

*Supporting Information*

**Pd-Catalyzed Allylic Alkylation of Dienyl Carbonates with  
Nitromethane in High C-5 Regioselectivity**

Xiao-Fei Yang,<sup>†</sup> Xiao-Hui Li,<sup>†</sup> Chang-Hua Ding,<sup>\*\*†</sup> Li-Xin Dai,<sup>†</sup> and Xue-Long Hou<sup>\*,†,‡</sup>

<sup>†</sup>State Key Laboratory of Organometallic Chemistry, <sup>‡</sup>Shanghai–Hong Kong Joint  
Laboratory in Chemical Synthesis, Shanghai Institute of Organic Chemistry, Chinese  
Academy of Sciences, 345 Lingling Road, Shanghai 200032, China

xlhou@sioac.ac.cn; dingch@sioac.ac.cn

<b>1. General.....</b>	<b>S-2</b>
<b>2. General Experimental Procedure for Table 2.....</b>	<b>S-2</b>
<b>3. Characterization of the products.....</b>	<b>S-3</b>
<b>4. Spectra of the products .....</b>	<b>S-9</b>

## 1. General Methods

The reactions were carried out in flame-dried glassware under a dry argon atmosphere. All solvents were purified and dried by using standard methods prior to use. Commercially available reagents were used without further purification.  $^1\text{H}$  NMR spectra were recorded on a NMR instrument operated at 400 MHz. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ( $\text{CDCl}_3$ :  $\delta$  7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet or unresolved), coupling constants (Hz), and integration.  $^{13}\text{C}$  NMR spectra were recorded on a NMR instrument operated at 100 MHz with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ( $\text{CDCl}_3$ :  $\delta$  77.1 ppm). Infrared spectra were recorded from thin films of pure samples. Mass and HRMS spectra were measured in EI or ESI mode and the mass analyzer type used for the HRMS was TOF. Thin layer chromatography was performed on pre-coated glassback plates and visualized with UV light at 254 nm. Flash column chromatography was performed on silica gel.

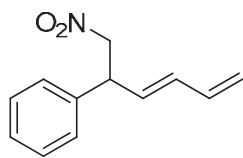
## 2. General Experimental Procedure for Table 2

To a flame dried Schlenk tube were added  $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$  (5.2 mg, 0.005 mmol), ligand  $^i\text{Pr}-(S_C, S_{\text{phos}}, R_a)\text{-L4}$  (6.84 mg, 0.010 mmol), freshly distilled anhydrous THF (1.0 mL). The resulting mixture was allowed to stir for 30 mins. The dienyl ester **1** (0.15 mmol) and DABCO (0.15 mmol) were added subsequently, then distilled

anhydrous THF (1.0 mL) and nitromethane 0.5 mL was added. The resulting reaction mixture was stirred at room temperature overnight (TLC control). After the ratio of compound **2**, **3**, **4** was determined by GC, the volatile was removed in vacuo. The resulting residue was purified by flash chromatography (FC) on silica gel with petroleum ether and EtOAc as eluent to give product **4**.

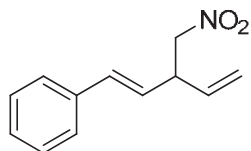
### 3. Characterization of the products

#### (*E*)-(1-nitrohexa-3,5-dien-2-yl)benzene (**4a**)



colorless oil, 87% yield (26.5 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.25 (q,  $J = 7.8$  Hz, 1H), 4.64 (dd,  $J = 8, 12.4$  Hz, 1H), 4.66 (dd,  $J = 7.6, 12$  Hz, 1H), 5.11 (d,  $J = 10.2$  Hz, 1H), 5.20 (d,  $J = 16.8$  Hz, 1H), 5.82 (dd,  $J = 7.8, 15.3$  Hz, 1H), 6.15 (dd,  $J = 10.5, 15$  Hz, 1H), 6.28 (dt,  $J = 10.2, 16.8$  Hz, 1H), 7.21-7.36 (m, 5H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  46.9, 79.5, 118.3, 127.5, 127.8, 129.1, 130.8, 133.6, 135.9, 138.2; MS (EI) 77 (30), 91 (100), 115 (51), 128 (55), 156 (81), 203 ( $\text{M}^+$ , 0.1); HRMS Calcd. for  $\text{C}_{12}\text{H}_{13}\text{NO}_2$ : 203.0946; Found: 203.0949; IR (film)  $\nu_{\text{max}}$  798, 1014, 1090, 1260, 1548, 2962  $\text{cm}^{-1}$ .

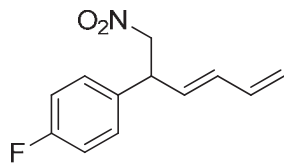
#### (*E*)-(3-(nitromethyl)penta-1,4-dienyl)benzene (**3a**)



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.79 (q,  $J = 7.6$  Hz, 1H), 4.49 (d,  $J = 7.6$  Hz, 2H), 5.24 (d,  $J = 11.6$  Hz, 1H), 5.25 (d,  $J = 16.4$  Hz, 1H), 5.83 (ddd,  $J = 7.6, 10.4, 17.6$  Hz, 1H), 6.07 (dd,  $J = 7.6, 15.6$  Hz, 1H), 6.53 (d,  $J = 16$  Hz, 1H), 7.25-7.37 (m, 5H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  45.5, 78.9, 118.4, 125.5, 126.4, 128.0, 128.6, 133.4, 134.7, 136.2; MS (EI) 77 (26), 91 (100), 115 (60), 128 (79), 156 (70), 203 ( $\text{M}^+$ , 0.3); HRMS Calcd. for  $\text{C}_{12}\text{H}_{13}\text{NO}_2$ : 203.0946; Found: 203.0944; IR (film)  $\nu_{\text{max}}$  798, 1014, 1090,

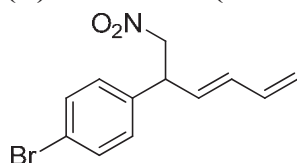
1260, 1548, 2962  $\text{cm}^{-1}$ .

**(E)-1-fluoro-4-(1-nitrohexa-3,5-dien-2-yl)benzene (4b)**



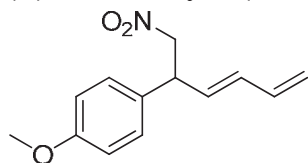
colorless oil, 91% yield (30.2 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.23 (q,  $J = 7.6$  Hz, 1H), 4.60 (dd,  $J = 8, 12.4$  Hz, 1H), 4.66 (dd,  $J = 7.6, 12$  Hz, 1H), 5.12 (d,  $J = 10$  Hz, 1H), 5.20 (d,  $J = 16.8$  Hz, 1H), 5.78 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.13 (dd,  $J = 10.4, 15.2$  Hz, 1H), 6.29 (dt,  $J = 10, 16.8$  Hz, 1H), 7.02-7.07 (m, 2H), 7.18-7.22 (m, 2H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  46.0, 79.5, 115.9 (d,  $J = 21.5$  Hz), 118.6, 129.1 (d,  $J = 8.2$  Hz), 130.5, 133.7, 133.9 (d,  $J = 3.3$  Hz), 135.7, 162.5 (d,  $J = 245$  Hz);  $^{19}\text{F}$  NMR (376 MHz)  $\delta$  -114.3 (m); MS (EI) 77 (11), 96 (8), 109 (100), 121 (13), 146 (34), 159 (33), 174 (53), 221 ( $\text{M}^+$ , 0.07); HRMS Calcd. for  $\text{C}_{12}\text{H}_{12}\text{NO}_2\text{F}$ : 221.0852; Found: 221.0854; IR (film)  $\nu_{\text{max}}$  832, 1003, 1223, 1508, 1548, 3016  $\text{cm}^{-1}$ .

**(E)-1-bromo-4-(1-nitrohexa-3,5-dien-2-yl)benzene (4c)**



colorless oil, 96% yield (40.5 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.19 (q,  $J = 8$  Hz, 1H), 4.62 (dd,  $J = 8, 12$  Hz, 1H), 4.65 (dd,  $J = 7.6, 12$  Hz, 1H), 5.12 (d,  $J = 10.4$  Hz, 1H), 5.20 (d,  $J = 16.8$  Hz, 1H), 5.75 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.12 (dd,  $J = 10.8, 15.2$  Hz, 1H), 6.29 (dt,  $J = 10.4, 17.2$  Hz, 1H), 7.10 (d,  $J = 8.4$  Hz, 2H), 7.47 (d,  $J = 8.4$  Hz, 2H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  46.2, 79.1, 118.8, 121.8, 129.2, 130.1, 132.2, 133.9, 135.7, 137.2; MS (EI) 77 (37), 115 (51), 141 (51), 155 (100), 169 (35), 234 (43), 281 ( $\text{M}^+$ , 0.2); HRMS Calcd. for  $\text{C}_{12}\text{H}_{12}\text{NO}_2\text{Br}$ : 281.0051; Found: 281.0047; IR (film)  $\nu_{\text{max}}$  755, 1002, 1374, 1548, 2916  $\text{cm}^{-1}$ .

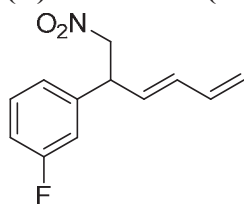
**(E)-1-methoxy-4-(1-nitrohexa-3,5-dien-2-yl)benzene (4d)**



colorless oil, 65% yield (22.7 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.79 (s, 3H), 4.19

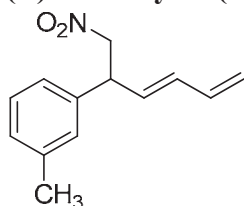
(q,  $J = 7.6$  Hz, 1H), 4.60 (dd,  $J = 8.4, 11.6$  Hz, 1H), 4.64 (dd,  $J = 7.6, 12$  Hz, 1H), 5.09 (d,  $J = 10$  Hz, 1H), 5.18 (d,  $J = 16.8$  Hz, 1H), 5.79 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.12 (dd,  $J = 10.8, 15.6$  Hz, 1H), 6.30 (dt,  $J = 10.4, 16.8$  Hz, 1H), 6.87 (d,  $J = 8.8$  Hz, 2H), 7.13 (d,  $J = 8.8$  Hz, 2H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  46.1, 55.3, 79.7, 114.4, 118.2, 128.6, 130.1, 131.2, 133.2, 135.9, 159.0; MS (EI) 77 (29), 91 (24), 121 (100), 128 (27), 158 (21), 186 (28), 233 ( $\text{M}^+$ , 8); HRMS Calcd. for  $\text{C}_{13}\text{H}_{15}\text{NO}_3$ : 233.1052; Found: 233.1051; IR (film)  $\nu_{\text{max}}$  828, 1004, 1376, 1511, 1548, 1609, 2962  $\text{cm}^{-1}$ ;

**(E)-1-fluoro-3-(1-nitrohexa-3,5-dien-2-yl)benzene (4e)**



colorless oil, 95% yield (31.5 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.24 (q,  $J = 8.0$  Hz, 1H), 4.64-4.66 (m, 2H), 5.13 (d,  $J = 10.4$  Hz, 1H), 5.22 (d,  $J = 16.8$  Hz, 1H), 5.80 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.13 (dd,  $J = 10.4, 14.4$  Hz, 1H), 6.29 (dt,  $J = 10.4, 17.2$  Hz, 1H), 6.92-7.02 (m, 3H), 7.30-7.38 (m, 1H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  46.4, 79.2, 114.6 (d,  $J = 20.5$  Hz), 114.8 (d,  $J = 19.4$  Hz), 118.8, 123.2 (d,  $J = 2.7$  Hz), 129.9, 130.7 (d,  $J = 7.9$  Hz), 134.0, 135.7, 140.7 (d,  $J = 6.8$  Hz), 163.5 (d,  $J = 246$  Hz);  $^{19}\text{F}$  NMR (376 MHz)  $\delta$  -111.7 (m); MS (EI) 77 (15), 96 (11), 109 (100), 133 (45), 146 (43), 174 (76), 221 ( $\text{M}^+$ , 0.06); HRMS Calcd. for  $\text{C}_{12}\text{H}_{12}\text{NO}_2\text{F}$ : 221.0852; Found: 221.0854; IR (film)  $\nu_{\text{max}}$  795, 1013, 1090, 1259, 1549, 2962  $\text{cm}^{-1}$ .

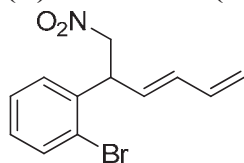
**(E)-1-methyl-3-(1-nitrohexa-3,5-dien-2-yl)benzene (4f)**



colorless oil, 94% yield (30.6 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.33 (s, 3H), 4.19 (q,  $J = 8.0$  Hz, 1H), 4.62 (d,  $J = 7.2$  Hz, 1H), 4.64 (d,  $J = 8.4$  Hz, 1H), 5.09 (d,  $J = 10$  Hz, 1H), 5.20 (d,  $J = 16.8$  Hz, 1H), 5.80 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.13 (dd,  $J = 10.4, 15.2$  Hz, 1H), 6.29 (dt,  $J = 10.4, 16.8$  Hz, 1H), 7.00-7.10 (m, 3H), 7.21-7.24 (m, 1H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  21.4, 46.9, 79.6, 118.2, 124.4, 128.2, 128.5, 128.9, 130.9, 133.4, 135.9, 138.2, 138.8; MS (EI) 77 (35), 91 (30), 105 (100), 115 (46), 129 (40), 142 (39), 155 (88), 170 (73), 217 ( $\text{M}^+$ , 0.12); HRMS Calcd. for  $\text{C}_{13}\text{H}_{15}\text{NO}_2$ :

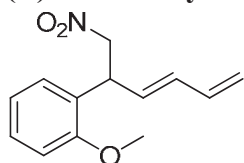
217.1103; Found: 217.1106; IR (film)  $\nu_{\max}$  794, 1014, 1085, 1258, 1548, 2962  $\text{cm}^{-1}$ .

**(E)-1-bromo-2-(1-nitrohexa-3,5-dien-2-yl)benzene (4g)**



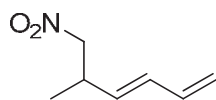
colorless oil, 93% yield (39.2 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  4.61-4.73 (m, 2H), 4.80 (q,  $J = 8.0$  Hz, 1H), 5.12 (d,  $J = 10.0$  Hz, 1H), 5.21 (d,  $J = 16.4$  Hz, 1H), 5.81 (dd,  $J = 7.6, 15.2$  Hz, 1H), 6.13 (dd,  $J = 10.4, 15.2$  Hz, 1H), 6.29 (dt,  $J = 10.4, 16.8$  Hz, 1H), 7.15 (t,  $J = 8.0$  Hz, 1H), 7.22 (t,  $J = 8.0$  Hz, 1H), 7.26 (t,  $J = 7.2$  Hz, 1H), 7.60 (d,  $J = 8.0$  Hz, 1H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  45.4, 77.9, 118.7, 124.4, 128.0, 128.5, 129.2, 129.3, 133.7, 134.4, 135.8, 137.3; MS (EI) 77 (36), 141 (42), 155 (100), 168 (36), 233 (47), 281 ( $\text{M}^+$ , 0.1); HRMS Calcd. for  $\text{C}_{12}\text{H}_{12}\text{NO}_2\text{Br}$ : 281.0051; Found: 281.0050; IR (film)  $\nu_{\max}$  755, 909, 1002, 1374, 1548, 2969  $\text{cm}^{-1}$ .

**(E)-1-methoxy-2-(1-nitrohexa-3,5-dien-2-yl)benzene (4h)**



colorless oil, 83% yield (29.0 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.86 (s, 3H), 4.52 (q,  $J = 8$  Hz, 1H), 4.68 (dd,  $J = 8.4, 12$  Hz, 1H), 4.72 (dd,  $J = 8, 13$  Hz, 1H), 5.08 (d,  $J = 9.2$  Hz, 1H), 5.20 (d,  $J = 16.4$  Hz, 1H), 5.90 (dd,  $J = 8, 14.8$  Hz, 1H), 6.13 (dd,  $J = 10.4, 15.6$  Hz, 1H), 6.29 (dt,  $J = 10.0, 16.8$  Hz, 1H), 6.88-6.95 (m, 2H), 7.13-7.16 (m, 1H), 7.24-7.35 (m, 1H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  42.6, 55.4, 78.3, 111.0, 117.7, 120.9, 126.4, 128.8, 128.9, 130.4, 133.6, 136.2, 156.8; MS (EI) 77 (27), 91 (56), 107 (14), 121 (100), 128 (28), 145 (13), 158 (16), 171 (25), 233 ( $\text{M}^+$ , 1.5); HRMS Calcd. for  $\text{C}_{13}\text{H}_{15}\text{NO}_3$ : 233.1052; Found: 233.1055; IR (film)  $\nu_{\max}$  752, 1005, 1024, 1243, 1547, 2963  $\text{cm}^{-1}$ .

