SUPPORTING INFORMATION

Ethylammonium Nitrate (EAN)/Tf_2O and EAN/TFAA; Ionic Liquid-Based Systems for Aromatic Nitration

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EXPERIMENTAL

NMR analysis and other characterization data for the nitro products:

Nitrobenzene **(1)**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.52-7.56 (m, 2H), 7.69 (tt, J = 1.3 Hz; J = 7.5 Hz, 1H), 8.21-8.23 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 123.5, 129.4, 134.7, 148.3; GC/MS (EI) m/z 123 (M^+), 93, 77 (100%), 74, 65, 51, 46, 39.

Nitrotoluenes **(2)**: **4-Nitro:** off-white solid, m.p. 52 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.46 (s, 3H), 7.32 (d, J = 8.3 Hz, 2H), 8.11 (d, J = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 21.7, 123.7, 129.9, 146.1, 146.3; GC/MS (EI) m/z 137 (M^+), 107, 91, 77, 65 (100%), 50, 46, 39; **2-Nitro:** GC/MS (EI) m/z 137 (M^+), 120, 92, 77, 65 (100%), 51, 46, 39; GC/MS for **3-Nitro:** (EI) m/z 137 (M^+), 91, 77, 65, 50, 46 (100%), 39.

Nitroanisoles **(6)**: **4-nitro:** off-white solid, m.p. 54 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 3.9 (s, 3H), 6.95 (d, J = 9.3 Hz, 2H), 8.19 (d, J = 9.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 56.1, 114.1, 126.0, 141.6, 164.7; GC/MS (EI) m/z 153 (M^+), 123, 106, 92, 77 (100%), 63, 51, 46, 38; **2-Nitro:** GC/MS (EI) m/z 153 (M^+), 123 (100%), 92, 77, 63, 50, 46, 38.

Fluoro-nitrobenzenes **(7)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture: **4-Nitro.** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.17-7.21 (m, 2H); 8.24 (dd, J = 4.7 Hz, J = 9.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 116.5 (d, $J_{C\text{-}F}$ = 24.8 Hz), 126.4 (d, $J_{C\text{-}F}$ = 10.13 Hz), 144.5, 166.3 (d, $J_{C\text{-}F}$ = 255.38 Hz); ^{19}F NMR (470.2 MHz, $CDCl_3$, 25 °C): δ -102.24 to -102.18 (m); GC/MS (EI) m/z 141 (M^+), 125, 111, 95, 83, 75 (100%), 69, 57, 50, 46, 37; **2-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.25-7.31 (m, 2H), 7.61-7.65 (m, 1H), 8.01-8.05 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 118.5 (d, $J_{C\text{-}F}$ = 20.38 Hz), 124.7 (d, $J_{C\text{-}F}$ = 4.63 Hz), 126.2 (d, $J_{C\text{-}F}$ = 2.76 Hz); 135.7 (d, $J_{C\text{-}F}$ = 9.25 Hz), 137.6, 155.6 (d, $J_{C\text{-}F}$ = 263.87 Hz); ^{19}F NMR (470.2 MHz,

$CDCl_3$, 25 °C): δ -117.93 to -117.88 (m); GC/MS (EI) *m/z* 141 (M^+), 111, 95, 83, 75 (100%), 69, 62, 57, 50, 46, 37.

Chloro-nitrobenzenes **(8)**: **4-Nitro:** pale-yellow solid, m.p. 84-85 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.52 (d, J = 9.2 Hz, 2H), 8.19 (d, J = 9.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 125.1, 129.7, 141.5, 146.6; GC/MS (EI) *m/z* 157 (M^+), 127, 111, 75 (100%), 50; **2-Nitro:** GC/MS (EI) *m/z* 157 (M^+), 127, 111, 99, 75 (100%), 61, 46.

Nitrophenylacetonitrile **(11)**: NMR chemical shift values for this isomer were determined directly from the isomeric mixture. **4-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 3.89 (s, 2H), 7.55 (d, J = 8.8 Hz, 2H), 8.26 (d, J = 8.8 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 23.7, 116.6, 124.5, 129.1, 137.1, 147.9; GC/MS (EI) *m/z* 162 (M^+), 132, 116, 104, 89 (100%), 77, 63, 50, 46, 39. **3-Nitro**: GC/MS (EI) *m/z* 162 (M^+), 132, 116, 104, 89 (100%), 75, 63, 50, 46, 39. **2-Nitro**: GC/MS (EI) *m/z* 162 (M^+, not detected), 145, 135, 114, 89 (100%), 79, 74, 63, 50, 46, 39. (NMR data for 2 and 3-nitro derivatives could not be determined due to overlap)

Methyl nitrophenylacetate **(12)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture. **4-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 3.67 (s, 3H), 3.72 (s, 2H), 7.43 (d, J = 8.6 Hz, 2H), 8.13 (d, J = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 40.7, 52.3, 123.7, 130.3, 141.4, 147.2, 170.4; GC/MS (EI) *m/z* 195 (M^+, not detected), 179, 164, 149 (100%), 136, 121, 89, 78, 63, 51, 46, 39; **2-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 3.68 (s, 3H), 3.99 (s, 2H), 7.33 (d, J = 7.5 Hz, 1H), 7.42-7.46 (m, 1H), 7.55-7.58 (m, 1H), 8.05-8.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 39.5, 52.2, 125.2, 128.6, 133.4, 133.6, 135.7, 148.8, 170.6; GC/MS (EI) *m/z* 195 (M^+), 136, 121, 106, 89 (100%), 78, 59, 51, 46, 39; **3-Nitro**: NMR data for this minor isomer could not be determined due to sever overlap with the other two isomers; GC/MS (EI) *m/z* 195 (M^+), 136, 120, 105, 89 (100%), 78, 59, 51, 46, 39.

Methyl 3-nitrobenzoate **(13)**: off-white crystalline powder, m.p. 77-79 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 3.99 (s, 3H), 7.66 (t, J = 8.1 Hz, 1H), 8.37 (dt, J = 1.3 Hz, J = 7.6 Hz, 1H), 8.42 (ddd, J = 1.1

Hz, J = 2.2 Hz, J = 8.4 Hz, 1H), 8.87 (t, J = 2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 52.9, 124.8, 127.5, 129.8, 132.0, 135.4, 148.4, 165.1; GC/MS (EI) m/z 181 (M^+), 150 (100%), 120, 104, 76, 50.

3-Nitrobenzonitrile **(14)**: yellow crystalline solid, m.p. 114-115 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.74 (t, J = 8.1 Hz, 1H), 7.99 (dt, J = 1.5 Hz, J = 7.8 Hz, 1H), 8.48 (ddd, J = 1.1 Hz, J = 2.2 Hz, J = 8.3 Hz, 1H), 8.54 (t, J = 1.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 114.3, 116.7, 127.4, 127.7, 130.8, 137.7, 148.4; GC/MS (EI) m/z 148 (M^+), 102 (100%), 90, 75, 63, 50, 46, 38.

3-Nitrobenzenetrifluoride **(16)**: NMR chemical shift values were determined directly out of the crude reaction mixture. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.75 (t, J = 7.95 Hz, 1H), 7.98 (d, J = 7.6 Hz, 1H), 8.44 (d, J = 8.0 Hz, 1H), 8.49 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 120.9 (q, $J_{C\text{-}F}$ = 3.75 Hz), 121.4 (q, $J_{C\text{-}F}$ = 160.63 Hz), 126.8, 130.5, 131.3 (q, $J_{C\text{-}F}$ = 3.25 Hz), 132.4 (q, $J_{C\text{-}F}$ = 34.25 Hz), 148.4; ^{19}F NMR (470.2 MHz, $CDCl_3$, 25 °C): δ -63.03 (m); GC/MS (EI) m/z 191 (M^+), 172, 145 (100%), 125, 95, 75, 69, 46, 38.

3-Nitroacetophenone **(17)**: pale-yellow crystalline solid, m.p. 79-80 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.67 (s, 3H), 7.67 (t, J = 8.0 Hz, 1H), 8.26 (dt, J = 1.4 Hz, J = 7.9 Hz, 1H), 8.37-8.4 (m, 1H), 8.72 (t, J = 1.7 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 26.8, 123.2, 127.5, 130.0, 133.9, 138.3, 148.5, 195.8; GC/MS (EI) m/z 165 (M^+), 150 (100%), 104, 76, 63, 50, 43, 38.

Nitrobenzaldehyde **(18)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture. **3-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.76 (t, J = 8.0 Hz, 1H), 8.22 (d, J = 7.5 Hz, 1H), 8.46 (dd, J = 1.5 Hz, J = 8 Hz, 1H), 8.67 (s, 1H), 10.10 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 124.4, 128.6, 130.5, 134.8, 137.4, 148.8, 189.9; GC/MS (EI) m/z 151 (M^+, 100%), 105, 77, 63, 51, 38; **2-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.74-7.81 (m, 2H), 7.91 (dd, J = 1.5 Hz; J = 7.5 Hz, 1H), 8.08 (dd, J = 1.0 Hz, J = 7.5 Hz, 1H), 10.37 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 124.5, 129.7, 131.4, 133.8, 134.6, 149.6, 188.2. GC/MS (EI) m/z 134 ($M^{+\cdot}$ not detected), 121 (100%), 104, 93, 76, 65, 50, 46, 39. **4-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 8.06 (d, J = 8.5 Hz, 2H), 8.36

(d, J = 8.5 Hz, 2H), 10.14 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 124.3, 130.5, 141.1, 151.5, 190.5; GC/MS (EI) m/z 151 (M^+, 100%), 121, 104, 77, 65, 51, 37.

4-Chloro-3-methyl-6-nitrophenol **(21)**: red color solid, m.p. 130-132 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.42 (s, 3H), 7.05 (s, 1H), 8.09 (s, 1H), 10.43 (s, 1H, OH); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 20.9, 121.6, 124.7, 125.9, 132.0, 147.7, 153.6; GC/MS (EI) m/z 187 (M^+,100%), 157, 129, 113, 77, 65, 51, 46, 39.

4-Methoxy-3-nitrobenzaldehyde **(24)**: off-white crystalline solid, m.p. 99-101 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 4.07 (s, 3H, OMe), 7.24 (d, J = 8.8 Hz, 1H), 8.09 (dd, J = 2.1 Hz, J = 8.7 Hz, 1H), 8.35 (d, J = 2.2 Hz, 1H), 9.94 (s, 1H, CHO); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 57.2, 113.9, 122.1, 127.6, 129.2, 134.8, 157.3, 188.9; GC/MS (EI) m/z 181 (M^+), 151, 134, 119 (100%), 104, 95, 77, 63, 51, 46, 38.

2-Fluoro-5-nitrobenzaldehyde **(25)**: pale-orange solid, m.p. 58-59 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.4 (t, J = 9 Hz, 1H), 8.48-8.52 (m, 1H), 8.76 (dd, J = 2.8 Hz, J = 6 Hz, 1H), 10.38 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 118.3 (d, $J_{C\text{-}F}$ = 23.12 Hz), 124.6 (d, $J_{C\text{-}F}$ = 10.13 Hz), 124.9 (d, $J_{C\text{-}F}$ = 3.75 Hz), 131.1 (d, $J_{C\text{-}F}$ = 11.13 Hz), 144.9, 167.3 (d, $J_{C\text{-}F}$ = 267.5 Hz), 184.9 (d, $J_{C\text{-}F}$ = 5.5 Hz; ^{19}F NMR (470.2 MHz, $CDCl_3$, 25 °C): -111.28 to -111.24 (quintet, $J_{C\text{-}F}$ = 5.33 Hz); GC/MS (EI) m/z 169 (M^+, 100%), 153, 139, 122, 95, 75, 57, 46.

2-Hydroxy-nitrobenzaldehydes **(26)**: NMR chemical shift values of the respective isomers were determined directly from the isomeric mixture. **3-Nitro:** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.14 (t, J = 7.95 Hz, 1H), 8.11 (dd, J = 1.7 Hz, J = 7.6 Hz, 1H), 8.41 (dd, J = 2.9 Hz, J = 9.2 Hz, 1H), 10.41 (s, 1H), 11.44 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 119.5, 125.6, 131.5, 135.5, 137.3, 156.7, 189.5; GC/MS (EI) m/z 167 (M^+, 100%), 149, 137, 120, 109, 92, 81, 65, 46. **5-Nitro:** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.13 (d, J = 9.3 Hz, 1H), 8.35 (dd, J = 1.7 Hz, J = 8.3 Hz, 1H), 8.57 (d, J = 2.7 Hz, 1H), 10.00 (s, 1H), 11.60 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 119.2, 119.9, 129.9, 131.8, 140.8, 166.3, 195.6; GC/MS (EI) m/z 167 (M^+), 149 (100%), 120, 91, 77, 63, 39.

4-Methoxy-3-nitroacetophenone **(27)**: beige solid, m.p. 97-99 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.59 (s, 3H), 4.03 (s, 3H), 7.16 (d, J = 8.8 Hz, 1H), 8.15 (dd, J = 2.2 Hz, J = 8.8 Hz, 1H), 8.40 (d, J = 2.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 26.4, 57.0, 113.4, 126.3, 129.7, 134.1, 139.3, 156.3, 194.9; GC/MS (EI) m/z 195 (M^+), 180, 119, 105, 91, 76, 63, 50, 43 (100%), 37.

4-Methoxy-3-nitrobenzonitrile **(28)**: white solid, m.p. 150-151 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 4.05 (s, 3H), 7.2 (d, J = 8.8 Hz, 1H), 7.83 (dd, J = 1.9 Hz; J = 8.8 Hz, 1H), 8.15 (d, J = 2.2 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 57.2, 104.4, 114.6, 116.9, 129.8, 134.1, 137.8, 156.1; GC/MS (EI) m/z 178 (M^+), 148, 131 (100%), 117, 102, 89, 75, 62, 51, 46, 38.

4-Fluoro-3-nitrobenzonitrile **(29)**: NMR chemical shift values were determined directly out of the crude reaction mixture. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.48 (dd, J = 8.75 Hz; J = 9.73 Hz, 1H), 7.96 (ddd, J = 2.13 Hz; J = 4 Hz; J = 4 Hz, J = 8.5 Hz, 1H), 8.42 (dd, J = 2.0 Hz; J = 6.5 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 109.8 ($J_{C\text{-}F}$ = 4.62 Hz), 115.8, 120.4 ($J_{C\text{-}F}$ = 21.25 Hz), 130.7 ($J_{C\text{-}F}$ = 1.9 Hz), 137.9 (broad), 139.0 ($J_{C\text{-}F}$ = 10.13 Hz), 157.9 ($J_{C\text{-}F}$ = 273.88 Hz); ^{19}F NMR (470.2 MHz, $CDCl_3$, 25 °C): δ -107.36 to -107.31 (m); GC/MS (EI) m/z 166 (M^+, 100%), 136, 120, 100, 75, 61, 46.

2,4-Dibromonitrobenzene **(30)**: pale-yellow crystalline solid, m.p. 60-61 °C**.** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.60 (dd, J = 2.0 Hz, J = 8.5 Hz, 1H), 7.76 (d, J = 8.5 Hz, 1H), 7.93 (d, J = 1.9 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 115.9, 126.9, 127.5, 131.7, 137.8, 148.8; GC/MS (EI) m/z 281 (M^+), 265, 251 (100%), 235, 223, 154, 74, 46, 37.

Dinitrobenzenes **(31)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture. **1,3-Nitro:** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.83 (t, J = 8.2 Hz, 1H), 8.59 (dd, J = 2.05 Hz, J = 8.25 Hz, 2H), 9.07 (t, J = 2.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 119.2, 129.0, 130.9, 148.7; GC/MS (EI) m/z 168 (M^+), 122, 92, 76 (100%), 63, 50, 38. **1,2-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.79 (dd, J = 3.25 Hz, J = 5.75 Hz, 2H), 7.95 (dd, J = 3.75 Hz, J = 6.25 Hz, 2H); GC/MS (EI) m/z 168 (M^+), 122, 92, 76, 63, 50 (100%), 46, 38; **1,4-Nitro**: ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 8.43 (s, 4H); GC/MS (EI) m/z 168 (M^+, 100%), 122, 92, 75, 63, 50, 46, 38.

1-Chloro-2,4-dinitrobenzene **(32)**: NMR chemical shift values were determined directly out of the crude reaction mixture. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.82 (d, J = 8.99 Hz, 1H), 8.40 (dd, J = 2.48 Hz, J = 9 Hz, 1H), 8.72 (d, J = 2.5 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 121.6, 127.5, 133.4, 133.9, 146.4, 147.8; GC/MS (EI) m/z 202 (M^+), 172, 126, 110, 84, 75 (100%), 63, 46, 37.

2,4-Dinitrotoluene **(33)**: beige solid, m.p. 68-70 °C.^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.74 (s, 3H), 7.58 (d, J = 8.6 Hz, 1H), 8.36 (dd, J = 2.5 Hz, J = 8.55 Hz, 1H), 8.84 (d, J = 2.5 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 20.8, 120.4, 127.1, 134.1, 140.8, 146.6, 149.3; GC/MS (EI) m/z 182 (M^+), 165 (100%), 119, 89, 77, 63, 51, 46, 39.

1,3-Dimethyl-2,4-dinitrobenzene **(34)**: white crystalline solid, m.p. 82-84 °C.^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.38 (s, 3H), 2.45 (s, 3H), 7.32 (d, J = 8.6 Hz, 1H), 7.94 (d, J = 8.3 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 14.4, 17.7, 125.5, 125.8, 129.6, 134.9, 148.2, 153.2; GC/MS (EI) m/z 196 (M^+), 179 (100%), 162, 149, 103, 91, 78, 63, 51, 46, 39.

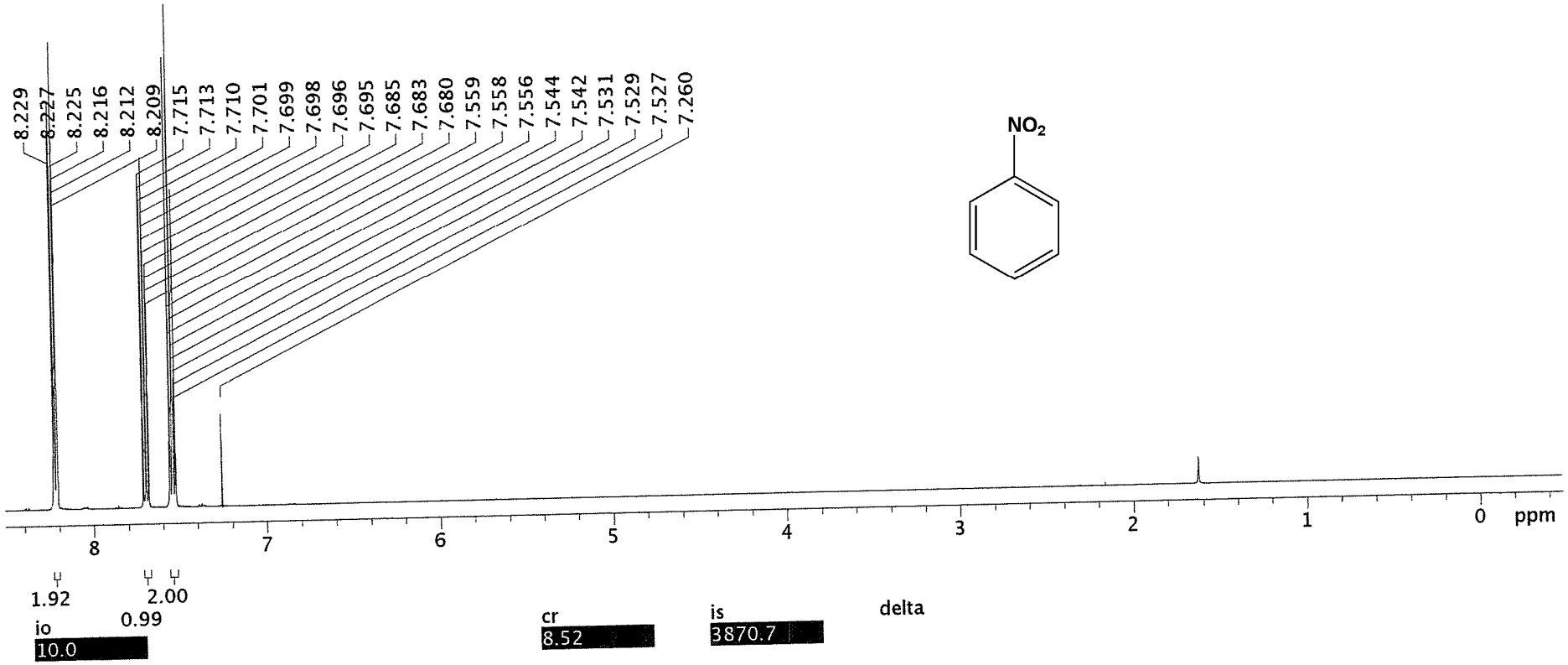
2,4-Dinitroanisole **(35)**: white solid, m.p. 93-95 °C.^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 4.10 (s, 3H), 7.24 (d, J = 10.25 Hz, 1H), 8.45 (dd, J = 2.7 Hz, J = 9.3 Hz, 1H), 8.75 (d, J = 2.9 Hz; 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 57.6, 113.7, 122.1, 129.3, 139.1, 140.4, 157.4; GC/MS (EI) m/z 198 (M^+), 168, 151, 107, 79 (100%), 63, 46.

2-Acetyl-5-nitrofuran **(36)**: oil. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.58 (s, 3H), 7.27 (d, J = 3.9 Hz, 1H), 7.36 (d, J = 3.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 26.4, 112.1, 117.1, 145.1, 151.5, 186.9; GC/MS (EI) m/z 155 (M^+), 140, 97, 82, 66, 54, 43 (100%), 38.

Nitro-2-acetylthiophene **(37)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture. **4-Nitro (major isomer):** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.61 (s, 3H), 8.15 (d, J = 1.4 Hz, 1H), 8.53 (d, J = 1.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 26.6, 126.1, 133.6, 145.0, 148.4, 190.5; GC/MS (EI) m/z 171 (M^+), 156 (100%), 110, 82, 69, 43, 38; **5-Nitro (minor isomer):** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 2.62 (s, 3H), 7.58 (d, J = 4.1 Hz, 1H), 7.89 (d, J =

4.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 26.7, 128.4, 130.2, 148.3, 156.6, 189.9; GC/MS (EI) *m*/*z* 171 (M^+), 156 (100%), 110, 98, 81, 69, 43.

