H, 0, -2.3234552455, -1.3870194527, -0.2055613314
O, 0, -2.978148692, 0.581788879, -0.3637387643
C, 0, -4.2842116305, 0.3411825946, 0.0874354686
H, 0, -4.6601127105, -0.6462438401, -0.2356748682
H, 0, -4.9292011571, 1.1177493627, -0.3373774808
H, 0, -4.357719731, 0.3839999261, 1.1884032069

F2 Vinyl MEM monomer 20e

-1811.653066

Zn, 0, 0.7365596569, 0.1443851607, -0.4009294826
C, 0, 0.5277359545, 2.0315123658, 0.1518143798
C, 0, 1.5084722885, 2.890022568, 0.4229550778
O, 0, -0.1171968901, -1.1094986967, 1.1732863973
O, 0, -0.7587018918, 2.5318117496, 0.458133418
O, 0, 2.7822128852, -0.5422328049, 0.1627079335
Cl, 0, 0.5853103547, -1.166297903, -2.2096833137
C, 0, 3.8606205384, -0.1799073151, -0.7483579172
H, 0, 3.4181824327, 0.1641651042, -1.6864788604
H, 0, 4.4137103202, 0.6422895221, -0.2854156746
C, 0, 2.9600274085, -1.9044757159, 0.6200517419
H, 0, 2.3213468295, -2.565912839, 0.0221367856
H, 0, 2.6439245143, -1.9422848766, 1.6649409857
C, 0, 4.7096501011, -1.4439020349, -0.915242569
H, 0, 4.3551615355, -2.0275899935, -1.7717004786
H, 0, 5.7676315408, -1.2130474287, -1.0712605607
C, 0, 4.4389315046, -2.2045342476, 0.3925375046
H, 0, 4.640022054, -3.2775710131, 0.3174639827
H, 0, 5.0438615271, -1.7967446462, 1.2109940104
C, 0, -0.7991737826, -0.4483075397, 2.2795208893
H, 0, -0.845261001, 0.6169759609, 2.0539647058
H, 0, -0.2026194678, -0.6087984568, 3.187097928
C, 0, -0.792251272, -2.360401855, 0.8479020437
H, 0, -0.0349184085, -3.1481266227, 0.8036014412
H, 0, -1.2453822939, -2.2543610745, -0.1404251963
C, 0, -1.8341349476, -2.5660826648, 1.9492151887
H, 0, -2.7057037932, -3.1170913908, 1.583973407
H, 0, -1.4057027924, -3.122970454, 2.7915064424
C, 0, -2.1644032173, -1.1236343107, 2.3631980548
H, 0, -2.8498566917, -0.6728507332, 1.6389558857
H, 0, -2.6014782679, -1.0517992491, 3.3642276274
O, 0, -1.9421425291, 0.8502593133, -0.5572914078

C, 0, -1.7245723698, 2.2537693788, -0.4997944949
H, 0, -2.6304873655, 2.7804275094, -0.1728955842
H, 0, -1.4202945332, 2.6105096549, -1.4984642079
C, 0, -2.7226474505, 0.4057619537, -1.6623823338
H, 0, -2.3759831217, -0.6033917301, -1.8981140833
H, 0, -2.5354728219, 1.0374631476, -2.5434799224
C, 0, -4.2145012471, 0.3851360766, -1.3628951353
H, 0, -4.761542894, 0.1657267684, -2.296929697
H, 0, -4.557563986, 1.3719173123, -1.0071090642
O, 0, -4.4783639984, -0.6085080898, -0.3914369752
C, 0, -5.8449766149, -0.6852603401, -0.0458256482
H, 0, -5.9460490922, -1.4756666566, 0.7024079251
H, 0, -6.4712830279, -0.9358208162, -0.9172371444
H, 0, -6.211450714, 0.2616716635, 0.3824768047
F, 0, 2.8090777769, 2.5987567522, 0.2808460246
F, 0, 1.3784587603, 4.1312071372, 0.8936418662

F2 Vinyl MEM anion

-659.2788145

C, 0, 3.2309406686, 0.3778994625, -0.1033840046
C, 0, 2.2179872787, 1.1469942808, 0.2941653326
O, 0, 1.02751205, 0.4603327066, 0.746919217
C, 0, 0.7167835348, -0.8071924887, 0.2652345092
H, 0, 0.9915103315, -0.8957628384, -0.8008161259
H, 0, 1.1964189741, -1.6214130909, 0.8270945483
O, 0, -0.6813986882, -1.0461102435, 0.4281273822
C, 0, -1.4867293373, -0.1480226737, -0.3086437254
H, 0, -1.133044366, 0.8814821374, -0.1898140686
H, 0, -1.4752933748, -0.3928490346, -1.3860609454
C, 0, -2.9016801507, -0.2916678333, 0.2299303529
H, 0, -2.9278050768, 0.0196836263, 1.2868514231
H, 0, -3.2123066311, -1.3500270762, 0.1890019323
O, 0, -3.7789192073, 0.5106741451, -0.5499188423
C, 0, -5.1032789448, 0.4606075229, -0.0893085724
H, 0, -5.5168059126, -0.5632010126, -0.1250689546
H, 0, -5.7039768913, 1.1042959989, -0.7405014639
H, 0, -5.1950193123, 0.8238123189, 0.9492621069
F, 0, 4.418433527, 0.8907551841, -0.5614443666
F, 0, 3.4126761287, -1.0209316919, -0.1699409346

Phenyl dimer 21

-2303.033331

Zn, 0, 1.5851032181, 0.4274009879, 0.0765331908
O, 0, 1.4166744445, 2.5567188565, 0.2828760325
C, 0, 2.4848105288, 3.4432252641, -0.1522610704
H, 0, 3.146782396, 3.618532872, 0.7033983865
H, 0, 3.0493971936, 2.9370092967, -0.9383425947
C, 0, 0.1535207106, 3.2771470105, 0.3722829059

H, 0, -0.4740905731, 2.9711863173, -0.4711981099
H, 0, -0.328439808, 2.9799335999, 1.3053725924
C, 0, 1.7810098072, 4.7214864657, -0.6082894324
H, 0, 2.4185379196, 5.6040113533, -0.5013461853
H, 0, 1.4834417306, 4.6397139042, -1.6599799015
C, 0, 0.5397559076, 4.7533504894, 0.2985433639
H, 0, 0.8009764043, 5.1335111378, 1.2929867658
H, 0, -0.2700179554, 5.3706863988, -0.1009000348
Cl, 0, -0.0181593754, 0.1723598123, -1.7312082785
Cl, 0, -0.062578364, -0.1242144037, 1.7229350914
Zn, 0, -1.6657858025, -0.3792669779, -0.0849167008
O, 0, -1.4971124438, -2.5086483005, -0.2912335085
C, 0, -2.5651851537, -3.395208259, 0.1439446235
H, 0, -3.1296935585, -2.8890655636, 0.9301307245
H, 0, -3.2272582557, -3.570441547, -0.7116509591
C, 0, -0.2339547426, -3.2290200835, -0.3807863864
H, 0, 0.2479392821, -2.9317137841, -1.3138816144
H, 0, 0.3937020915, -2.923110513, 0.462685315
C, 0, -1.861311545, -4.673492018, 0.5997866041
H, 0, -2.498817766, -5.5560278823, 0.4928051824
H, 0, -1.5636578458, -4.5918252221, 1.651462147
C, 0, -0.6201181719, -4.7052480393, -0.3071435318
H, 0, -0.8813846218, -5.0853429723, -1.3016000014
H, 0, 0.1896990598, -5.3225820624, 0.0922129601
C, 0, -3.5170778764, 0.2648337427, 0.0467403902
C, 0, -6.1859970017, 1.2056410911, 0.2486397952
C, 0, -4.0960476488, 0.5732244615, 1.2932745265
C, 0, -4.3216777827, 0.4454826268, -1.0954543632
C, 0, -5.6374255766, 0.9088232674, -1.0007773775
C, 0, -5.4112668821, 1.0367617544, 1.3978243347
H, 0, -3.5118242741, 0.456228679, 2.2048869549
H, 0, -3.9185679413, 0.2267597126, -2.0831499723
H, 0, -6.2331014773, 1.040240305, -1.901781404
H, 0, -5.8297128838, 1.267783012, 2.3753070157
H, 0, -7.2087257735, 1.5672067237, 0.3256737497
C, 0, 3.4363069432, -0.2170592464, -0.054635652
C, 0, 6.1052266143, -1.1580271914, -0.2558139355
C, 0, 4.0155557188, -0.525608976, -1.3010059385
C, 0, 4.2406305266, -0.3976284912, 1.0877656223
C, 0, 5.556374247, -0.8610545167, 0.9934438878
C, 0, 5.3307742192, -0.9892318786, -1.4051985984
H, 0, 3.4315528526, -0.4086923906, -2.2127696217
H, 0, 3.8372942277, -0.1787898911, 2.0753432019
H, 0, 6.1518299496, -0.9924116347, 1.8946021542
H, 0, 5.7494375937, -1.2203777135, -2.3825589194
H, 0, 7.1279572147, -1.5196464842, -0.3325697265