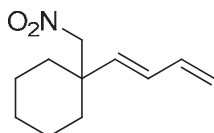
**(E)-5-methyl-6-nitrohexa-1,3-diene (4i)**



colorless oil, 63% yield (13.3 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.15 (d,  $J = 6.8$  Hz, 3H), 3.09 (q,  $J = 7.2$  Hz, 1H), 4.27 (dd,  $J = 7.2, 11.6$  Hz, 1H), 4.34 (dd,  $J = 7.6, 12$  Hz,

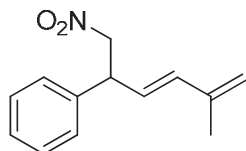
1H), 5.08 (d,  $J = 9.6$  Hz, 1H), 5.19 (d,  $J = 16.8$  Hz, 1H), 5.55 (dd,  $J = 8, 15.2$  Hz, 1H), 6.14 (dd,  $J = 10.4, 14.8$  Hz, 1H), 6.28 (dt,  $J = 10.4, 17.2$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  17.3, 35.9, 80.8, 117.7, 132.6, 132.8, 136.1; MS (EI) 55 (40), 67 (38), 79 (100), 94 (49), 106 (0.14), 141 ( $\text{M}^+$ , 0.39); HRMS Calcd. for  $\text{C}_7\text{H}_{11}\text{NO}_2$ : 141.0790; Found: 141.0796; IR (film)  $\nu_{\text{max}}$  797, 1015, 1089, 1259, 1552, 2917  $\text{cm}^{-1}$ .

**(E)-1-(buta-1,3-dienyl)-1-(nitromethyl)cyclohexane (4j)**



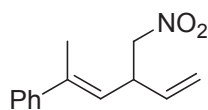
colorless oil, 64% yield (18.7 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.31-1.35 (m, 1H), 1.49-1.57 (m, 7H), 1.75-1.78 (m, 2H), 4.31 (s, 2H), 5.09 (d,  $J = 10$  Hz, 1H), 5.21 (d,  $J = 16.8$  Hz, 1H), 5.54 (d,  $J = 15.6$  Hz, 1H), 6.10 (dd,  $J = 10.4, 15.6$  Hz, 1H), 6.34 (dt,  $J = 10, 16.8$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  21.8, 25.7, 33.7, 40.9, 85.2, 117.2, 132.2, 136.4, 136.7; MS (EI) 67 (100), 79 (33), 91 (26), 123 (7), 165 (2), 195 ( $\text{M}^+$ , 1.6); HRMS Calcd. for  $\text{C}_{11}\text{H}_{17}\text{NO}_2$ : 195.1259; Found: 195.1255; IR (film)  $\nu_{\text{max}}$  797, 902, 1005, 1260, 1376, 1544, 2856, 2930  $\text{cm}^{-1}$ .

**(E)-(5-methyl-1-nitrohexa-3,5-dien-2-yl)benzene (4k)**



colorless oil, 56% yield (18.2 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  1.82 (s, 3H), 4.25 (q,  $J = 7.6$  Hz, 1H), 4.66 (d,  $J = 7.6$  Hz, 1H), 4.68 (d,  $J = 8.4$  Hz, 1H), 4.97 (d,  $J = 11.2$  Hz, 2H), 5.73 (dd,  $J = 7.6, 15.6$  Hz, 1H), 6.24 (d,  $J = 16$  Hz, 1H), 7.22-7.41 (m, 5H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  18.4, 47.1, 79.7, 117.7, 126.8, 1127.5, 127.7, 129.1, 135.7, 138.6, 140.9; MS (EI) 65 (14), 77 (28), 91 (100), 129 (36), 155 (76), 170 (49), 217 ( $\text{M}^+$ , 0.27); HRMS Calcd. for  $\text{C}_{13}\text{H}_{15}\text{NO}_2$ : 217.1103; Found: 217.1104; IR (film)  $\nu_{\text{max}}$  796, 1016, 1086, 1259, 1549, 2962  $\text{cm}^{-1}$ .

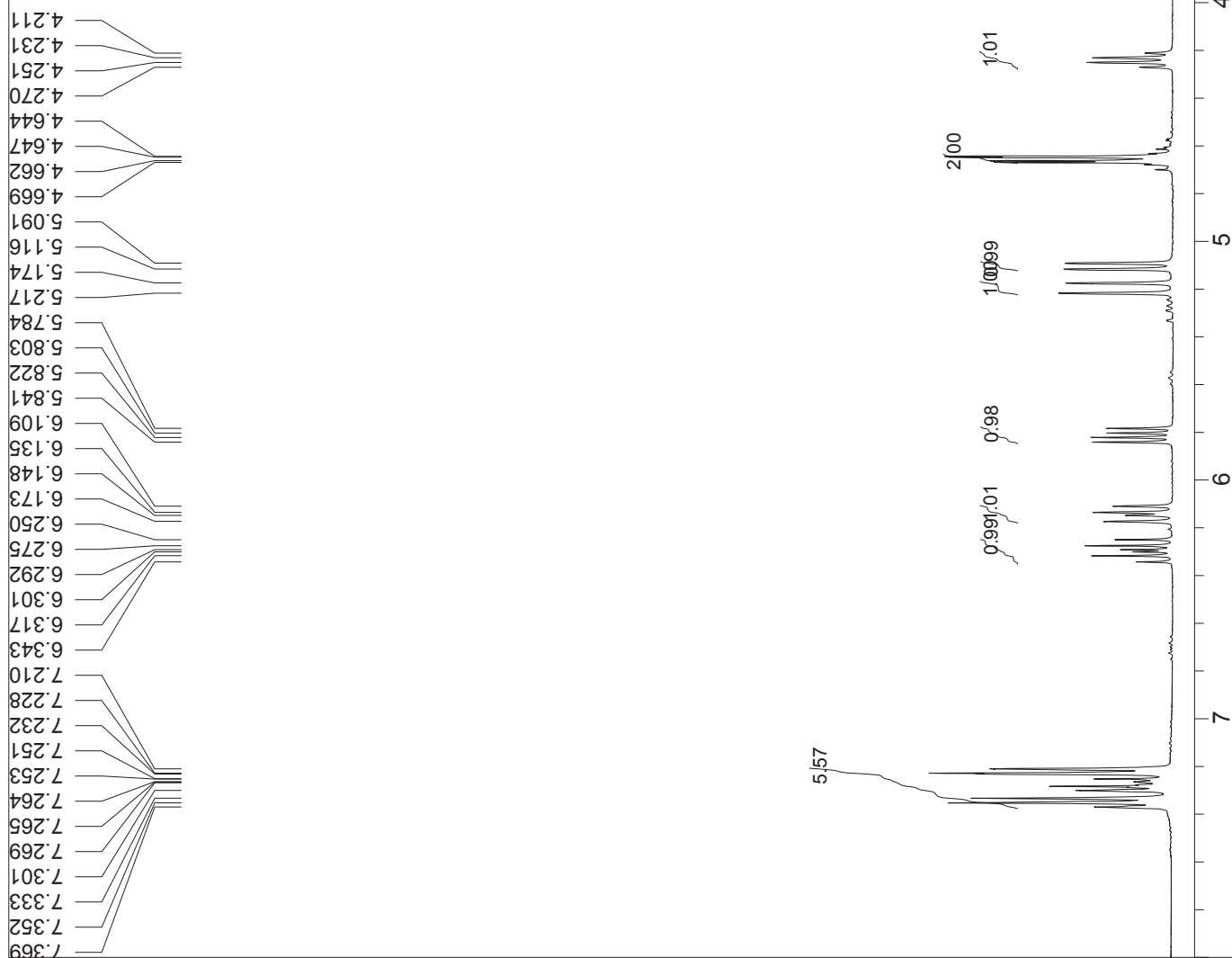
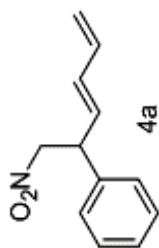
**(E)-(4-(nitromethyl)hexa-2,5-dien-2-yl)benzene (3m)**



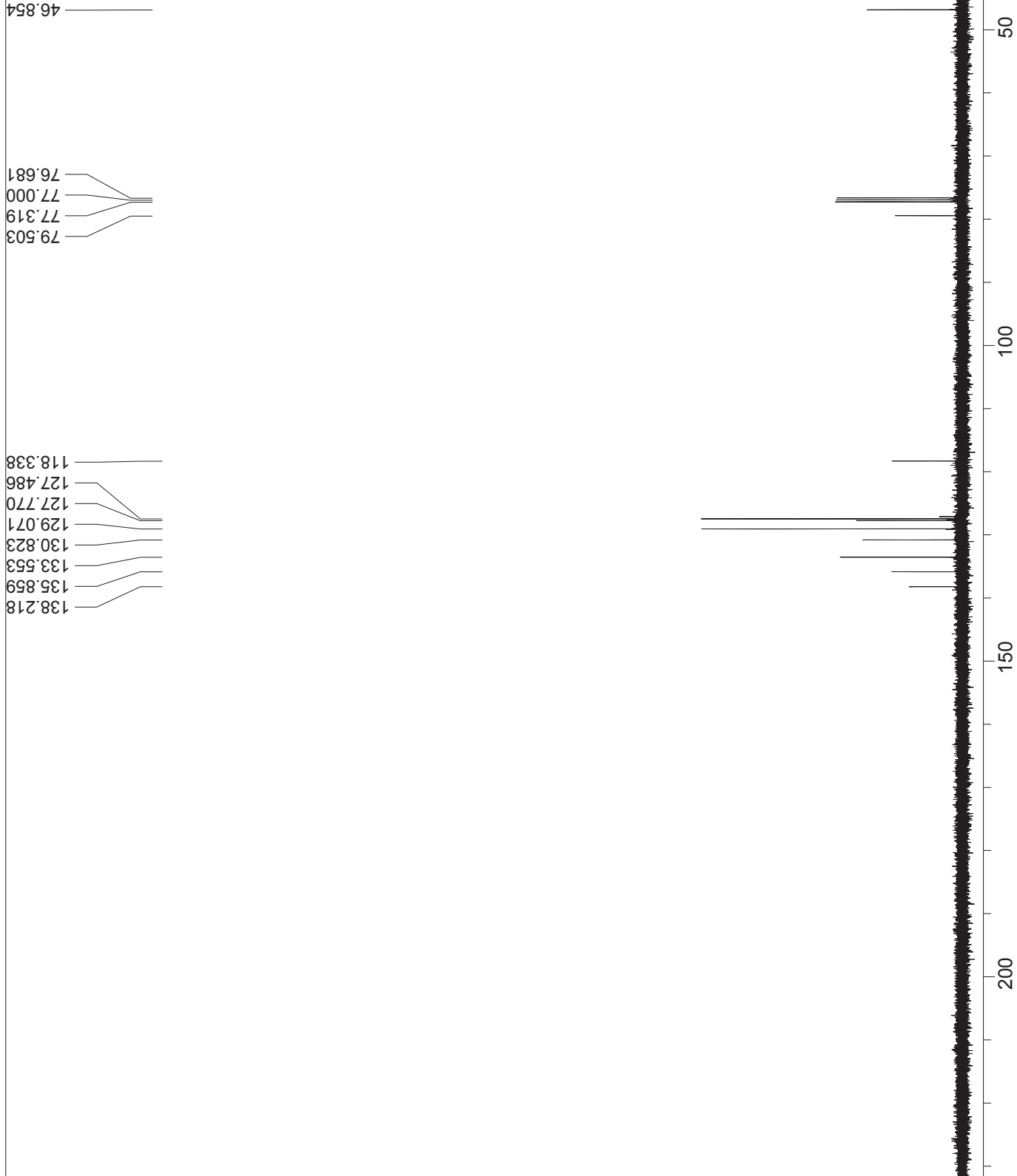
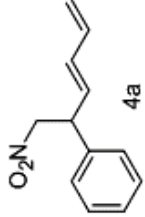
colorless oil, 56% yield (18.2 mg),  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.10 (s, 3H), 4.02

(q,  $J = 8.4$  Hz, 1H), 4.40 (dd,  $J = 7.8, 11.7$  Hz, 1H), 4.47 (dd,  $J = 7.5, 11.7$  Hz, 1H), 5.19 (d,  $J = 9.3$  Hz, 1H), 5.23 (d,  $J = 16.5$  Hz, 1H), 5.54 (d,  $J = 9.3$  Hz, 1H), 5.77 (ddd,  $J = 7.2, 10.5, 16.9$  Hz, 1H) 7.25-7.37 (m, 5H);  $^{13}\text{C}$  NMR (100 M Hz,  $\text{CDCl}_3$ )  $\delta$  16.3, 42.0, 79.0, 117.6, 123.2, 125.9, 127.4, 128.3, 134.8, 139.7, 142.8; MS (EI) 77 (61), 91 (81), 105 (100), 129 (96), 141 (34), 187 (24), 217 ( $\text{M}^+$ , 10); HRMS Calcd. for  $\text{C}_{13}\text{H}_{15}\text{NO}_2$ : 217.1103; Found: 217.1105; IR (film)  $\nu_{\text{max}}$  694, 757, 1376, 1547, 2918  $\text{cm}^{-1}$ ; Chiral HPLC: Chiralcel OJ, 0.46 cm  $\times$  250 mm, *n*-hexane/2-propanol 80/20, flow rate 0.5 mL/min, UV 230 nm):  $t_{\text{R}} = 25.5$  min (major), 33.7 min (minor).

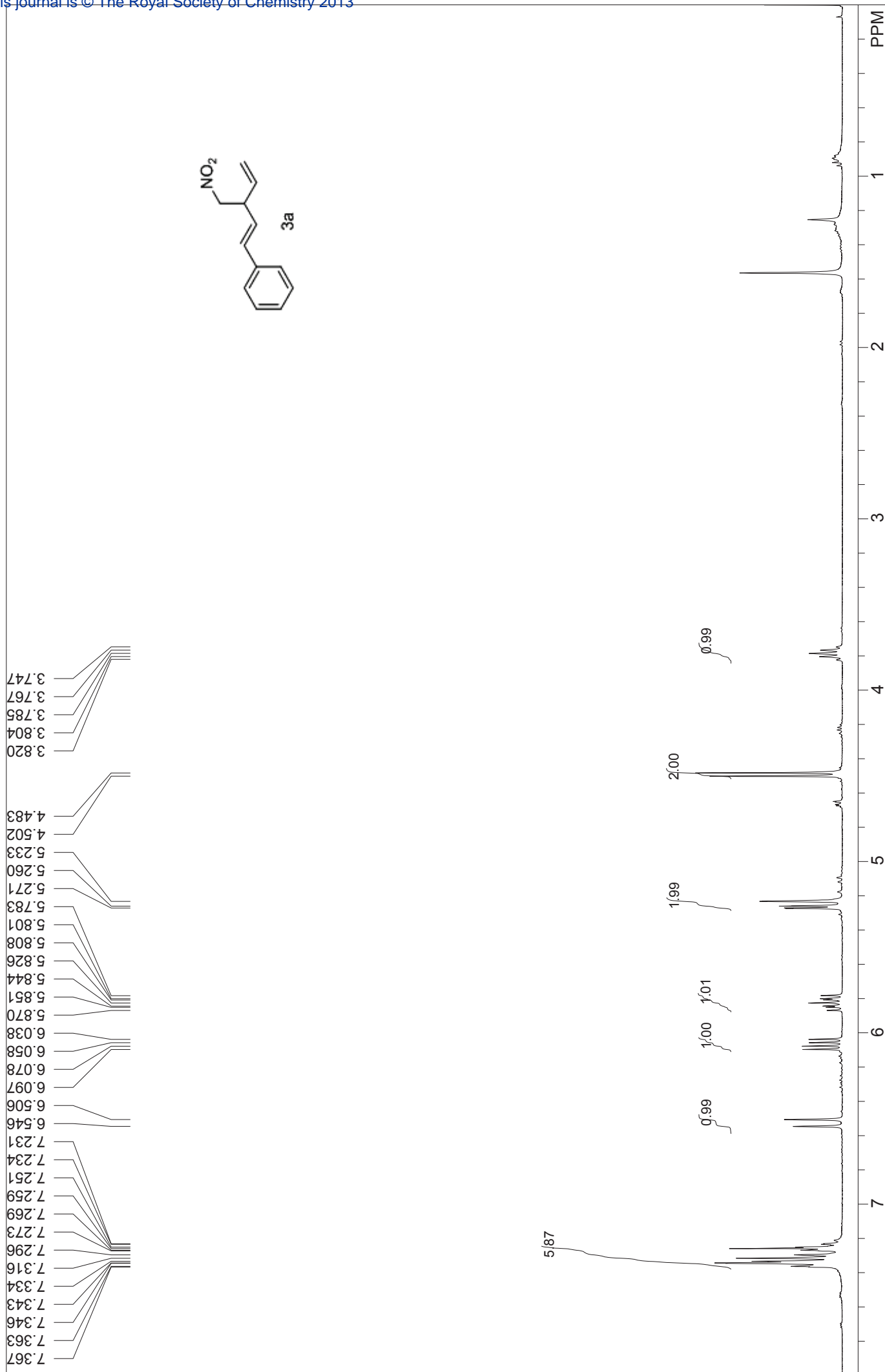
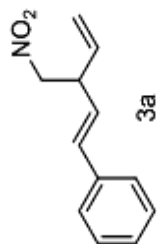