Nitrothiophene-2-carboxaldehyde **(38)**: NMR chemical shift values for the respective isomers were determined directly from the isomeric mixture. **4-Nitro (major isomer):** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 8.26 (d, J = 1.5 Hz, 1H), 8.64 (t, J = 1.5 Hz, 1H), 9.95 (s, 1H, CHO); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 129.5, 134.5, 143.6, 148.7, 182.1; GC/MS (EI) *m*/*z* 157 (M^+,100%), 127, 110, 82, 57, 39; **5-Nitro (minor isomer):** ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 7.74 (d, J = 4.0 Hz, 1H), 7.96 (d, J = 4.5 Hz, 1H), 9.92 (s, 1H, CHO); ^{13}C NMR (125 MHz, $CDCl_3$, 25 °C): δ 128.4, 133.7, 146.7, 157.4, 183.4; GC/MS (EI) *m*/*z* 157 (M^+,100%), 127, 112, 99, 82, 71, 57, 39.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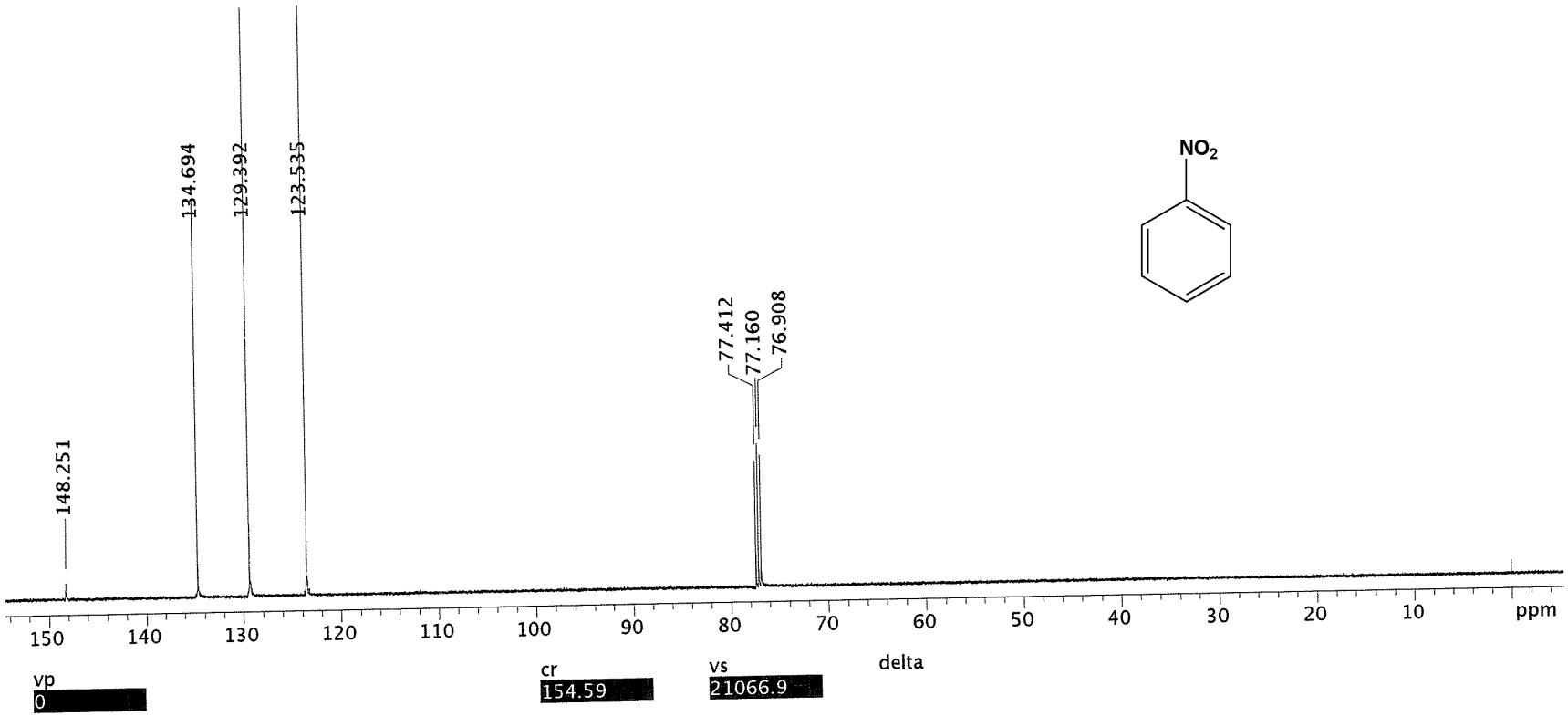
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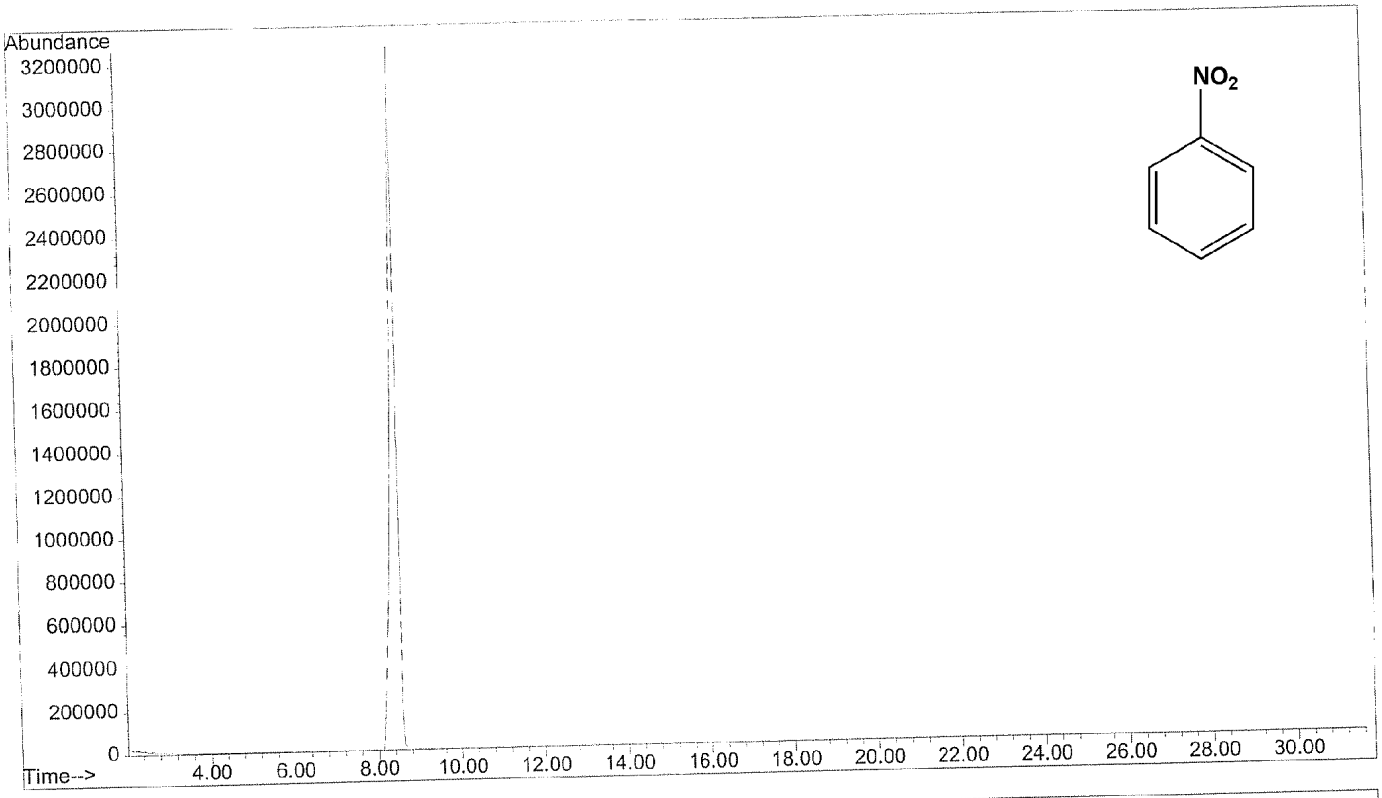
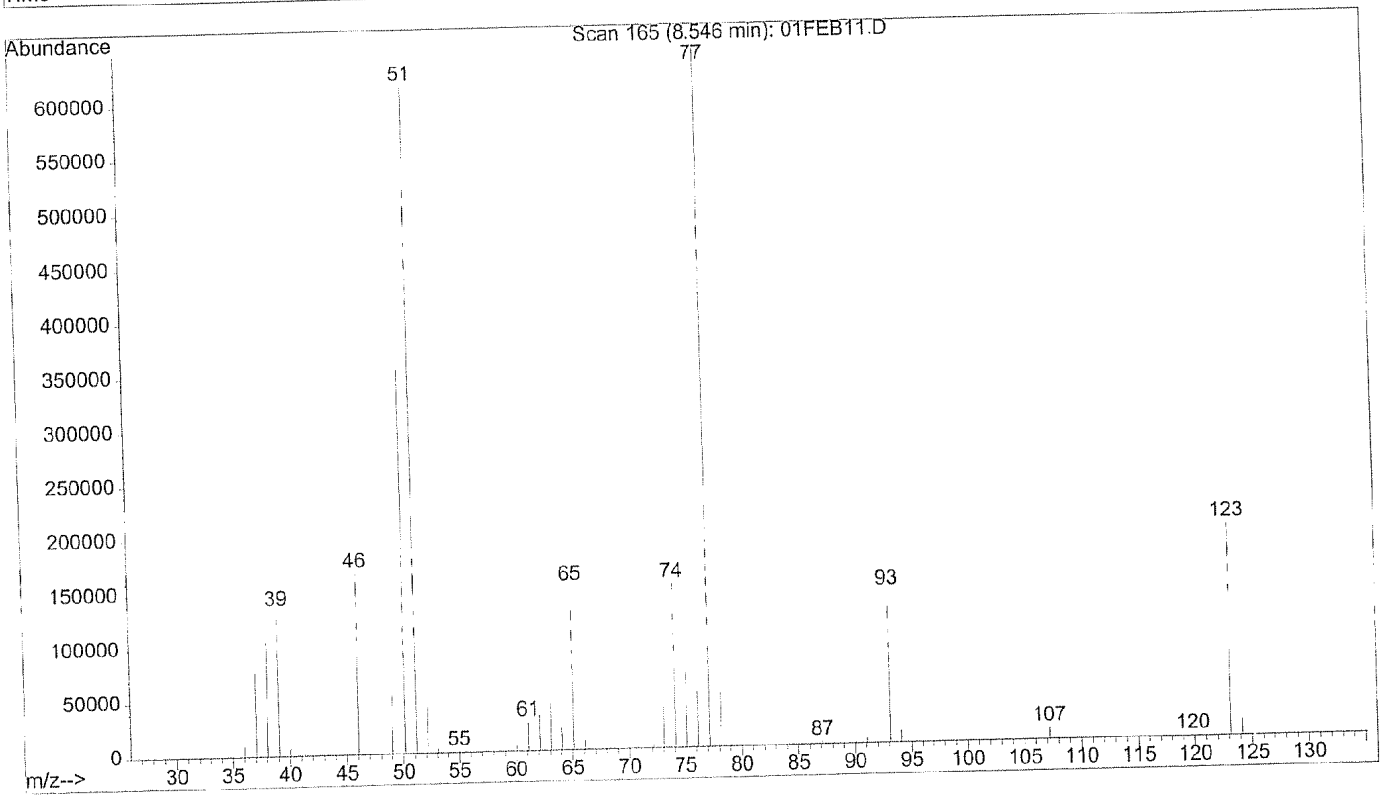
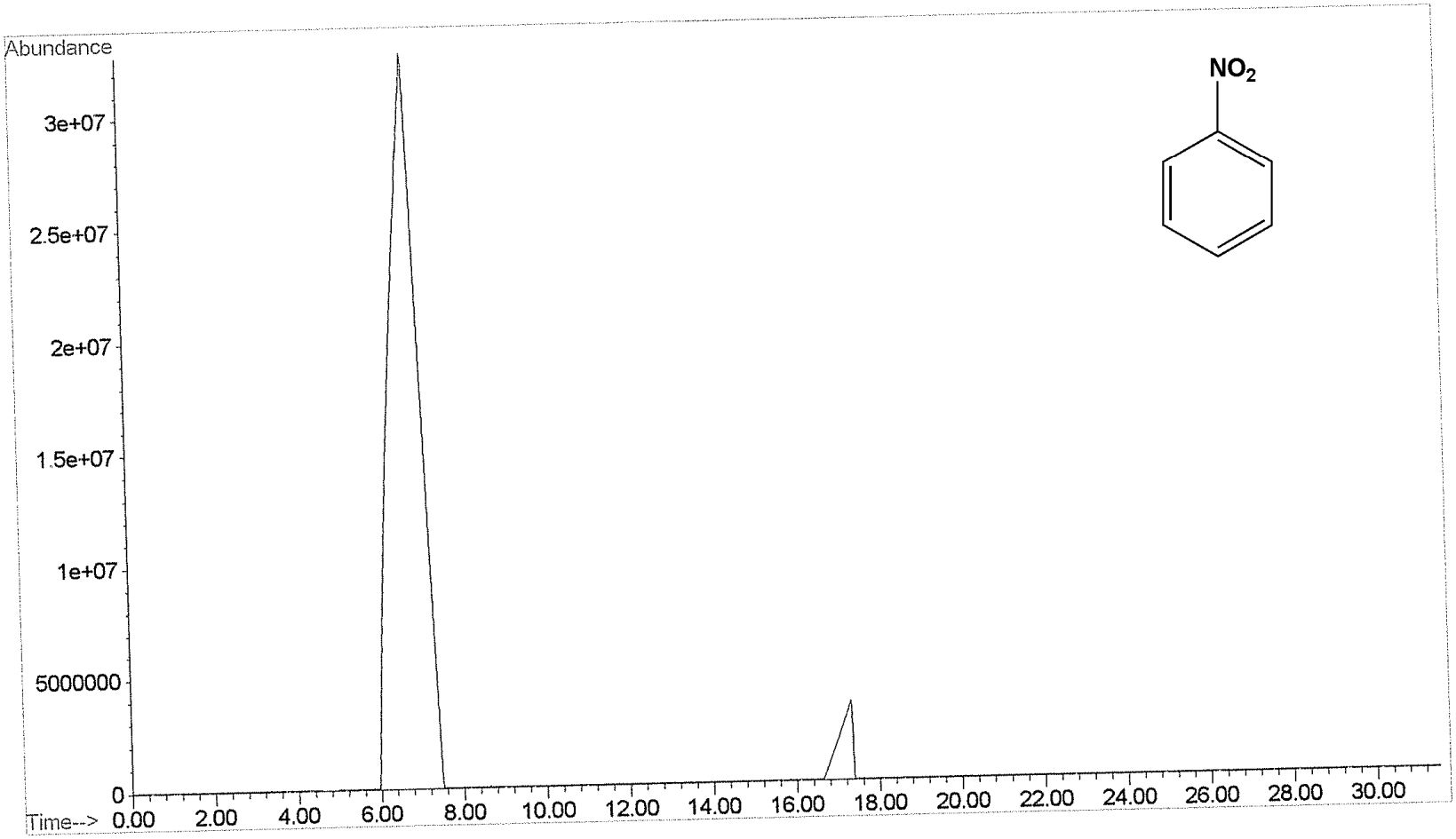
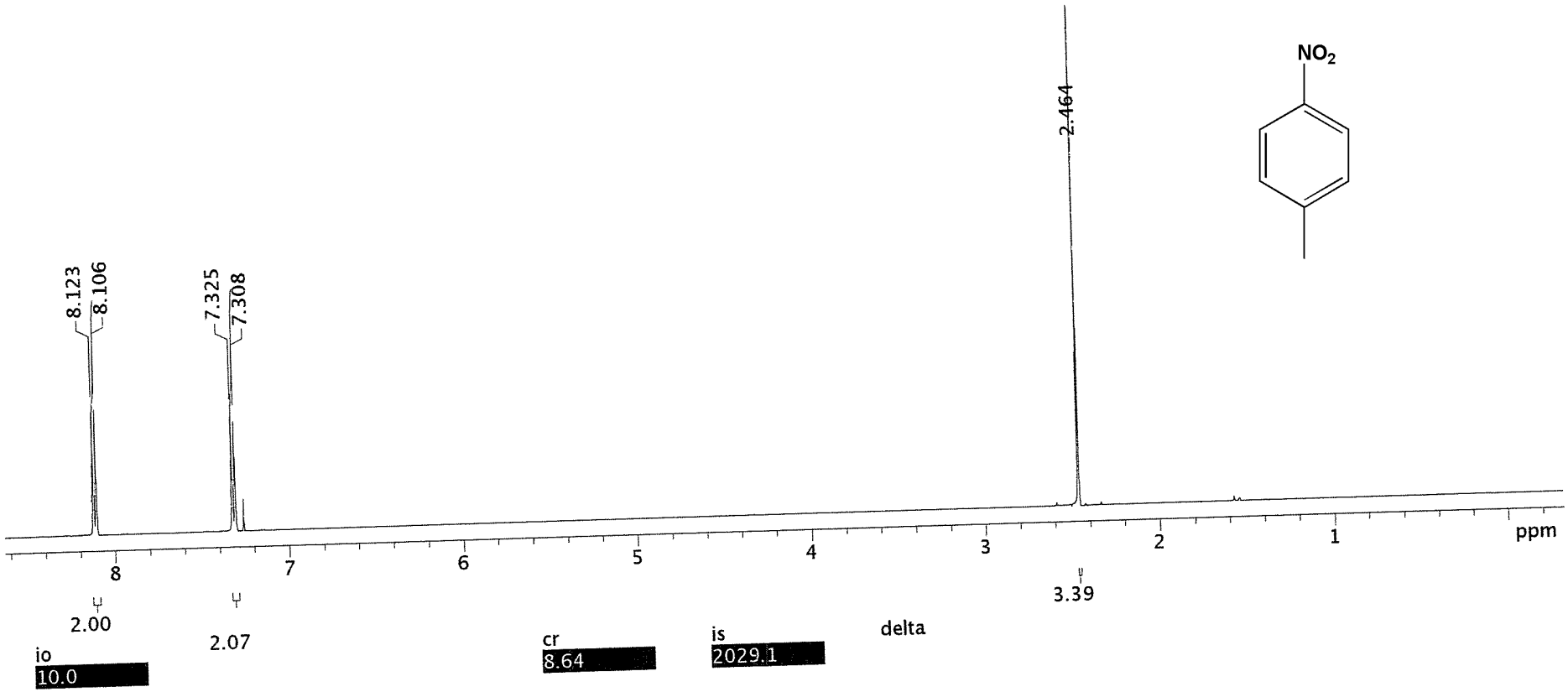
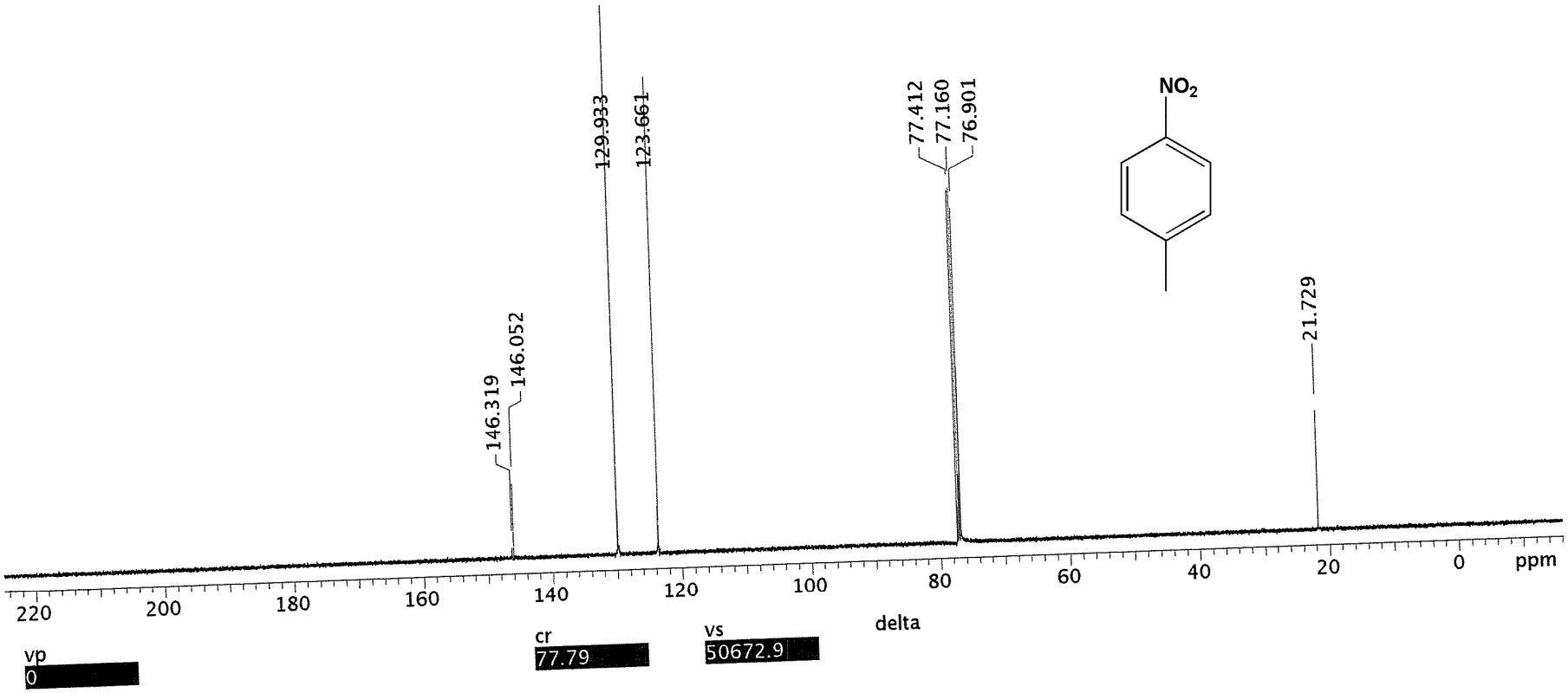
cr
154.59
vs
21066.9

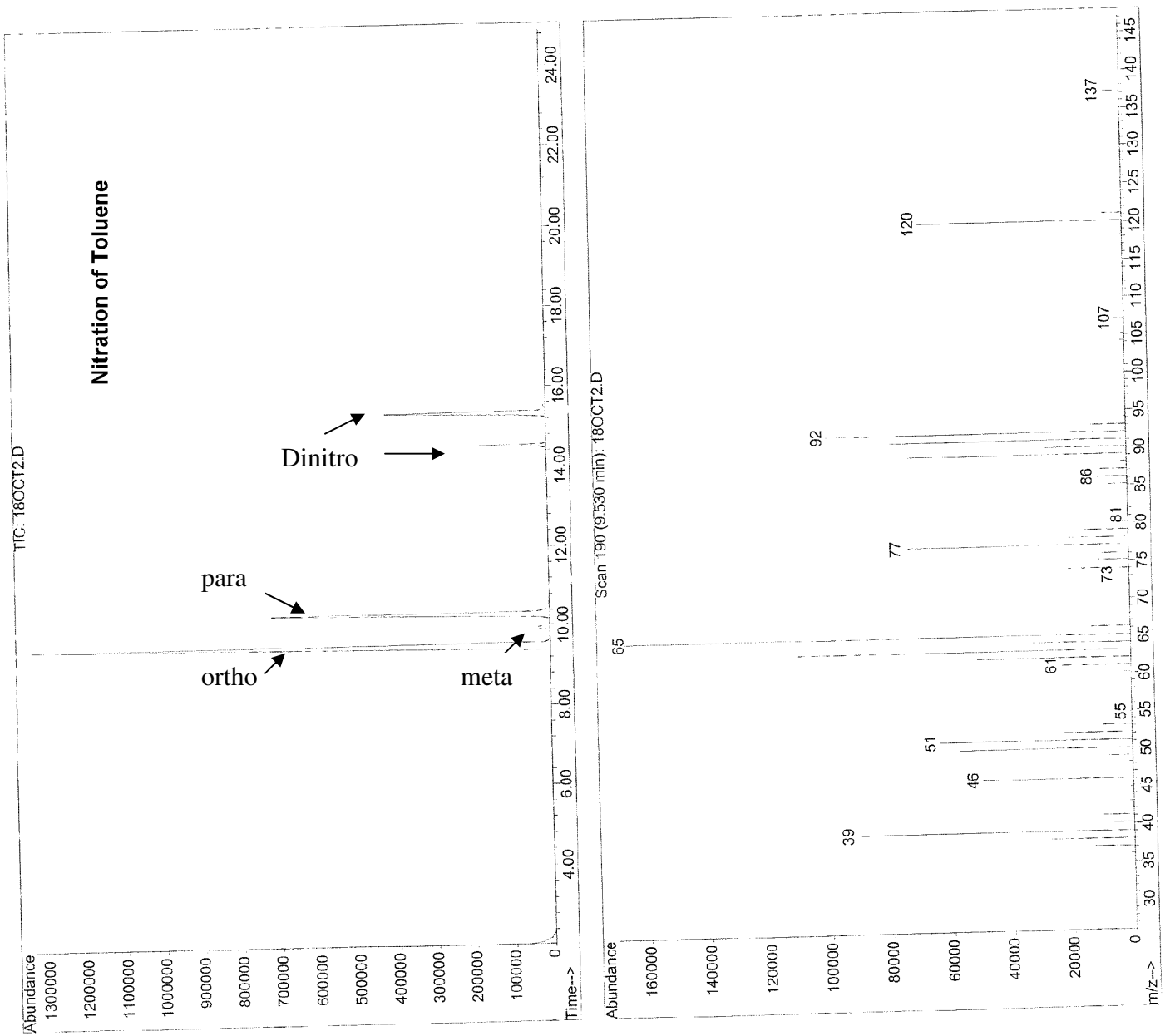

Abundance
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00
NO2

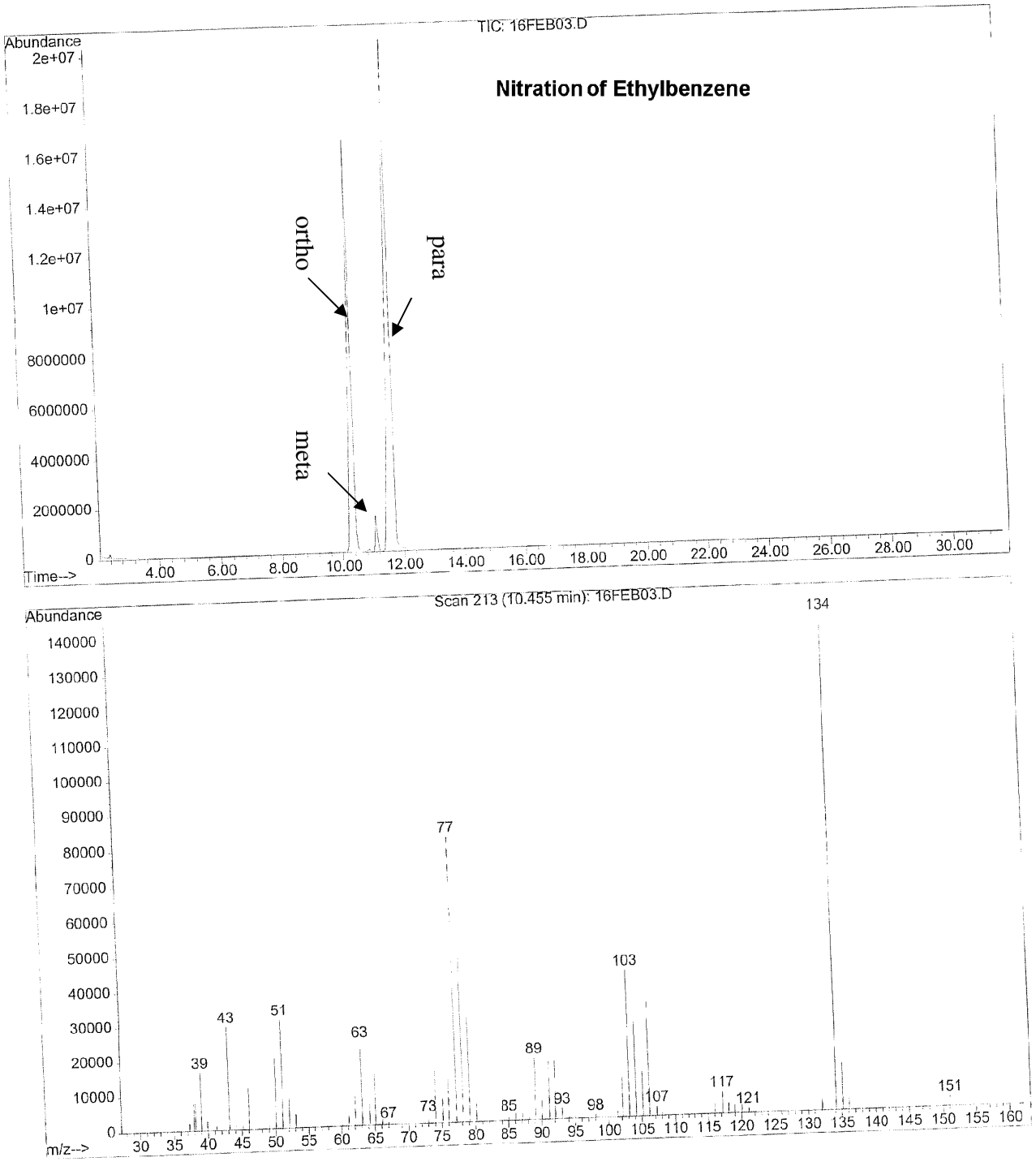

Scan 165 (8.546 min): 01FEB11.D
Abundance
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
m/z-->
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
110
115
120
125
130
39
46
51
55
61
65
74
77
87
93
107
120
123