Phenyl dimer cation 23
-2071.175625

Zn, 0, 1.5817622275, -0.0449143428, 0.1678289024

O, 0, 2.4621325804, 1.7468504365, 0.1938955088
C, 0, 3.9278747009, 1.8606307909, 0.0599014913
H, 0, 4.3646483531, 1.6196705513, 1.0334675077
H, 0, 4.2496181917, 1.1264967506, -0.6815065954
C, 0, 1.8353313698, 3.0793749602, 0.1961349677
H, 0, 1.3158321778, 3.19648884, -0.7591049067
H, 0, 1.1163750565, 3.0967356827, 1.0166175339
C, 0, 4.1578335513, 3.3117461274, -0.3455304277
H, 0, 5.1423010691, 3.6682417133, -0.031734718
H, 0, 4.0837522335, 3.422771471, -1.432638968
C, 0, 3.0033997475, 4.0468970446, 0.3568361837
H, 0, 3.2316078141, 4.2009559187, 1.4168938326
H, 0, 2.7862630268, 5.0203564728, -0.0905179944
Cl, 0, -0.3239845805, 0.5992869968, -1.7445981027
Cl, 0, -0.4071810207, 0.5782650175, 1.8917509966
Zn, 0, -1.586440054, 0.3927416173, 0.0386128733
O, 0, -3.5051433553, 0.0589274012, 0.014669676
C, 0, -4.3672938951, 0.0101210676, 1.2208167647
H, 0, -3.8184099321, -0.5342857152, 1.9909388922
H, 0, -4.5326387807, 1.0433766439, 1.5375636072
C, 0, -4.2825864969, -0.2820381298, -1.2018178304
H, 0, -4.0213863951, 0.4506614786, -1.9670424883
H, 0, -3.968702418, -1.2809565931, -1.5162161844
C, 0, -5.6393147068, -0.6735607509, 0.7366183791
H, 0, -6.5082666513, -0.3654421313, 1.323573519
H, 0, -5.5436051874, -1.7617685585, 0.8122055995
C, 0, -5.7319983271, -0.2341299284, -0.7360491576
H, 0, -6.1273090742, 0.7841248621, -0.8136197769
H, 0, -6.3667682434, -0.893571422, -1.333317072
C, 0, 1.9708658194, -1.9374630087, 0.0787445597
C, 0, 2.5503707961, -4.6884040834, -0.0651309223
C, 0, 1.8985143794, -2.6234994642, -1.1470875306
C, 0, 2.336403904, -2.6559024102, 1.2319529796
C, 0, 2.6239401791, -4.021361194, 1.1595310171
C, 0, 2.1868916156, -3.9891218864, -1.2177128536
H, 0, 1.6136941071, -2.0992532916, -2.0563914941
H, 0, 2.39732298, -2.159292457, 2.1977436134
H, 0, 2.9055705632, -4.5622442893, 2.059078356
H, 0, 2.1284682579, -4.5047763009, -2.1726562694
H, 0, 2.7754333173, -5.7498433875, -0.1207541691

Vinyl dimer 22a

-1995.718924

Zn, 0, 0.7174065988, -1.4889811779, -0.2121033621
C, 0, 0.4702689151, -3.3447012198, -0.7748567787
H, 0, 0.4418593256, -3.5765012727, -1.8441542495
C, 0, 0.3036158885, -4.3811508937, 0.0604012908
H, 0, 0.1529728828, -5.4050445589, -0.2913177603
H, 0, 0.3060078843, -4.2653967748, 1.1443192561
O, 0, 2.7460339077, -0.9194379445, 0.2206209996

C, 0, 3.8279094907, -1.4666863482, -0.5834139882
H, 0, 4.2498591527, -2.3206664181, -0.041735725
H, 0, 3.4087080514, -1.8181450911, -1.5291989438
C, 0, 3.1206939816, 0.3791445717, 0.7657201766
H, 0, 2.5836409801, 1.152704282, 0.2069962591
H, 0, 2.8003552822, 0.401380324, 1.808739687
C, 0, 4.8325719621, -0.3250001827, -0.7389188273
H, 0, 5.8552939662, -0.6902923487, -0.8706767677
H, 0, 4.5750946501, 0.2942323192, -1.6055531498
C, 0, 4.6319706026, 0.4679575432, 0.5626927087
H, 0, 5.1616748544, -0.0145344515, 1.3924318262
H, 0, 4.9770580183, 1.5035856383, 0.4932310522
Cl, 0, 0.2564163528, 0.3980234011, -1.6939660657
Cl, 0, -0.2728341251, -0.3674563297, 1.6498752452
Zn, 0, -0.7340536851, 1.5194274135, 0.1678974898
O, 0, -2.7625958071, 0.9495976832, -0.2646306219
C, 0, -0.4867764372, 3.375114432, 0.7307060729
H, 0, -0.4583680843, 3.6067109576, 1.8000523342
C, 0, -0.3198130115, 4.4116887903, -0.1043303092
H, 0, -0.1689563327, 5.4354732159, 0.2476113911
H, 0, -0.3221626721, 4.2961564601, -1.1882727796
C, 0, -3.8445510226, 1.496629967, 0.539467748
H, 0, -3.425531062, 1.8475000303, 1.4855547538
H, 0, -4.2661515349, 2.3509933305, -0.0018685003
C, 0, -3.136964131, -0.3491046743, -0.8096055258
H, 0, -2.8159538925, -0.3716072173, -1.852410442
H, 0, -2.6003487865, -1.1225933032, -0.2503527149
C, 0, -4.8495228116, 0.355090412, 0.6941508432
H, 0, -5.872242908, 0.7205710758, 0.8253994073
H, 0, -4.5926973579, -0.2643773699, 1.5608118384
C, 0, -4.6483614386, -0.4376881251, -0.6074872664
H, 0, -5.1774560462, 0.0450638333, -1.4374620623
H, 0, -4.9936976008, -1.4732562787, -0.5383917398

Vinyl dimer cation 24a

-1917.518795

Zn, 0, 1.818493063, -1.3909725392, -0.0893495417
C, 0, 1.8207648046, -3.3155540252, -0.1927815652
H, 0, 2.1249059261, -3.7805337417, -1.1313574699
C, 0, 1.4589014045, -4.1073537946, 0.8253722471
H, 0, 1.4671533462, -5.1945800367, 0.7378450703
H, 0, 1.1408245665, -3.7209891114, 1.7920920639
O, 0, 3.0607920457, 0.1706994079, -0.0608317902
C, 0, 4.5226364471, -0.0310329925, -0.0564743882
H, 0, 4.8014673288, -0.3990779422, 0.9353350201
H, 0, 4.7524607233, -0.7873502253, -0.8096838733
C, 0, 2.7332081649, 1.6059579963, -0.0254309616
H, 0, 2.3389640257, 1.8732602356, -1.0097688564
H, 0, 1.9629763058, 1.7434335906, 0.7352084629
C, 0, 5.0934092862, 1.350328906, -0.3543545712