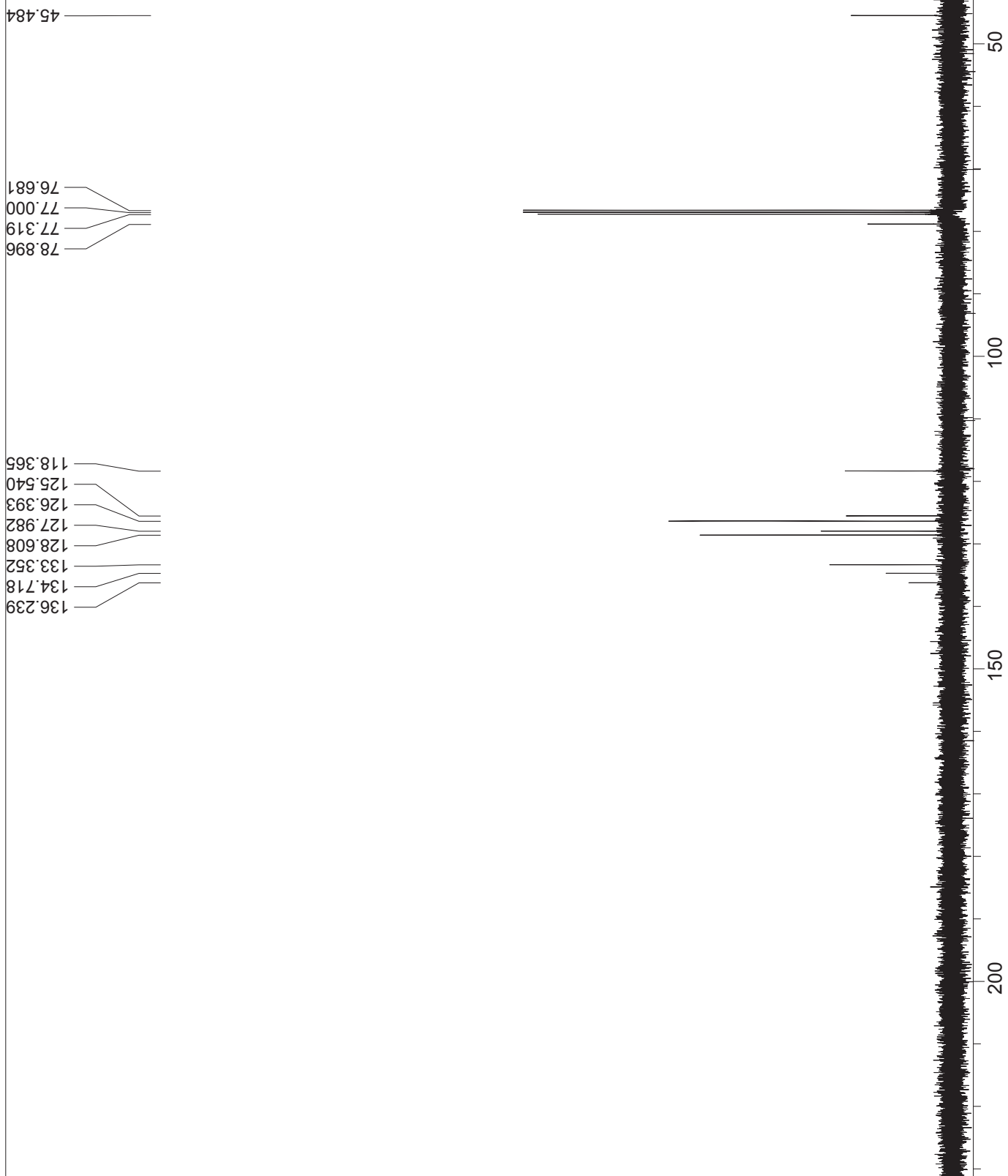
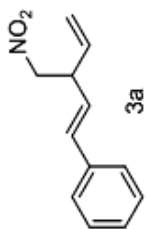
:blank line:blank line		USER: -- DATE: Dec 19 2012	
F1: 400.032	F2: 100.597	PTSIId: 21676	32768
EX: s2pul	PD: 1.0 sec	LB: 0.0	Nuts - \$yxf-1219.fid
SW1: 7225	NA: 12		
PW: 10.5 us			



Std carbon; blank line			USER: -- DATE: Nov 24 2011		
F1: 100.598	F2: 400.031	SW1: 25000	OF1: 10808.3	PTSId: 37500	65536
EX: s2pul	PW: 7.3 us	PD: 1.0 sec	NA: 60	LB: 0.0	Nuts - \$yxf-11-90-c.fid



:blank line		USER: -- DATE: Nov 25 2011	
F1: 400.032	F2: 100.597	PTSId: 21676	32768
EX: s2pul	PD: 1.0 sec	LB: 0.0	Nuts - \$yxf-11-92-b.fid
SW1: 7225	NA: 16		
PW: 10.3 us			



Std carbon,blank line

F1: 100.598 F2: 400.031

EX: s2pul

SW1: 25000

PW: 7.3 us

PD: 1.0 sec

NA: 380

OF1: 10812.9

NA: 380

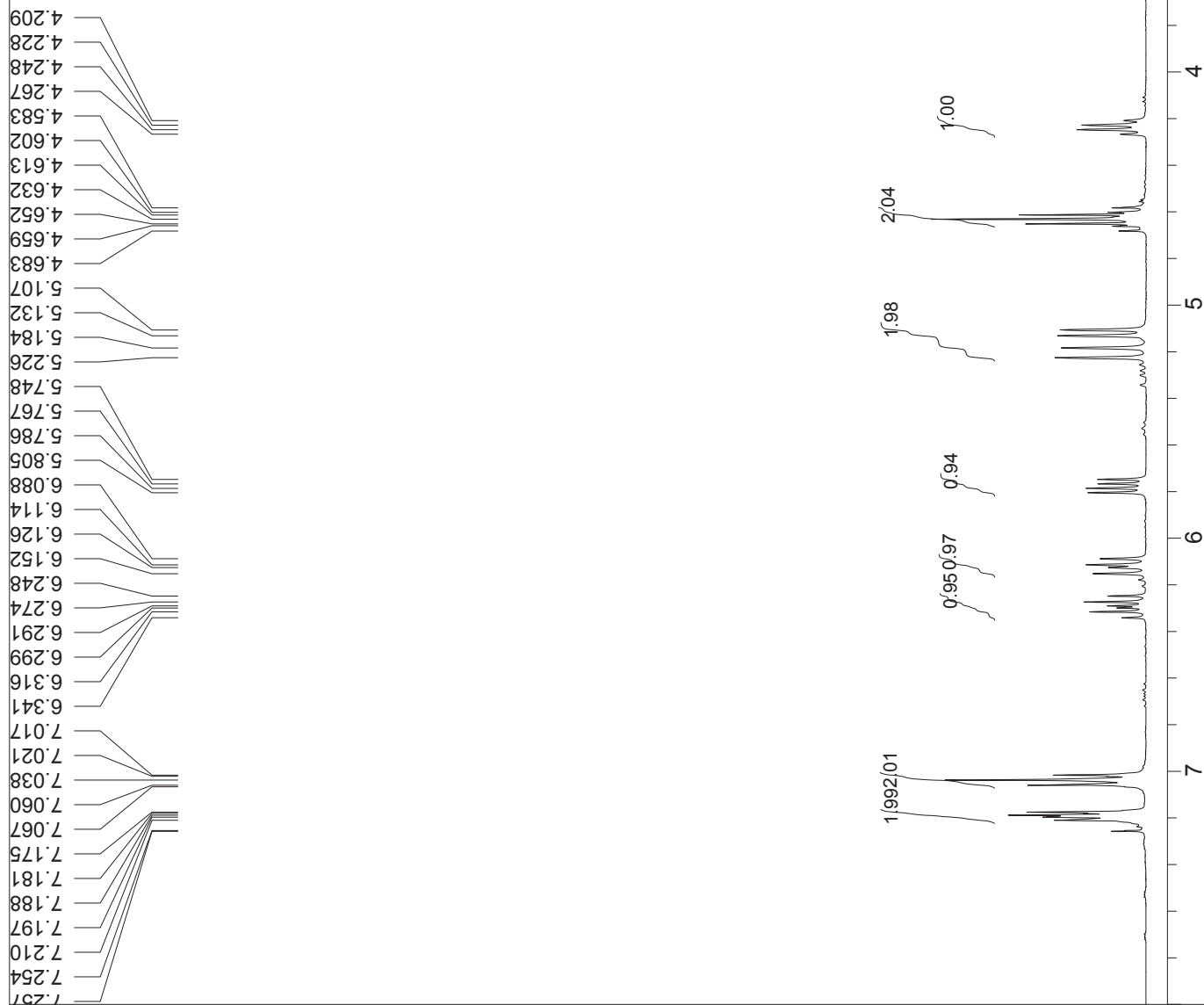
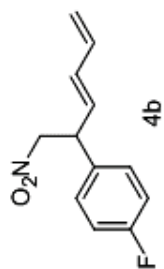
LB: 0.0

PTSlid: 37500

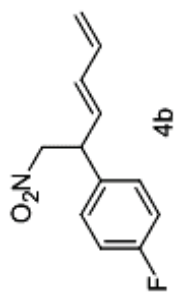
65536

USER: -- DATE: Nov 29 2011

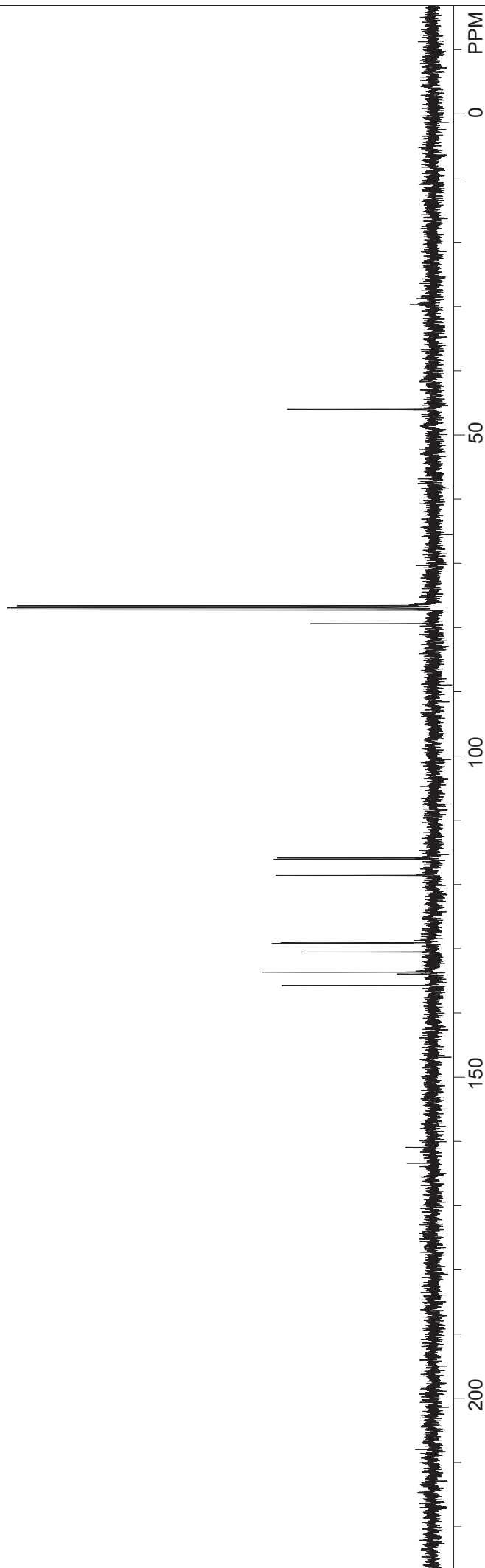
Nuts - \$20111128.fid



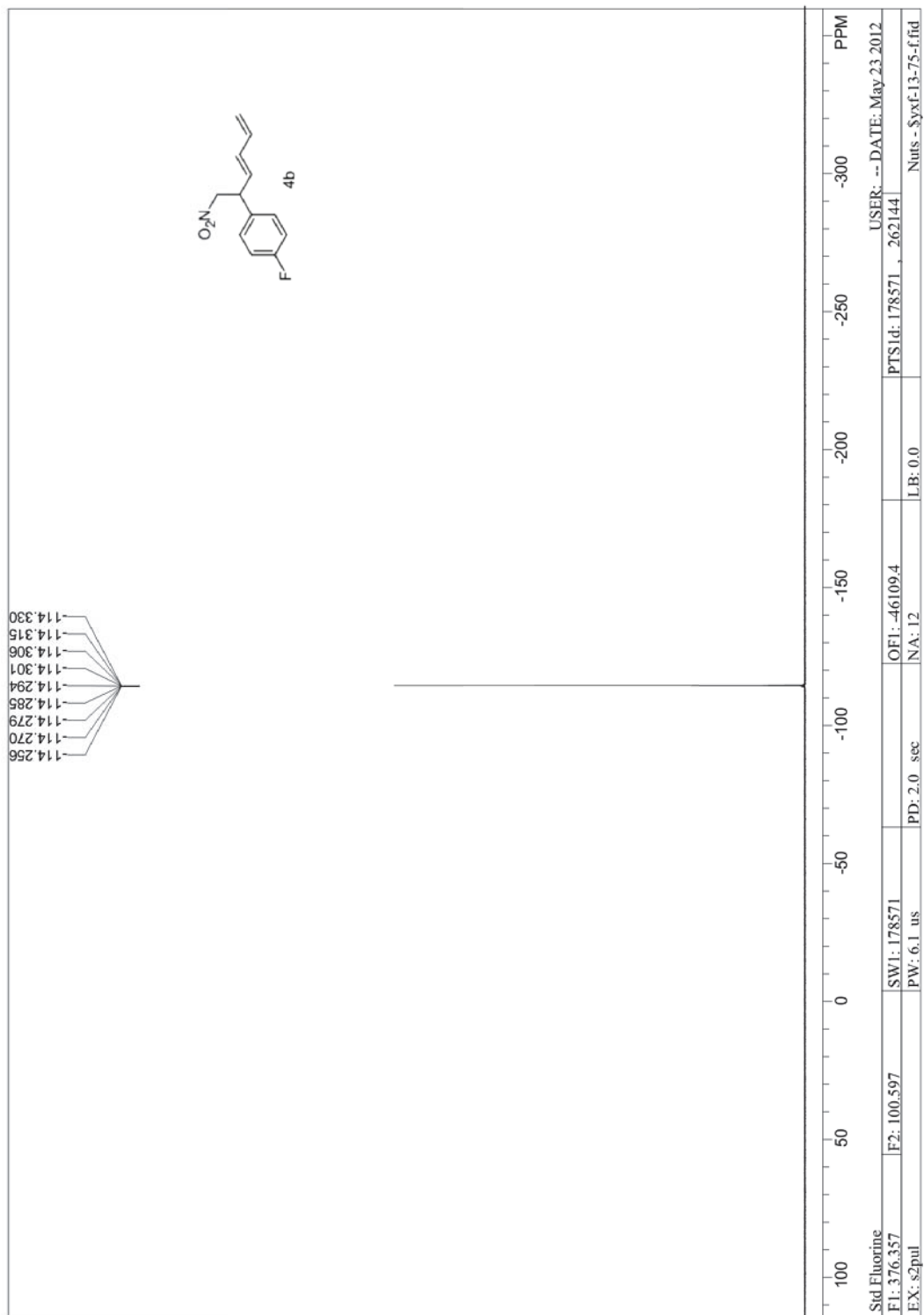
HP20120522-3,blank line		USER: -- DATE: May 22 2012	
F1: 400.032	F2: 100.597	PTSId: 21429	32768
EX: s2pul	PW: 10.3 us	LB: 0.0	Nuts - \$yxf-13-75-h.fid
	PD: 1.0 sec	NA: 24	
	SW1: 7143	OF1: 2766.2	