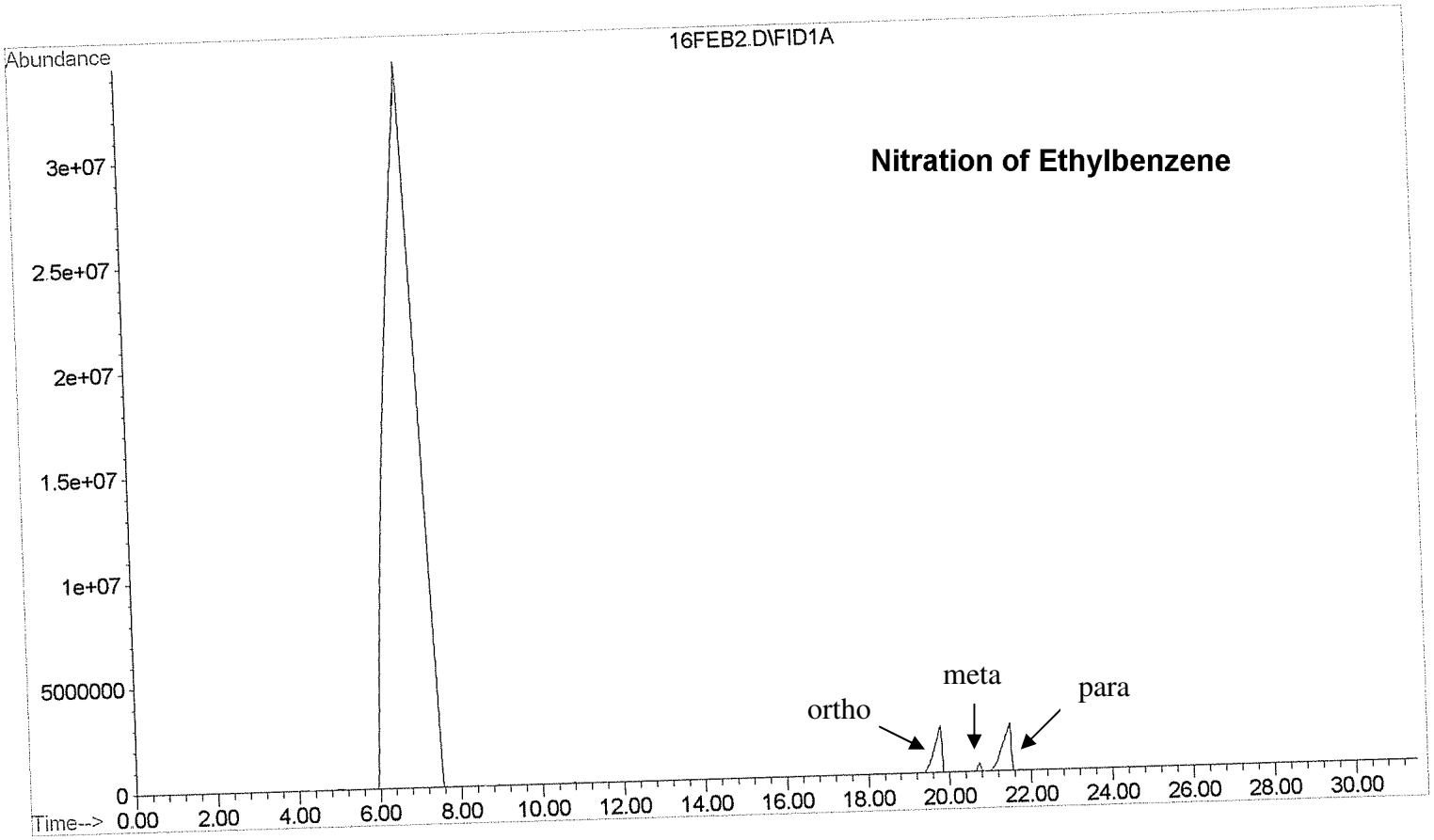

Abundance
3e+07
2.5e+07
2e+07
1.5e+07
1e+07
5000000
0
Time-->
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00
NO2

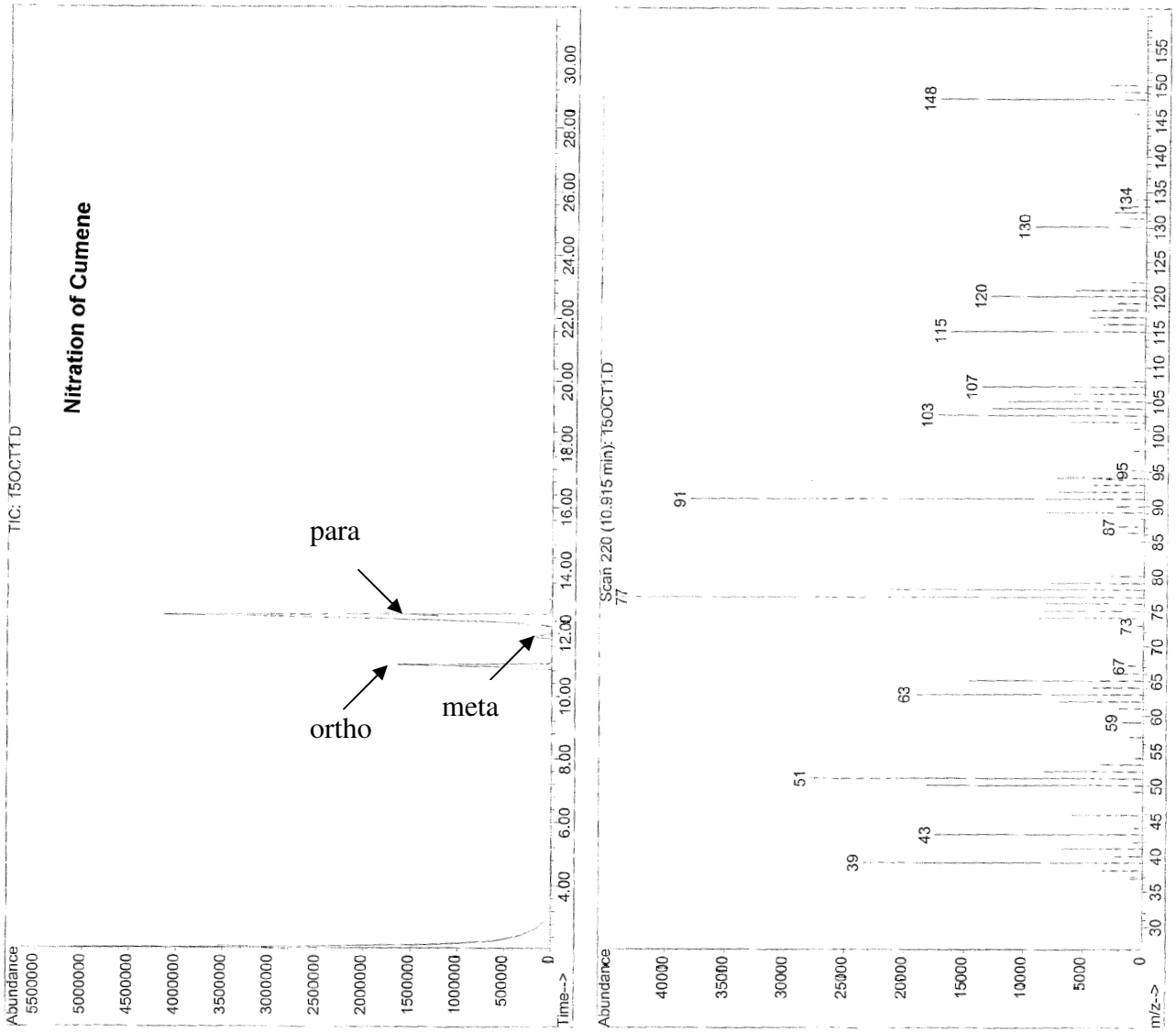

NO2
8.123
8.106
7.325
7.308
2.464
8
7
6
5
4
3
2
1
ppm
2.00
2.07
3.39
io
10.0
cr
8.64
is
2029.1
delta

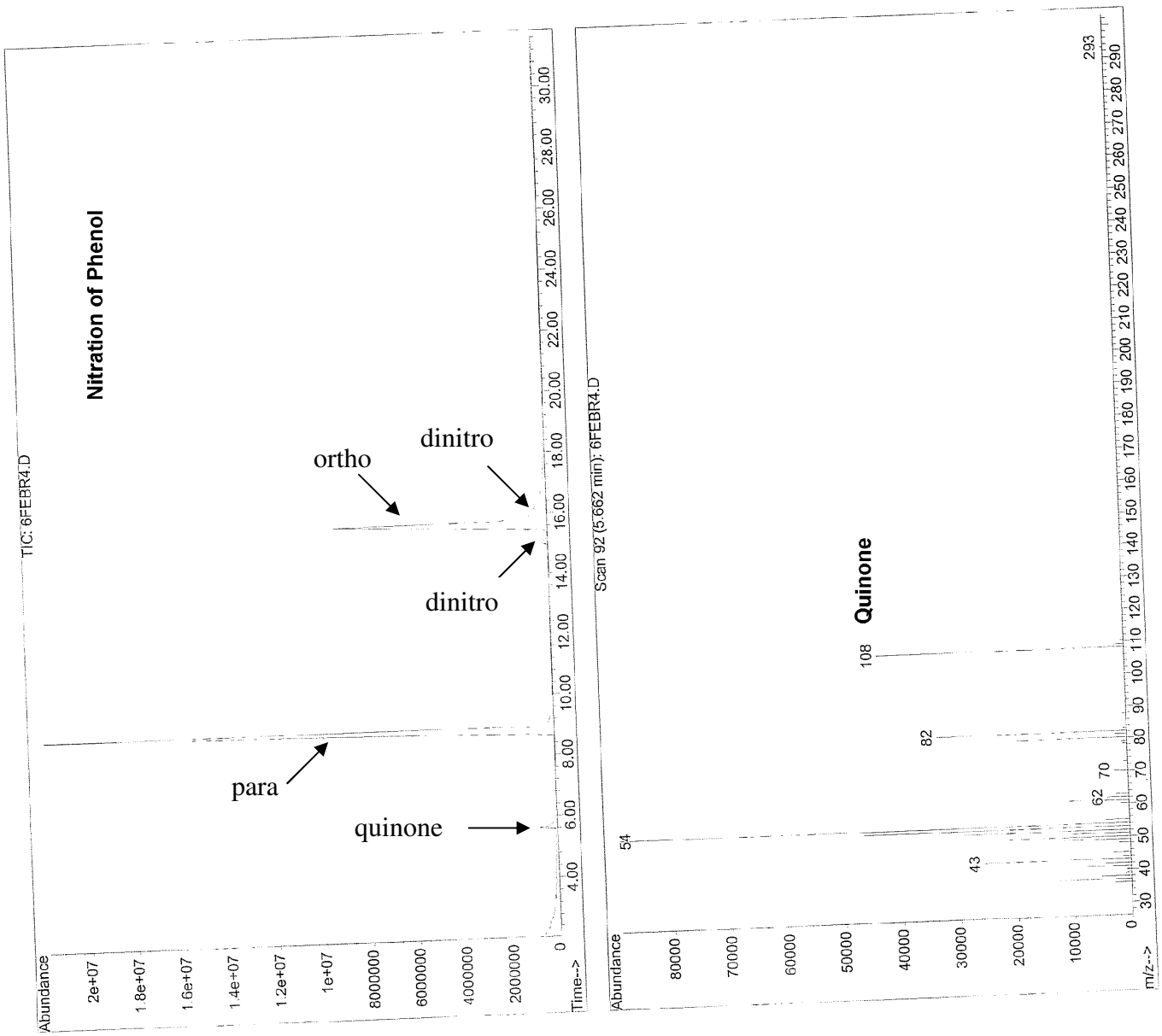

146.319
146.052
129.933
123.661
77.412
77.160
76.901
21.729
NO2
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
77.79
vs
50672.9

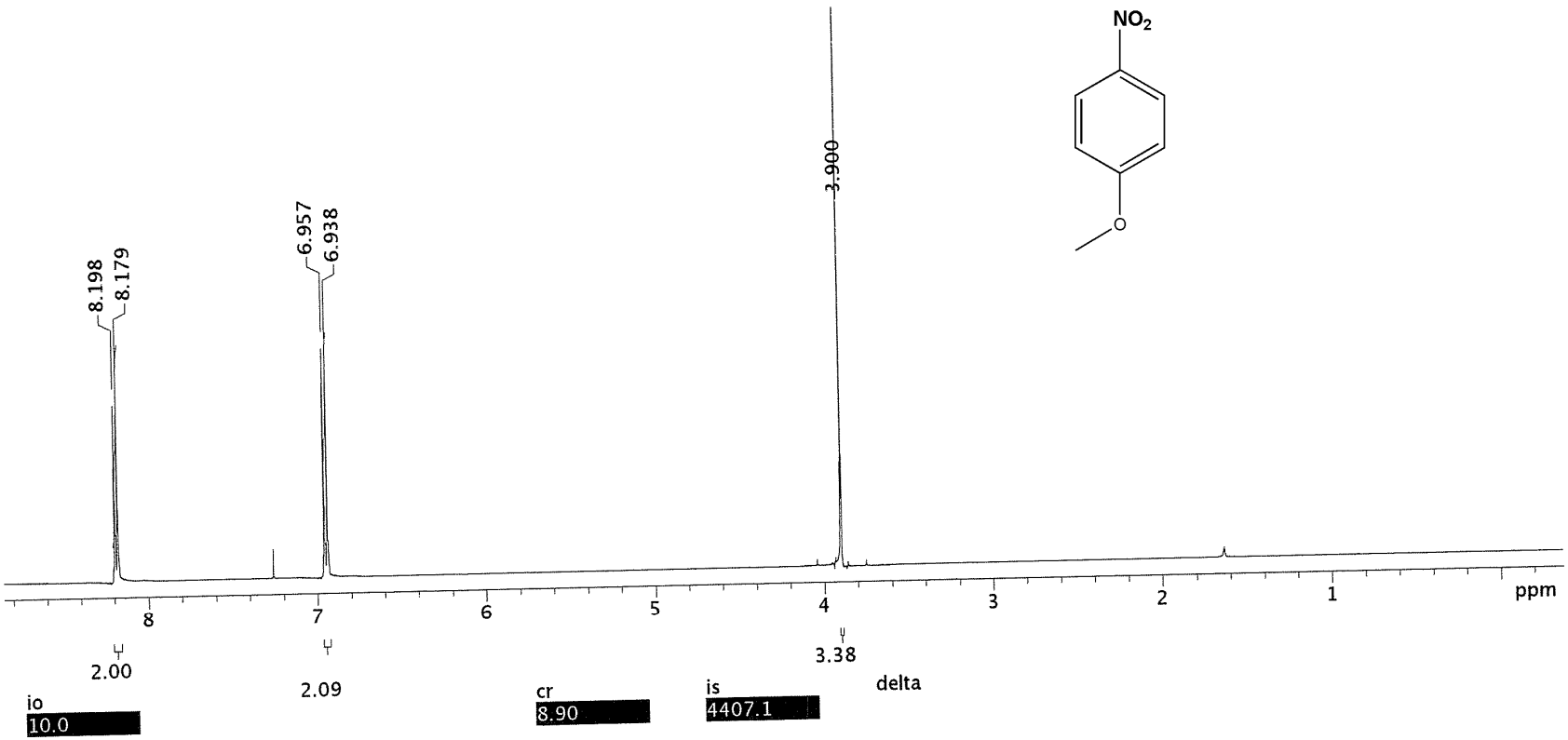

Nitration of Toluene
TIC: 18OCT2.D
Abundance
Time-->
Dinitro
para
ortho
meta
Scan 190 (9.530 min): 18OCT2.D
Abundance
m/z-->

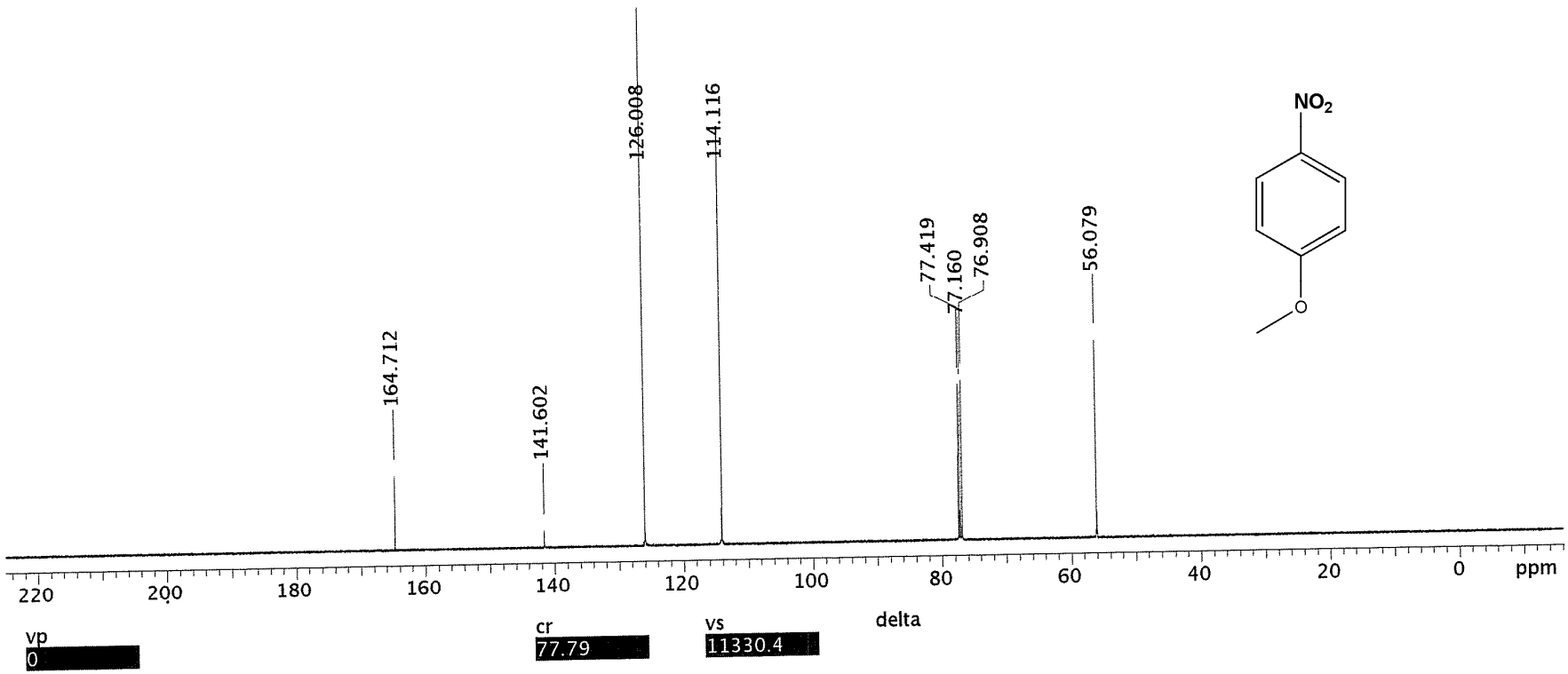

TIC: 16FEB03.D
Abundance
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00
Nitration of Ethylbenzene
ortho
para
meta
Scan 213 (10.455 min): 16FEB03.D
Abundance
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
m/z-->
30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160
39
43
51
63
67
73
77
85
89
93
98
103
107
117
121
134
151

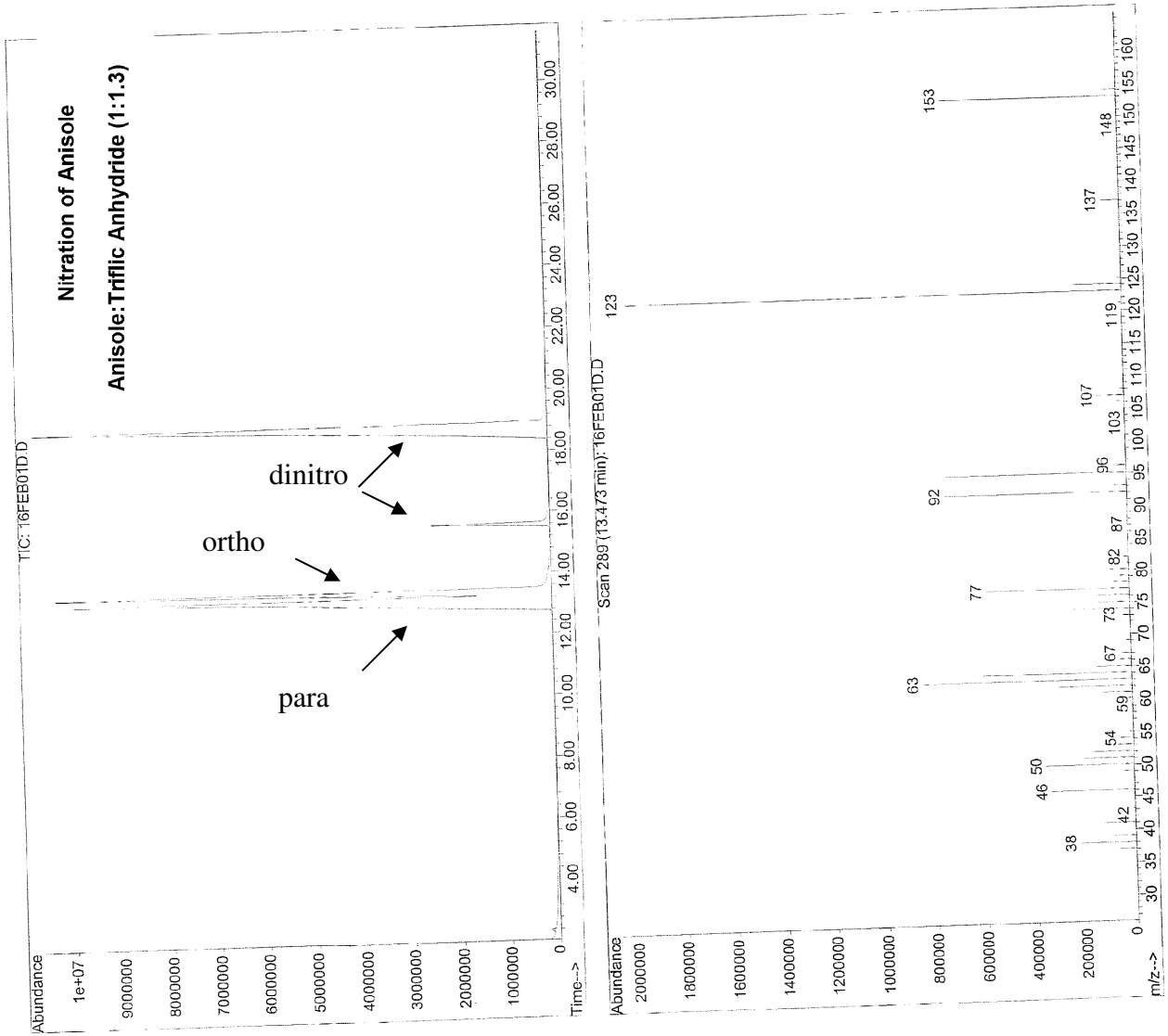

16FEB2.D\FID1A
Abundance
Nitration of Ethylbenzene
3e+07
2.5e+07
2e+07
1.5e+07
1e+07
5000000
0
ortho
meta
para
Time-->
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00

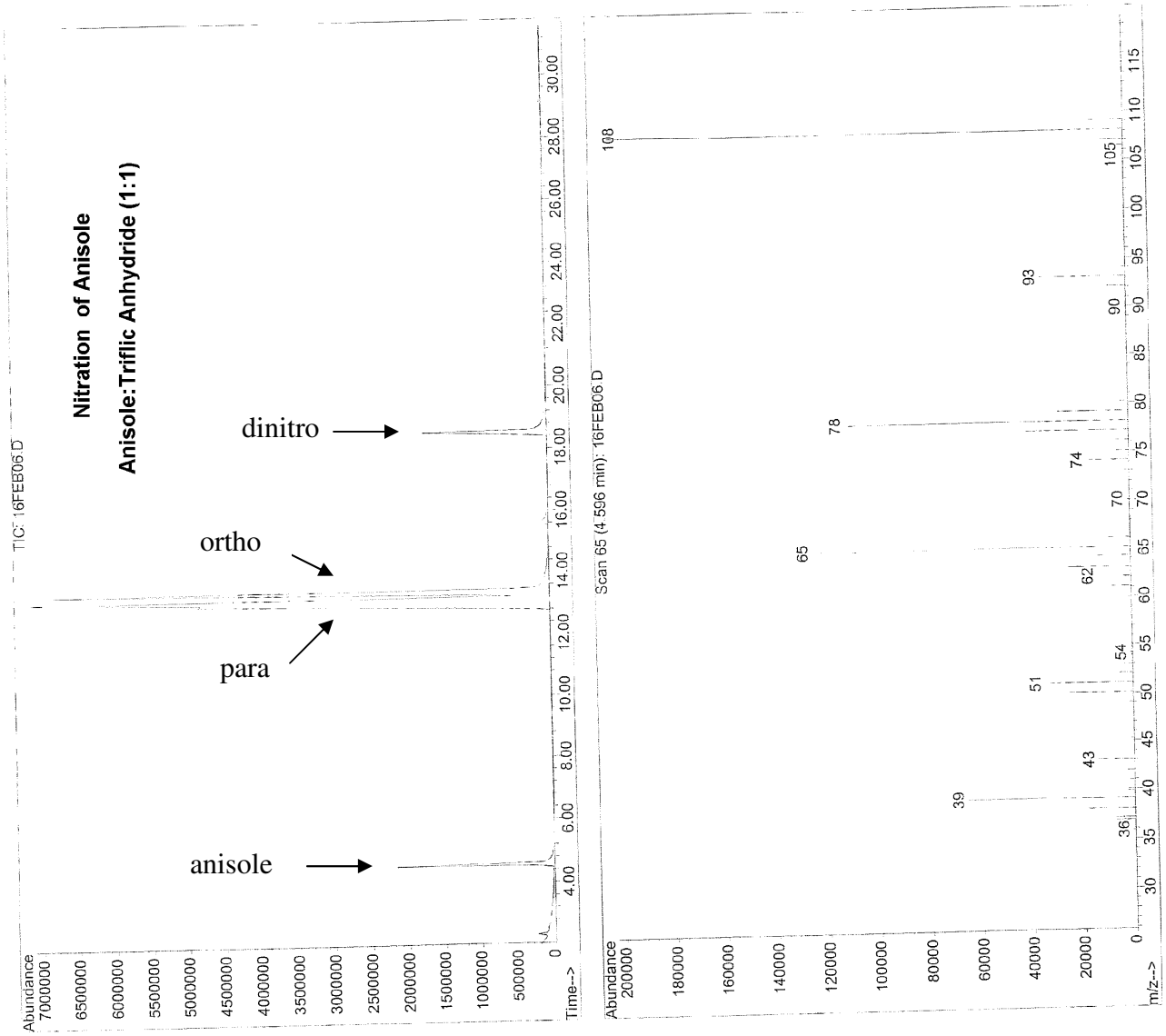

Nitration of Cumene
TIC: 150CT1.D
Abundance
Time-->
para
ortho
meta
Scan 220 (10.915 min): 150CT1.D
Abundance
m/z-->