H, 0, 6.0963058547, 1.4721532826, 0.0627643779
H, 0, 5.1490290913, 1.517347204, -1.4353332219
C, 0, 4.0596265302, 2.2902762246, 0.2893838401
H, 0, 4.2135881826, 2.3498303492, 1.3721013887
H, 0, 4.0980784198, 3.304205778, -0.1171758584
Cl, 0, 0.0600165731, -0.2886934435, -1.934269668
Cl, 0, 0.0532694844, -0.4483144999, 1.6870480787
Zn, 0, -1.1862573129, -0.259289806, -0.1324495596
O, 0, -3.125696206, -0.1106557539, -0.084648711
C, 0, -3.9359170827, 0.0027650227, 1.1533891915
H, 0, -3.5165444745, -0.693474632, 1.8814345867
H, 0, -3.8293232032, 1.0300367185, 1.5118442966
C, 0, -4.0017509058, -0.1998902458, -1.2795206689
H, 0, -3.5902369918, 0.4746232137, -2.0320885422
H, 0, -3.9570532335, -1.2324733013, -1.6358831679
C, 0, -5.3522516011, -0.3234950915, 0.697605557
H, 0, -6.0988631305, 0.1646872125, 1.3290812668
H, 0, -5.5279793497, -1.4037638838, 0.7322257813
C, 0, -5.3775865568, 0.1874705757, -0.7545534486
H, 0, -5.5081566862, 1.2743489681, -0.7823752178
H, 0, -6.1750766399, -0.2676830196, -1.3473445474

Vinyl DMC dimer 22b

-2640.837329

Zn, 0, -1.5658447874, 0.0941134772, 0.5199064488
Cl, 0, -0.0601782983, -0.2269080665, -1.2907672295
Cl, 0, 0.3974214068, -0.3238230871, 2.1584873543
Zn, 0, 1.7513244173, -0.5960245575, 0.2818328181
O, 0, 1.3237851573, -2.9268055922, 0.1306479626
C, 0, 0.4712714712, -3.6610834377, 1.0397156145
H, 0, -0.5086561207, -3.1728001437, 1.0975644347
H, 0, 0.93771193, -3.6281807712, 2.0270227191
C, 0, 1.3238145289, -3.5589338645, -1.1730309755
H, 0, 2.3487257411, -3.884737292, -1.3862648649
H, 0, 1.0246124625, -2.8176307074, -1.918232122
C, 0, 0.3676357919, -5.0585278016, 0.4324393145
H, 0, -0.5228911299, -5.5971627128, 0.7708991245
H, 0, 1.2502805816, -5.656363313, 0.6900602028
C, 0, 0.3498815624, -4.7399064464, -1.0712670784
H, 0, -0.6560432836, -4.4324922946, -1.3793966019
H, 0, 0.6537261795, -5.583378767, -1.698873901
C, 0, 3.7034223764, -0.7628285431, -0.0239529025
O, 0, 2.4820790004, 1.6463489781, 0.1160885587
O, 0, 4.4007665207, 0.4630893862, -0.2293951484
C, 0, 3.6929553759, 1.6027438638, -0.1365011722
N, 0, 4.4552300419, 2.7128103229, -0.3462044629
C, 0, 3.8402998225, 4.0275091131, -0.2941119193
H, 0, 2.8000781945, 3.9212763555, 0.0083292997
H, 0, 3.8839887598, 4.5160125654, -1.2773451448
H, 0, 4.3669640005, 4.6633346155, 0.429432297

C, 0, 5.8710195176, 2.6724816578, -0.6821308011
H, 0, 6.2258107713, 1.6450337339, -0.6743006378
H, 0, 6.4467755046, 3.2580745057, 0.0464796209
H, 0, 6.0388015735, 3.1039292443, -1.6783138053
C, 0, 4.4983297424, -1.8362138648, -0.0487630873
H, 0, 5.5747911695, -1.7753107846, -0.2074460086
H, 0, 4.0655735128, -2.8181171853, 0.1062530892
O, 0, -1.4166352294, 2.2023196132, 0.6858759094
C, 0, -0.6248659335, 2.9044000547, 1.6875673709
H, 0, -1.0610760062, 2.6771808045, 2.6626137541
H, 0, 0.4003888411, 2.5277119072, 1.6524566058
C, 0, -1.5688709497, 3.0234123791, -0.5101704174
H, 0, -1.2443083851, 2.4353573044, -1.3697210766
H, 0, -2.6333862435, 3.2541404011, -0.6121165043
C, 0, -0.714620949, 4.370827689, 1.2765204492
H, 0, 0.119170107, 4.9604149381, 1.6699249473
H, 0, -1.6500149476, 4.8180517634, 1.6336025683
C, 0, -0.7145278755, 4.2670412524, -0.2570760257
H, 0, -1.1210682926, 5.1541560267, -0.7523502317
H, 0, 0.3046952894, 4.1034993096, -0.6243051902
C, 0, -3.0326646981, -1.0086583427, 1.2773352624
C, 0, -3.0792754588, -1.7978712913, 2.3540785507
H, 0, -3.972113169, -2.3499287952, 2.6473632136
H, 0, -2.1963169484, -1.8955873305, 2.9764017823
O, 0, -4.2578306888, -0.9687420206, 0.5456619854
O, 0, -3.3667851433, 0.5631701421, -0.8886880542
C, 0, -4.3084225793, -0.1541498988, -0.5227211951
N, 0, -5.5065665338, -0.194344998, -1.1664386943
C, 0, -5.709229365, 0.6142786757, -2.3577591185
H, 0, -5.9316252186, -0.0267814184, -3.2210524159
H, 0, -4.8047395146, 1.1858370637, -2.5580533536
H, 0, -6.5528061637, 1.3020119467, -2.2128276174
C, 0, -6.6185374921, -1.039402011, -0.7562611918
H, 0, -6.8622313493, -1.7590900779, -1.5492614703
H, 0, -7.5079552257, -0.4243884405, -0.5664096686
H, 0, -6.3596645719, -1.5813700334, 0.1499503304

Vinyl DMC dimer cation 24b

-2240.107586

Zn, 0, -0.637376877, 1.7020206346, 0.2600710412
Cl, 0, 0.4301545256, 0.6142254124, -1.724028924
Cl, 0, 1.2537194828, 0.9645725377, 1.6572485433
O, 0, -0.2700631218, 3.6554926349, -0.0230420757
O, 0, -0.8571888631, -1.5767205148, 0.5054303085
C, 0, -2.337710333, 0.8434299238, 0.755777967
C, 0, -3.2476505189, 1.3801818007, 1.5715590687
H, 0, -4.1933285089, 0.8920581592, 1.8001999401
H, 0, -3.0574543662, 2.3389367436, 2.0437369091
O, 0, -2.7837688098, -0.3802889635, 0.1523902386
C, 0, -2.0341735634, -1.4705057827, 0.0496722274