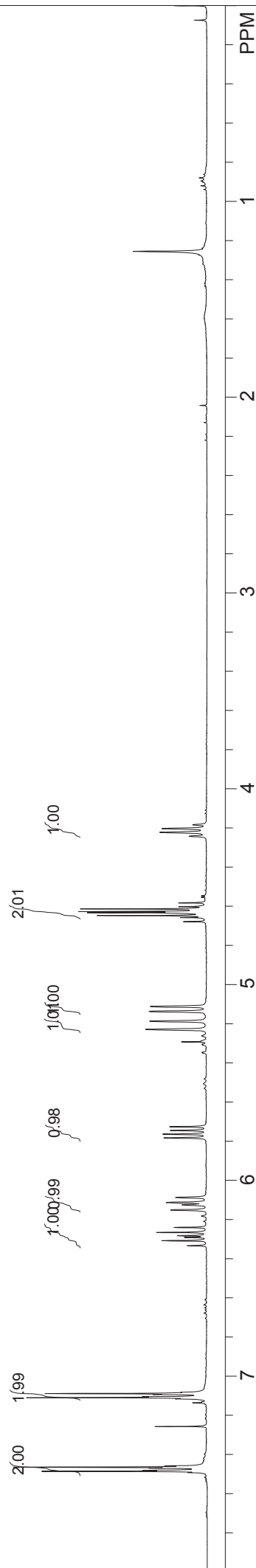
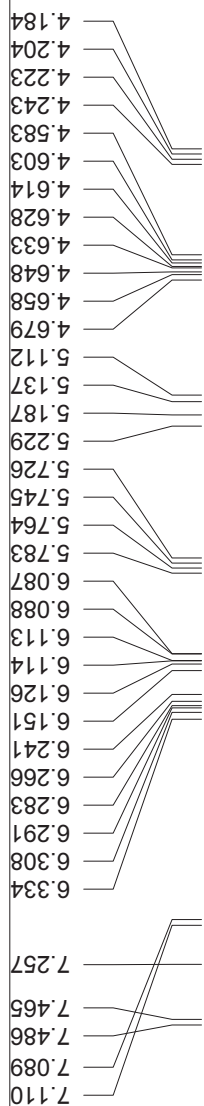
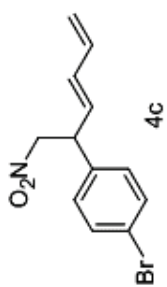


163.383  
160.929  
135.731  
133.980  
133.947  
133.657  
130.530  
129.188  
129.106  
118.598  
116.107  
115.892  
79.465  
77.320  
77.000  
76.684  
46.039



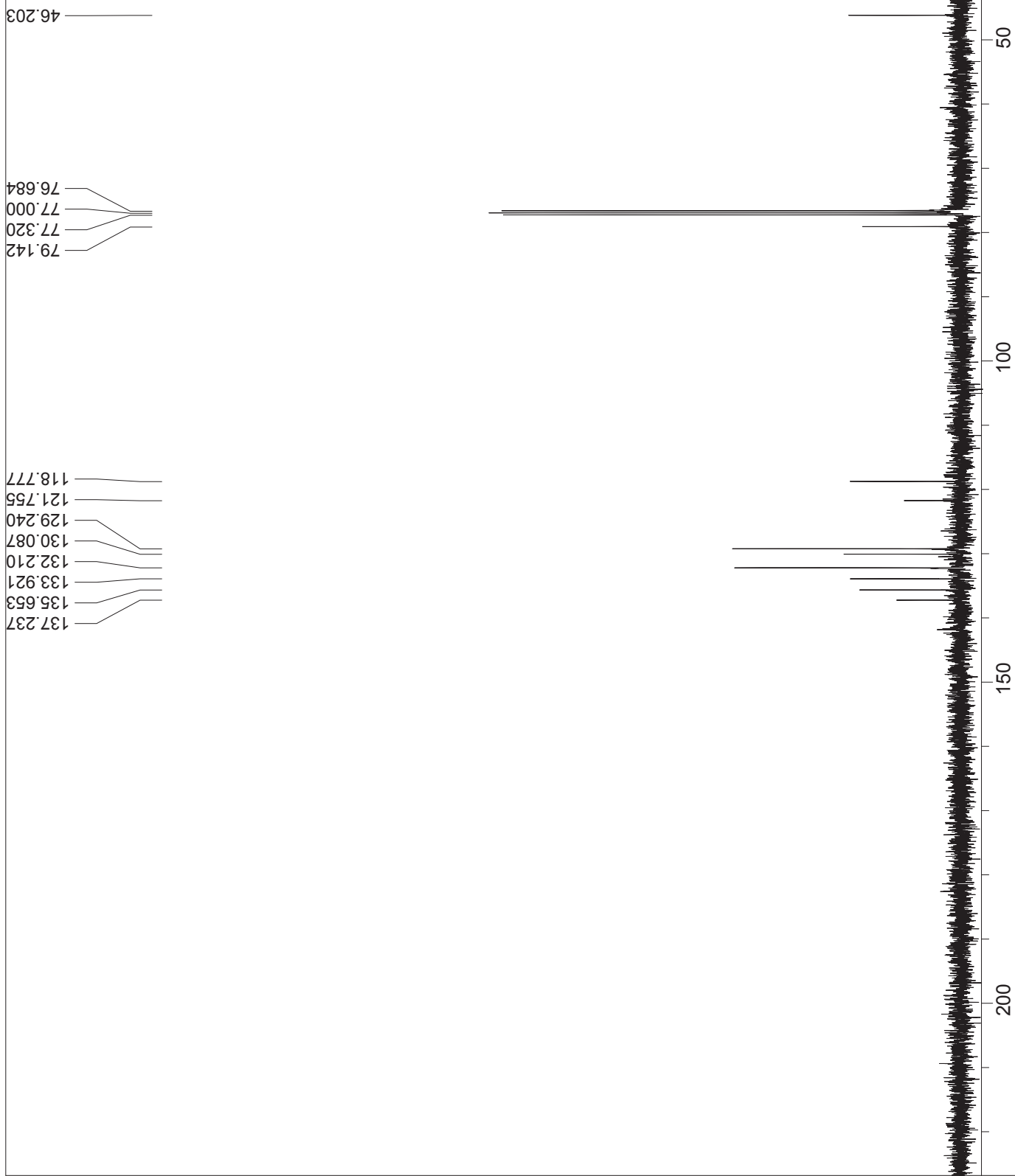
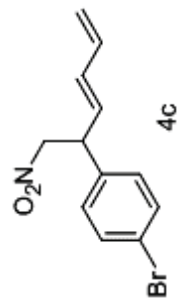
Std carbon, blank line		USER: -- DATE: May 22 2012	
F1: 100.598	F2: 400.031	PTSID: 39216	65536
EX: s2pul	SW1: 24510	OF1: 10559.7	LB: 1.6
	PW: 7.6 us	NA: 36	Nuts - \$yxf-13-75-c.fid
	PD: 1.0 sec		



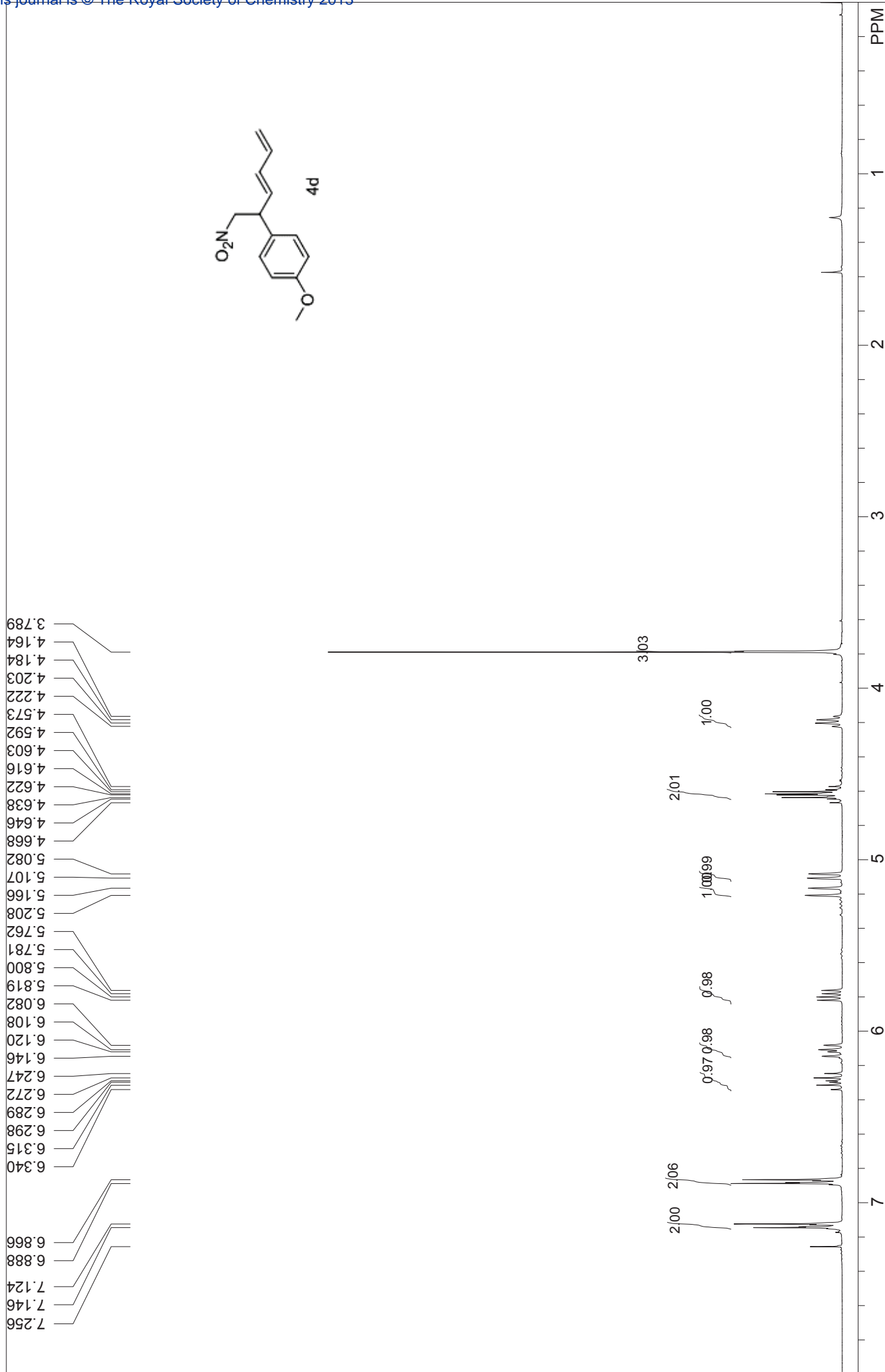
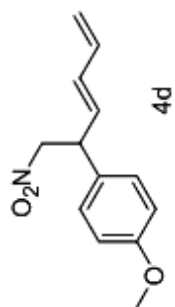


:blank line		USER: -- DATE: May 23 2012	
F1: 400.032	F2: 100.597	PTSIId: 21429	32768
EX: s2pul	PW: 10.3 us	LB: 0.0	Nuts - \$yxf-13-76-hh.fid
	PD: 1.0 sec	NA: 16	
	SW1: 7143	OF1: 2766.4	

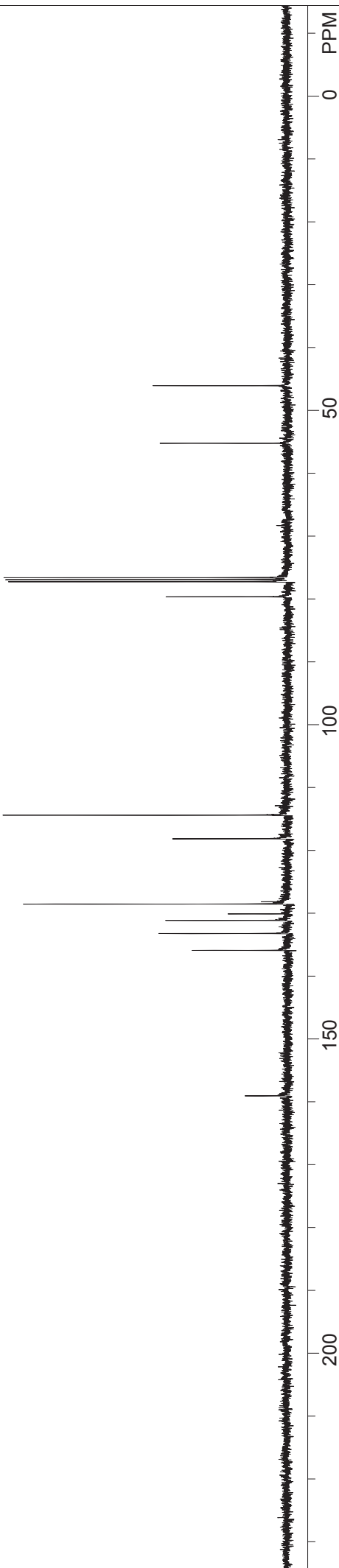
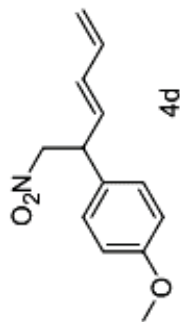




Std carbon, blank line	OF1: 10559.7	PTSID: 39216	USER: -- DATE: May 27 2012
F1: 100.598	SW1: 24510	65536	
EX: s2pul	PW: 7.6 us	LB: 1.4	Nuts - \$yxf13-76-ccc.fid
	PD: 1.0 sec	NA: 40	



:blank line;blank line		USER: -- DATE: Dec 8 2012	
F1: 400.032	F2: 100.597	PTSID: 21676	32768
EX: s2pul	PD: 1.0 sec	LB: 0.0	Nuts - \$yxf-15-58.fid
SW1: 7225	NA: 12	OF1: 2805.9	