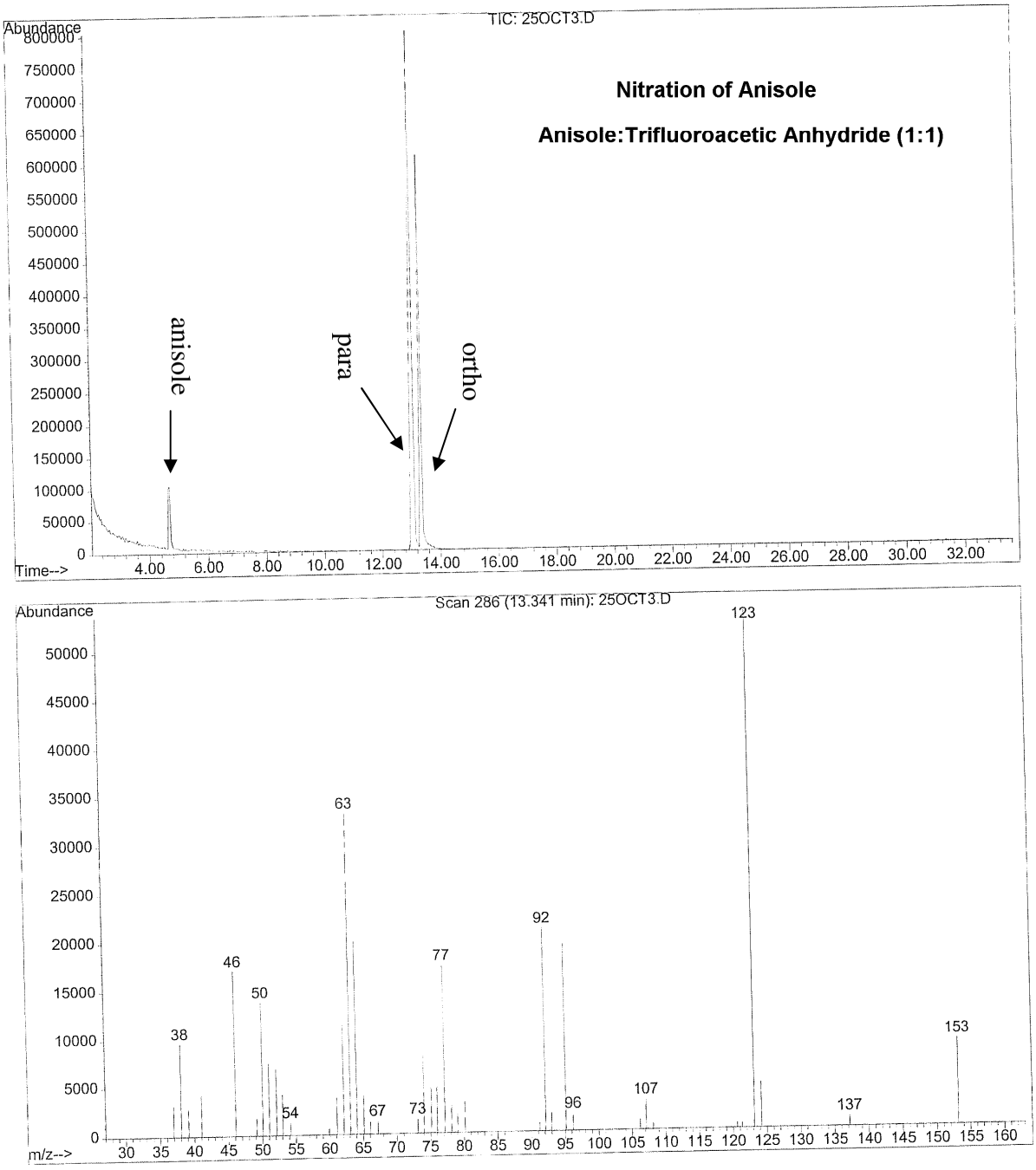

Nitration of Phenol
TIC: 6FEBR4.D
Abundance
Time-->
ortho
dinitro
dinitro
para
quinone
Scan 92 (5.662 min): 6FEBR4.D
Quinone
m/z-->

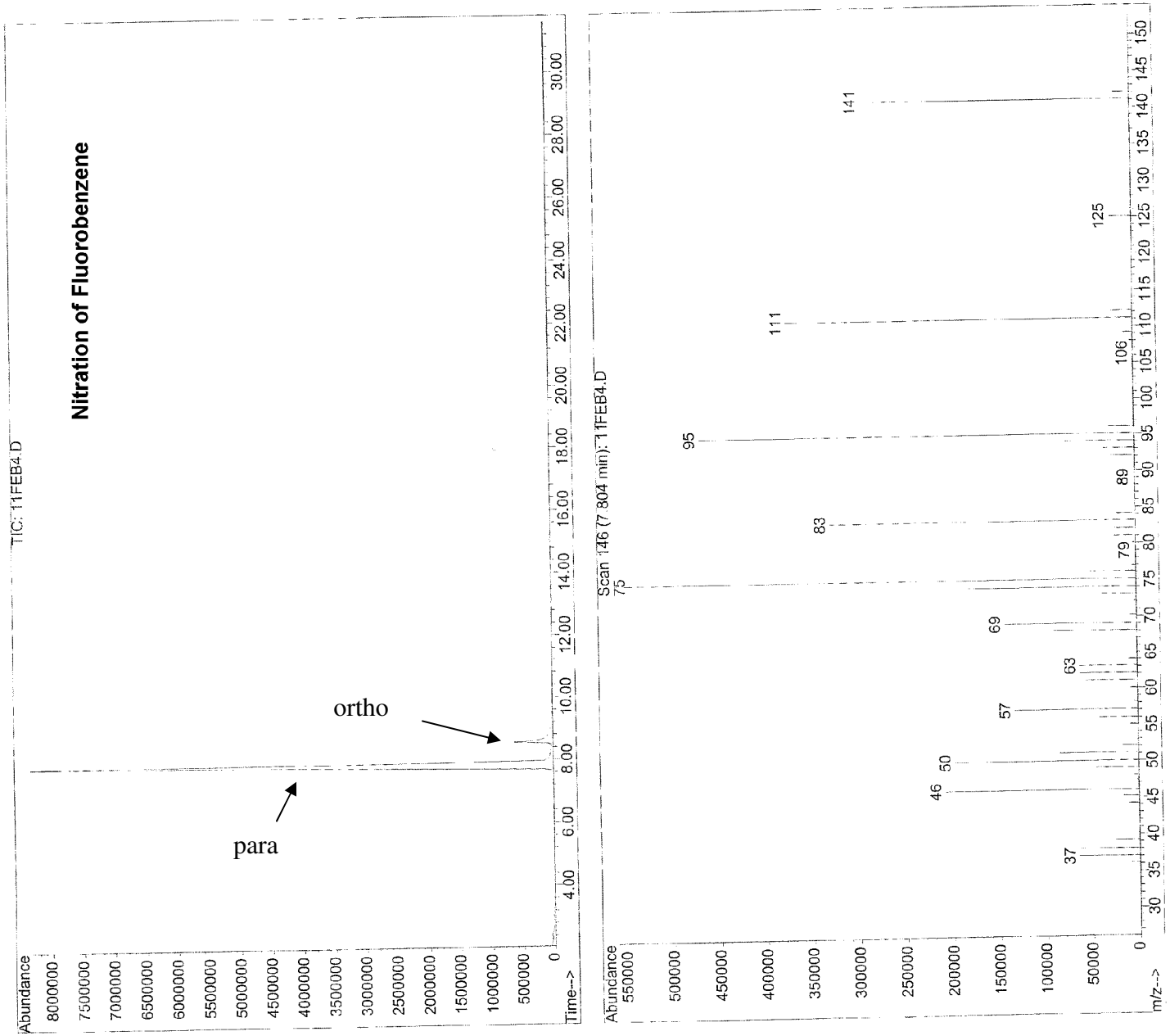

NO2
O
8.198
8.179
6.957
6.938
3.900
8
7
6
5
4
3
2
1
ppm
2.00
2.09
3.38
delta
io
10.0
cr
8.90
is
4407.1

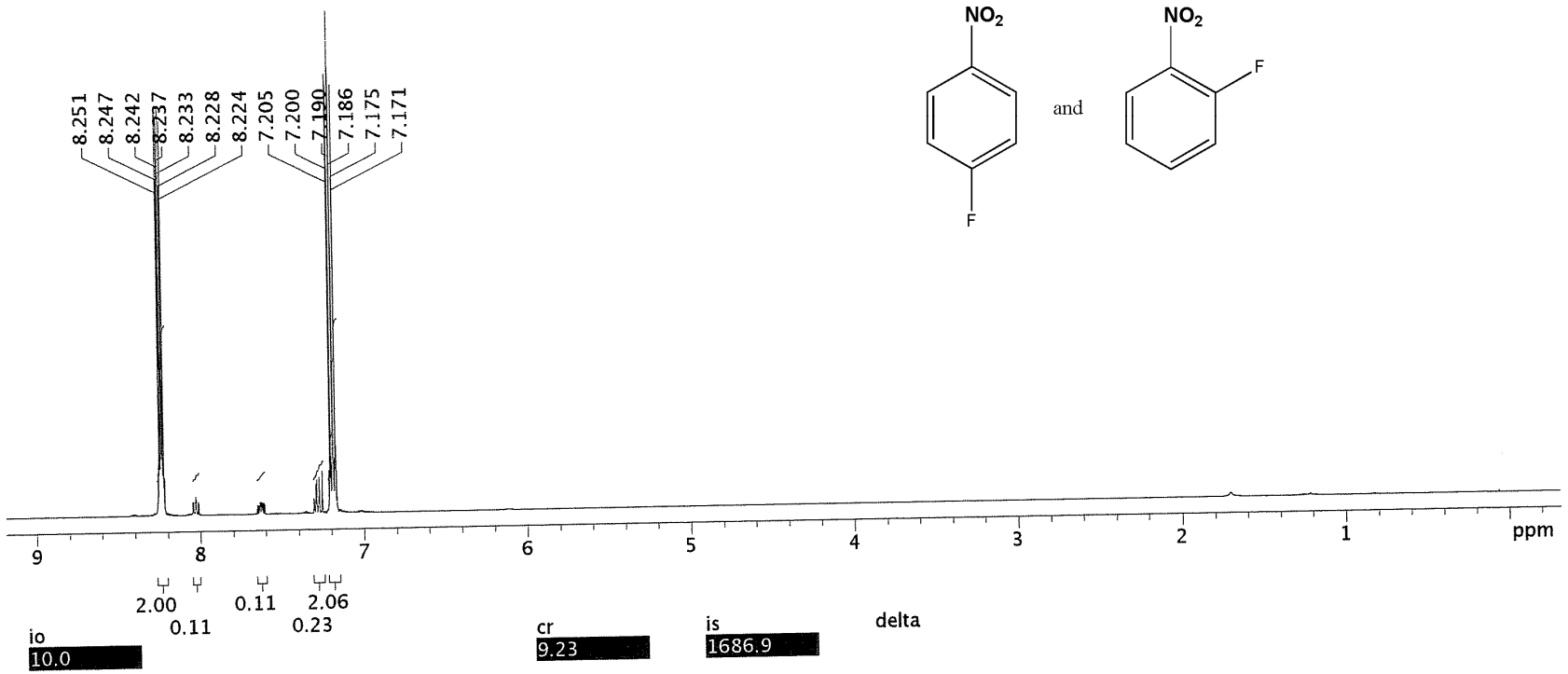

164.712
141.602
126.008
114.116
77.419
77.160
76.908
56.079
NO2
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
77.79
vs
11330.4

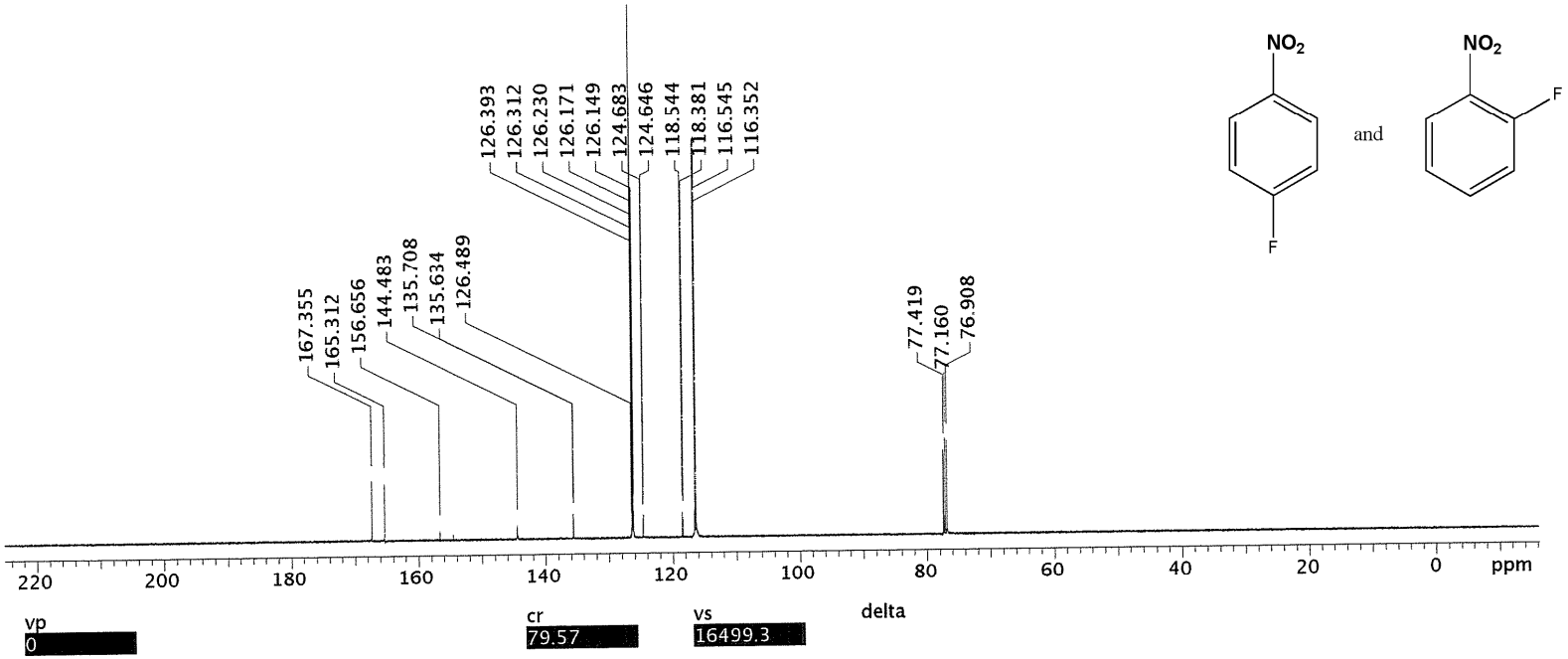

Nitration of Anisole
Anisole:Triflic Anhydride (1:1.3)
TIC: 16FEB01D.D
dinitro
ortho
para
Abundance
Time-->
Scan 289 (13.473 min): 16FEB01D.D
m/z-->

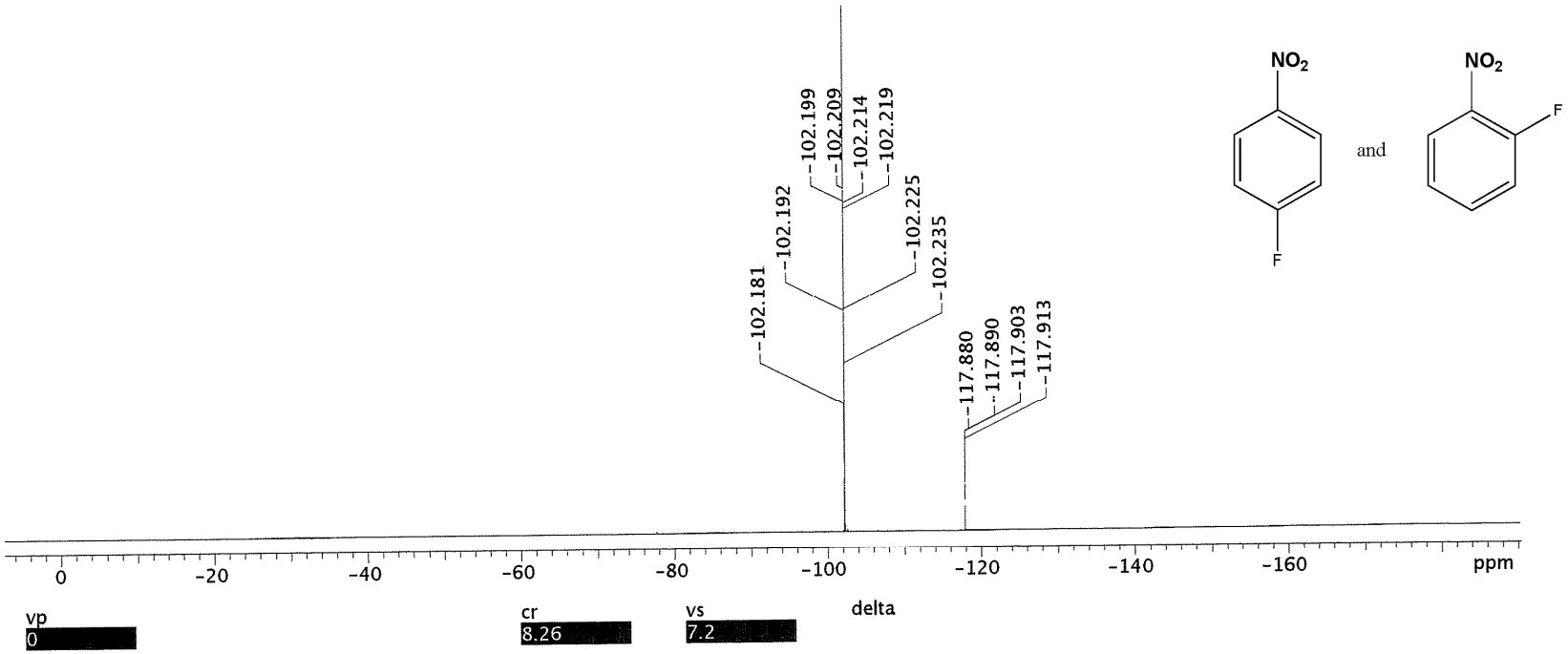

Nitration of Anisole
Anisole:Triflic Anhydride (1:1)
TIC: 16FEB06.D
dinitro
ortho
para
anisole
Abundance
Time-->
Scan 65 (4.596 min): 16FEB06.D
m/z-->

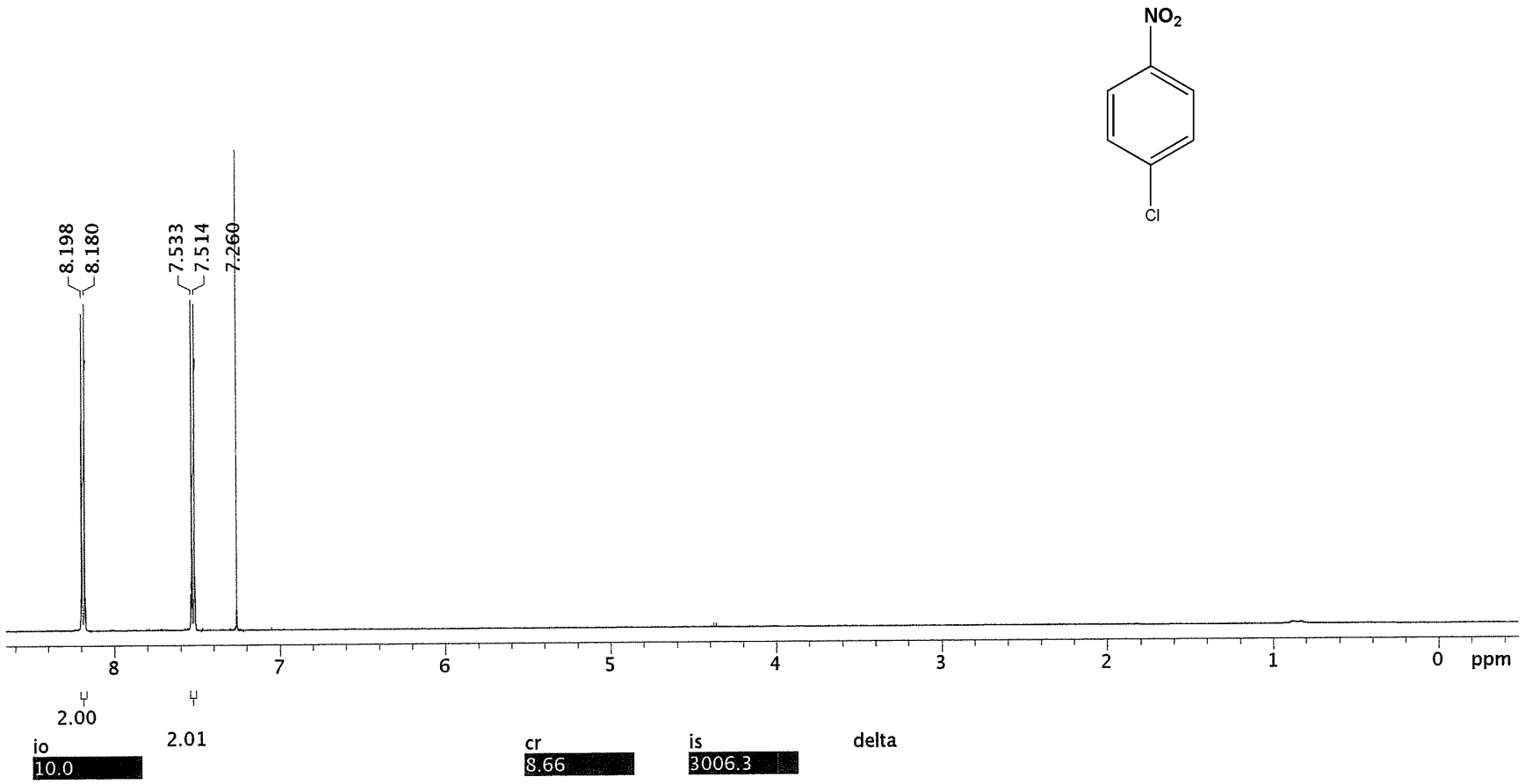

TIC: 25OCT3.D
Abundance
Nitration of Anisole
Anisole:Trifluoroacetic Anhydride (1:1)
anisole
para
ortho
Time-->
Scan 286 (13.341 min): 25OCT3.D
Abundance
m/z-->

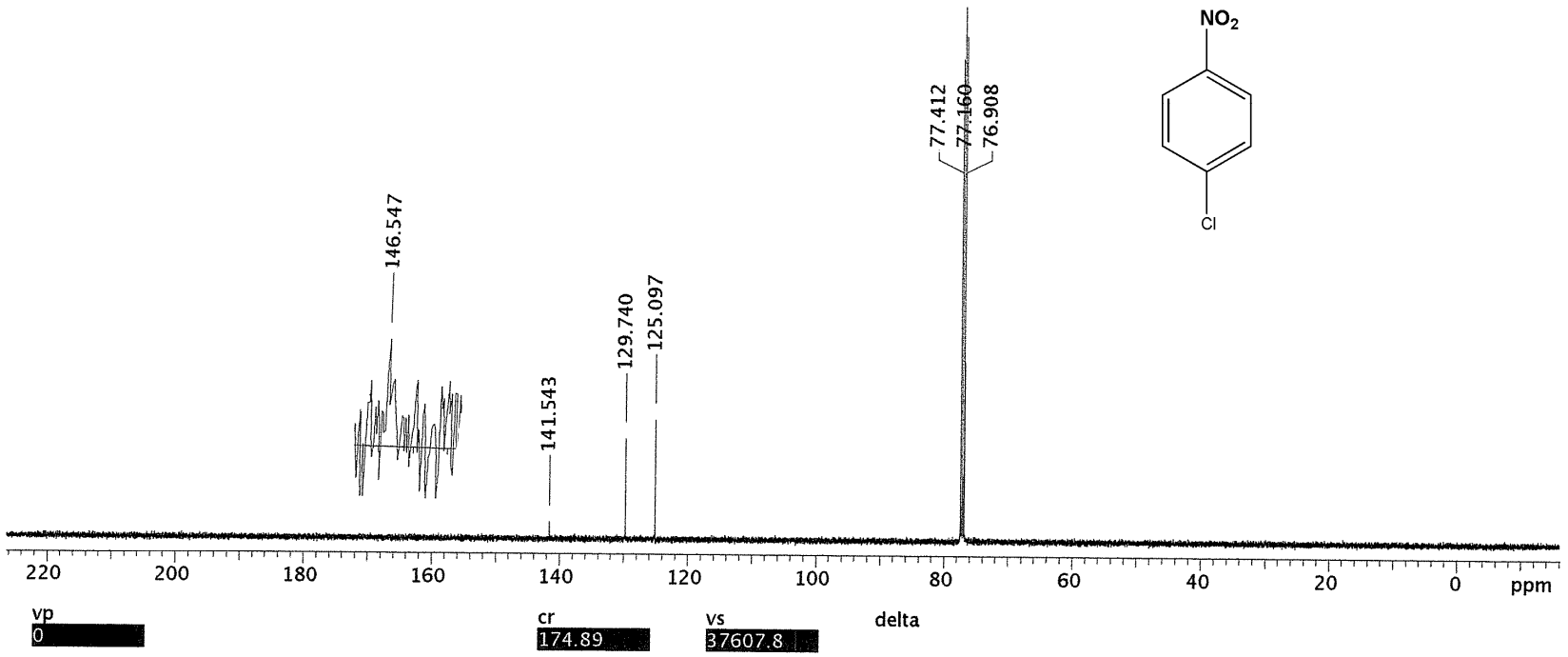

Nitration of Fluorobenzene
TIC: 11FEB4.D
Abundance
Time-->
ortho
para
Scan 146 (7.804 min): 11FEB4.D
Abundance
m/z-->

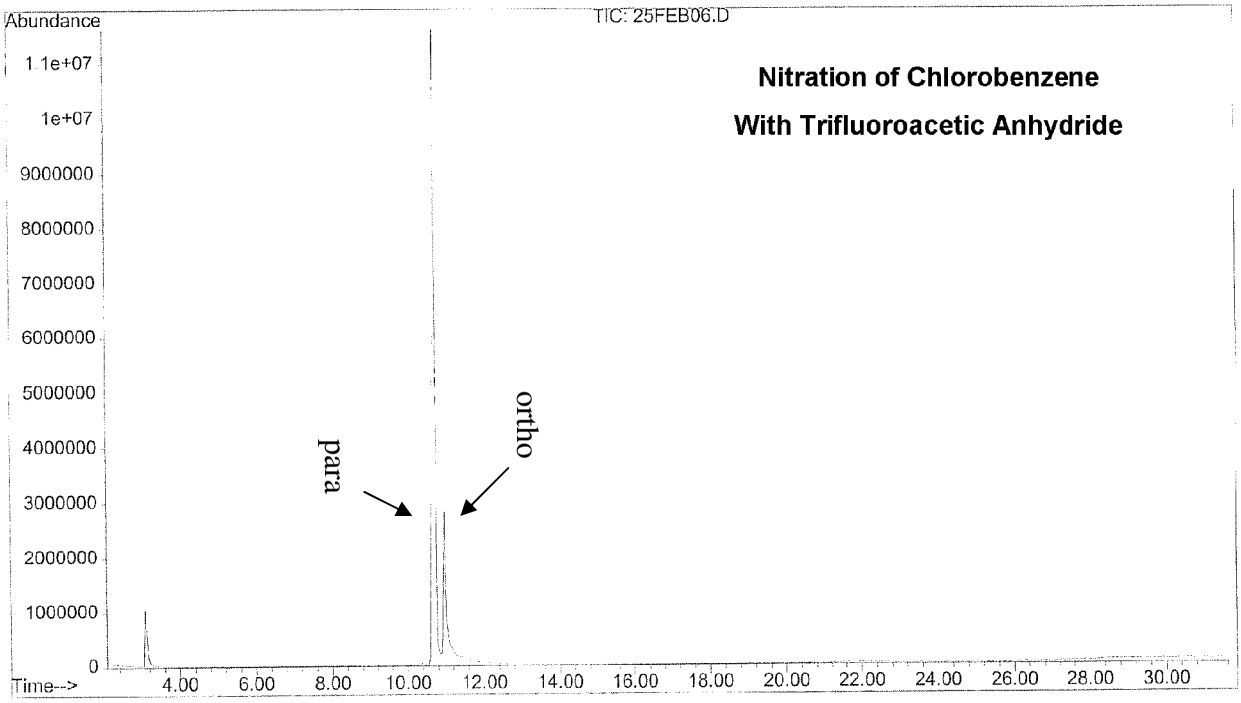

8.251
8.247
8.242
8.237
8.233
8.228
8.224
7.205
7.200
7.190
7.186
7.175
7.171
NO2
F
and
NO2
F
9
8
7
6
5
4
3
2
1
ppm
2.00
0.11
0.11
2.06
0.23
io
10.0
cr
9.23
is
1686.9
delta