N, 0, -2.6529258408, -2.500902065, -0.5451808463
C, 0, -1.9922410708, -3.7982484054, -0.6770562167
H, 0, -2.6506087239, -4.5785973761, -0.2813148545
H, 0, -1.0602734843, -3.7982823971, -0.1162535613
H, 0, -1.7893732183, -4.0128616003, -1.7326212356
C, 0, -4.0257369716, -2.4305099716, -1.0537025157
H, 0, -4.6881478077, -3.0406326122, -0.4291875959
H, 0, -4.0450218301, -2.8228830051, -2.0753390471
H, 0, -4.3767457759, -1.4021615261, -1.0570751752
C, 0, 0.9516593512, 4.3582283896, 0.3980710893
H, 0, 1.8037774828, 3.878695065, -0.0926459881
H, 0, 1.0354543755, 4.2390396777, 1.4791896429
C, 0, -0.9955282798, 4.4390176661, -1.0375053004
H, 0, -1.9335898837, 4.7653516196, -0.5796077415
H, 0, -1.2065213985, 3.7803666758, -1.8830104208
C, 0, -0.0626451366, 5.6003798408, -1.3737330062
H, 0, 0.6060023196, 5.3278553611, -2.1971870928
H, 0, -0.6186819886, 6.494286721, -1.6678167267
C, 0, 0.7342608762, 5.7909428474, -0.0717205158
H, 0, 1.6806569172, 6.3156352791, -0.226762802
H, 0, 0.1480254171, 6.3515053831, 0.6644052596
Zn, 0, 0.8620991588, -0.7051074013, 0.118792581
O, 0, 2.3270856882, -2.0461556953, 0.0019082867
C, 0, 3.1068549558, -2.2974736614, -1.2261840952
H, 0, 3.0732337472, -1.3908687964, -1.8334166606
H, 0, 2.6109707764, -3.1158201754, -1.7560584639
C, 0, 3.0862737076, -2.4695895042, 1.1938186152
H, 0, 2.3878950435, -2.9945480916, 1.8484760915
H, 0, 3.4567499339, -1.5686205007, 1.6917603958
C, 0, 4.2077007548, -3.3350467392, 0.6328494854
H, 0, 5.0787421735, -3.3468056635, 1.2930669853
H, 0, 3.8664556686, -4.3669692178, 0.4976930142
C, 0, 4.4976865686, -2.6743202633, -0.7261697021
H, 0, 5.1145290999, -1.7786924203, -0.5957193931
H, 0, 5.0101053479, -3.3428423228, -1.4227313335

F2 Vinyl DMC dimer 22c

-3037.765927

Zn, 0, -1.5495595247, 0.455266391, 0.2460631853
Cl, 0, -0.0403265419, 0.4008904505, -1.6043056142
Cl, 0, 0.3718477205, -0.028234514, 1.8205863978
Zn, 0, 1.6617075556, -0.3789060345, -0.1024988412
O, 0, 0.7317626585, -2.4700036733, -0.3126586665
C, 0, 0.6924799051, -3.4229292203, 0.7833183917
H, 0, -0.1773421882, -3.1787064619, 1.3985145397
H, 0, 1.5993372906, -3.3029473648, 1.3822027779
C, 0, 0.6127174586, -3.1520446613, -1.5786500985
H, 0, 1.6133446853, -3.2965605041, -2.0056019804
H, 0, 0.0252854395, -2.5117754202, -2.2396042014
C, 0, 0.5881195937, -4.8058100235, 0.1273163002

H, 0, -0.0038499565, -5.5036855775, 0.7270935821
H, 0, 1.5856840316, -5.2370847021, -0.0130256236
C, 0, -0.0454499149, -4.4870796925, -1.2372062599
H, 0, -1.1302374092, -4.3614773975, -1.1396787737
H, 0, 0.1459407142, -5.2555187968, -1.9926633825
C, 0, 3.5872244208, -0.7956607354, -0.3794504759
O, 0, 2.7177764358, 1.7112251687, -0.0892362006
O, 0, 4.4724965652, 0.3063463602, -0.4508124607
C, 0, 3.9234621608, 1.5266850758, -0.2887415828
N, 0, 4.8426723482, 2.5253681666, -0.3683394878
C, 0, 4.416014831, 3.906976634, -0.2221149976
H, 0, 3.3429326006, 3.930983887, -0.040748757
H, 0, 4.6432419612, 4.4764094081, -1.133090836
H, 0, 4.9383723857, 4.3798137787, 0.6198909458
C, 0, 6.2618473826, 2.3030125235, -0.6098166973
H, 0, 6.4647460291, 1.2381691369, -0.6939071655
H, 0, 6.8532267194, 2.7179373304, 0.2168619475
H, 0, 6.569944702, 2.8028358904, -1.5376534479
C, 0, 4.233056217, -1.9524426378, -0.4923228528
O, 0, -1.5159036283, 2.5372552871, 0.7144752264
C, 0, -1.0552869759, 3.1118010336, 1.9729980809
H, 0, -1.8354309598, 2.9461036465, 2.7217396408
H, 0, -0.1506098972, 2.5782976575, 2.2706401336
C, 0, -1.4167028585, 3.5158439743, -0.3572790144
H, 0, -1.0688402346, 2.9955717338, -1.2492845451
H, 0, -2.4176416815, 3.9235963748, -0.5404186866
C, 0, -0.7932545839, 4.5901135833, 1.6727694229
H, 0, 0.009926537, 4.9952235172, 2.2954487023
H, 0, -1.6941733159, 5.1901104261, 1.8476822972
C, 0, -0.449315041, 4.5675220433, 0.1748895862
H, 0, -0.577847769, 5.5384029371, -0.3135818042
H, 0, 0.5829230564, 4.2319917894, 0.0226851046
C, 0, -3.0998470093, -0.7128933415, 0.6721492144
C, 0, -3.2312013755, -1.7115197722, 1.541243121
O, 0, -4.2870285509, -0.5113705386, -0.0754344717
O, 0, -3.2726730569, 1.193121571, -1.1908819467
C, 0, -4.2597601009, 0.4767556327, -0.9893434697
N, 0, -5.4355092872, 0.6018212434, -1.6607060936
C, 0, -5.5520936422, 1.5900910136, -2.7210018156
H, 0, -5.735874992, 1.098251635, -3.685560346
H, 0, -4.6262618389, 2.1597467749, -2.7794393036
H, 0, -6.3887416673, 2.2701539131, -2.5153326568
C, 0, -6.5867896023, -0.2632996752, -1.4421518528
H, 0, -6.7821834492, -0.8748069901, -2.3335247845
H, 0, -7.4765621581, 0.3473182737, -1.2431753399
H, 0, -6.4063554547, -0.9186496823, -0.593358513
F, 0, 3.6290984956, -3.1471009761, -0.4549805319
F, 0, 5.5484082763, -2.1201692305, -0.6571792453
F, 0, -4.3245150143, -2.4584954917, 1.7286649911
F, 0, -2.2613694967, -2.1127791476, 2.3642712359

F2 Vinyl DMC dimer cation 24c

-2438.571770

Zn, 1.4266642307, -0.1801766394, -0.0898566568
Cl, -0.172109605, -0.8424234297, -1.8358717397
Cl, 0.0585274699, -1.380659084, 1.6038102609
O, 3.0146702183, -1.3597462066, -0.3234375577
O, -1.5362475716, 1.4915325689, 0.2787867337
C, 1.302242902, 1.7517381116, 0.2395272415
C, 2.2076833703, 2.4002624637, 0.9716961914
O, 0.3618381556, 2.6350093538, -0.3546689469
C, -0.9560500232, 2.5133952953, -0.1846731767
N, -1.6329157518, 3.6076755967, -0.5511919626
C, -3.0950587245, 3.6122378085, -0.5882810012
H, -3.4789589666, 4.3753878233, 0.0967141604
H, -3.4744775012, 2.6377773072, -0.2889902993
H, -3.4364543292, 3.8445745189, -1.6029778031
C, -0.9610311003, 4.8366605264, -0.9911194167
H, -1.559427614, 5.689726747, -0.6615920984
H, -0.8749134651, 4.8623166616, -2.0831827491
H, 0.0315651983, 4.9013824337, -0.5497259376
C, 2.9699832141, -2.8297987921, -0.3708022226
H, 2.5747876935, -3.1144210312, -1.350491212
H, 2.2866882453, -3.1574494699, 0.4139907659
C, 4.3981391778, -0.8716106223, -0.4483300513
H, 4.6903615272, -0.4615995543, 0.522318406
H, 4.4009205757, -0.0790478988, -1.1997085577
C, 5.2033635623, -2.1076555512, -0.8385917726
H, 5.2140950351, -2.2305542357, -1.9268616685
H, 6.2380698833, -2.0421150921, -0.492428819
C, 4.420754314, -3.2526651395, -0.1721136742
H, 4.6259041711, -4.2258967876, -0.6255369664
H, 4.6589272336, -3.3145014412, 0.8952006235
Zn, -1.4005394881, -0.4616264017, 0.0884860098
O, -3.2297223925, -1.2495432404, 0.1479729234
C, -3.8821082379, -1.8802709955, -1.0154838098
H, -3.0971730153, -2.1967373674, -1.7048719004
H, -4.5034507803, -1.1141935985, -1.4886404368
C, -3.8206280549, -1.7460079883, 1.4059267898
H, -3.994020587, -0.8773558982, 2.044239236
H, -3.0910057277, -2.411838287, 1.8759313143
C, -5.0862098001, -2.4737435806, 0.9664323637
H, -5.363649871, -3.2622585882, 1.6706838038
H, -5.9252946999, -1.7741295588, 0.8885788536
C, -4.7023776751, -3.0187999676, -0.4202417574
H, -4.0912091856, -3.92272413, -0.3246870441
H, -5.5718816269, -3.2579276553, 1.0379604553
F, 3.2365803793, 1.7731234435, 1.5387717584