mx-13-26-p1-C400

F1: 100.521

F2: 399.722

SW1: 25000

PW: 6.8 us

PD: 1.0 sec

OF1: 11052.6

NA: 124

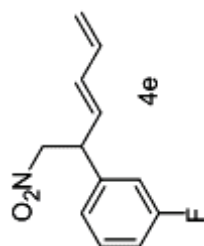
LB: 1.4

PTSIId: 37500

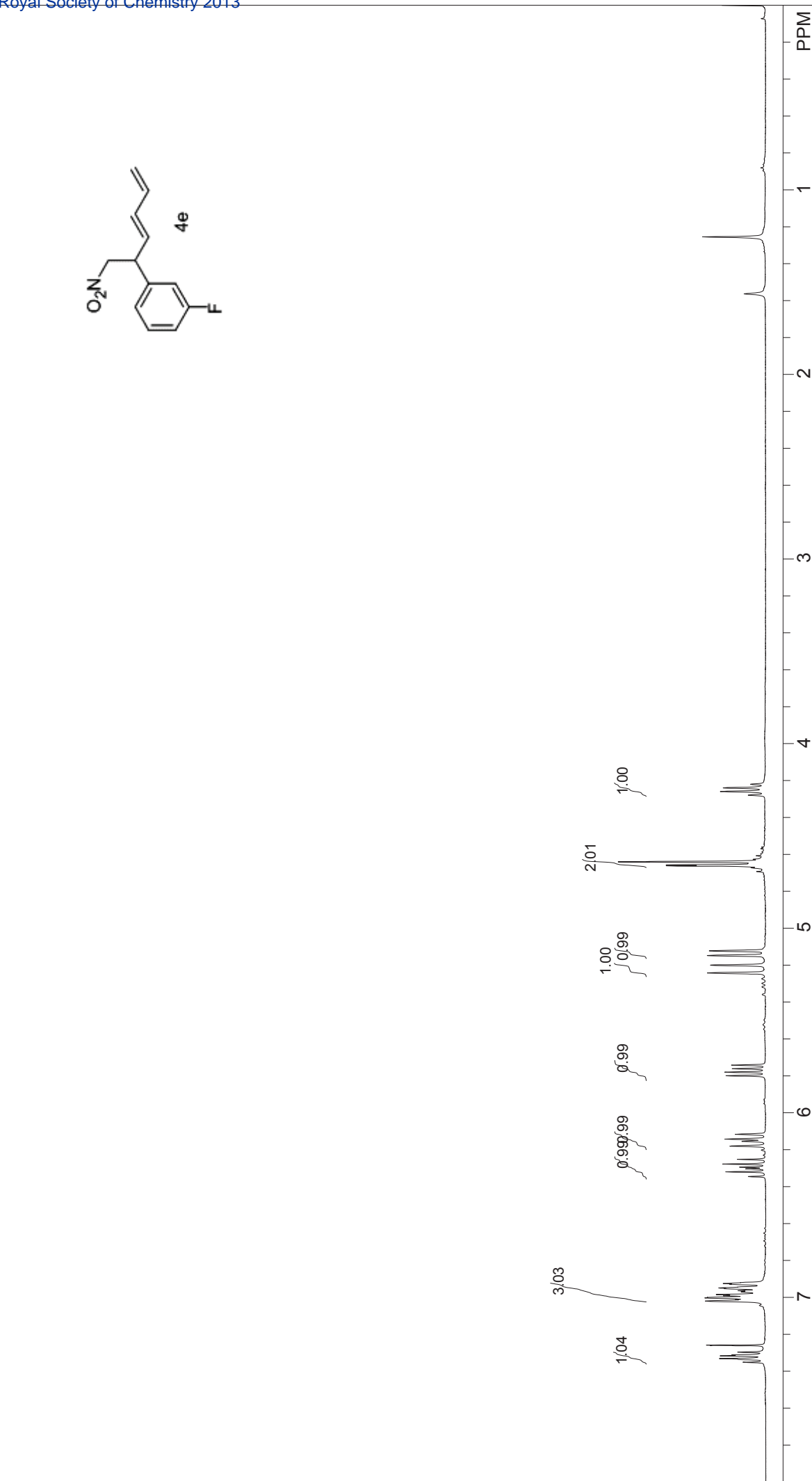
65536

USER: -- DATE: Dec 8 2012

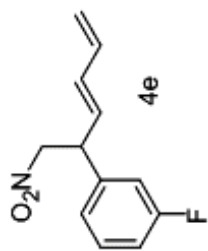
Nuts - \$yxf-15-58-c.fid



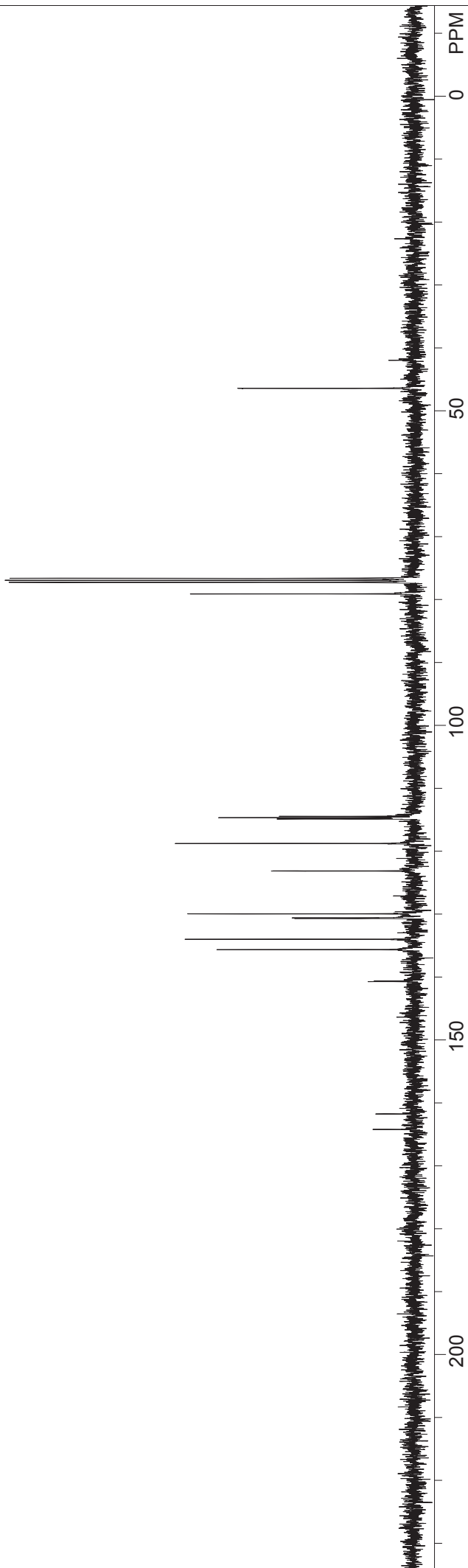
7.332  
7.317  
7.312  
7.297  
7.260  
7.021  
7.012  
6.985  
6.925  
6.920  
6.346  
6.320  
6.303  
6.295  
6.278  
6.252  
6.181  
6.179  
6.155  
6.153  
6.143  
6.117  
5.799  
5.780  
5.761  
5.742  
5.243  
5.242  
5.200  
5.148  
5.123  
4.662  
4.657  
4.641  
4.639  
4.279  
4.259  
4.240  
4.220



:blank line;blank line		USER: -- DATE: Dec 21 2012	
F1: 400.032	F2: 100.597	PTSIId: 21676	32768
EX: s2pul	SW1: 7225	LB: 0.0	
	PW: 10.5 us		
	PD: 1.0 sec		
	NA: 24		
			Nuts - \$yxf-3-f-h.fid



164.219  
161.759  
140.736  
140.668  
135.658  
134.015  
130.701  
130.618  
129.980  
123.183  
123.156  
118.803  
114.905  
114.700  
114.491  
79.163  
77.319  
77.000  
76.681  
46.436



mx-13-26-p2-C400

F1: 100.521

F2: 399.722

SW1: 25000

PW: 6.8 us

PD: 1.0 sec

OF1: 11052.2

NA: 44

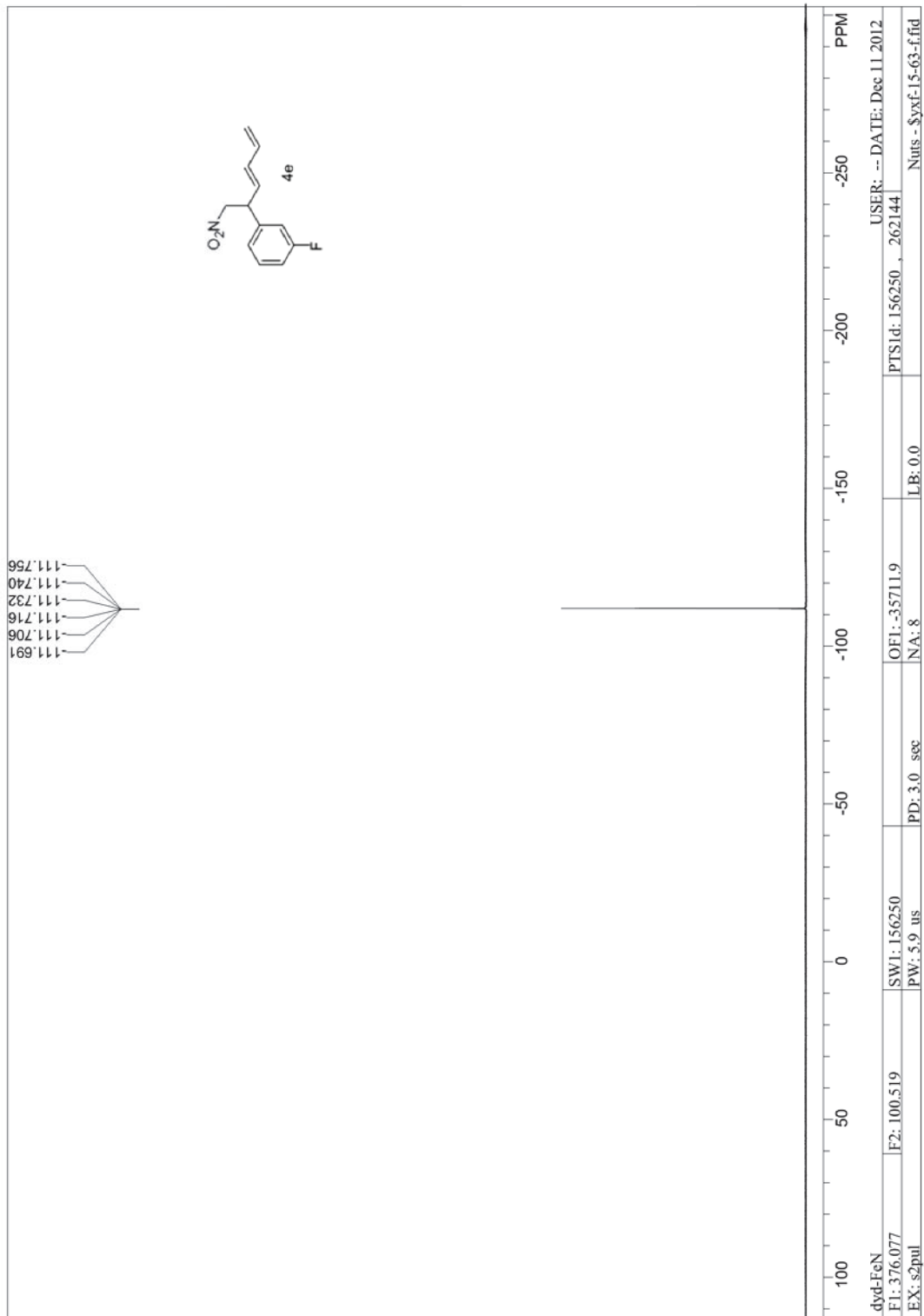
LB: 2.0

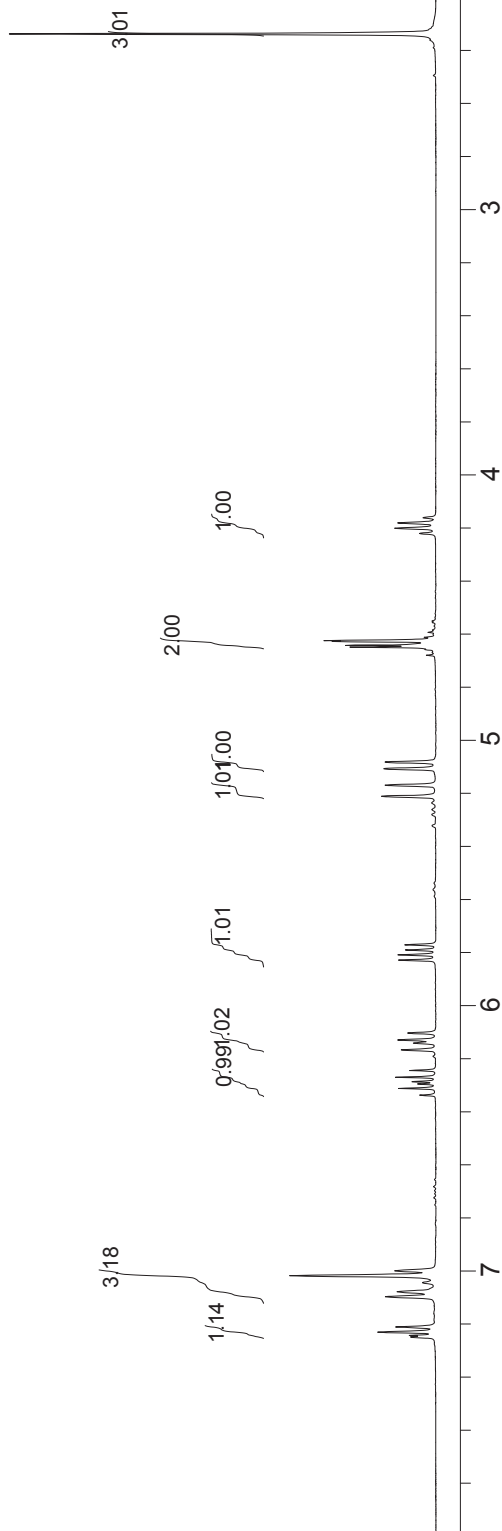
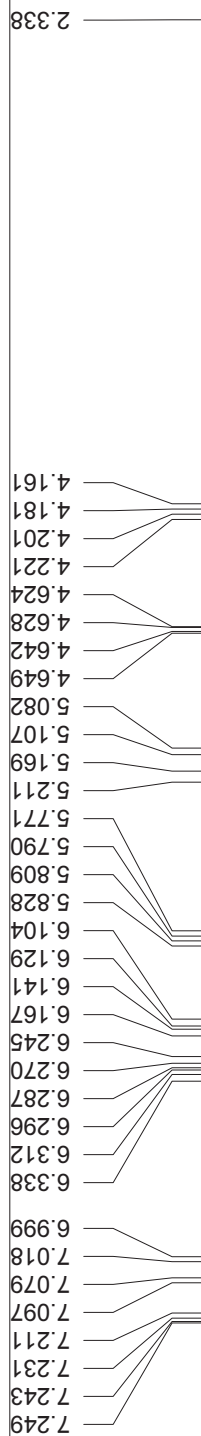
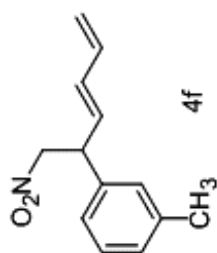
PTSIId: 37500