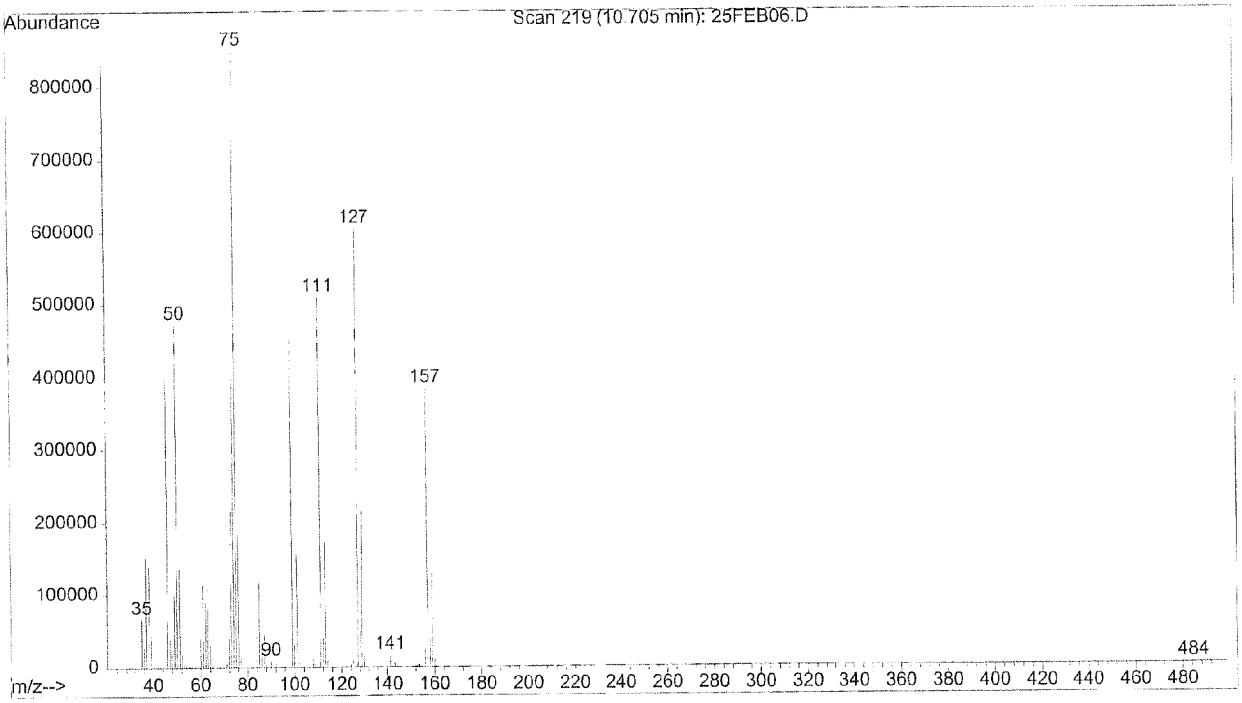

126.393
126.312
126.230
126.171
126.149
124.683
124.646
118.544
118.381
116.545
116.352
167.355
165.312
156.656
144.483
135.708
135.634
126.489
77.419
77.160
76.908
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
79.57
vs
16499.3
NO2
F
and
NO2
F

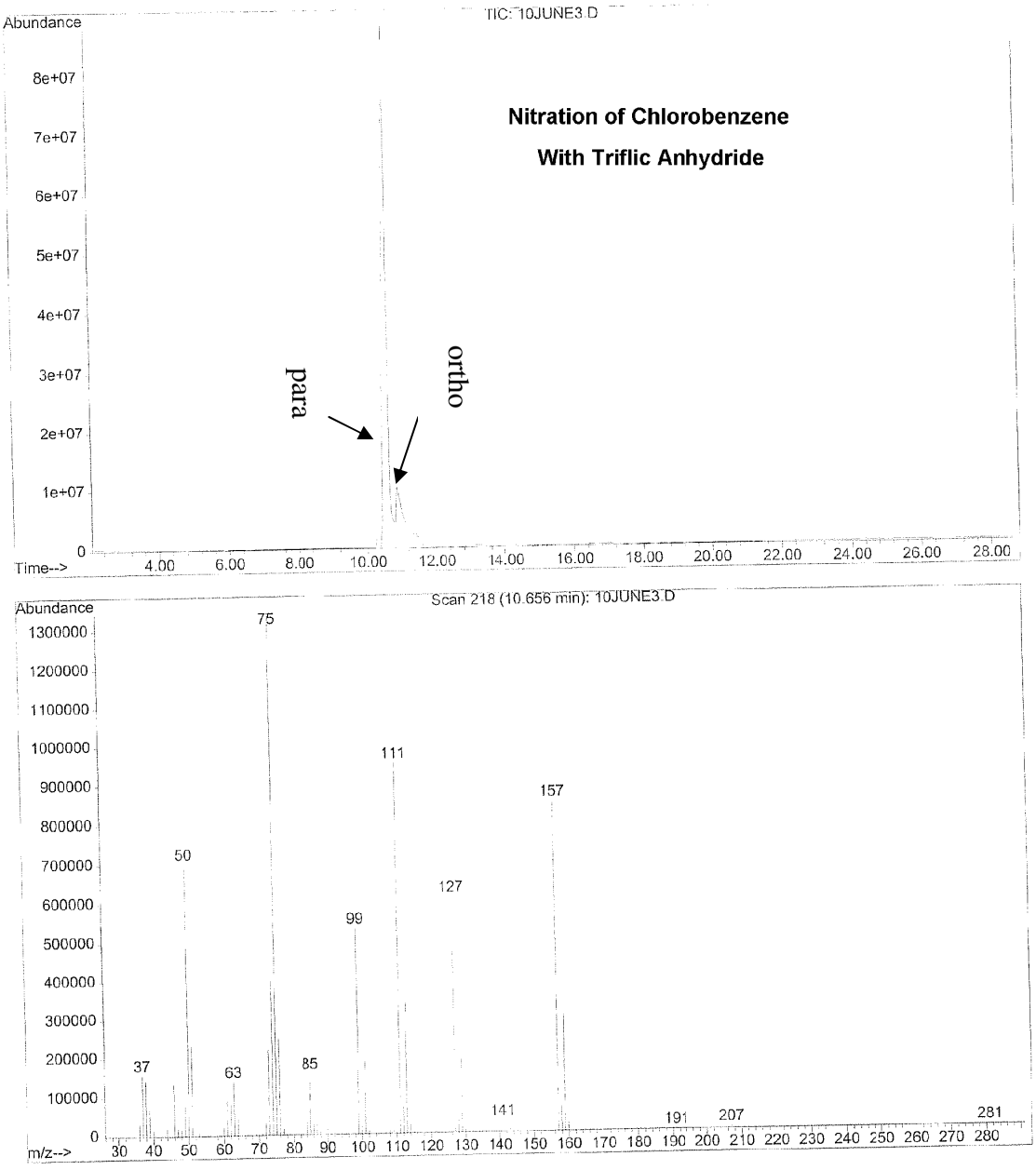

-102.181
-102.192
-102.199
-102.209
-102.214
-102.219
-102.225
-102.235
-117.880
-117.890
-117.903
-117.913
0
-20
-40
-60
-80
-100
-120
-140
-160
ppm
delta
vp
0
cr
8.26
vs
7.2
NO2
F
and
NO2
F

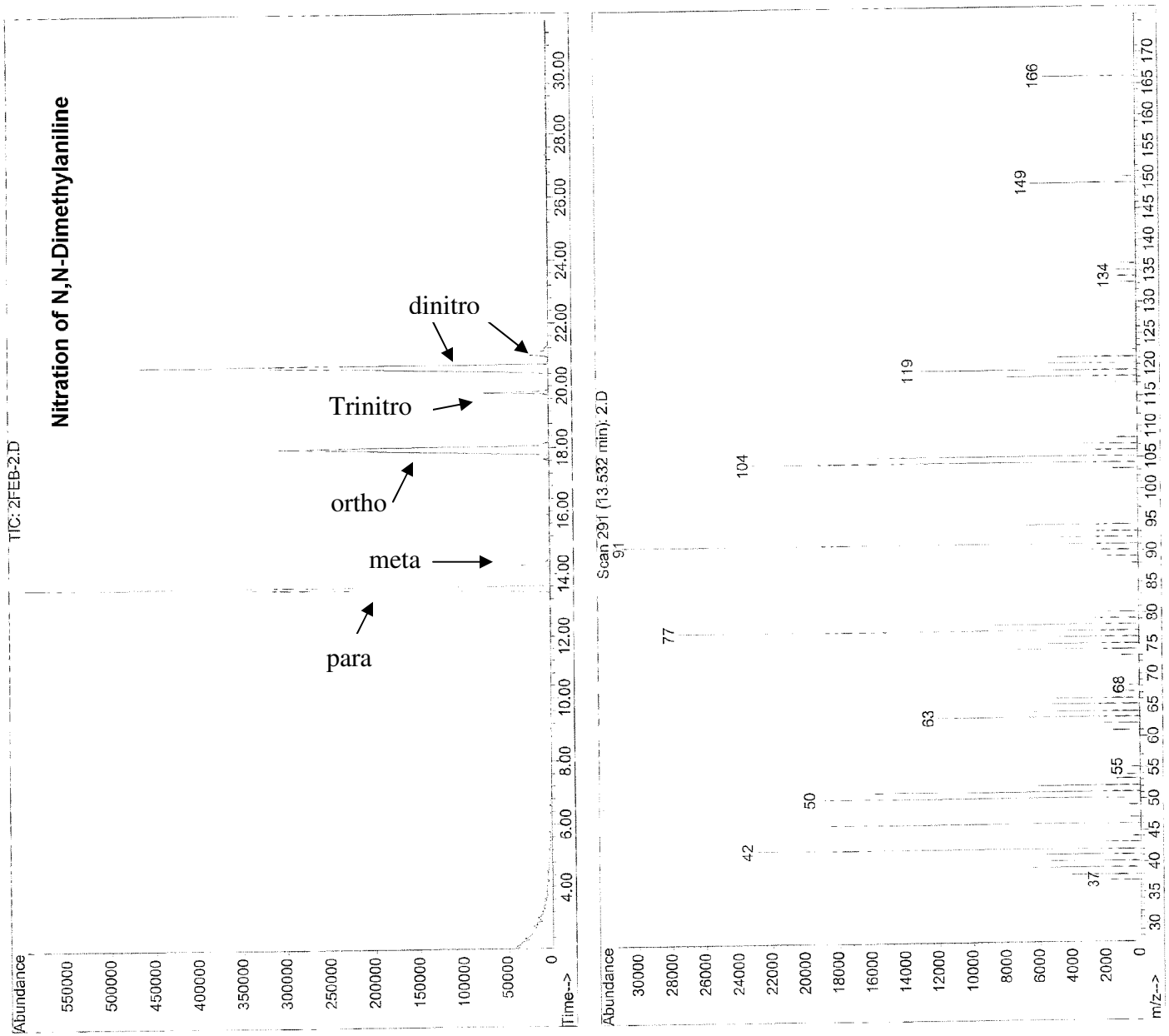

NO2
Cl
8.198
8.180
7.533
7.514
7.260
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
io
10.0
cr
8.66
is
3006.3
delta

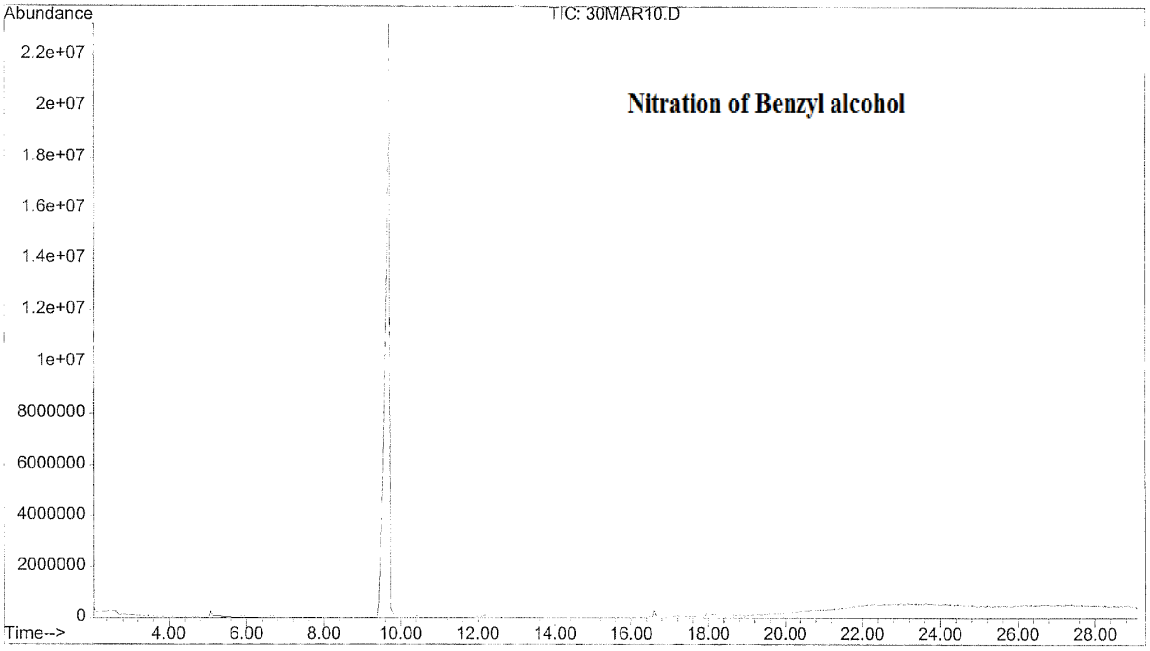

146.547
141.543
129.740
125.097
77.412
77.160
76.908
NO2
Cl
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
174.89
vs
37607.8
delta

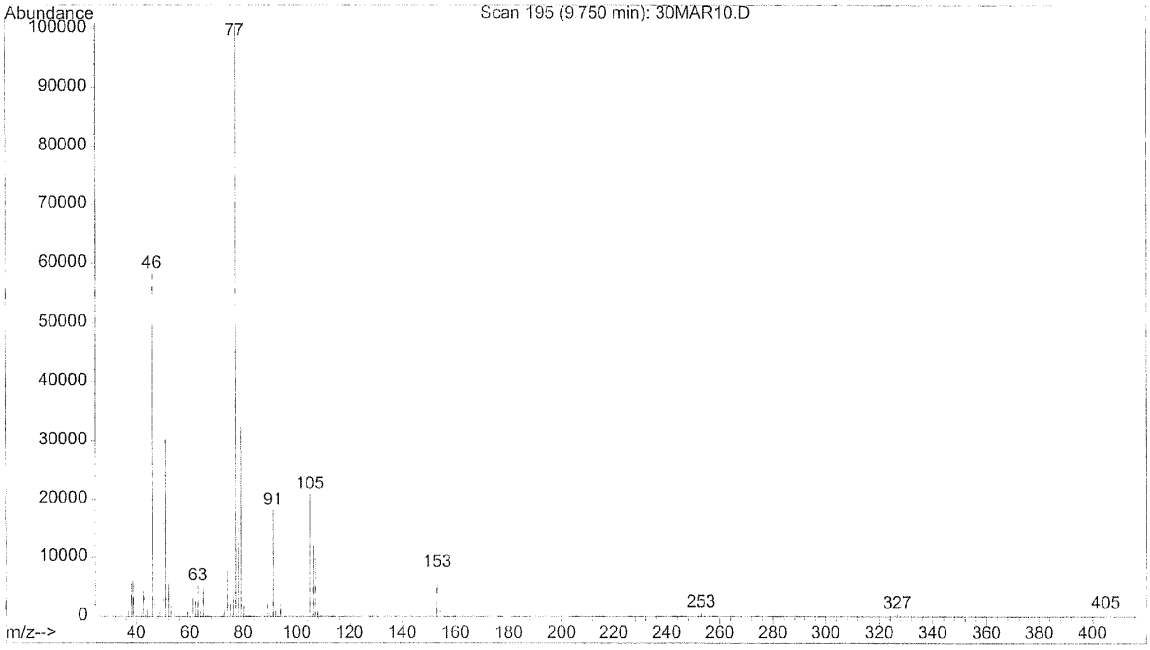

TIC: 25FEB06.D
Abundance
Nitration of Chlorobenzene
With Trifluoroacetic Anhydride
para
ortho
Time-->

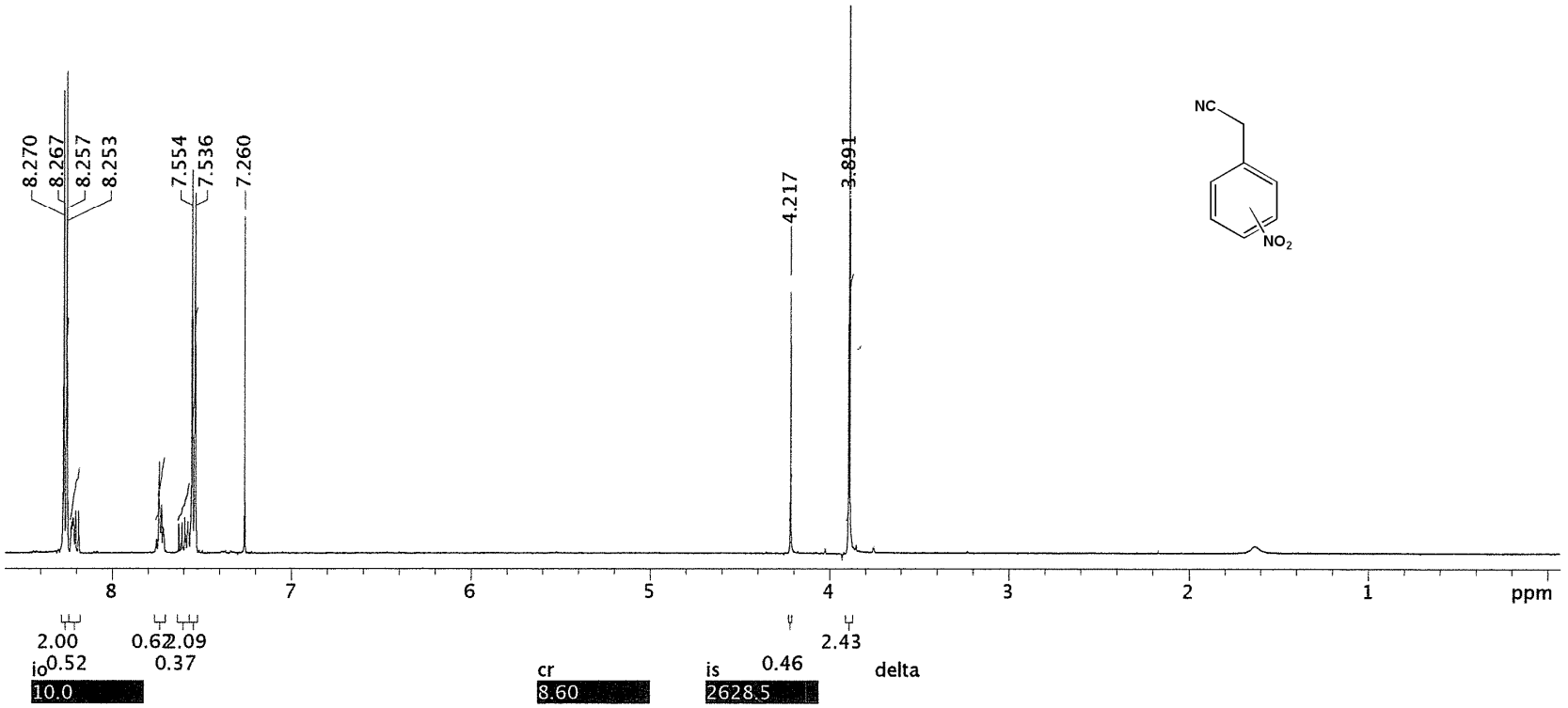

Scan 219 (10.705 min): 25FEB06.D
Abundance
m/z-->

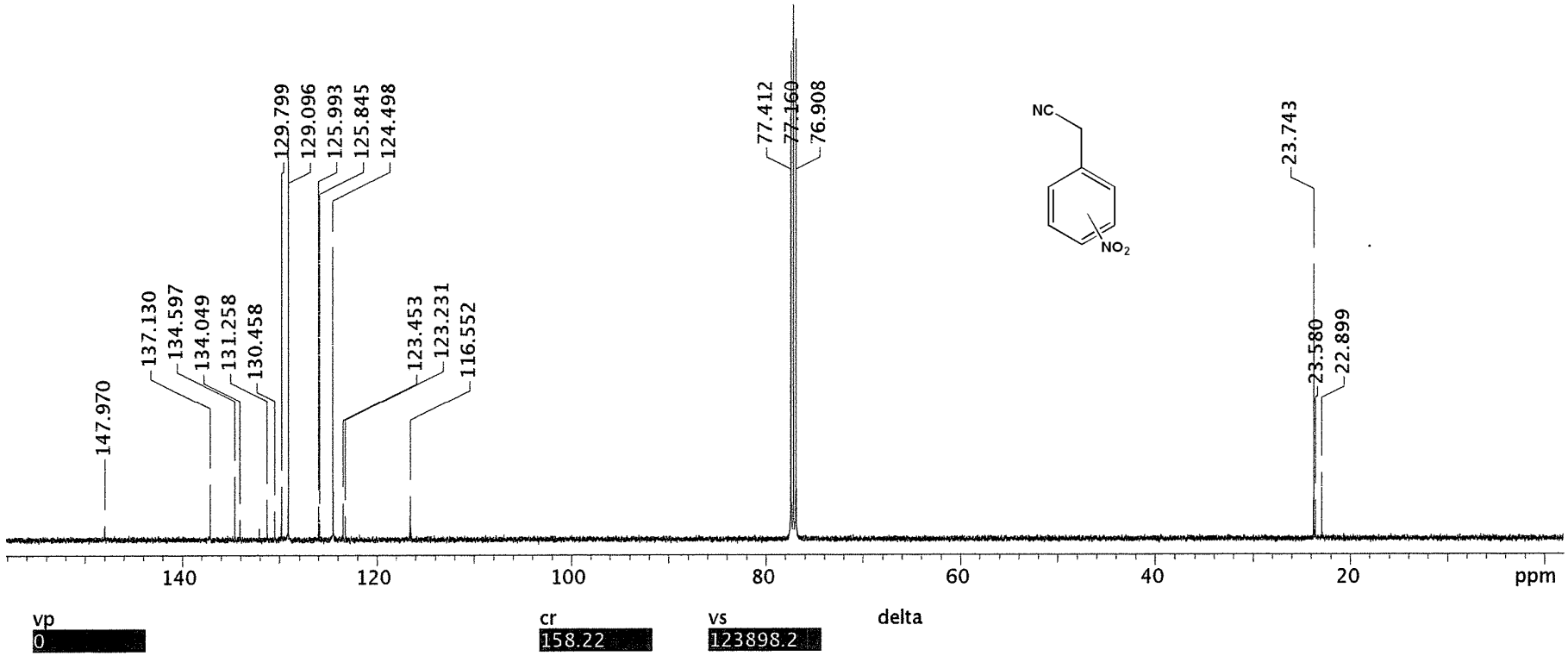

TIC: 10JUNE3.D
Abundance
Nitration of Chlorobenzene
With Triflic Anhydride
para
ortho
Time-->
Scan 218 (10.656 min): 10JUNE3.D
Abundance
m/z-->

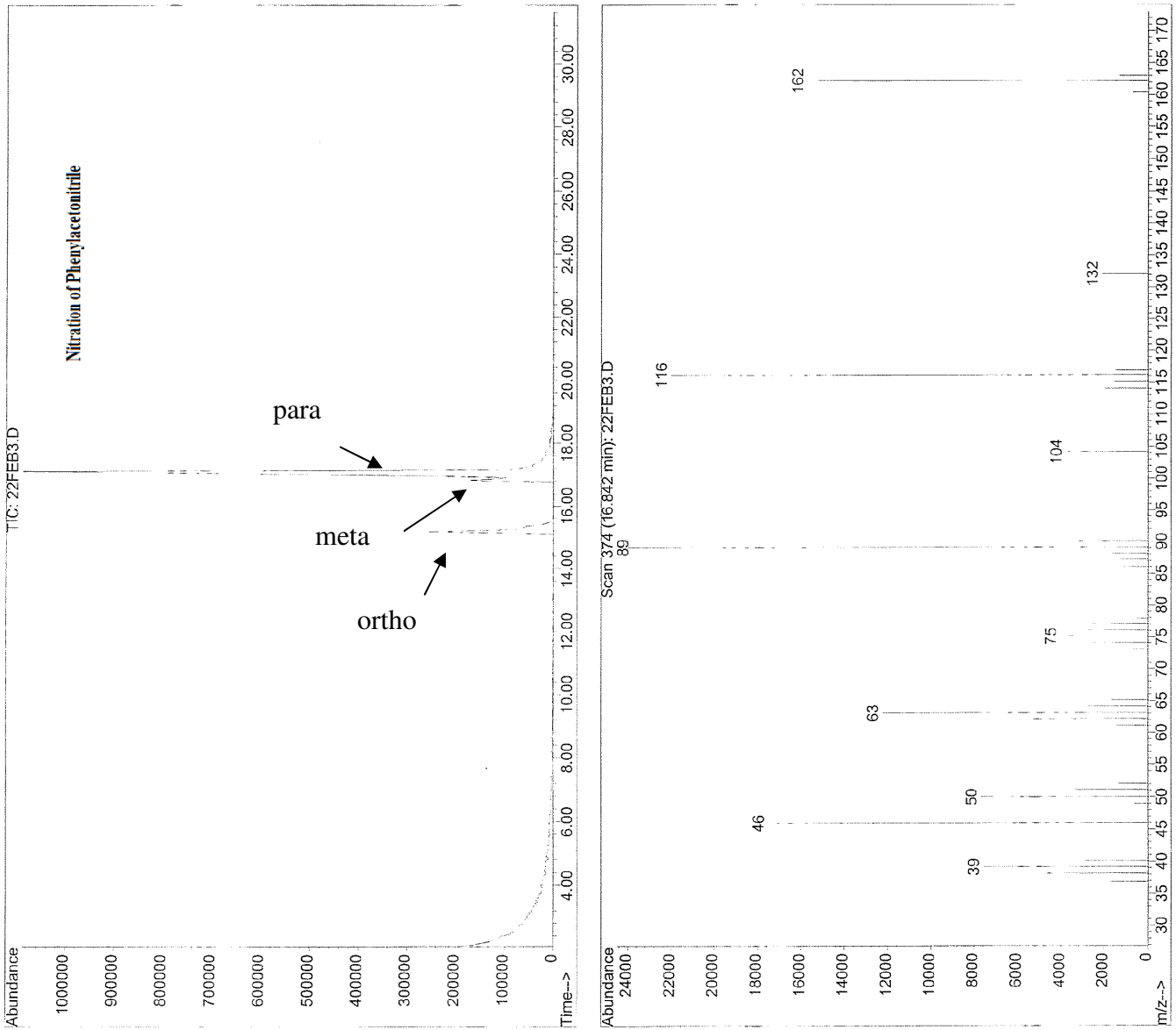

Nitration of N,N-Dimethylaniline
TIC: 2FEB-2.D
Abundance
Time-->
dinitro
Trinitro
ortho
meta
para
Scan 291 (13.532 min): 2.D
m/z-->