F, 2.240917161, 3.6949991566, 1.2329917517

Vinyl MEM dimer 22d

-2761.481006

Zn, 0, -1.5658447874, 0.0941134772, 0.5199064488
Cl, 0, -0.0601782983, -0.2269080665, -1.2907672295
Cl, 0, 0.3974214068, -0.3238230871, 2.1584873543
Zn, 0, 1.7513244173, -0.5960245575, 0.2818328181
O, 0, 1.3237851573, -2.9268055922, 0.1306479626
C, 0, 0.4712714712, -3.6610834377, 1.0397156145
H, 0, -0.5086561207, -3.1728001437, 1.0975644347
H, 0, 0.93771193, -3.6281807712, 2.0270227191
C, 0, 1.3238145289, -3.5589338645, -1.1730309755
H, 0, 2.3487257411, -3.884737292, -1.3862648649
H, 0, 1.0246124625, -2.8176307074, -1.918232122
C, 0, 0.3676357919, -5.0585278016, 0.4324393145
H, 0, -0.5228911299, -5.5971627128, 0.7708991245
H, 0, 1.2502805816, -5.656363313, 0.6900602028
C, 0, 0.3498815624, -4.7399064464, -1.0712670784
H, 0, -0.6560432836, -4.4324922946, -1.3793966019
H, 0, 0.6537261795, -5.583378767, -1.698873901
C, 0, 3.7034223764, -0.7628285431, -0.0239529025
O, 0, 2.4820790004, 1.6463489781, 0.1160885587
O, 0, 4.4007665207, 0.4630893862, -0.2293951484
C, 0, 3.6929553759, 1.6027438638, -0.1365011722
N, 0, 4.4552300419, 2.7128103229, -0.3462044629
C, 0, 3.8402998225, 4.0275091131, -0.2941119193
H, 0, 2.8000781945, 3.9212763555, 0.0083292997
H, 0, 3.8839887598, 4.5160125654, -1.2773451448
H, 0, 4.3669640005, 4.6633346155, 0.429432297
C, 0, 5.8710195176, 2.6724816578, -0.6821308011
H, 0, 6.2258107713, 1.6450337339, -0.6743006378
H, 0, 6.4467755046, 3.2580745057, 0.0464796209
H, 0, 6.0388015735, 3.1039292443, -1.6783138053
C, 0, 4.4983297424, -1.8362138648, -0.0487630873
H, 0, 5.5747911695, -1.7753107846, -0.2074460086
H, 0, 4.0655735128, -2.8181171853, 0.1062530892
O, 0, -1.4166352294, 2.2023196132, 0.6858759094
C, 0, -0.6248659335, 2.9044000547, 1.6875673709
H, 0, -1.0610760062, 2.6771808045, 2.6626137541
H, 0, 0.4003888411, 2.5277119072, 1.6524566058
C, 0, -1.5688709497, 3.0234123791, -0.5101704174
H, 0, -1.2443083851, 2.4353573044, -1.3697210766
H, 0, -2.6333862435, 3.2541404011, -0.6121165043
C, 0, -0.714620949, 4.370827689, 1.2765204492
H, 0, 0.119170107, 4.9604149381, 1.6699249473
H, 0, -1.6500149476, 4.8180517634, 1.6336025683
C, 0, -0.7145278755, 4.2670412524, -0.2570760257
H, 0, -1.1210682926, 5.1541560267, -0.7523502317

H, 0, 0.3046952894, 4.1034993096, -0.6243051902
C, 0, -3.0326646981, -1.0086583427, 1.2773352624
C, 0, -3.0792754588, -1.7978712913, 2.3540785507
H, 0, -3.972113169, -2.3499287952, 2.6473632136
H, 0, -2.1963169484, -1.8955873305, 2.9764017823
O, 0, -4.2578306888, -0.9687420206, 0.5456619854
O, 0, -3.3667851433, 0.5631701421, -0.8886880542
C, 0, -4.3084225793, -0.1541498988, -0.5227211951
N, 0, -5.5065665338, -0.194344998, -1.1664386943
C, 0, -5.709229365, 0.6142786757, -2.3577591185
H, 0, -5.9316252186, -0.0267814184, -3.2210524159
H, 0, -4.8047395146, 1.1858370637, -2.5580533536
H, 0, -6.5528061637, 1.3020119467, -2.2128276174
C, 0, -6.6185374921, -1.039402011, -0.7562611918
H, 0, -6.8622313493, -1.7590900779, -1.5492614703
H, 0, -7.5079552257, -0.4243884405, -0.5664096686
H, 0, -6.3596645719, -1.5813700334, 0.1499503304

Vinyl MEM dimer cation 24d

-2300.437232

Zn, 0, -1.5956093079, -0.9482206195, -0.0125488956
Cl, 0, -0.1706103697, 0.4325023249, -1.4954606991
Cl, 0, -0.0298999292, -0.4302470639, 1.8510179214
O, 0, -3.1351673228, 0.3113267358, 0.4003905324
C, 0, -1.7785283621, -2.8565122062, -0.4512173474
C, 0, -2.8702542394, -3.5602136009, -0.12835675
H, 0, -2.936845521, -4.6337774843, -0.298338172
H, 0, -3.7291389933, -3.0738170822, 0.3223688634
O, 0, -0.7223206133, -3.6221317773, -0.9904776541
C, 0, 0.2851271403, -2.981251799, -1.6679442028
C, 0, -3.9787069103, 0.9041315941, -0.6460981644
H, 0, -4.6973174571, 0.1399687259, -0.9571934304
H, 0, -3.3319973407, 1.1660896445, -1.4862776411
C, 0, -3.4024596277, 0.9346187184, 1.701005853
H, 0, -2.5728581747, 1.611073217, 1.9275196524
H, 0, -3.4349902016, 0.1366002052, 2.4452614994
C, 0, -4.723438256, 1.6687426187, 1.5000915653
H, 0, -5.5677618769, 0.9894383929, 1.6597104158
H, 0, -4.82946433, 2.5124232429, 2.1871549246
C, 0, -4.6459496763, 2.1021909228, 0.0260454755
H, 0, -5.6261996808, 2.3172284978, -0.4071558693
H, 0, -4.0228230922, 2.9968936028, -0.0797448935
Zn, 0, 1.4256730288, -0.4224844295, 0.0580399152
O, 0, 2.6292223687, 1.2601261327, -0.0504935274
C, 0, 2.1335532113, 2.5089779659, 0.5455941446
H, 0, 1.0927811519, 2.6454475167, 0.2365601212
H, 0, 2.1840593428, 2.3842536494, 1.6289019785
C, 0, 3.3846631758, 1.5576515553, -1.2790922751
H, 0, 2.9352812611, 0.9976913673, -2.1029219917
H, 0, 4.4079507157, 1.2093827143, -1.110227435