65536

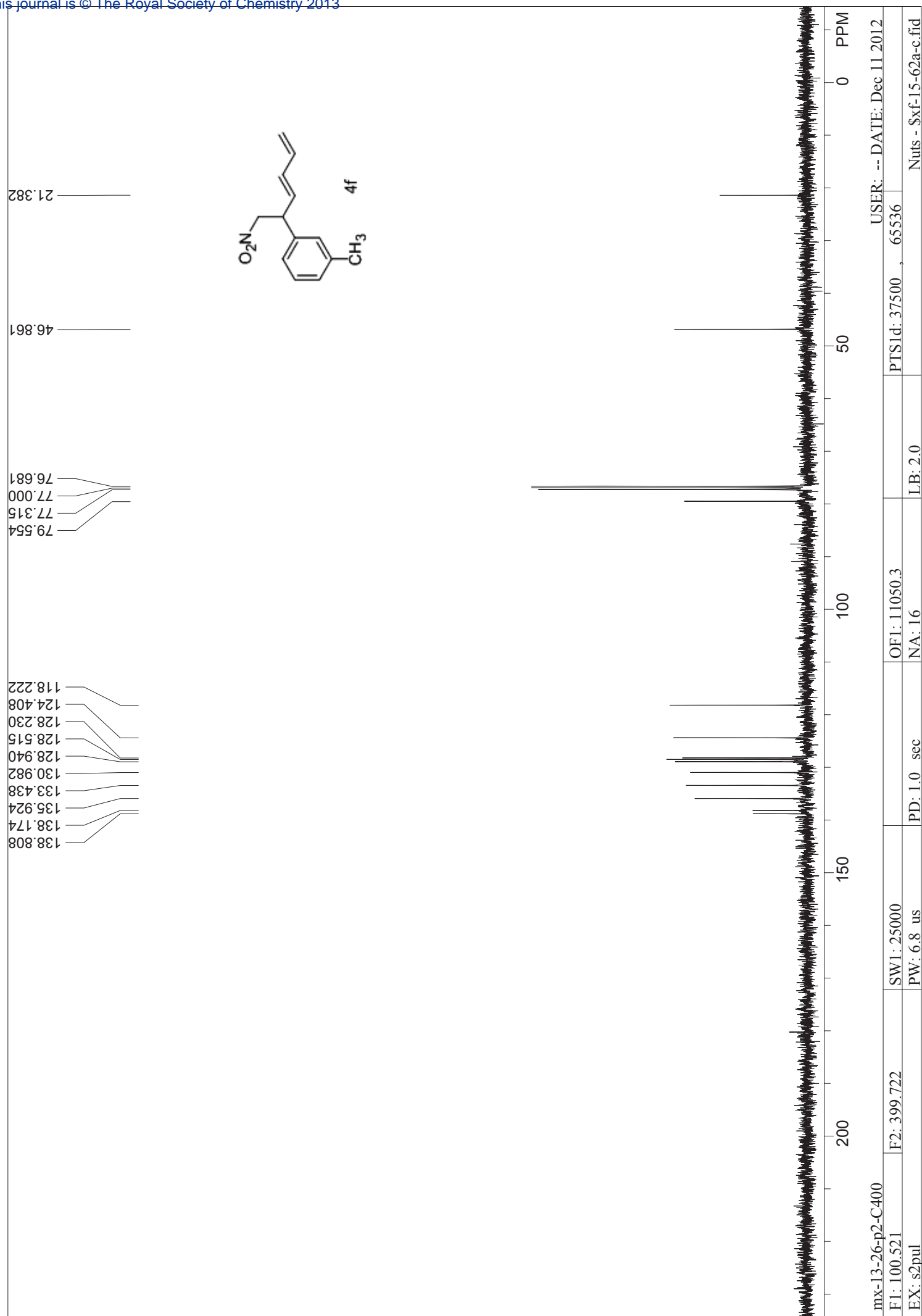
USER: -- DATE: Dec 11 2012

Nuts - \$yxf-15-63-c.fid

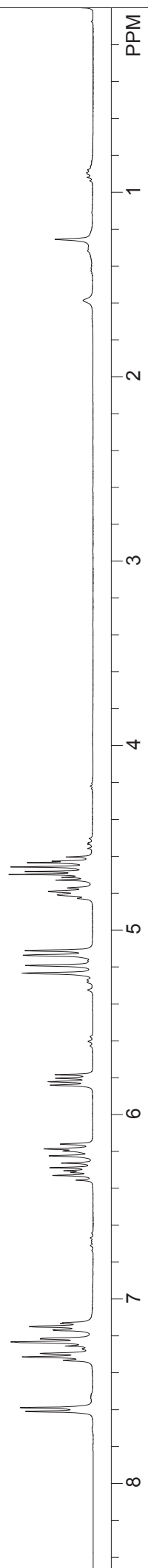
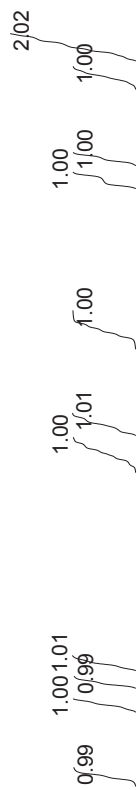
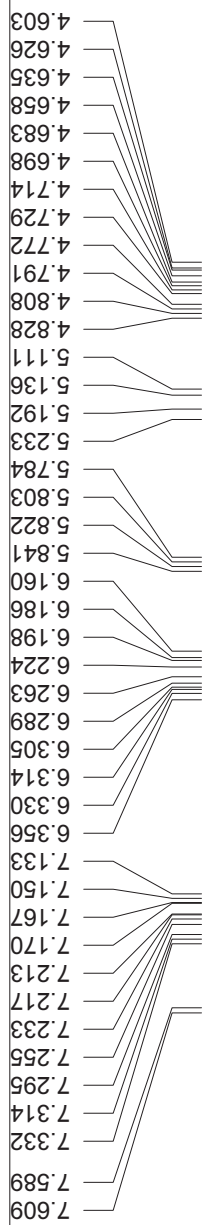
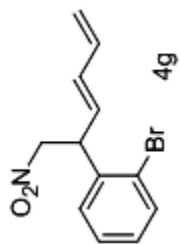




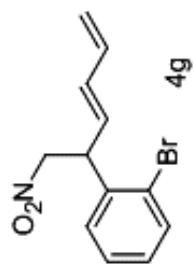
mx-13-26-p2-h,blank line	OF1: 2791.7	PTSID: 21552	USER: -- DATE: Dec 11 2012
F1: 399.723	NA: 12	LB: 0.0	32768
EX: s2pul	PD: 1.0 sec	Nuts - \$yxf-15-62-h.fid	







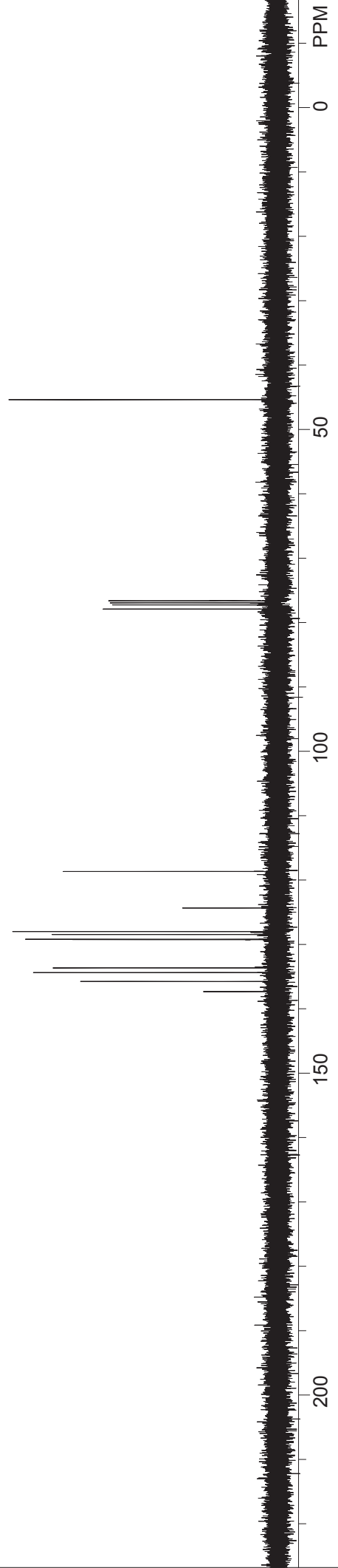
:blank line		USER: -- DATE: May 23 2012	
F1: 400.031	F2: 100.597	SW1: 6410	OF1: 2405.6
EX: s2pul	PW: 10.3 us	PD: 1.0 sec	NA: 28
		LB: 0.0	PTSId: 19231
			32768
			Nuts - \$yxf-13-78-h.fid



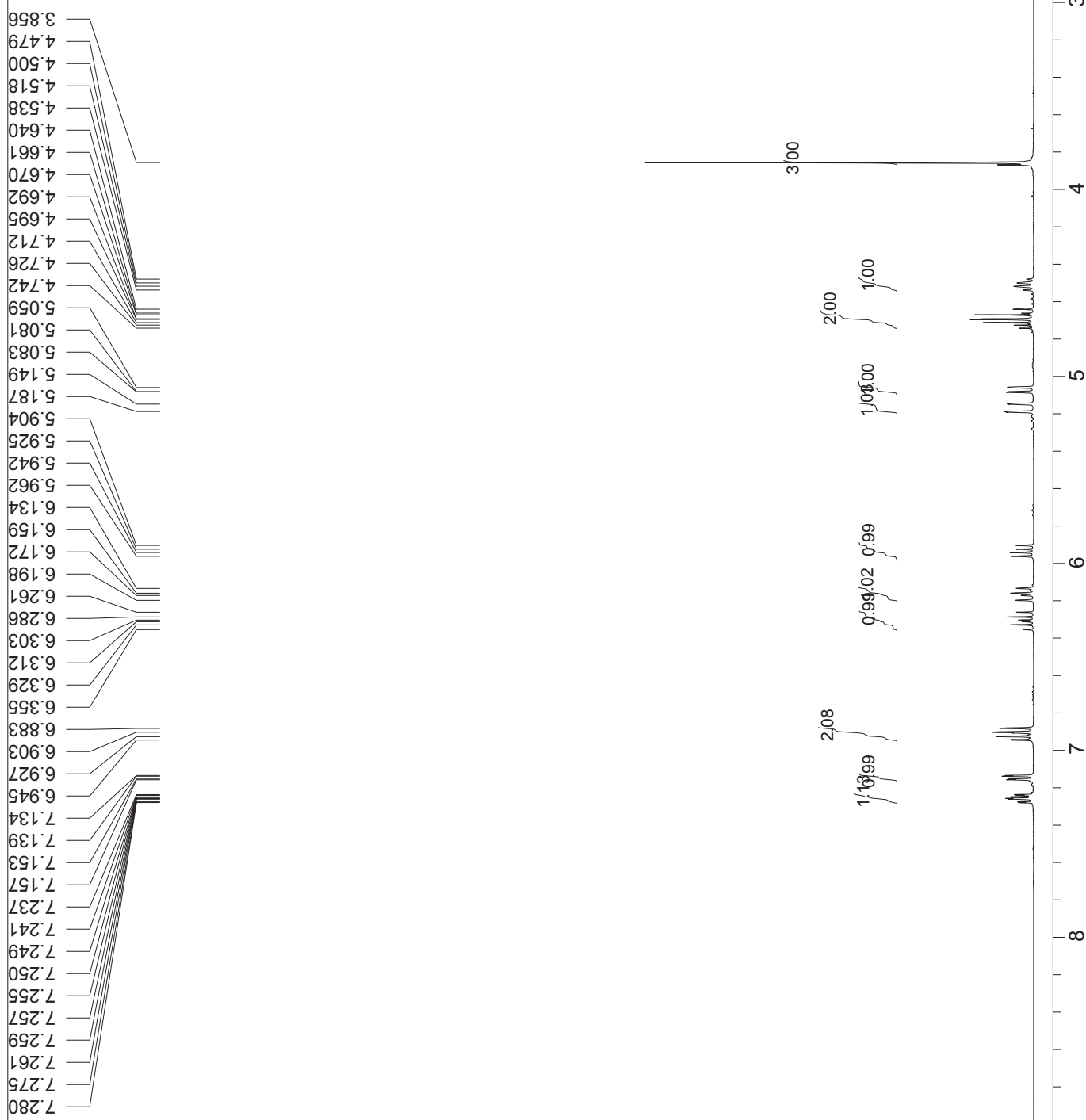
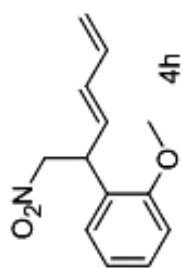
45.385

76.684  
77.000  
77.316  
77.959

118.691  
124.361  
128.016  
128.470  
129.214  
129.269  
133.660  
134.378  
135.761  
137.334

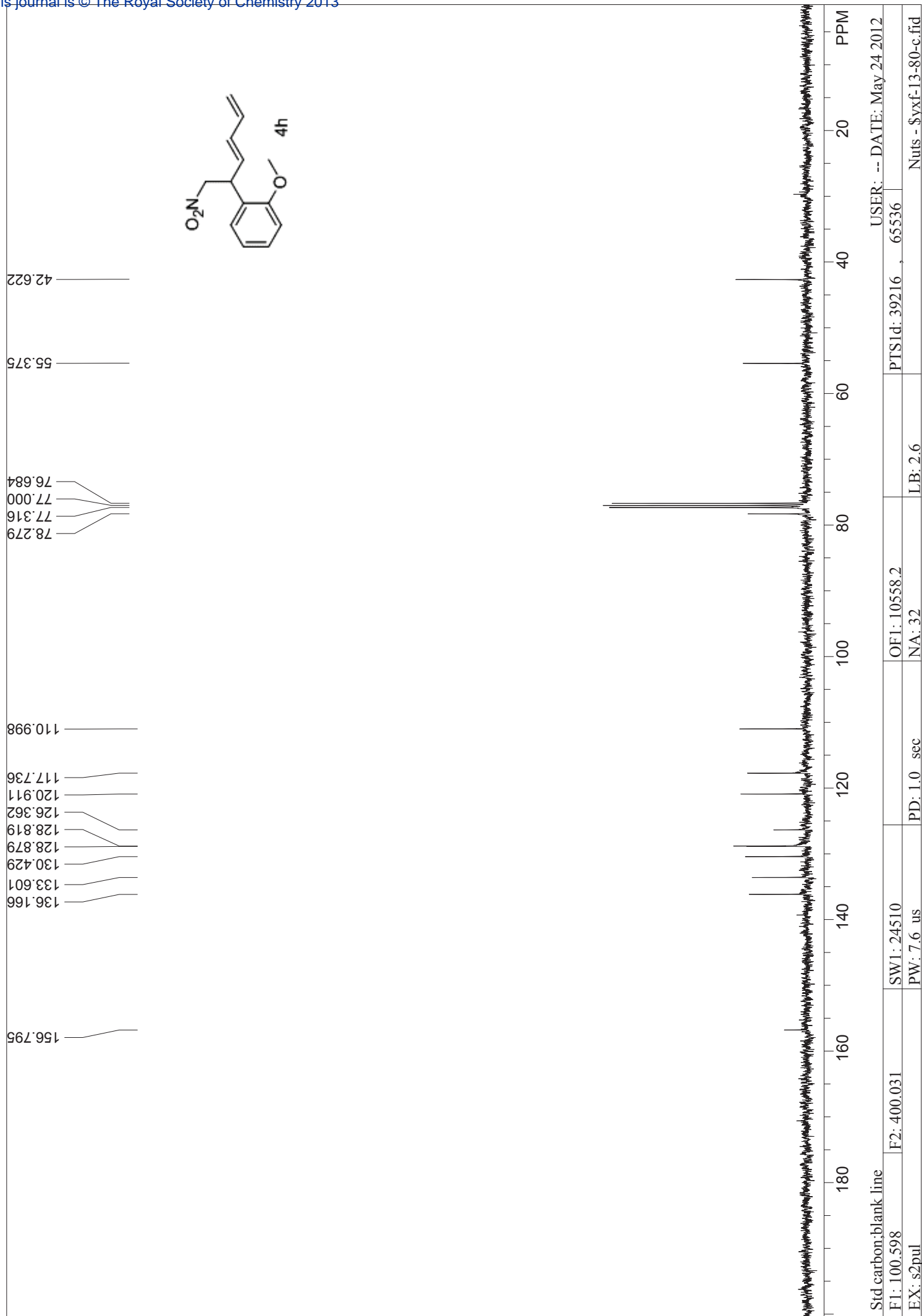
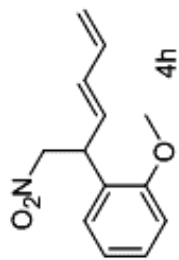


Std carbon, blank line				USER: -- DATE: May 23 2012
F1: 100.598	F2: 400.031	SW1: 24510	OF1: 10557.9	PTSId: 39216 , 65536
EX: s2pul	PW: 7.6 us	PD: 1.0 sec	NA: 32	LB: 0.0
				Nuts - \$yxf-13-78-c.fid

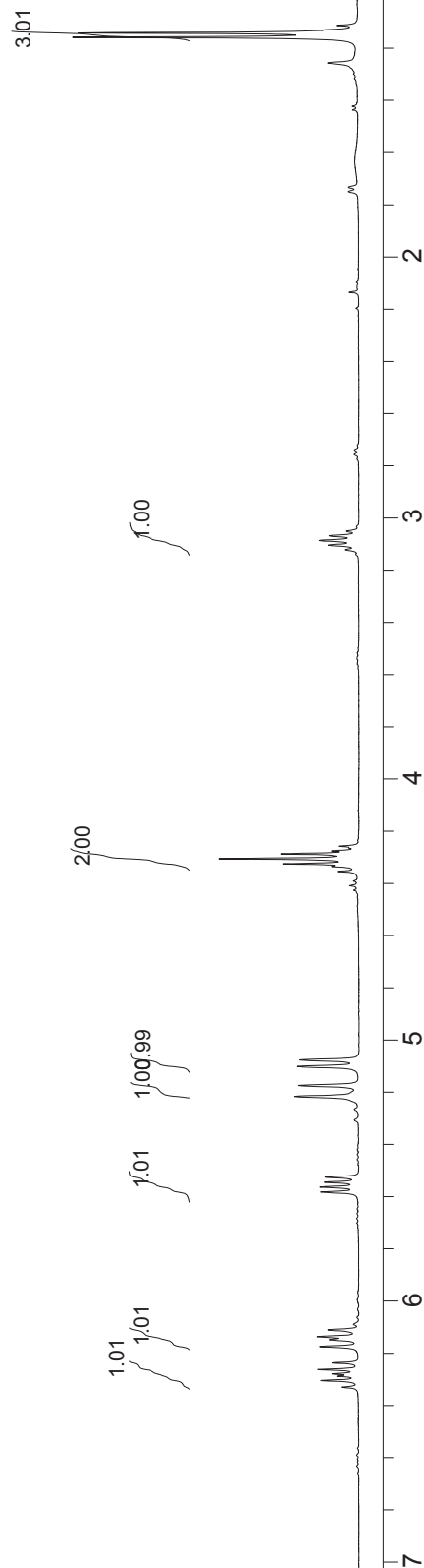
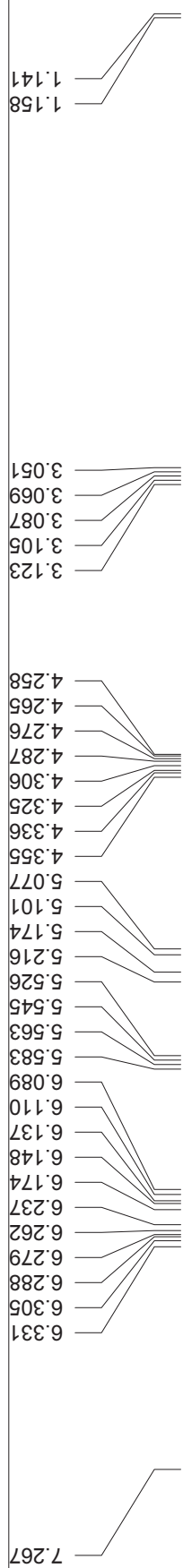
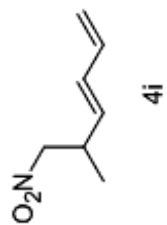