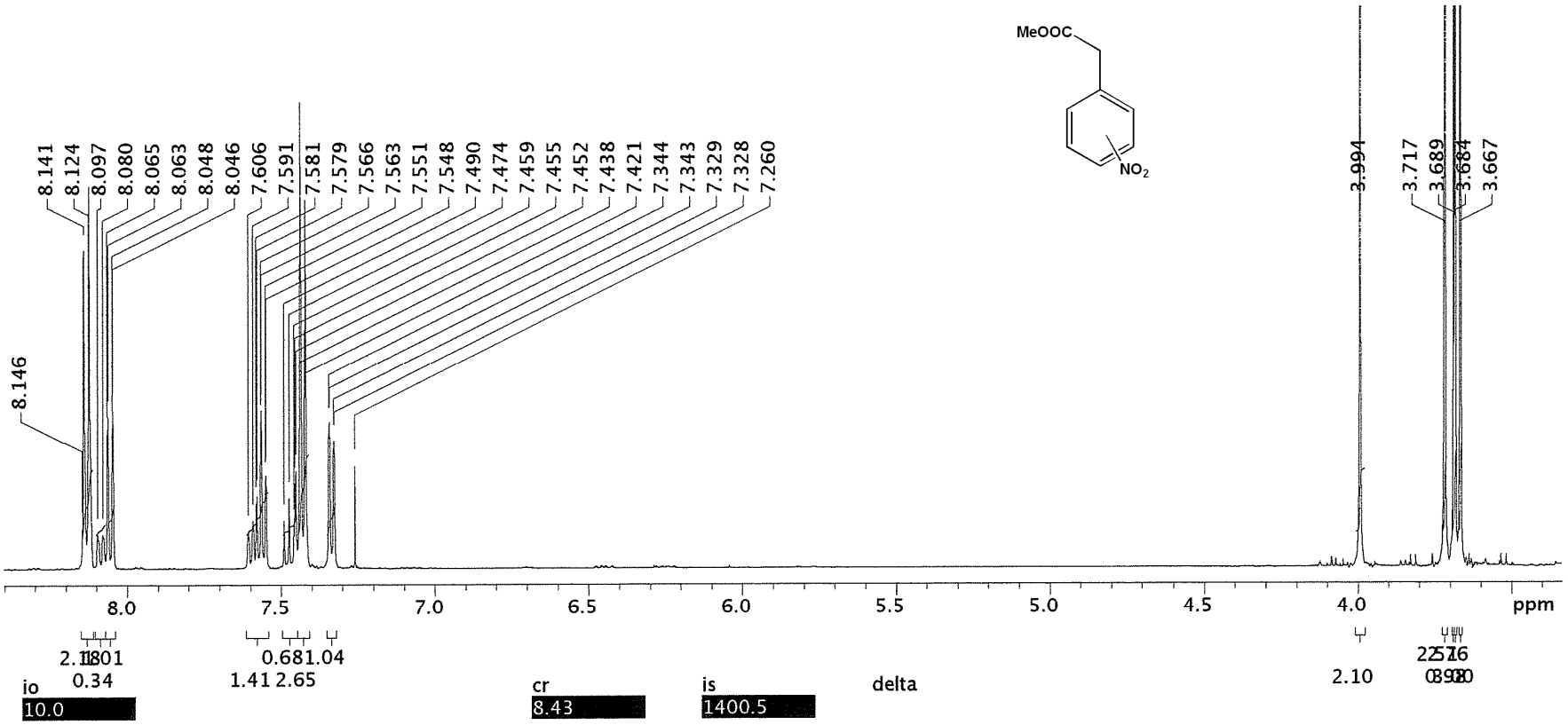

Abundance
TIC: 30MAR10.D
Nitration of Benzyl alcohol
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00

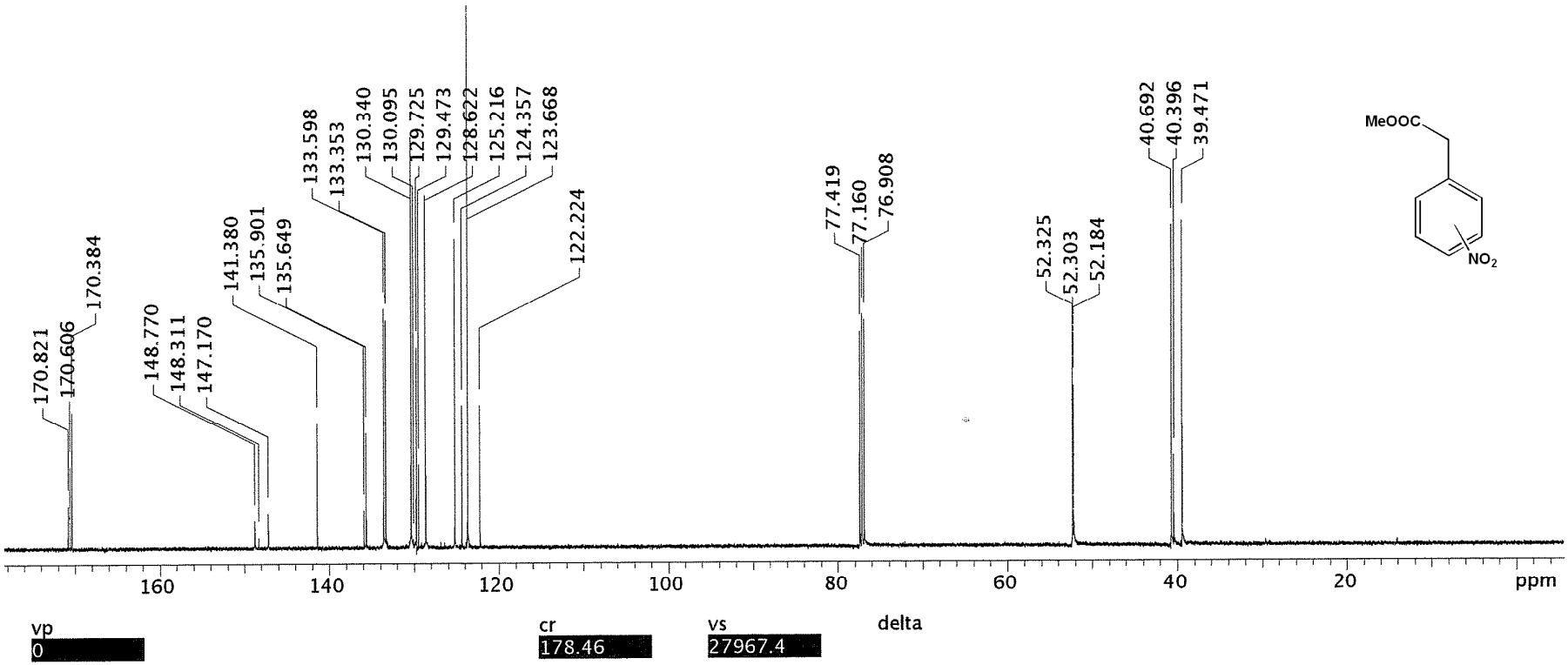

Abundance
Scan 195 (9.750 min): 30MAR10.D
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
77
46
105
91
63
153
253
327
405
m/z-->
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400

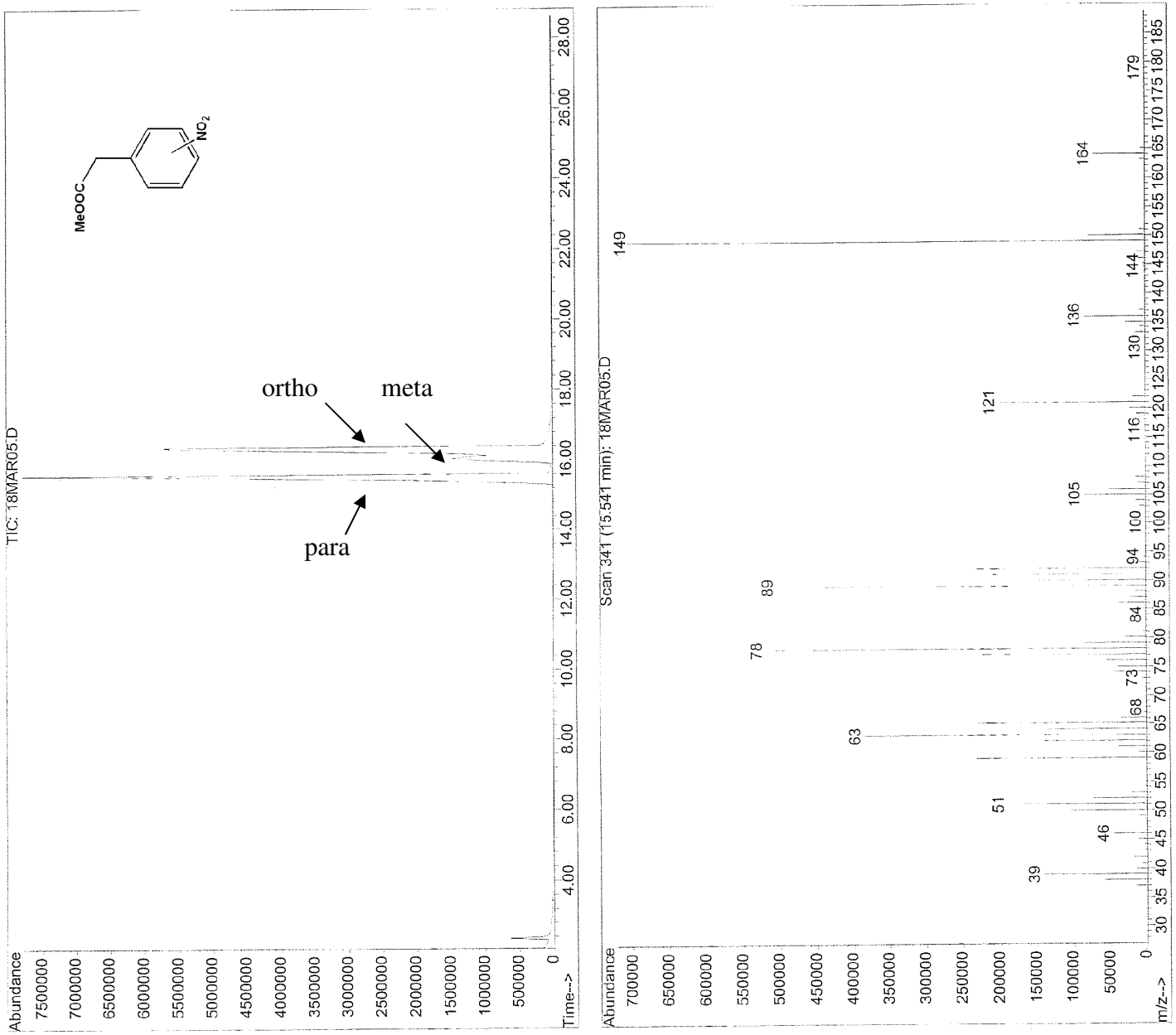

8.270
8.267
8.257
8.253
7.554
7.536
7.260
4.217
3.891
NC
NO2
8
7
6
5
4
3
2
1
ppm
2.00
0.62
2.09
2.43
io 0.52
0.37
cr
is 0.46
delta
10.0
8.60
2628.5

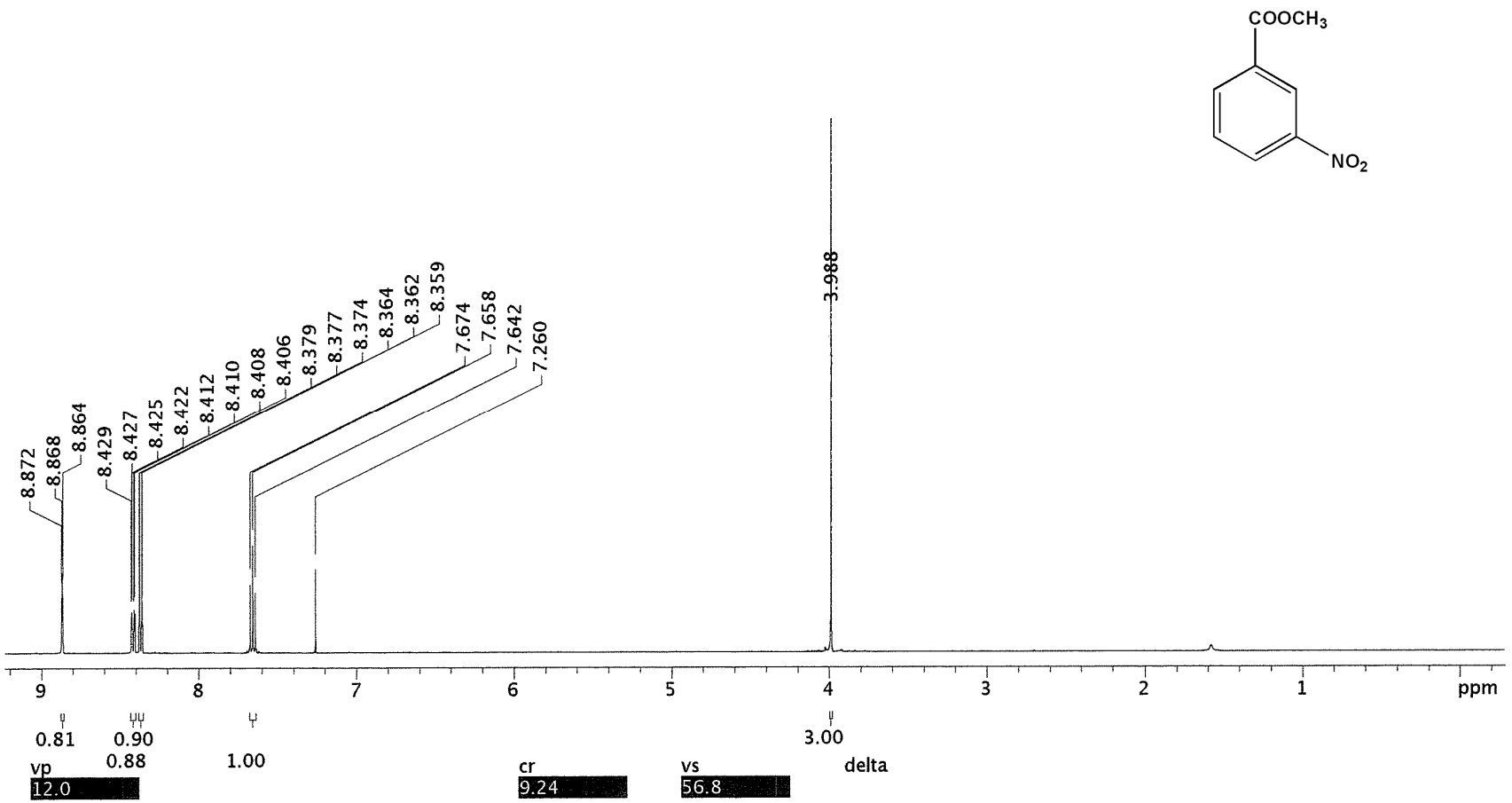

147.970
137.130
134.597
134.049
131.258
130.458
129.799
129.096
125.993
125.845
124.498
123.453
123.231
116.552
77.412
77.160
76.908
23.743
23.580
22.899
NC
NO2
140
120
100
80
60
40
20
ppm
vp
0
cr
158.22
vs
123898.2
delta

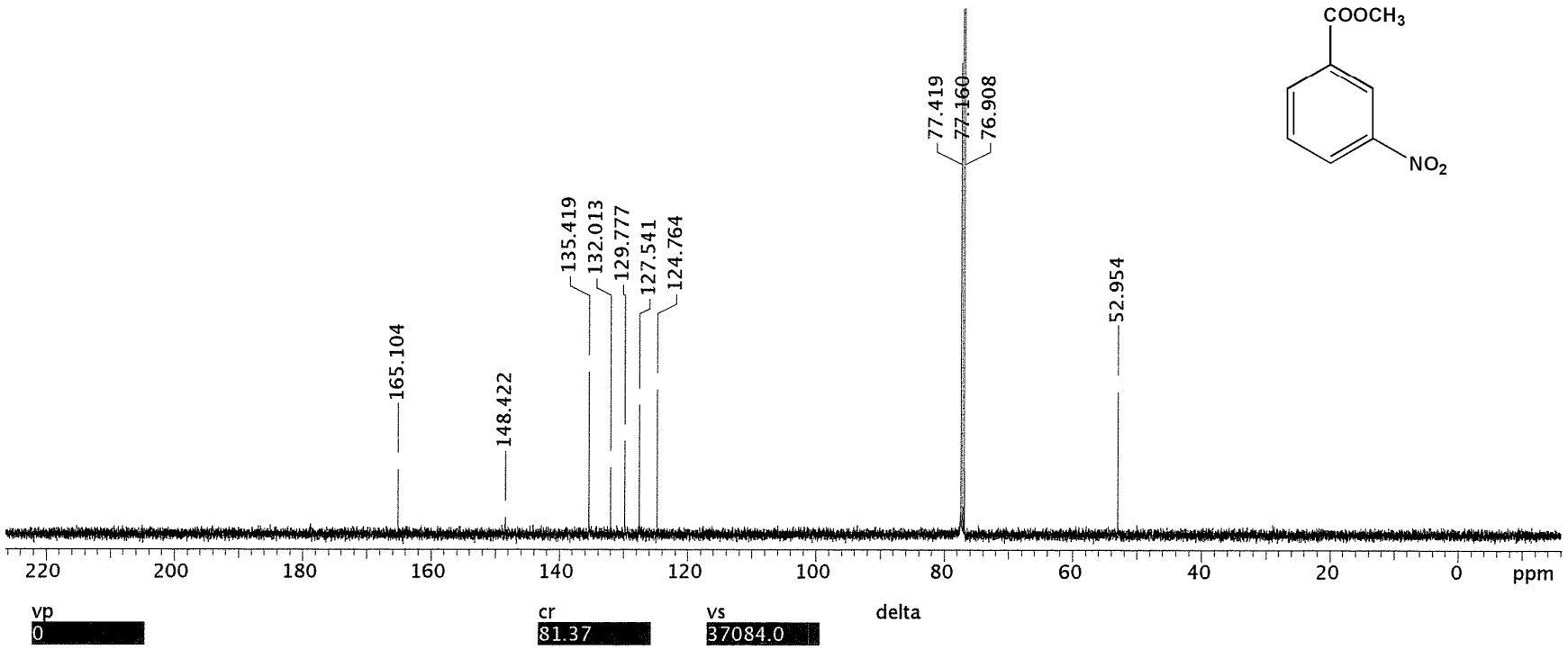

Nitration of Phenylacetonitrile
TIC: 22FEB3.D
Abundance
Time-->
para
meta
ortho
Scan 374 (16.842 min): 22FEB3.D
m/z-->

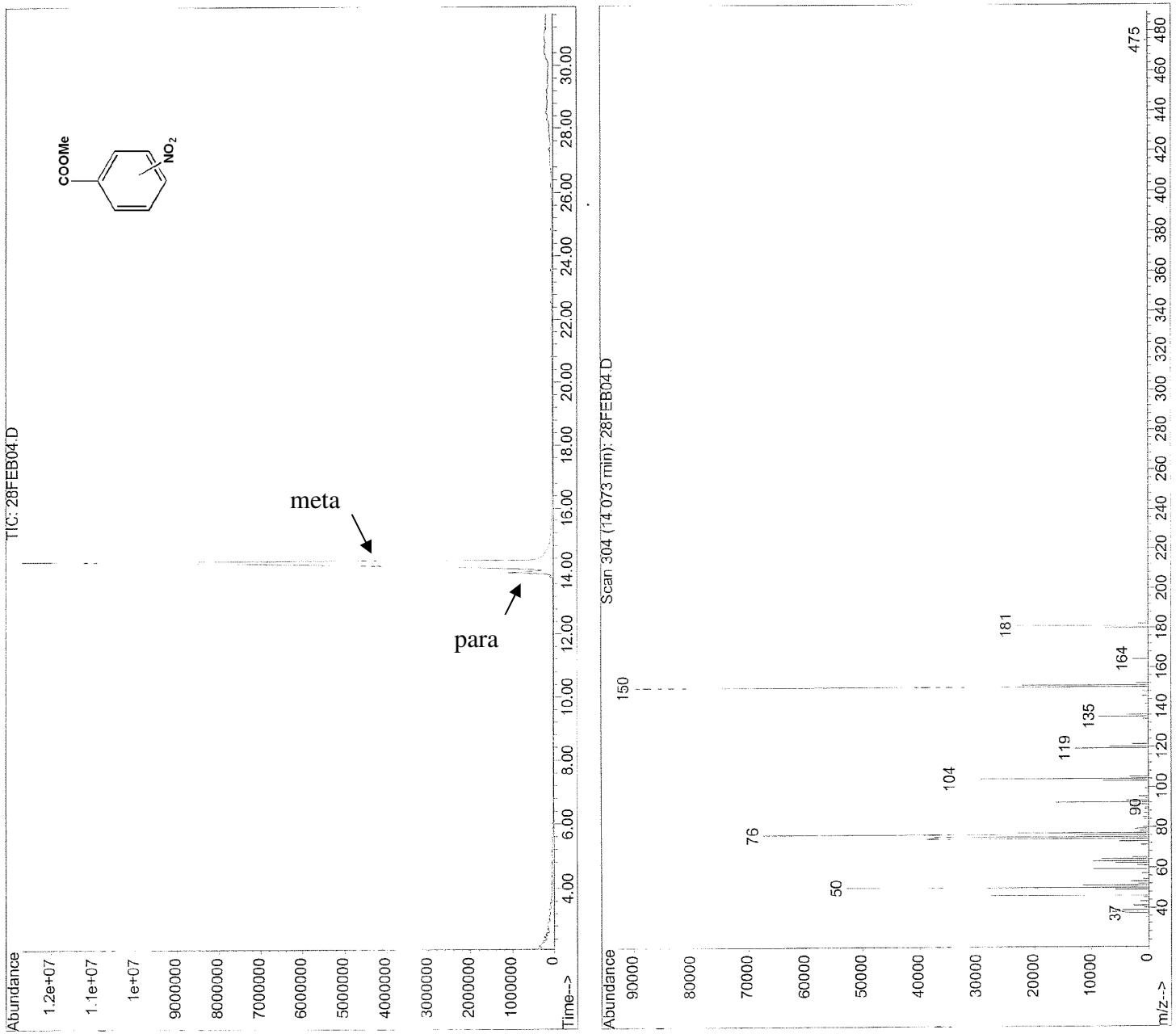

MeOOC
NO2
8.141
8.124
8.097
8.080
8.065
8.063
8.048
8.046
7.606
7.591
7.581
7.579
7.566
7.563
7.551
7.548
7.490
7.474
7.459
7.455
7.452
7.438
7.421
7.344
7.343
7.329
7.328
7.260
8.146
3.994
3.717
3.689
3.684
3.667
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
0.34
1.41
2.65
0.68
1.04
2.10
io
10.0
cr
8.43
is
1400.5
delta

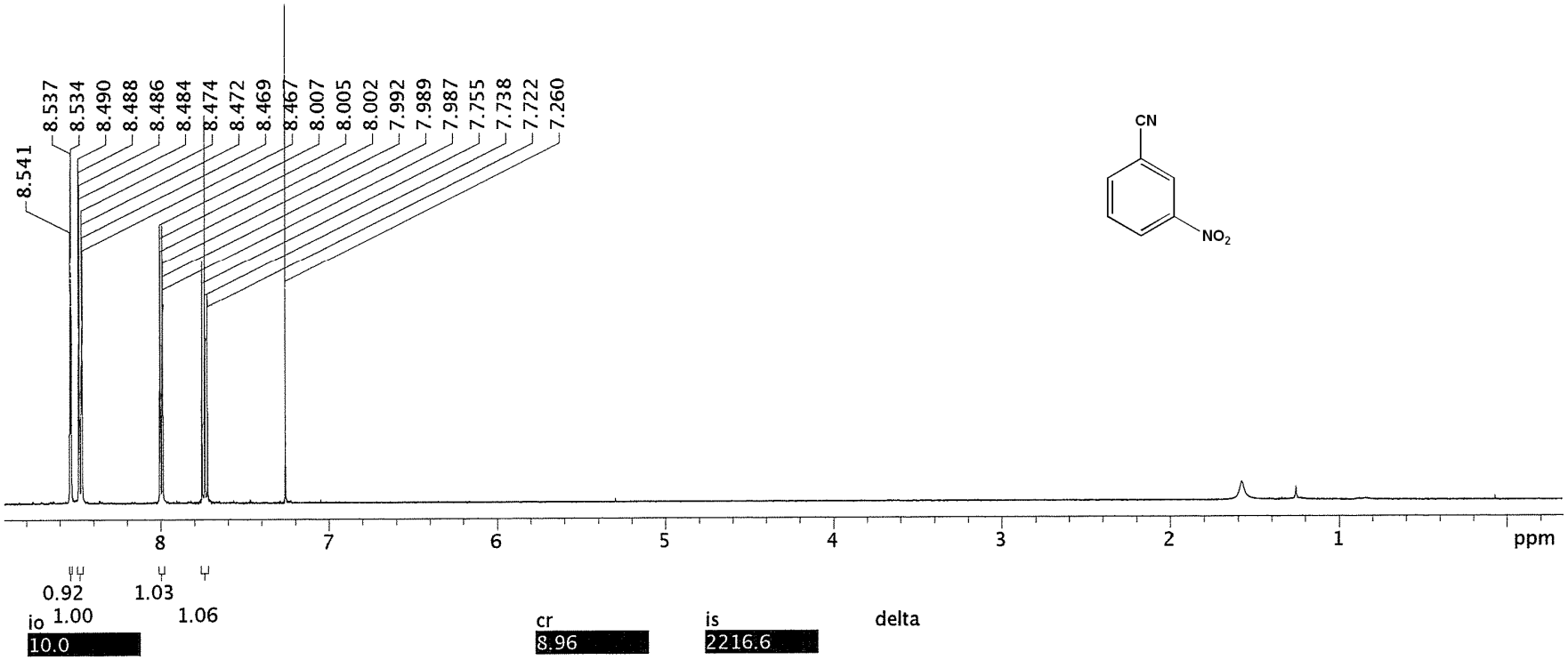

170.821
170.606
170.384
148.770
148.311
147.170
141.380
135.901
135.649
133.598
133.353
130.340
130.095
129.725
129.473
128.622
125.216
124.357
123.668
122.224
77.419
77.160
76.908
52.325
52.303
52.184
40.692
40.396
39.471
MeOOC
NO2
160
140
120
100
80
60
40
20
ppm
vp
0
cr
178.46
vs
27967.4
delta