C, 0, 3.2946775291, 3.0743580145, -1.4564871066
H, 0, 4.2022495174, 3.4846528681, -1.9066472846
H, 0, 2.4478663187, 3.331867257, -2.1006842253
C, 0, 3.0520811002, 3.5806799061, -0.0244531207
H, 0, 3.9897293787, 3.6258310898, 0.540353953
H, 0, 2.589605718, 4.5708984739, 0.0015459247
H, 0, 0.7902007521, -3.7328895341, -2.2801407556
H, 0, -0.0489640595, -2.1317644938, -2.2645433286
O, 0, 1.3078871955, -2.4152708431, -0.7804184496
C, 0, 1.8916657642, -3.3746544713, 0.1252815665
H, 0, 1.2500568716, -3.4788282211, 1.0047235521
H, 0, 1.9777477063, -4.3473156637, -0.3704279249
C, 0, 3.2663896485, -2.8563890166, 0.4939148065
H, 0, 3.9581103903, -2.9119831894, -0.3567817273
H, 0, 3.6752236338, -3.4388561277, 1.3283244971
O, 0, 3.119289201, -1.4840859599, 0.8899859713
C, 0, 4.2911935826, -0.9312479154, 1.5099998103
H, 0, 4.0734954056, 0.112746269, 1.7265471482
H, 0, 5.1486162637, -1.0011300141, 0.8302122361
H, 0, 4.5055564689, -1.4728528108, 2.4371583438

F2 Vinyl MEM dimer 22e

-3158.410144

Zn, 0, 1.8696254222, -0.8412182708, -0.1977563636
C, 0, 3.7222324296, -0.6456573106, -0.8607223946
C, 0, 4.5943262125, -1.6530136378, -0.8464456515
O, 0, 1.3026211969, -2.9066564437, -0.0173007945
C, 0, 1.3444789996, -3.7783415372, -1.1802578311
H, 0, 0.4051219884, -3.645727543, -1.7265789763
H, 0, 2.1785892493, -3.4641502714, -1.8113130359
C, 0, 1.2472756223, -3.683491983, 1.2120421951
H, 0, 2.2433687623, -3.6780737502, 1.6702677051
H, 0, 0.5340924804, -3.1979064152, 1.8783717976
C, 0, 1.5075294242, -5.1917366137, -0.6185384023
H, 0, 2.5706585343, -5.4322865335, -0.5062324416
H, 0, 1.0510898744, -5.947840295, -1.2640927121
C, 0, 0.8357882393, -5.0827715737, 0.7600139045
H, 0, -0.2543000484, -5.1450307776, 0.6645769248
H, 0, 1.1629912208, -5.8562340241, 1.4610998561
C, 0, 3.3412809508, 1.5796139165, -1.5773960609
O, 0, 4.2719533395, 0.574715519, -1.2709562412
H, 0, 2.6162489453, 1.2476427586, -2.3281550676
H, 0, 3.9451067504, 2.4097392329, -1.9637492825
O, 0, 2.558431182, 1.9745876252, -0.4717858705
C, 0, 3.2961542279, 2.5434528261, 0.615513359
H, 0, 4.2706303592, 2.0498977214, 0.7044491503
H, 0, 2.7163205361, 2.3272060525, 1.516568948
C, 0, 3.4948317545, 4.0438677009, 0.4791421115
H, 0, 4.1966947796, 4.3776895652, 1.2636242598
H, 0, 3.9529124522, 4.2923974492, -0.4932692217

O, 0, 2.2516117477, 4.7082059647, 0.6183526098
 C, 0, 2.378446119, 6.1118278904, 0.5267977648
 H, 0, 3.0406902712, 6.5125864948, 1.3110421238
 H, 0, 1.380134704, 6.538494936, 0.6551271104
 H, 0, 2.7762665239, 6.421377894, -0.4528889285
 Cl, 0, -0.0809356795, -0.3215028864, -1.5218649886
 Cl, 0, 0.8669037871, -0.1845097675, 1.8254114527
 Zn, 0, -1.263690364, -0.1751848288, 0.5455168368
 C, 0, -2.6852166491, -1.4200953152, 1.1240534679
 C, 0, -2.5836676677, -2.2149765933, 2.189281167
 O, 0, -3.9256828825, -1.4813863852, 0.4796774009
 O, 0, -1.4782868047, 1.9138965843, 0.7355988138
 C, 0, -1.4796521052, 2.5486375558, 2.0497406909
 H, 0, -2.5135154248, 2.5315235051, 2.4101070601
 H, 0, -0.8510942188, 1.9585735673, 2.7206410459
 C, 0, -0.9513043783, 2.8375305788, -0.2664674551
 H, 0, -1.4767294131, 2.6210155832, -1.1981457698
 H, 0, 0.1196968848, 2.6556376088, -0.3935601777
 C, 0, -0.9525901543, 3.9714124588, 1.8215874894
 H, 0, -1.4457315867, 4.697755939, 2.4747583165
 H, 0, 0.1256927728, 4.0176230492, 2.0003401625
 C, 0, -1.2280098787, 4.2121456279, 0.3275831001
 H, 0, -2.2715602007, 4.5060727721, 0.1604227368
 H, 0, -0.575323093, 4.9762940618, -0.1022871203
 O, 0, -3.564983732, 0.2933094175, -1.01507547
 C, 0, -3.9079628817, -1.0720480564, -0.8647748953
 H, 0, -4.9119757297, -1.2654784306, -1.2470844516
 H, 0, -3.1489898524, -1.6159496274, -1.4377088023
 C, 0, -4.5679444045, 1.2118134208, -0.575649602
 H, 0, -5.1626788138, 0.7700844696, 0.2323983493
 H, 0, -4.0355681, 2.0797937113, -0.1741299128
 C, 0, -5.4688326843, 1.656599123, -1.7158329017
 H, 0, -4.8483379397, 1.9825567763, -2.5672602922
 H, 0, -6.0716917837, 2.5229607327, -1.387472257
 O, 0, -6.3098521412, 0.5843867531, -2.0950043469
 C, 0, -7.1215182859, 0.8876841739, -3.2092203333
 H, 0, -7.7888486431, 1.7408477417, -3.0052758976
 H, 0, -7.7297851576, 0.00360405, -3.4164631969
 H, 0, -6.5178739571, 1.1250427241, -4.0998740399
 F, 0, 4.2844874942, -2.9003486942, -0.4446523994
 F, 0, 5.8817822333, -1.6021547559, -1.1926568217
 F, 0, -3.52236041, -3.0418341097, 2.6559338118
 F, 0, -1.4969849061, -2.2763747023, 2.9765888853

F2 Vinyl MEM dimer cation 24e

-2498.901129

Zn, 0, -1.4708455429, 0.1744821637, -0.0255429575
 Cl, 0, 0.2953304831, 0.9572899595, -1.5161895447
 Cl, 0, 0.1266585718, 0.2991249057, 1.8723920643
 O, 0, -2.6131306901, 1.8045877184, 0.2996788603

C, 0, -2.1145166609, -1.6384860781, -0.4163557849
C, 0, -3.4007178628, -1.9468249795, -0.2497270827
O, 0, -1.303462427, -2.7394936105, -0.7561737056
C, 0, -0.1442954672, -2.4856108489, -1.4510368311
C, 0, -2.9502938067, 2.8103327417, -0.7133167766
H, 0, -3.5095985488, 2.3133972698, -1.5131262538
H, 0, -2.0105018859, 3.2000236786, -1.1080807807
C, 0, -3.4924557507, 1.9293594059, 1.4731916445
H, 0, -2.8701882158, 2.2713273528, 2.3049908813
H, 0, -3.8970683973, 0.9396655166, 1.6918342744
C, 0, -4.5472579065, 2.9527034854, 1.058620006
H, 0, -5.3978955801, 2.4530786292, 0.5830044827
H, 0, -4.9206911086, 3.5201669064, 1.9149565766
C, 0, -3.7979109307, 3.828850835, 0.0401505039
H, 0, -4.4702508213, 4.3734172919, -0.6279493694
H, 0, -3.1576704866, 4.556213606, 0.5510400652
Zn, 0, 1.573191585, -0.1978686389, 0.1555350847
O, 0, 3.2206247484, 1.0110537589, -0.1142424637
C, 0, 3.1454035893, 2.417623143, 0.3134501116
H, 0, 2.1780129166, 2.8188231709, -0.0031823845
H, 0, 3.2086494068, 2.422011628, 1.4035148673
C, 0, 4.0252081689, 0.9021711554, -1.3429432804
H, 0, 3.4372773206, 0.3646520793, -2.0909163512
H, 0, 4.9167216992, 0.3218577427, -1.0865655381
C, 0, 4.3505719117, 2.3406737487, -1.7422931267
H, 0, 5.3184417903, 2.4132949735, -2.2450043662
H, 0, 3.5830291617, 2.7300105375, -2.4189756289
C, 0, 4.3125935415, 3.0881987757, -0.3988342132
H, 0, 5.2435749343, 2.9376094245, 0.1584337563
H, 0, 4.1544395919, 4.163435411, -0.5163454342
H, 0, 0.1325529476, -3.4112558024, -1.9622198158
H, 0, -0.2170203289, -1.6446726816, -2.141282835
O, 0, 0.9805719143, -2.145120695, -0.5759447314
C, 0, 1.277886043, -3.165396137, 0.4033148644
H, 0, 0.5971964966, -3.0618912183, 1.2526089894
H, 0, 1.1420587728, -4.1549939254, -0.04577925
C, 0, 2.7206301737, -2.9777556163, 0.8212092681
H, 0, 3.4115782237, -3.2276563715, 0.0052192164
H, 0, 2.9437145954, -3.6124374675, 1.6874724844
O, 0, 2.8860882029, -1.5982086996, 1.176274492
C, 0, 4.1299135742, -1.3106717243, 1.8338225186
H, 0, 4.1419722073, -0.2423055943, 2.041678208
H, 0, 4.9746964662, -1.5753527252, 1.1868724254
H, 0, 4.186768263, -1.874809745, 2.7704872088
F, 0, -4.3096769749, -1.0343728937, 0.1237957907
F, 0, -3.9660737082, -3.1319110626, -0.397101339