:blank line		USER: -- DATE: May 24 2012	
F1: 400.032	F2: 100.597	OF1: 2763.1	PTSId: 21429 , 32768
EX: s2pul	PW: 10.3 us	NA: 16	LB: 0.0
	PD: 1.0 sec		Nuts - \$yxf-13-80-h.fid

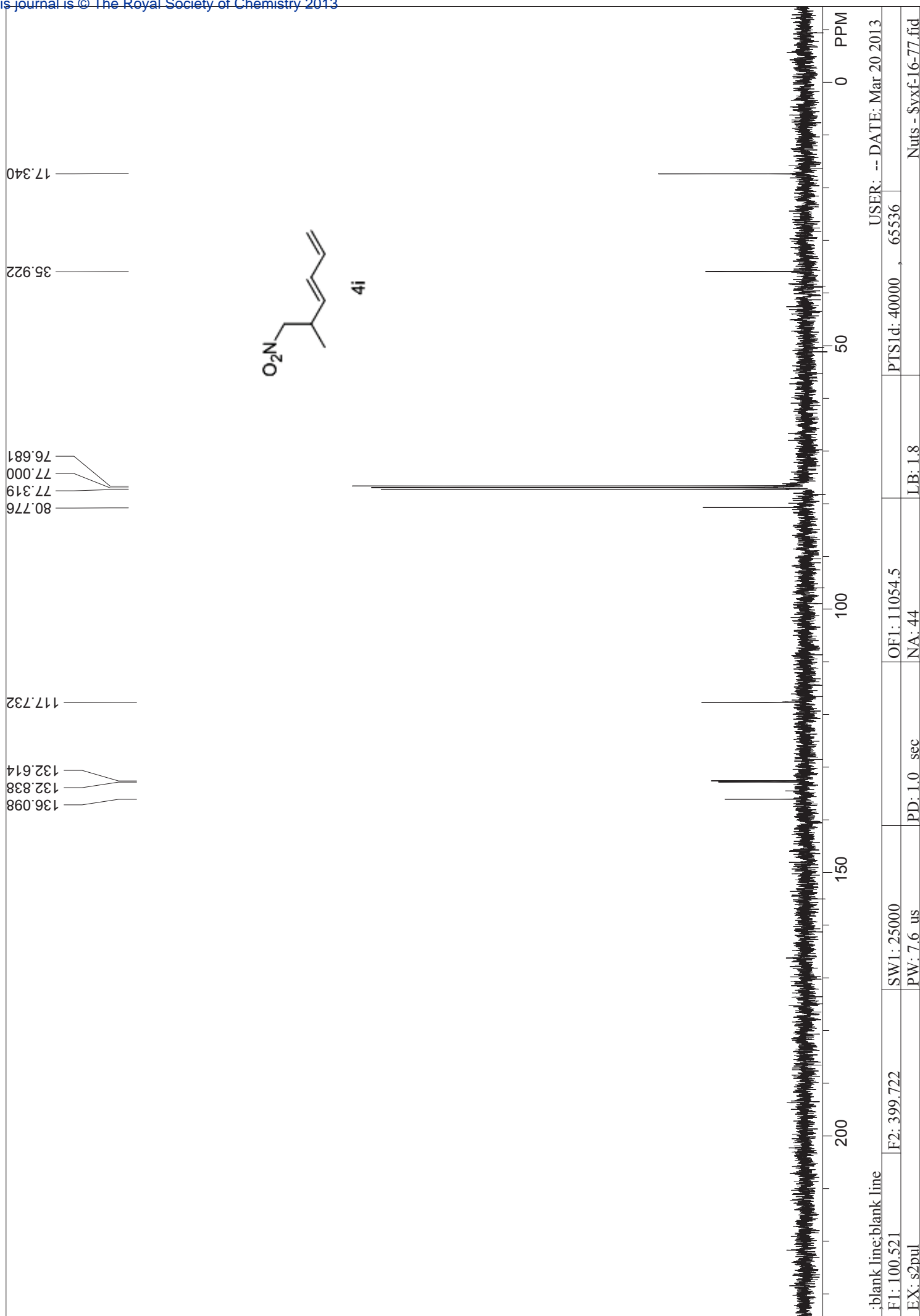
**S-27**

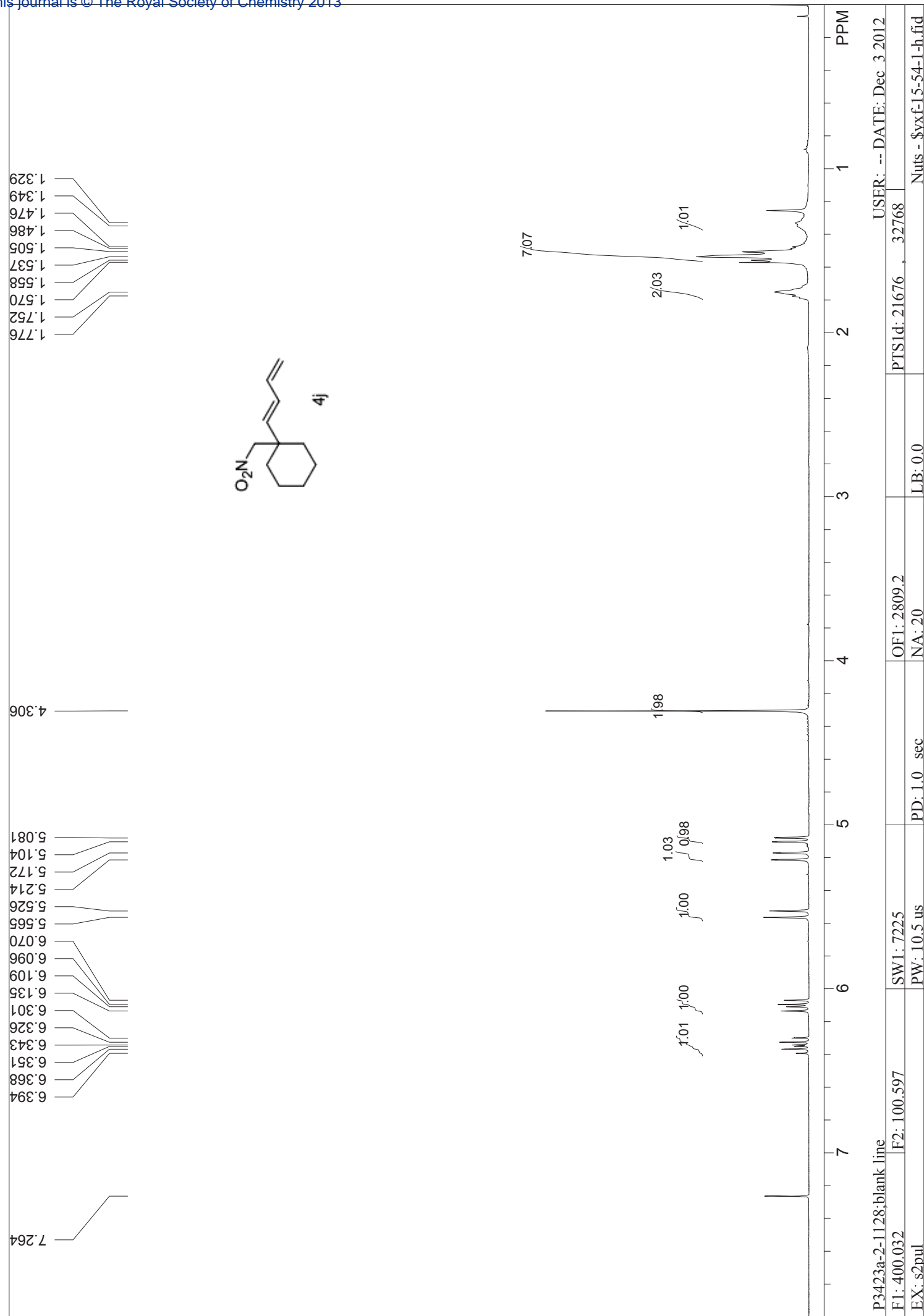


Std carbon, blank line  
 F1: 100.598 F2: 400.031 SW1: 24510  
 EX: s2pul PD: 1.0 sec NA: 32 OF1: 10558.2  
 USER: -- DATE: May 24 2012  
 PTSId: 39216 , 65536  
 LB: 2.6  
 Nuts - \$yxf-13-80-c.fid  
**S-28**



:blank line		USER: -- DATE: Jun 4 2012	
F1: 400.032	F2: 100.597	OF1: 2766.2	PTSIId: 23571, 32768
EX: s2pul	PW: 10.3 us	NA: 16	LB: 0.0
	PD: 1.0 sec		Nuts - \$yxf-14-4-h.fid





P3423a-2-1128;blank line

F1: 400.032 F2: 100.597

EX: s2pul

SW1: 7225

PW: 10.5 us

PD: 1.0 sec

NA: 20

OF1: 2809.2

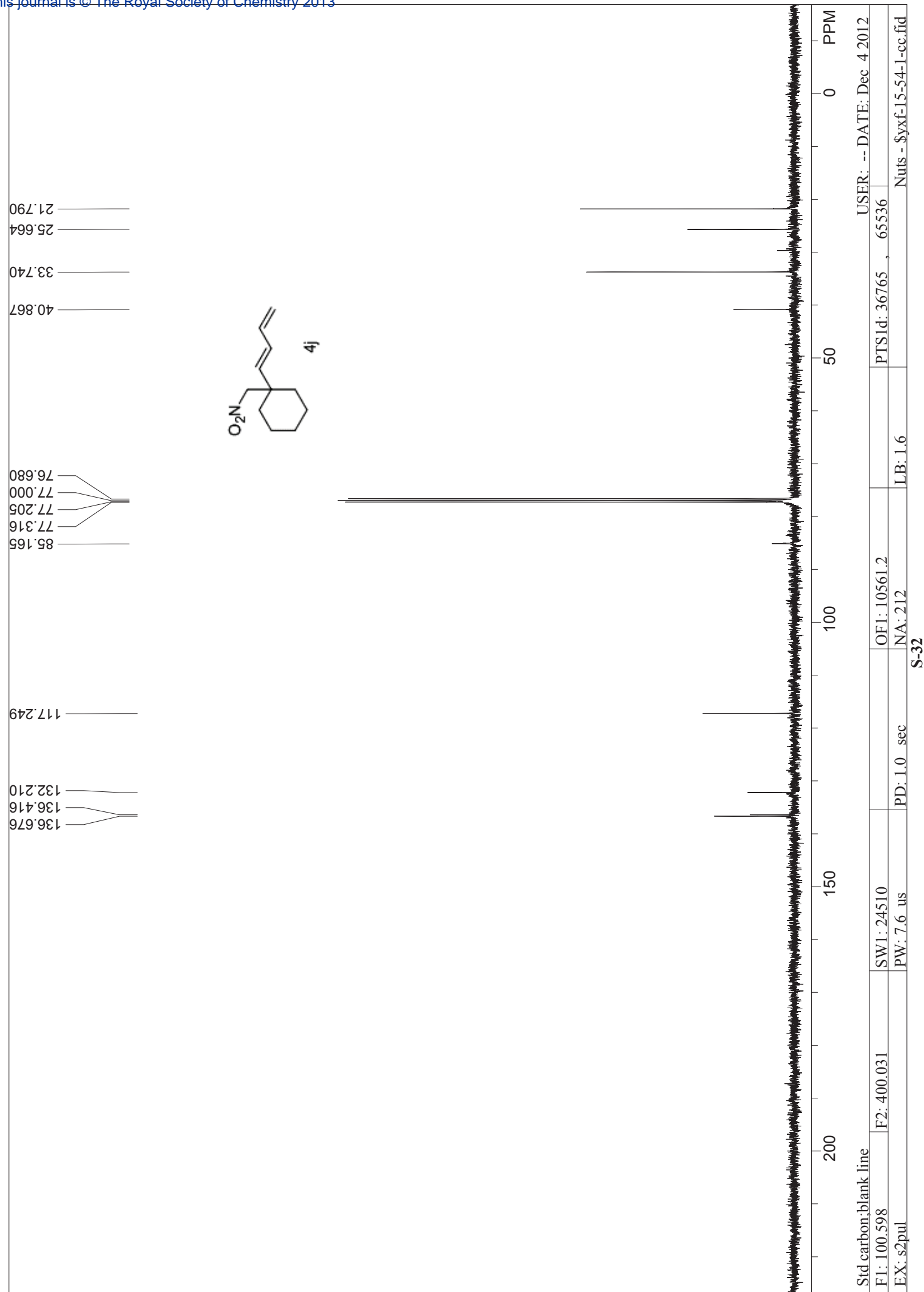
LB: 0.0

PTSlD: 21676

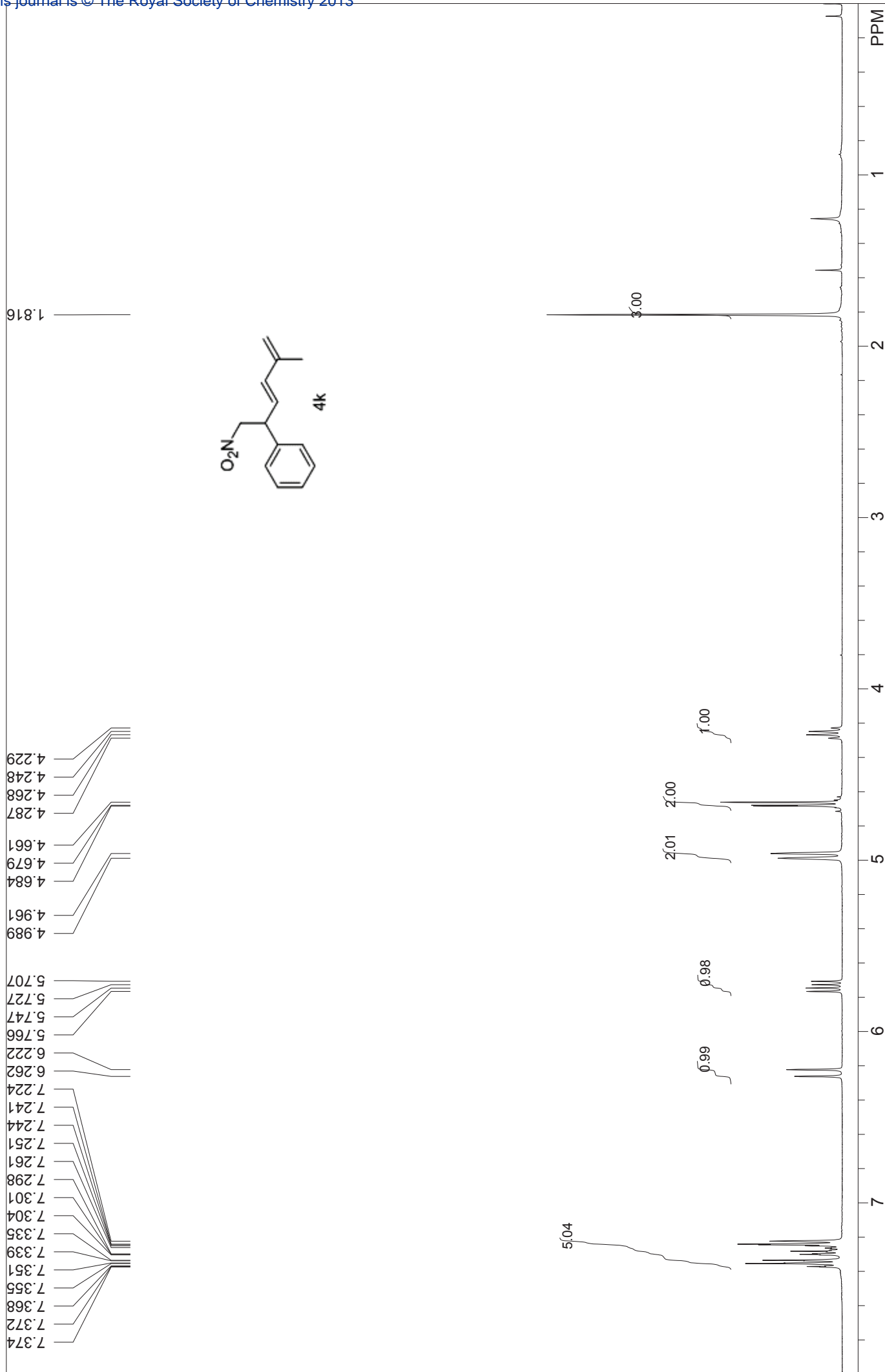
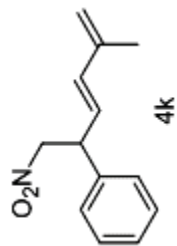
32768