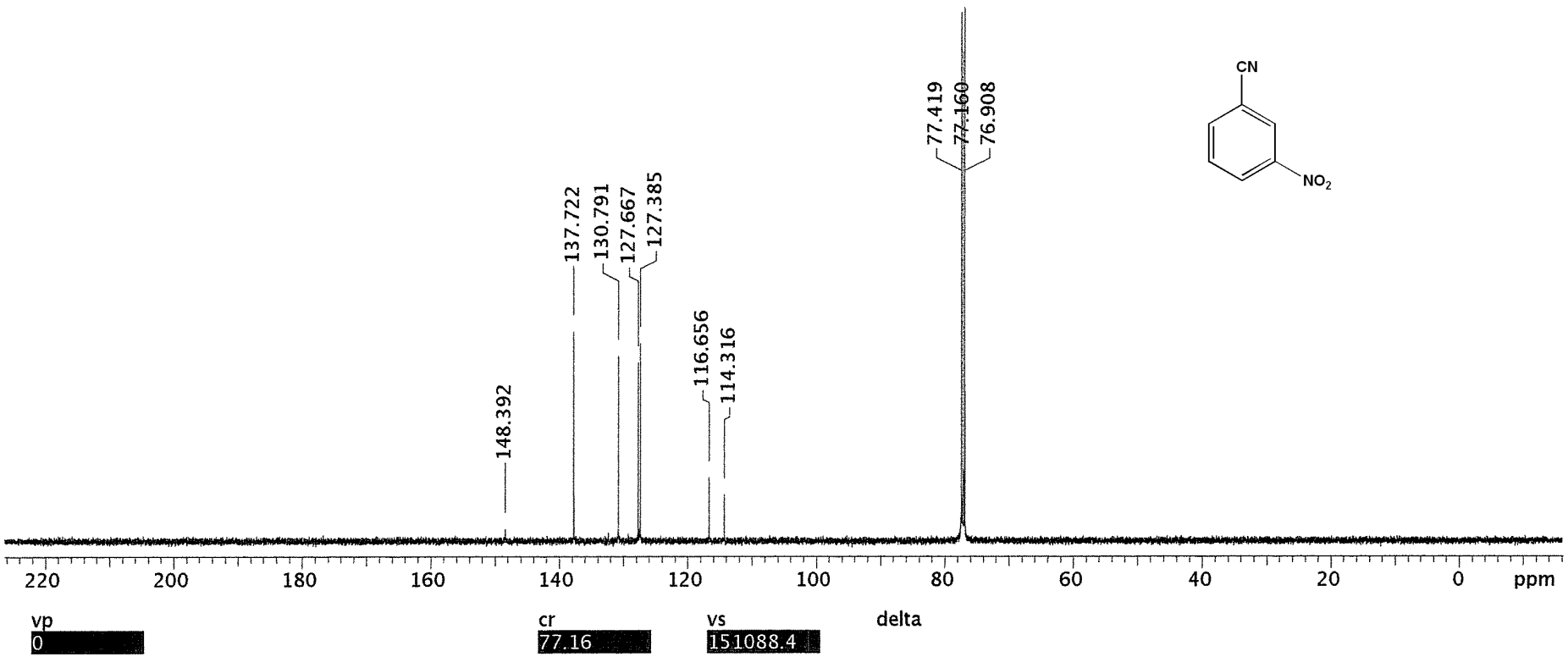

TIC: 18MAR05.D
Abundance
Time-->
MeOOC
NO2
ortho
meta
para
Scan 341 (15.541 min): 18MAR05.D
Abundance
m/z-->

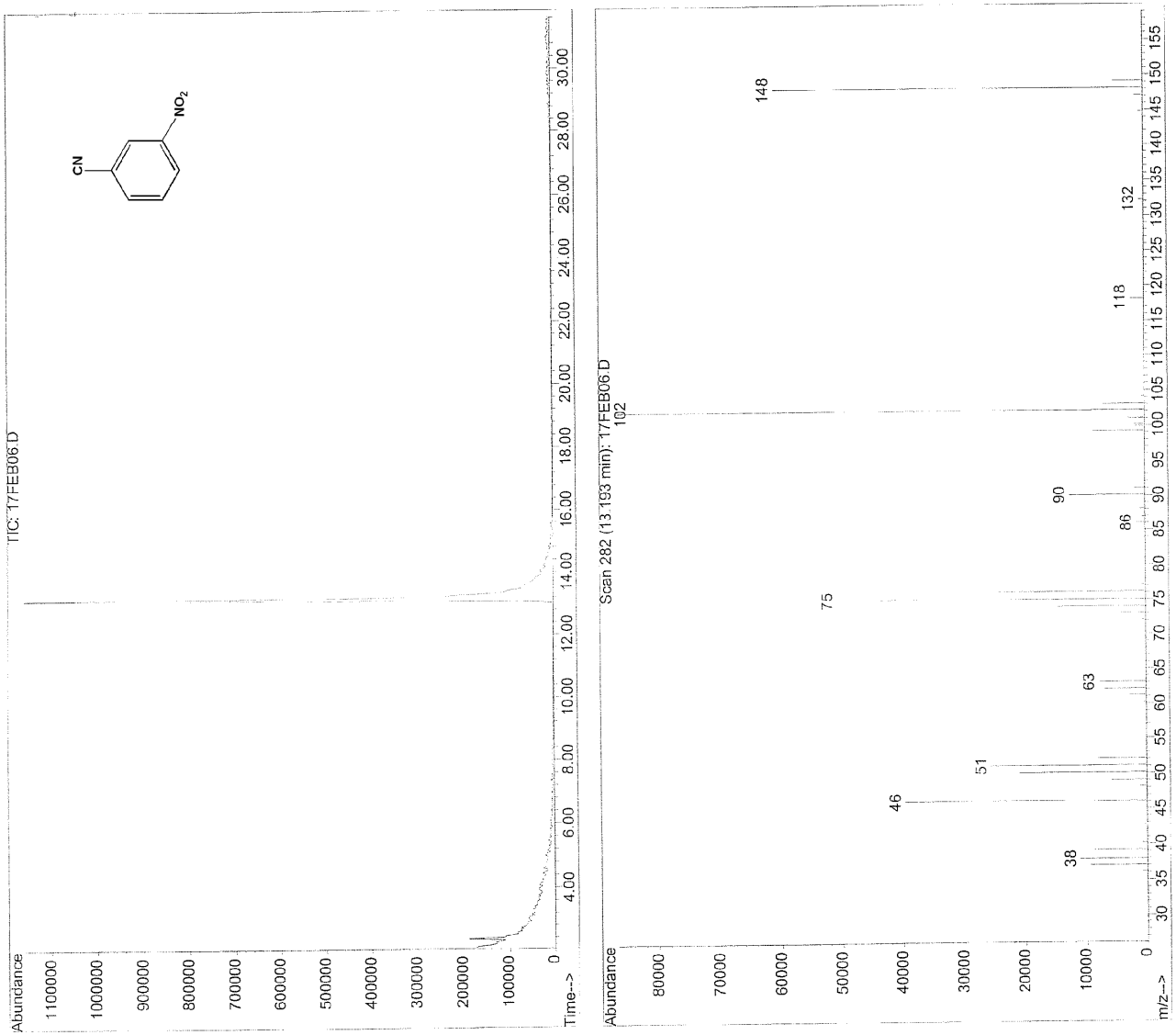

COOCH3
NO2
8.872
8.868
8.864
8.429
8.427
8.425
8.422
8.412
8.410
8.408
8.406
8.379
8.377
8.374
8.364
8.362
8.359
7.674
7.658
7.642
7.260
3.988
9
8
7
6
5
4
3
2
1
ppm
0.81
0.90
3.00
0.88
1.00
vp
12.0
cr
9.24
vs
56.8
delta

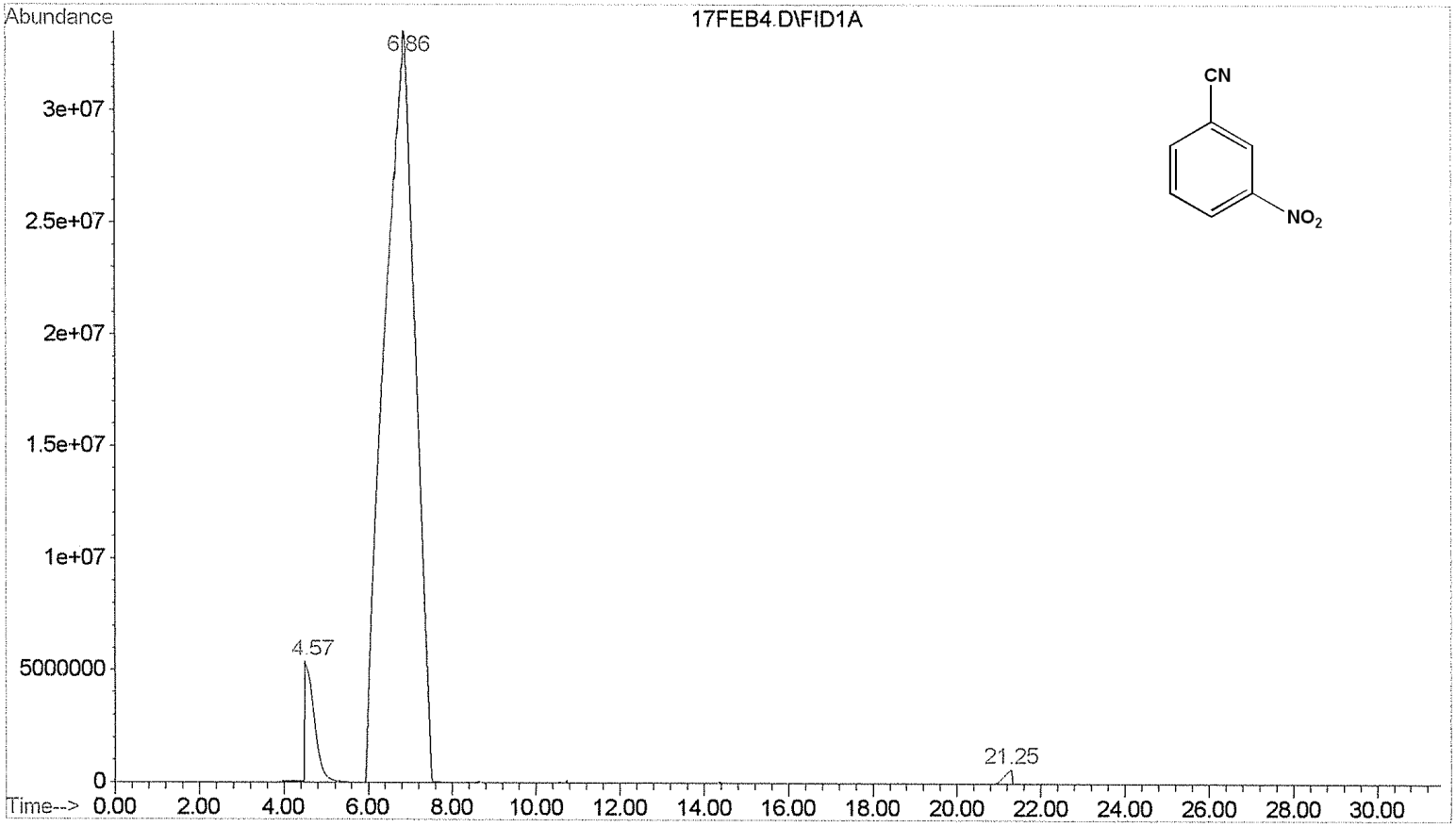

COOCH3
NO2
165.104
148.422
135.419
132.013
129.777
127.541
124.764
77.419
77.160
76.908
52.954
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
81.37
vs
37084.0
delta

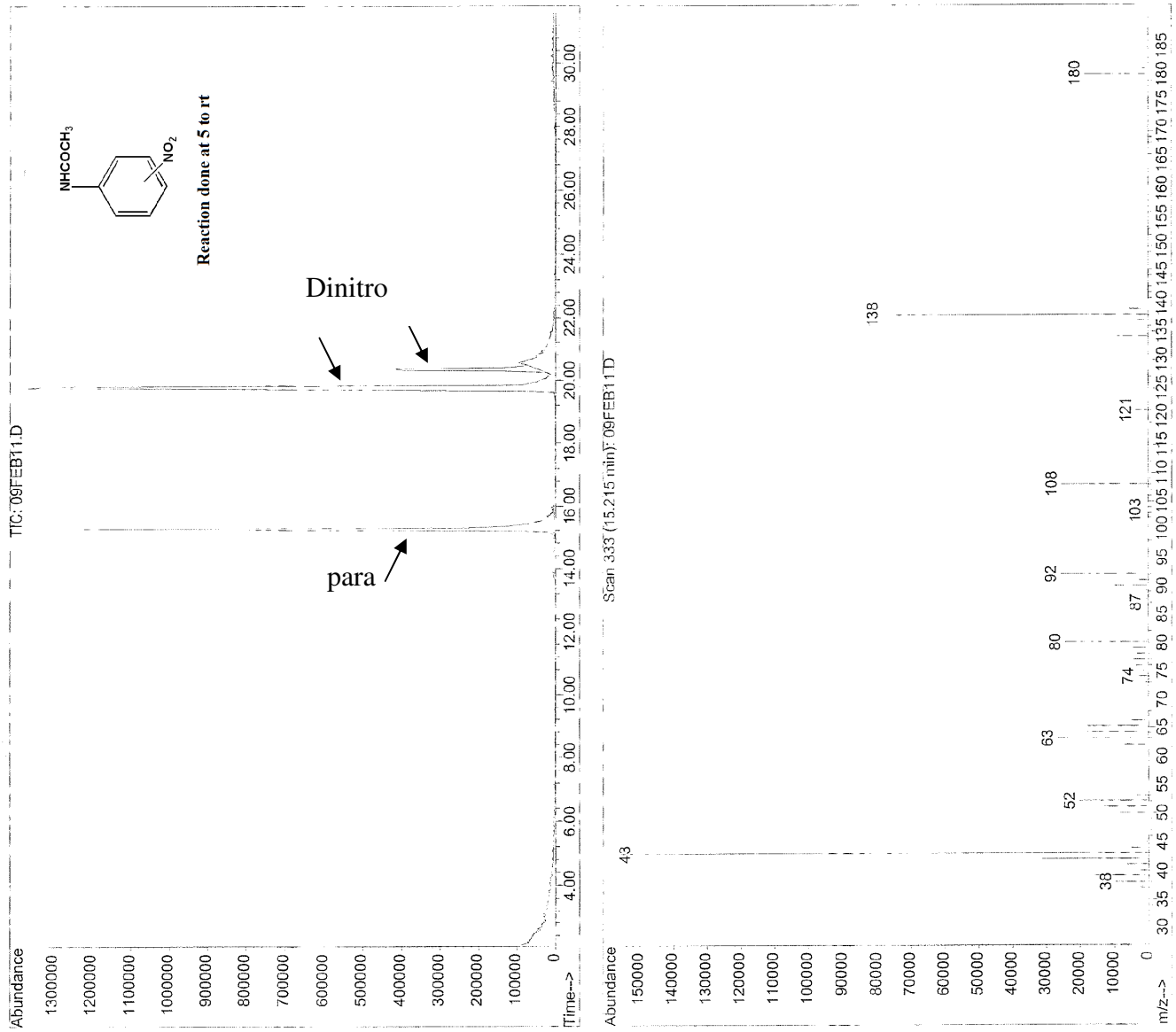

TIC: 28FEB04.D
Abundance
Time-->
meta
para
COOMe
NO2
Scan 304 (14.073 min): 28FEB04.D
Abundance
m/z-->

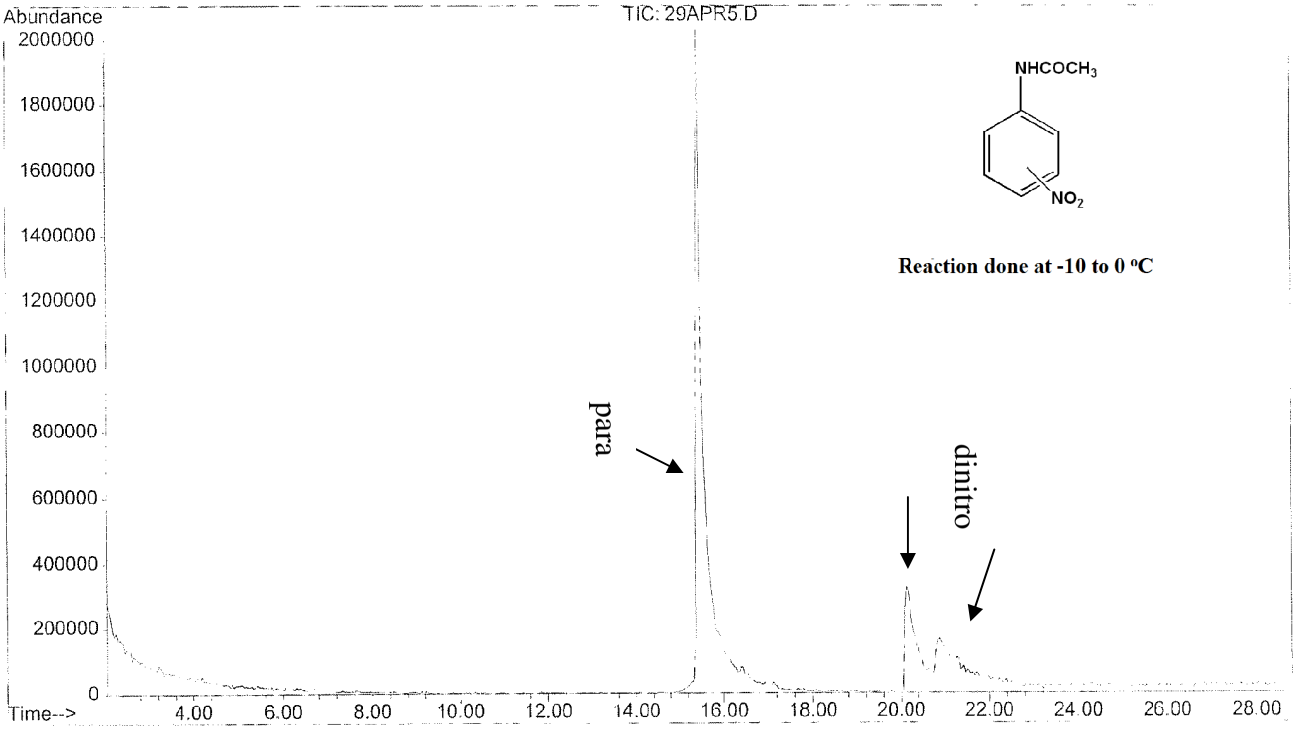

8.541
8.537
8.534
8.490
8.488
8.486
8.484
8.474
8.472
8.469
8.467
8.007
8.005
8.002
7.992
7.989
7.987
7.755
7.738
7.722
7.260
CN
NO2
8
7
6
5
4
3
2
1
ppm
0.92
1.00
1.03
1.06
io
10.0
cr
8.96
is
2216.6
delta

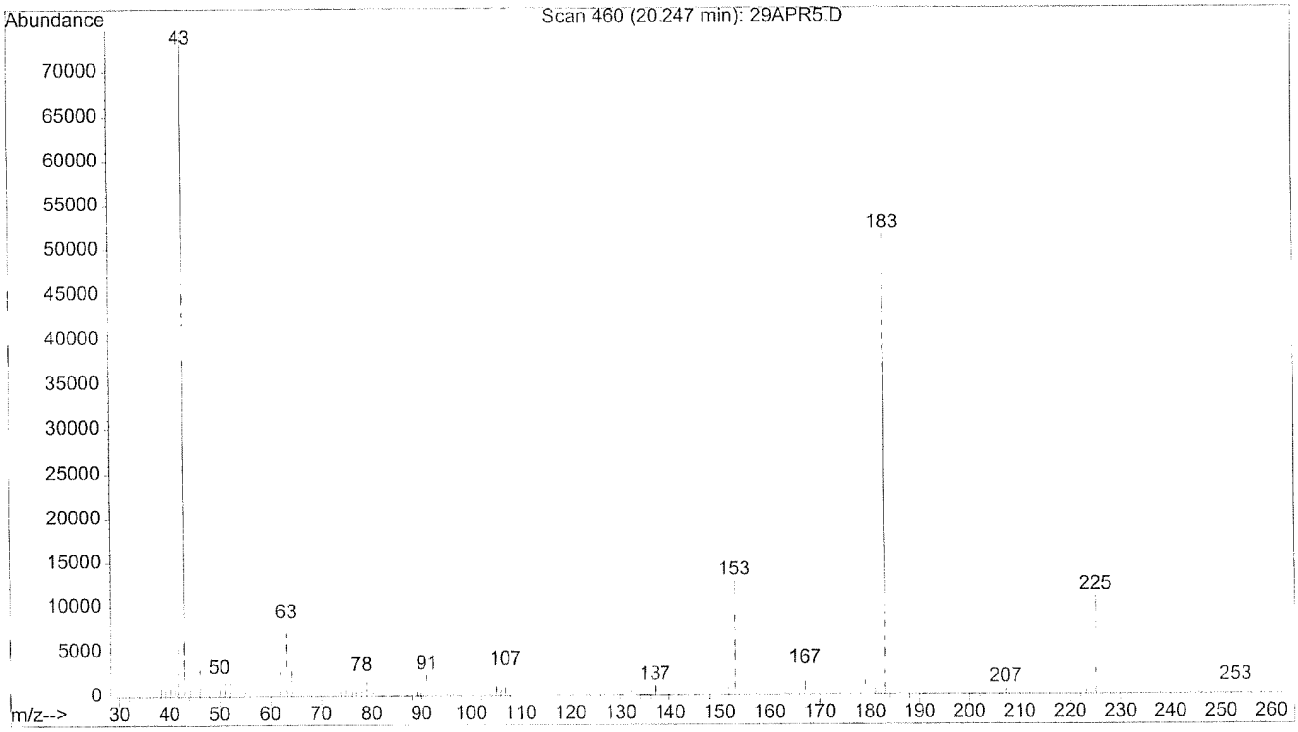

148.392
137.722
130.791
127.667
127.385
116.656
114.316
77.419
77.160
76.908
CN
NO2
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
77.16
vs
151088.4
delta

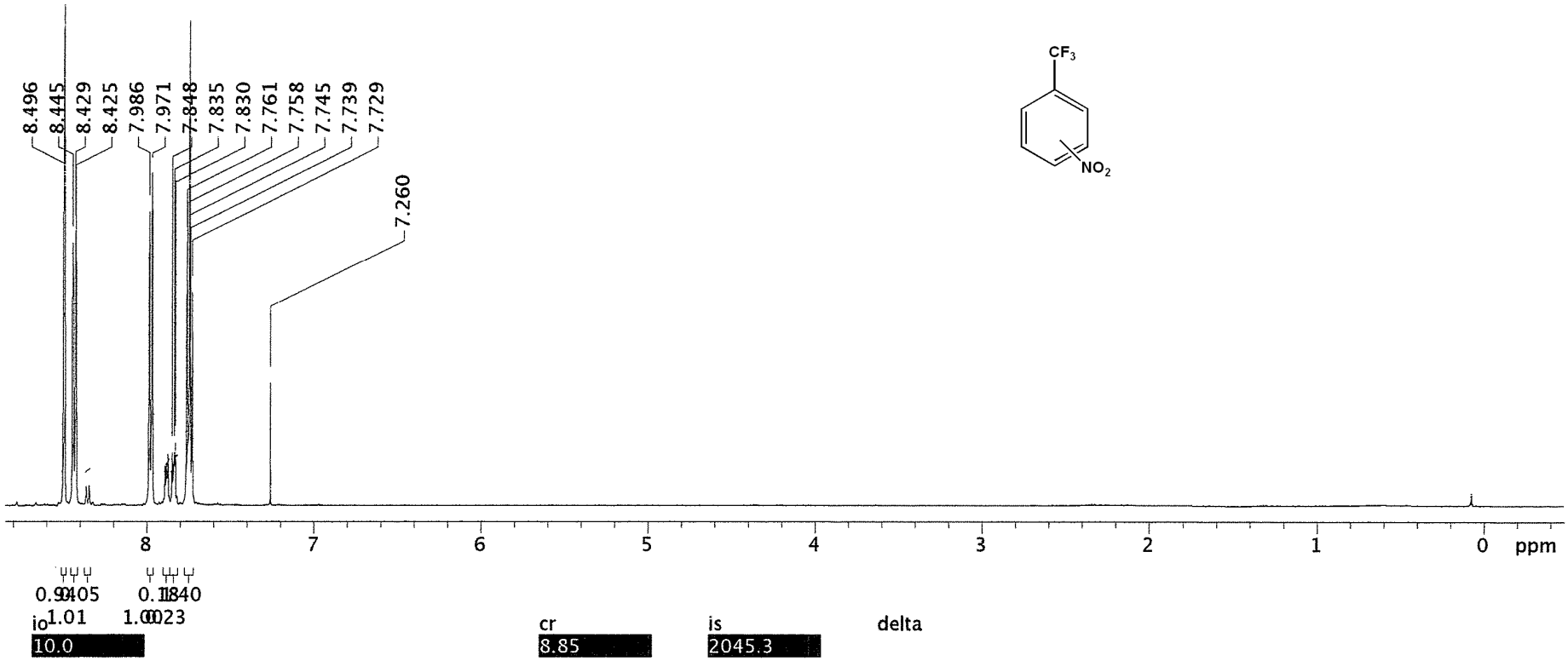

TIC: 17FEB06.D
Abundance
Time-->
CN
NO2
Scan 282 (13.193 min): 17FEB06.D
102
148
75
46
51
38
63
86
90
118
132
m/z-->