Vinyl DMC monomer (tetracoordinate) 25

-1553.13630221

Zn	0.92341100	-0.18392600	0.76738400
C	-0.92966100	-0.38603200	1.41798100
C	-1.27409200	-0.82119800	2.63289500
H	-2.29125400	-0.93546100	2.97791800
H	-0.46891500	-1.07838300	3.31232600
O	0.96148100	1.63635700	-0.47616000
O	1.19521100	-1.45016900	-1.02889900
C	0.55447700	2.87205100	0.17285600
H	0.30866000	2.64346300	1.21001300
H	-0.34354300	3.24550900	-0.33020900
C	2.09164900	1.88758100	-1.36316600
H	1.85027100	1.46469100	-2.33921300
H	2.95998400	1.37343700	-0.94605800
C	1.73699100	3.81834100	0.00219500
H	1.43970100	4.86734700	0.05176900
H	2.48432900	3.63120500	0.77721700
C	2.27610100	3.40565700	-1.37605200
H	1.67866700	3.86315700	-2.17013700
H	3.31866000	3.68847500	-1.52969300
C	2.29788500	-2.37514300	-1.17946700
H	2.68105600	-2.28278900	-2.20236300
H	3.06848800	-2.07523500	-0.47280600
C	0.04549800	-2.11163100	-1.60167900
H	-0.84222400	-1.59941600	-1.23729700
H	0.10224200	-2.01490400	-2.69280300
C	1.69498900	-3.76692300	-0.92355200
H	1.89237900	-4.09005600	0.09925200
H	2.12615100	-4.51069900	-1.59590300
C	0.16979200	-3.57385000	-1.15504100
H	-0.23085300	-4.25692800	-1.90603300
H	-0.38344700	-3.73250500	-0.22850000
Cl	3.01508500	-0.16517600	1.53190800
O	-1.85839800	0.02210300	0.42014600
C	-3.22021700	-0.07787900	0.51177200
O	-3.82708200	-0.64555200	1.39332000
N	-3.81764600	0.54052500	-0.55872800
C	-5.26776100	0.51900000	-0.65501000
H	-5.66655900	-0.05532700	0.17676800
H	-5.58344800	0.05851300	-1.59845400
H	-5.67347100	1.53707300	-0.61726400
C	-3.11280200	1.26491100	-1.60351300
H	-3.32252900	0.82182600	-2.58496800
H	-2.04289700	1.23711000	-1.42472500
H	-3.44346600	2.31077000	-1.63025100

Vinyl DMC 26

B3LYP/6-31G*

-401.133840464

C	2.95708000	-0.35729400	0.00509300
H	4.02674700	-0.17298100	0.00619000
H	2.59900300	-1.37495700	0.00824400
C	2.15689200	0.70619000	-0.00044500
H	2.54157800	1.72105100	-0.00359600
O	0.77516100	0.79116000	-0.00230200
C	-0.04331400	-0.31319600	-0.00445800
O	0.34823800	-1.46554800	-0.00115400
N	-1.35701700	0.06700800	-0.01469000
C	-1.83209500	1.44160500	0.00532300
H	-2.50120900	1.61958900	-0.84725400
H	-0.99460400	2.13214900	-0.05228400
H	-2.39637700	1.63958600	0.92746900
C	-2.37839700	-0.96760600	0.00494300
H	-3.03812700	-0.86862700	-0.86716300
H	-2.99227800	-0.88561000	0.91220600
H	-1.89379500	-1.94234500	-0.01607900

B3LYP/6-311G**

-401.248238904

C	2.95453900	-0.35832000	0.00146300
H	4.02166500	-0.17324300	0.00355700
H	2.59355400	-1.37272100	-0.00036100
C	2.15734000	0.70296500	0.00144100
H	2.54306200	1.71521400	0.00351200
O	0.77578500	0.78736800	-0.00073400
C	-0.04562100	-0.31563700	-0.00347900
O	0.34558900	-1.46081100	0.00082200
N	-1.35562000	0.06701500	-0.01419900
C	-1.82670900	1.44426100	0.00333600
H	-2.49304200	1.62206600	-0.84800400
H	-0.98940500	2.13072000	-0.05557100
H	-2.38770700	1.64507800	0.92370900
C	-2.37987700	-0.96613300	0.00463200
H	-3.03677000	-0.86677800	-0.86639700
H	-2.99173900	-0.88436500	0.91027100
H	-1.89930500	-1.94034100	-0.01638600

Vinyl DMC 27

B3LYP/6-31G*

-401.139789200

C	-3.25053500	0.46569800	0.00044800
H	-4.21858200	-0.02136800	0.00151500
H	-3.22021100	1.55042000	-0.00061000
C	-2.14498500	-0.27143400	0.00047500
H	-2.10963000	-1.35442900	0.00142900
O	-0.90325600	0.33312900	-0.00091400

C	0.19696800	-0.49849100	-0.00097700
O	0.11778300	-1.71395400	0.00055800
N	1.35488800	0.22006800	-0.00340400
C	1.43371900	1.67294300	0.00111200
H	1.97094100	2.02082700	0.89368700
H	0.43625100	2.10491100	-0.00299000
H	1.97987000	2.02467300	-0.88436800
C	2.61955900	-0.49807000	0.00097200
H	3.20062500	-0.24547300	0.89784400
H	3.21403300	-0.22932400	-0.88208300
H	2.41792400	-1.56799300	-0.00993000

Vinyl DMC 27

B3LYP/6-311G**

-401.253912049

C	-3.24744500	0.46391000	-0.00153500
H	-4.21249000	-0.02340700	-0.00072800
H	-3.21382700	1.54607000	-0.00460500
C	-2.14477900	-0.27139100	0.00109500
H	-2.11250600	-1.35254500	0.00387800
O	-0.90265500	0.33024900	0.00032000
C	0.19942500	-0.50033200	0.00007800
O	0.11883200	-1.70856200	0.00117800
N	1.35331800	0.21933400	-0.00244600
C	1.42864700	1.67361200	0.00181800
H	1.96156200	2.02155600	0.89388200
H	0.43262600	2.10243700	-0.00391400
H	1.97331800	2.02514600	-0.88154900
C	2.62008900	-0.49716600	-0.00124300
H	3.20291700	-0.24158300	0.89056600
H	3.20841300	-0.23284300	-0.88675600
H	2.42172500	-1.56547100	-0.00690800