USER: -- DATE: Dec 3 2012

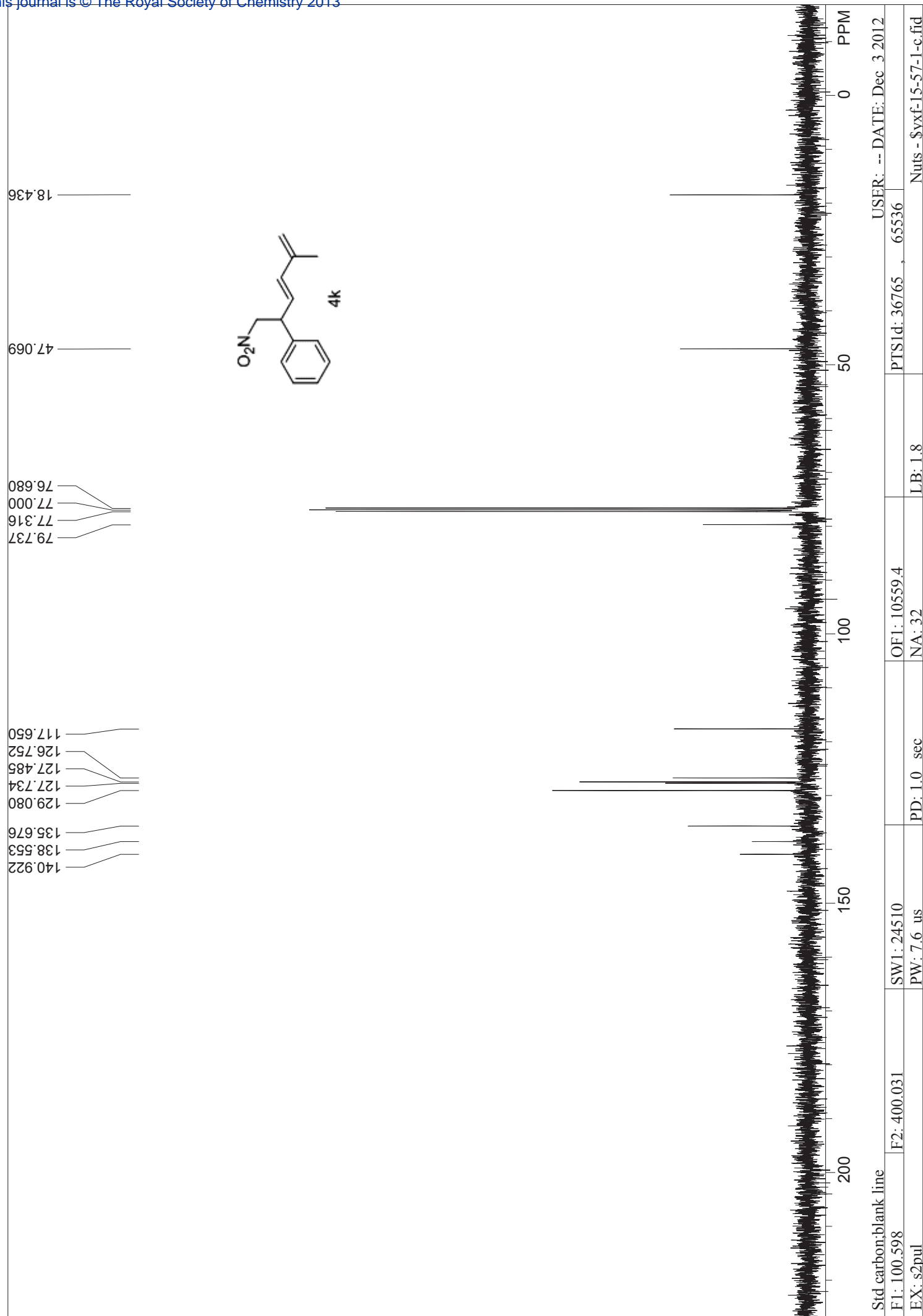
Nuts - \$yxf15-54-1-h.fid

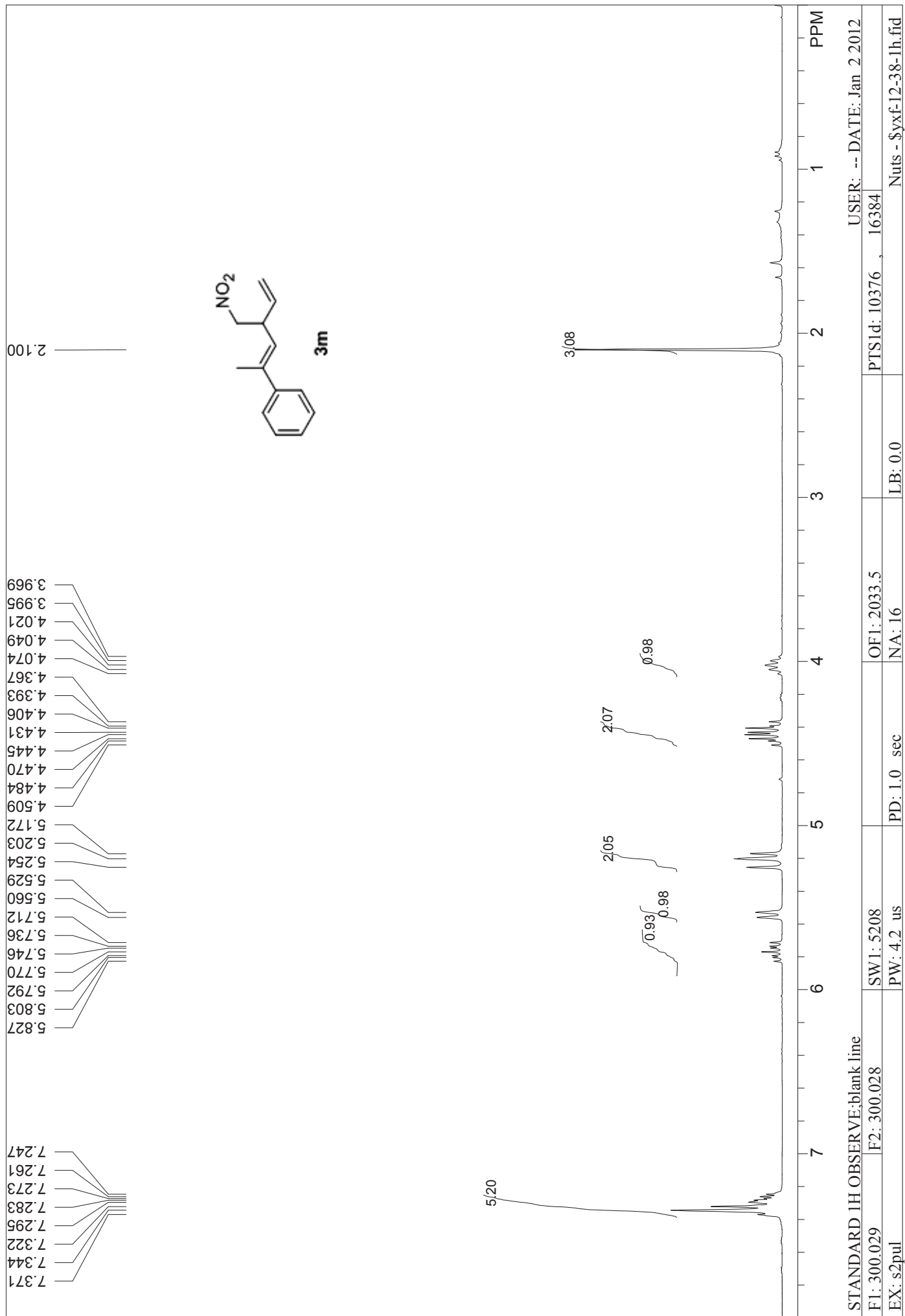


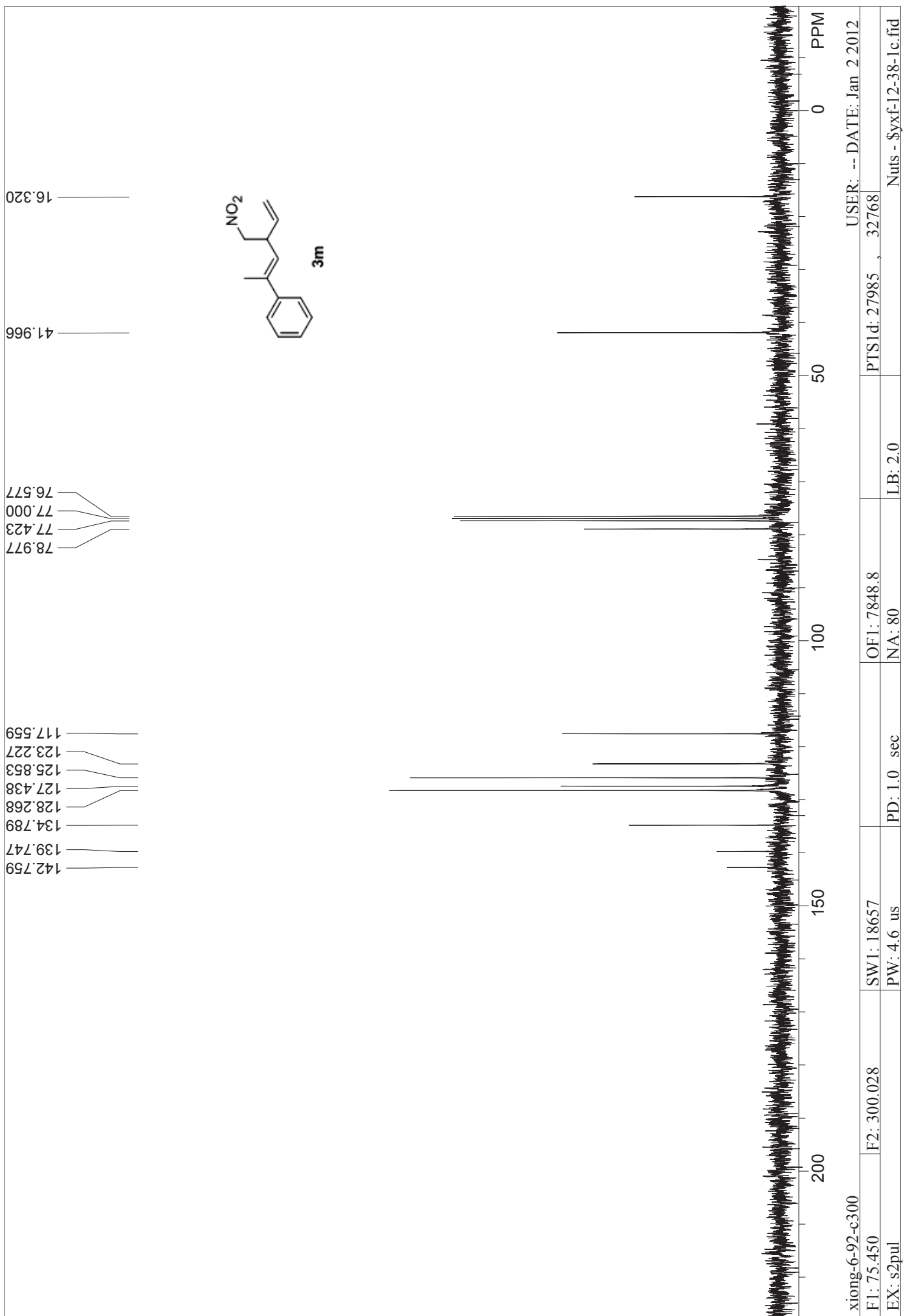




P3423a-2-1128; blank line	SW1: 7225	OF1: 2803.9	PTSID: 21676	USER: -- DATE: Dec 3 2012
F1: 400.032	F2: 100.597	PD: 1.0 sec	LB: 0.0	32768
EX: s2pul	PW: 10.5 us	NA: 8	Nuts - \$yxf-15-57-1-h.fid	







942

## HPLC REPORT

Sample Name: yxf-12-20-2-oj-8-2-0.5. che

Date: 2012-01-08

Time: 12:41

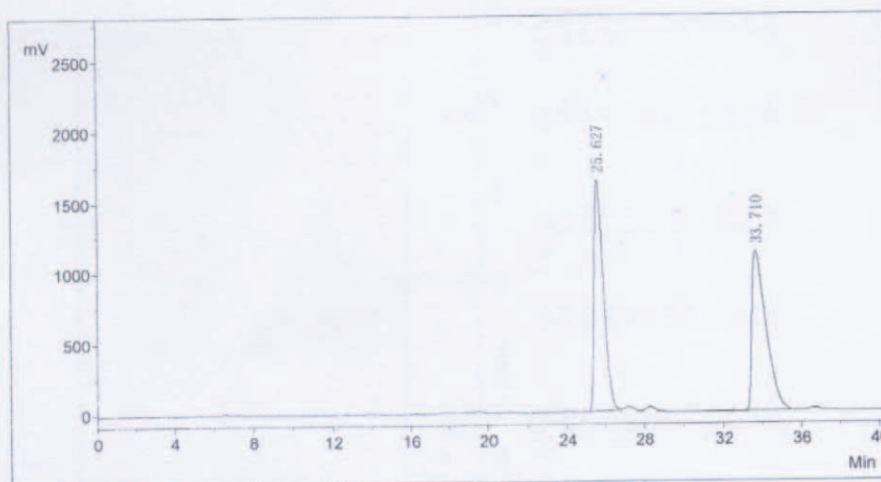
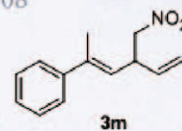
Method:

Column:

Flow Rate:

Wave Length:

Mobile Phase:



No.	PeakNo	ID. Name	R. Time	PeakHeight	PeakArea	PerCent
1	1	Unknown	25.627	1635638.3	54692147.1	49.3004
2	2	Unknown	33.710	1129347.8	56244312.8	50.6996
Total				2764986.2	110936459.9	100.0000

# HPLC REPORT

Sample Name: yxf-12-35-1. che

Date: 2012-01-08

Time: 14:02

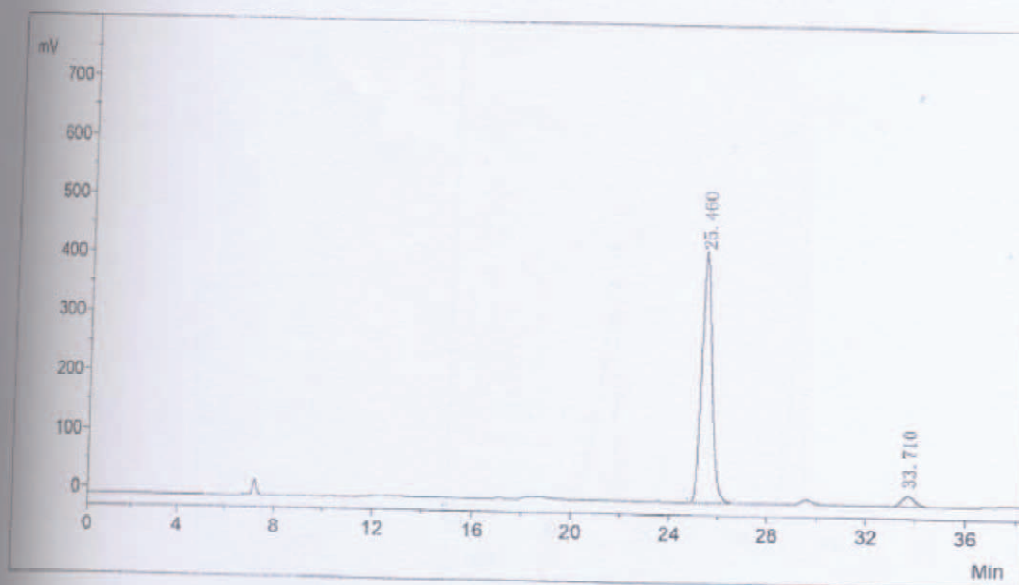
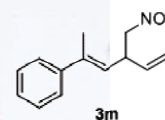
Method:

Column:

Flow Rate:

Wave Length:

Mobile Phase:



No.	PeakNo	ID. Name	R. Time	PeakHeight	PeakArea	PerCent
1	1	Unknown	25.460	414572.5	12319482.5	94.9375
2	2	Unknown	33.710	17064.2	656930.3	5.0625
Total				431636.7	12976412.8	100.0000