Vinyl DMC Monomer THF 28a

B3LYP/6-311G**

-1553.14680994

Zn	-0.68470500	0.12447800	0.73667500
C	0.98478300	0.18632600	1.81808400
C	0.97697500	0.42994100	3.12968500
H	1.88707700	0.47119200	3.72386500
H	0.03202200	0.59024800	3.63267300
O	-1.21394400	-1.51685400	-0.52206500
O	-1.12370800	1.59155200	-0.82847900
C	-0.46687200	-2.75863000	-0.53518700
H	0.16079700	-2.77894300	0.35530300
H	0.17536400	-2.76909200	-1.42084200
C	-2.56695600	-1.73011200	-1.02194900
H	-2.73298300	-1.03322800	-1.84539500

H	-3.25537100	-1.49579500	-0.21026500
C	-1.53180100	-3.84777000	-0.57544300
H	-1.15329000	-4.78530400	-0.98637400
H	-1.91397800	-4.03987500	0.43024000
C	-2.61753700	-3.19937100	-1.44895700
H	-2.36174500	-3.30598700	-2.50776800
H	-3.60637500	-3.63413900	-1.29474600
C	-1.94444000	2.75805900	-0.59403600
H	-2.76640300	2.74890200	-1.31989400
H	-2.35638400	2.67185600	0.40849600
C	-0.30340700	1.91267800	-1.97199000
H	0.52669500	1.21197700	-1.98044900
H	-0.91185400	1.77952600	-2.87521600
C	-1.00255300	3.94749300	-0.82309500
H	-0.55999300	4.27040200	0.12069700
H	-1.53479700	4.79933600	-1.24978900
C	0.08975500	3.38698600	-1.77770400
H	0.12210000	3.91611300	-2.73178300
H	1.07732600	3.46466100	-1.32063400
Cl	-2.68321700	0.34988000	1.81674700
O	2.29732700	-0.01118300	1.29976000
C	2.46512500	-0.29012700	-0.00373200
O	1.55138400	-0.36658100	-0.81810000
N	3.77789600	-0.48592300	-0.32088600
C	4.14322900	-0.78353300	-1.69552000
H	3.24051500	-0.85665200	-2.29547100
H	4.68942800	-1.73202000	-1.74711200
H	4.78622300	0.00459900	-2.10459300
C	4.87311700	-0.38827400	0.63386900
H	5.44552900	-1.32213100	0.64442000
H	4.48404400	-0.20004500	1.62845400
H	5.55165900	0.42606400	0.35434300

Vinyl DMC Monomer DMF 28b

B3LYP/6-311G**

-1585.29493817

Zn	0.21389600	-0.00008800	0.73734000
Cl	2.25653800	0.00210700	1.94765300
C	-1.44391600	-0.00453700	1.84214200
C	-1.54517700	-0.00701100	3.17098100
H	-2.50186600	-0.00971800	3.68911300
H	-0.64180400	-0.00624200	3.76744400
O	-2.70496100	-0.00564700	1.17476300
C	-2.70233400	-0.00401700	-0.17152100
O	-1.68999800	-0.00146100	-0.85965500
N	-3.96654000	-0.00613200	-0.69004000
C	-4.14136400	0.00003300	-2.13149300
H	-4.70431300	-0.88366600	-2.45476000
H	-3.16315000	-0.00444500	-2.60475000
H	-4.69341100	0.89243700	-2.45004000

C	-5.17826200	-0.00383300	0.11432800
H	-5.78802500	-0.88591900	-0.11461400
H	-5.77705000	0.88952100	-0.10062300
H	-4.92293500	-0.01416600	1.16875700
O	0.73854600	1.67163200	-0.47475700
C	1.68938800	2.42440000	-0.23007500
N	1.95148100	3.54076900	-0.92677100
C	1.10323900	3.94792200	-2.03982100
H	1.68704300	3.99247400	-2.96444300
H	0.67594400	4.93660200	-1.84645800
H	0.30301800	3.21939500	-2.14785500
O	0.74380600	-1.66830700	-0.47732100
C	1.69491500	-2.42042100	-0.23155100
N	1.96001300	-3.53523800	-0.92995400
C	1.11489200	-3.94098900	-2.04596300
H	0.68660700	-4.92975600	-1.85487800
H	1.70154900	-3.98492500	-2.96875300
H	0.31525700	-3.21204800	-2.15561800
H	2.38476200	2.20599900	0.58864600
H	2.38812200	-2.20264100	0.58928300
C	3.08680700	4.38586700	-0.59072000
H	3.77501000	4.46154700	-1.43849100
H	3.62160300	3.95888100	0.25758000
H	2.75160200	5.39318300	-0.32402900
C	3.09487200	-4.38043000	-0.59211700
H	3.78517300	-4.45477200	-1.43833500
H	2.75932300	-5.38810600	-0.32742900
H	3.62732700	-3.95424900	0.25792600

Viny1 DMC Monomer DMPU 28c

B3LYP/6-311G**

-1929.56962108

Zn	-0.03715500	-0.16189300	1.55193200
Cl	0.20363800	-1.77069400	3.18278400
C	-1.31991100	1.31253200	1.98818600
C	-1.97967400	1.35791400	3.14750800
H	-2.68464500	2.15018500	3.39167900
H	-1.80242700	0.58621700	3.88583600
O	-1.66700600	2.40159200	1.12866700
C	-1.04940300	2.56568400	-0.05058500
O	-0.16726800	1.84079000	-0.48958200
N	-1.53386600	3.65737900	-0.72504700
C	-0.91699400	4.04432500	-1.98081700
H	-1.67877200	4.15858800	-2.76026300
H	-0.20876200	3.27576200	-2.27820500
H	-0.38689900	5.00020700	-1.88019000
C	-2.52225700	4.57652900	-0.18104300
H	-2.06017500	5.53305700	0.09508800
H	-2.98679100	4.14457900	0.69885400
H	-3.29357400	4.77550000	-0.93292700

O	1.95400400	0.11527200	1.02755400
C	2.83793900	-0.10127600	0.17571700
N	3.20532100	-1.36626500	-0.17844800
N	3.48324800	0.95458900	-0.41585700
C	4.21671000	-1.67913000	-1.18657400
H	3.85020000	-2.51761100	-1.78819200
H	5.13246200	-2.02390000	-0.68564300
C	4.68804100	0.75707200	-1.21119100
H	4.83092800	1.64438800	-1.83209600
H	5.57769700	0.66305500	-0.56986300
C	4.52043500	-0.48348200	-2.07688000
H	3.69823900	-0.31774100	-2.77893000
H	5.42592700	-0.67542100	-2.65790000
C	3.17280700	2.30466400	0.04254900
H	3.36825200	3.00224300	-0.77517800
H	3.78360500	2.59336200	0.90703400
H	2.12197800	2.35662500	0.31081400
C	2.62863000	-2.51804900	0.51230300
H	3.43074800	-3.22286000	0.75300600
H	1.88846700	-3.01897600	-0.11868700
H	2.14166200	-2.20762000	1.43271600
O	-0.55635100	-1.36092600	-0.14261100
C	-1.57776900	-1.56110800	-0.83334100
N	-2.71836600	-2.09139400	-0.30411400
N	-1.56093500	-1.27263500	-2.17272500
C	-3.94980700	-2.15327200	-1.08318500
H	-4.46820600	-1.18340500	-1.07867800
H	-4.61262000	-2.87556900	-0.60286500
C	-2.63037900	-1.60535600	-3.11263900
H	-2.17809800	-2.03415900	-4.01387000
H	-3.14150800	-0.68233500	-3.42041800
C	-3.62649600	-2.58360600	-2.50739900
H	-3.20025500	-3.59062700	-2.48458500
H	-4.53156000	-2.61593300	-3.11901000
C	-2.80175200	-2.36920100	1.12927500
H	-1.80936500	-2.54082600	1.53818900
H	-3.40929900	-3.26553300	1.27706600
H	-3.25576400	-1.53489100	1.67393300
C	-0.39232300	-0.60931200	-2.73854600
H	-0.72634500	0.08697900	-3.51309400
H	0.29595500	-1.33220300	-3.19429100
H	0.12011800	-0.04767300	-1.96352400

Representative structures of complexes (fluorinated examples are not shown)