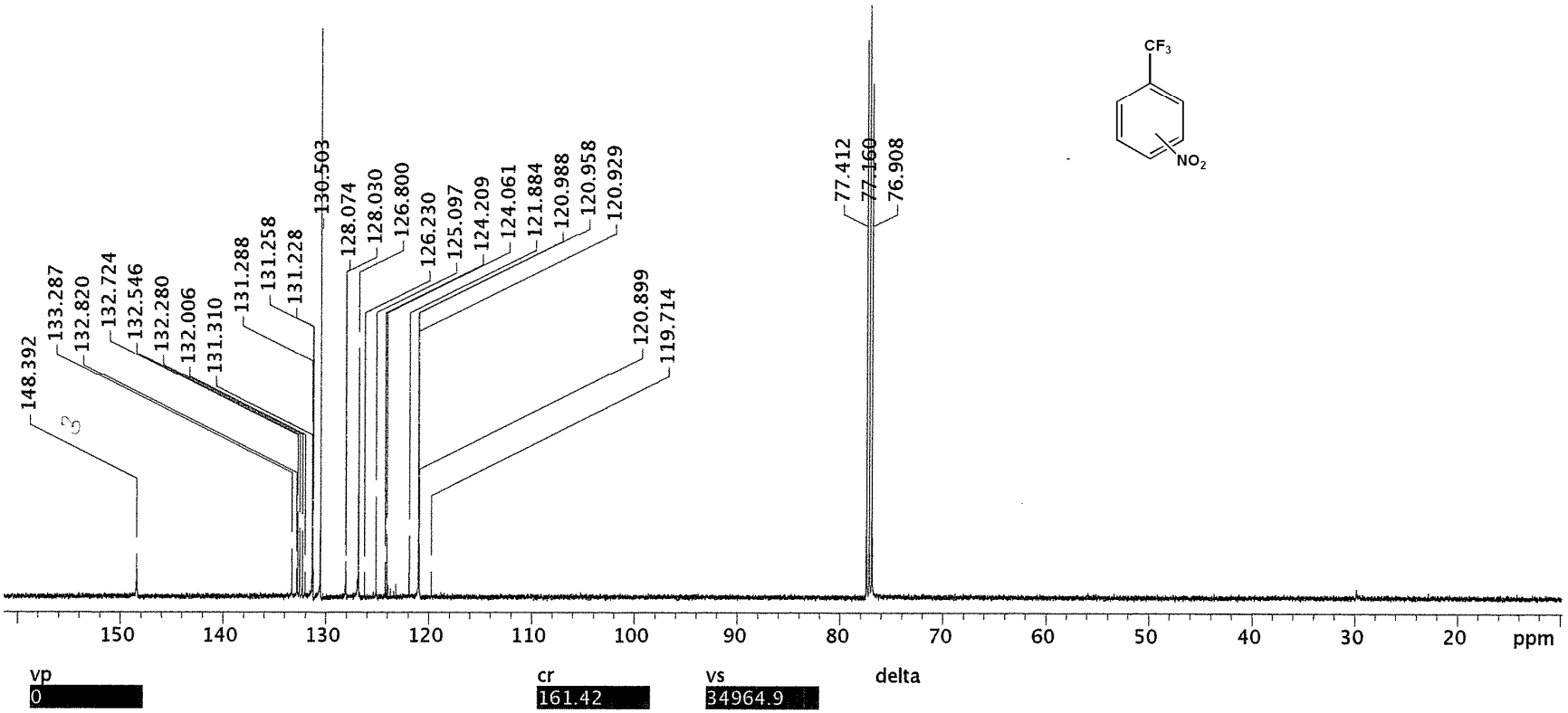

Abundance
17FEB4.D\FID1A
6.86
4.57
21.25
3e+07
2.5e+07
2e+07
1.5e+07
1e+07
5000000
0
Time-->
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00
CN
NO2

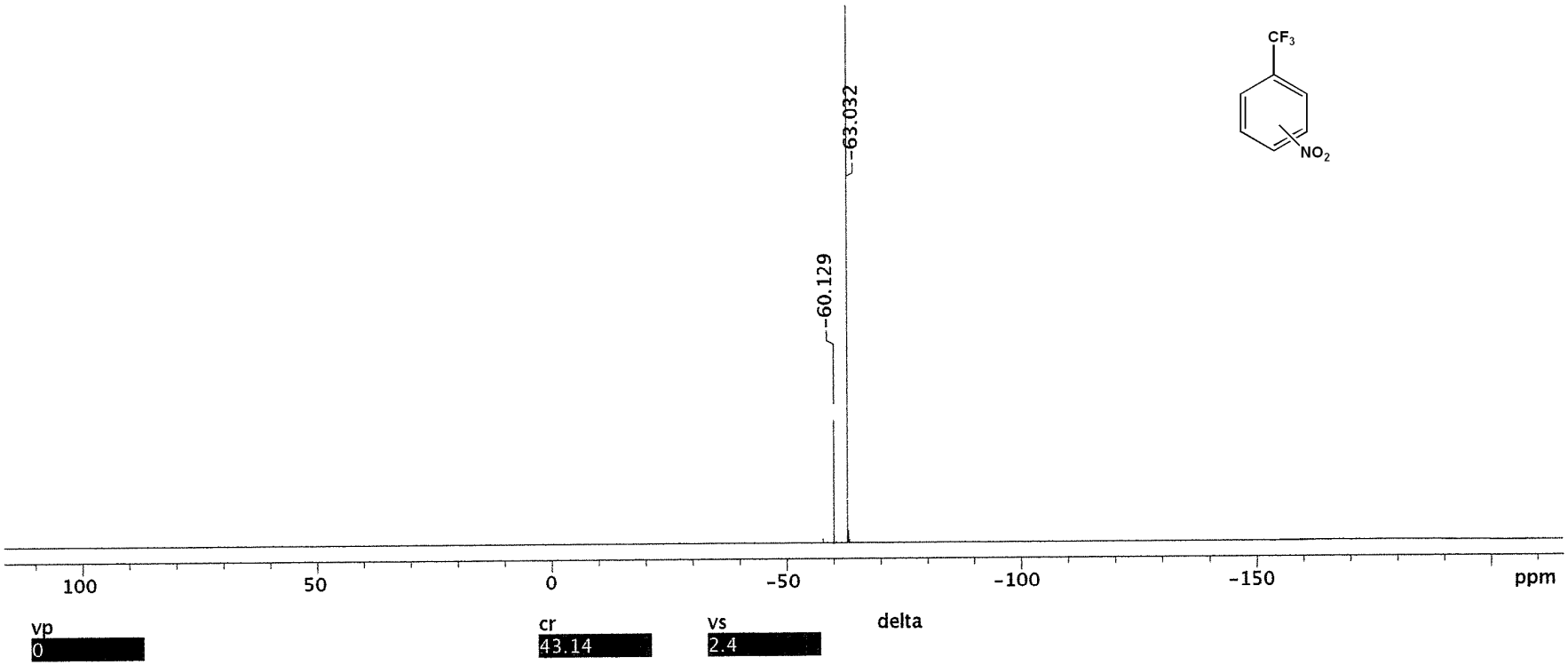

TIC: 09FEB11.D
Abundance
Time-->
Reaction done at 5 to rt
NHCOCH3
NO2
Dinitro
para
Scan 333 (15.215 min): 09FEB11.D
Abundance
m/z-->

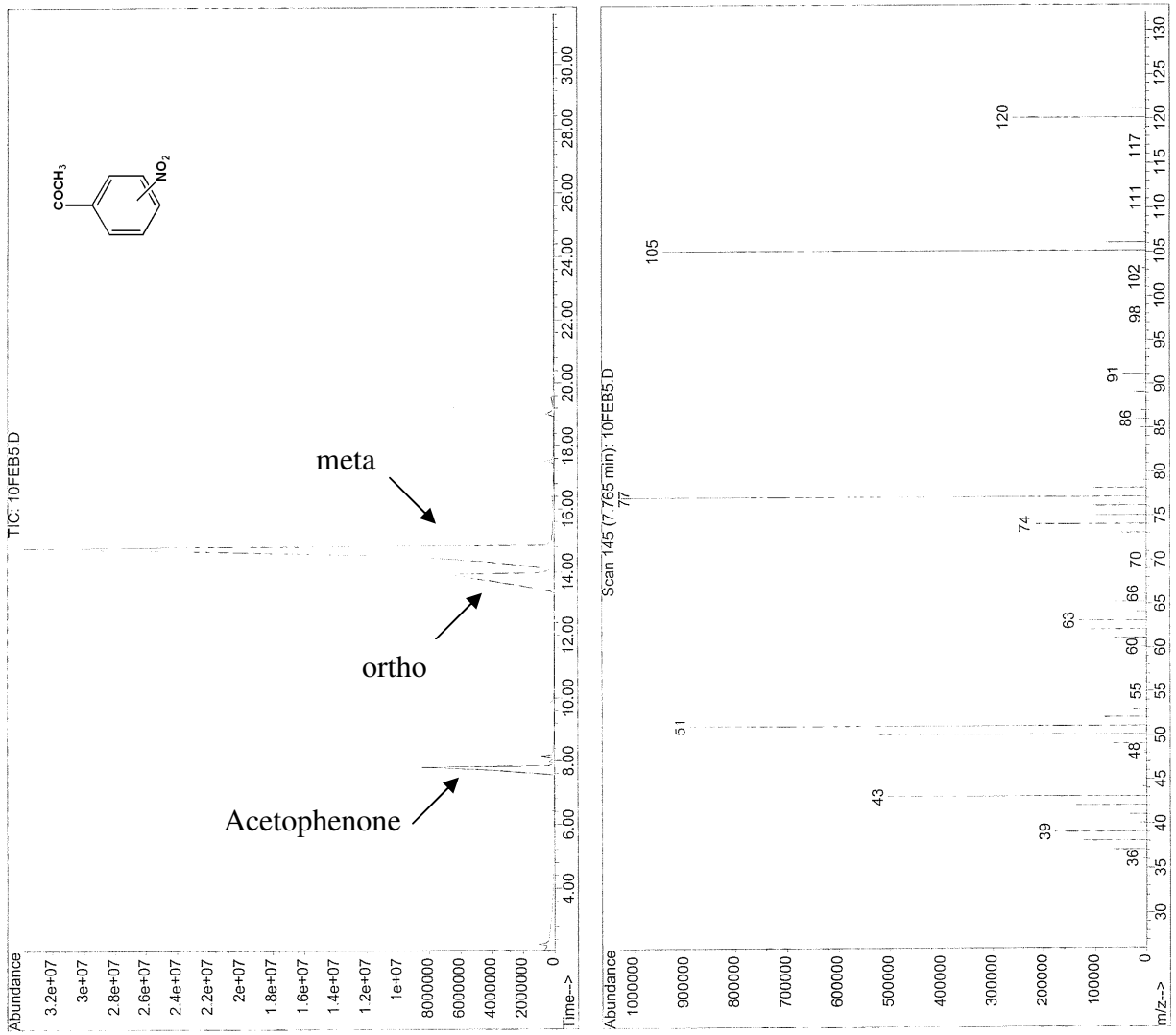

TIC: 29APR5.D
Abundance
Time-->
NHCOCH3
NO2
Reaction done at -10 to 0 °C
para
dinitro

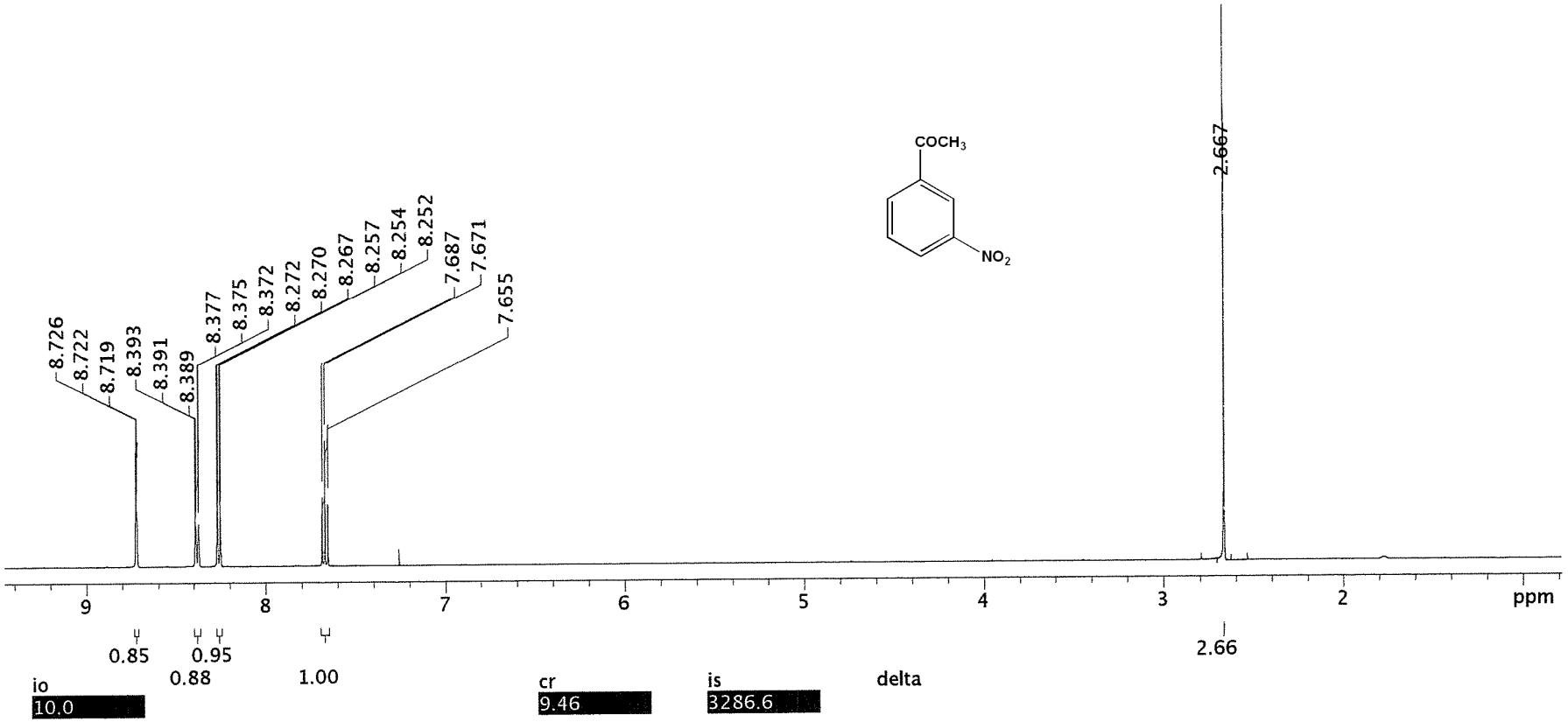

Scan 460 (20.247 min): 29APR5.D
Abundance
m/z-->

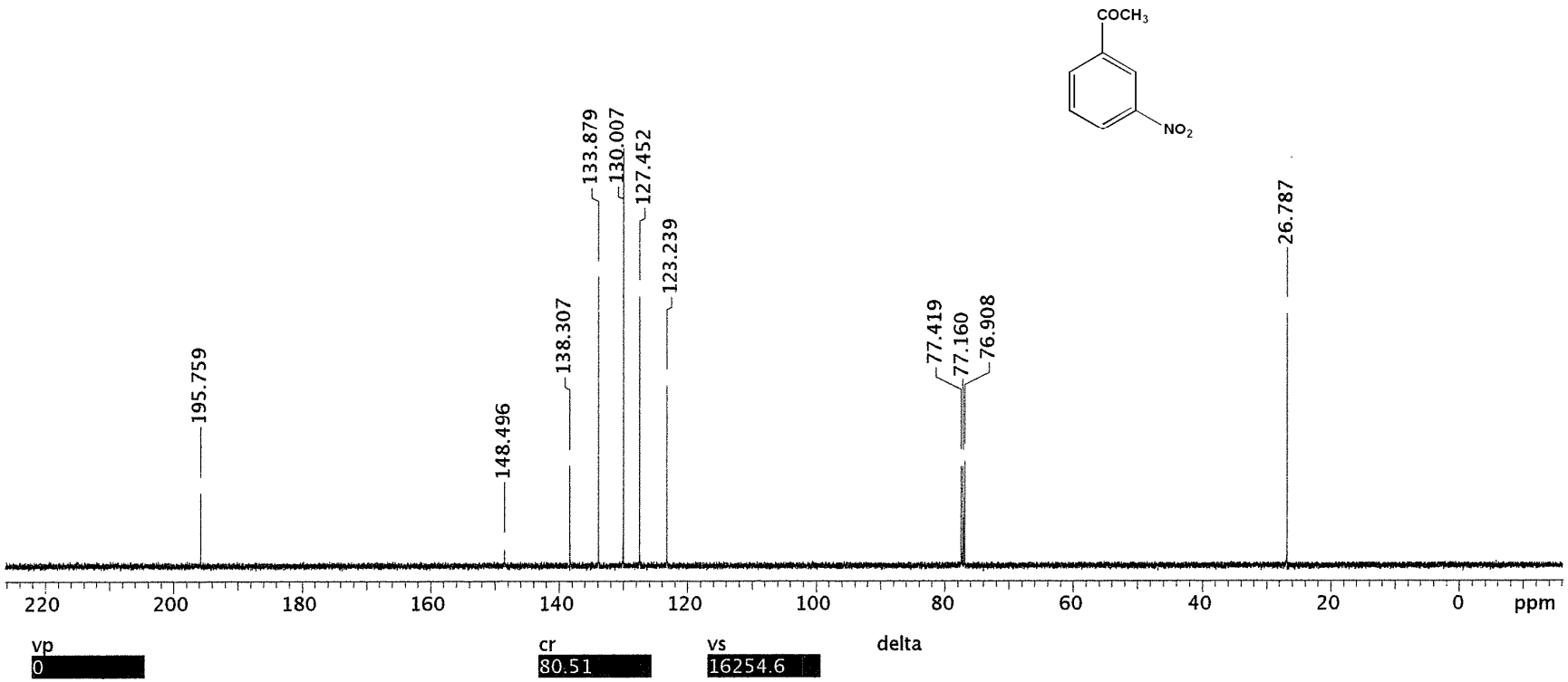

8.496
8.445
8.429
8.425
7.986
7.971
7.848
7.835
7.830
7.761
7.758
7.745
7.739
7.729
7.260
CF3
NO2
8
7
6
5
4
3
2
1
0
ppm
0.99
1.01
0.11
1.00
io
10.0
cr
8.85
is
2045.3
delta

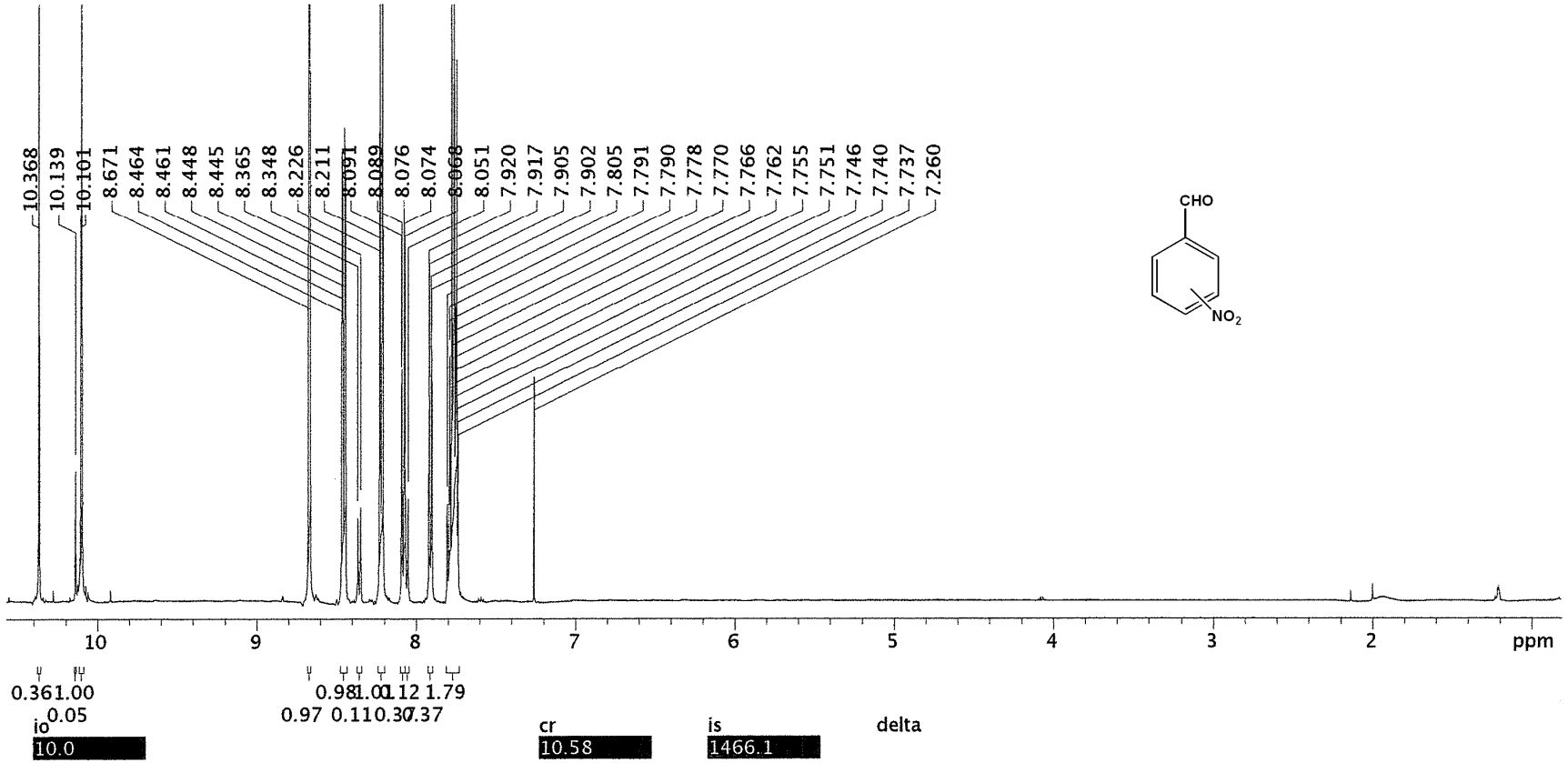

148.392
133.287
132.820
132.724
132.546
132.280
132.006
131.310
131.288
131.258
131.228
130.503
128.074
128.030
126.800
126.230
125.097
124.209
124.061
121.884
120.988
120.958
120.929
120.899
119.714
77.412
77.160
76.908
CF3
NO2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
vp
0
cr
161.42
vs
34964.9
delta

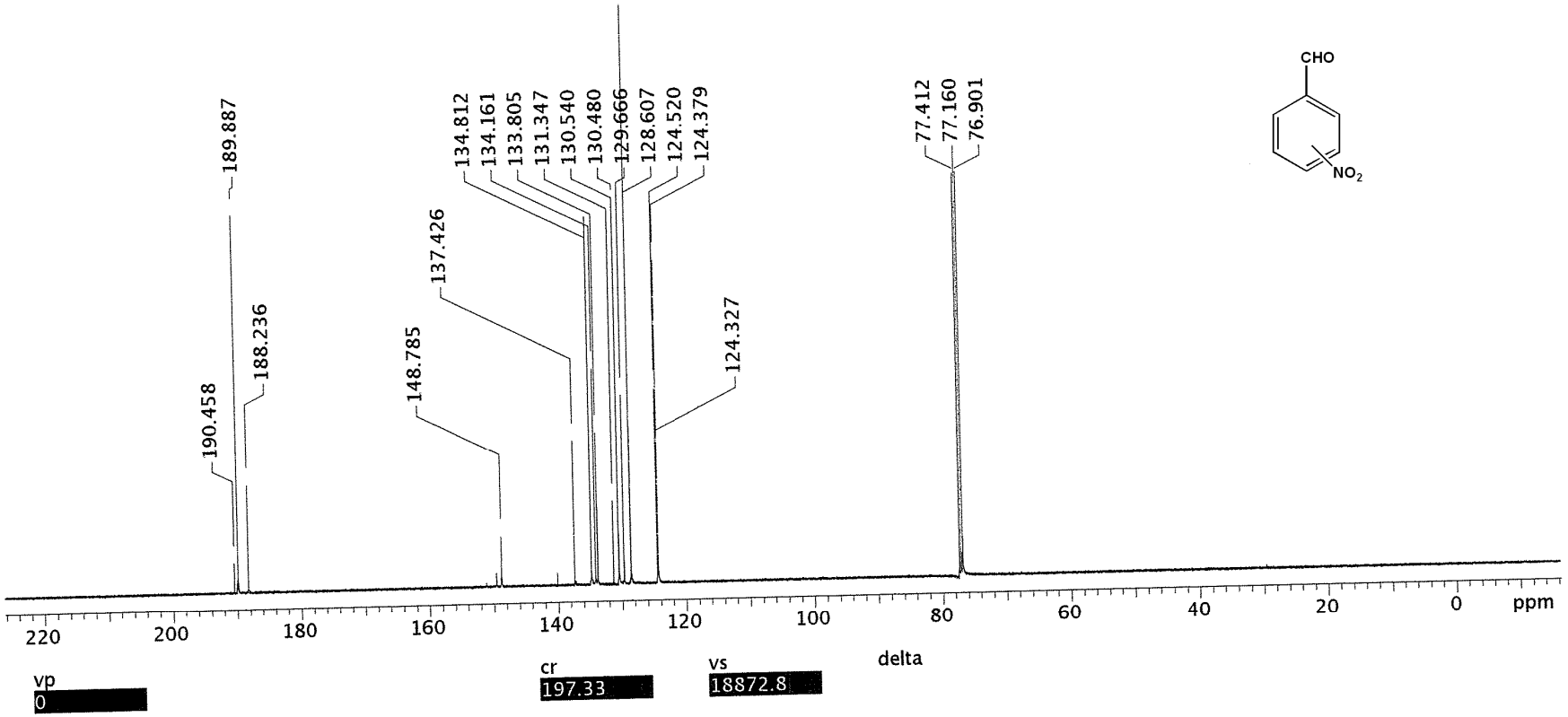

-63.032
-60.129
CF3
NO2
100
50
0
-50
-100
-150
ppm
vp
0
cr
43.14
vs
2.4
delta

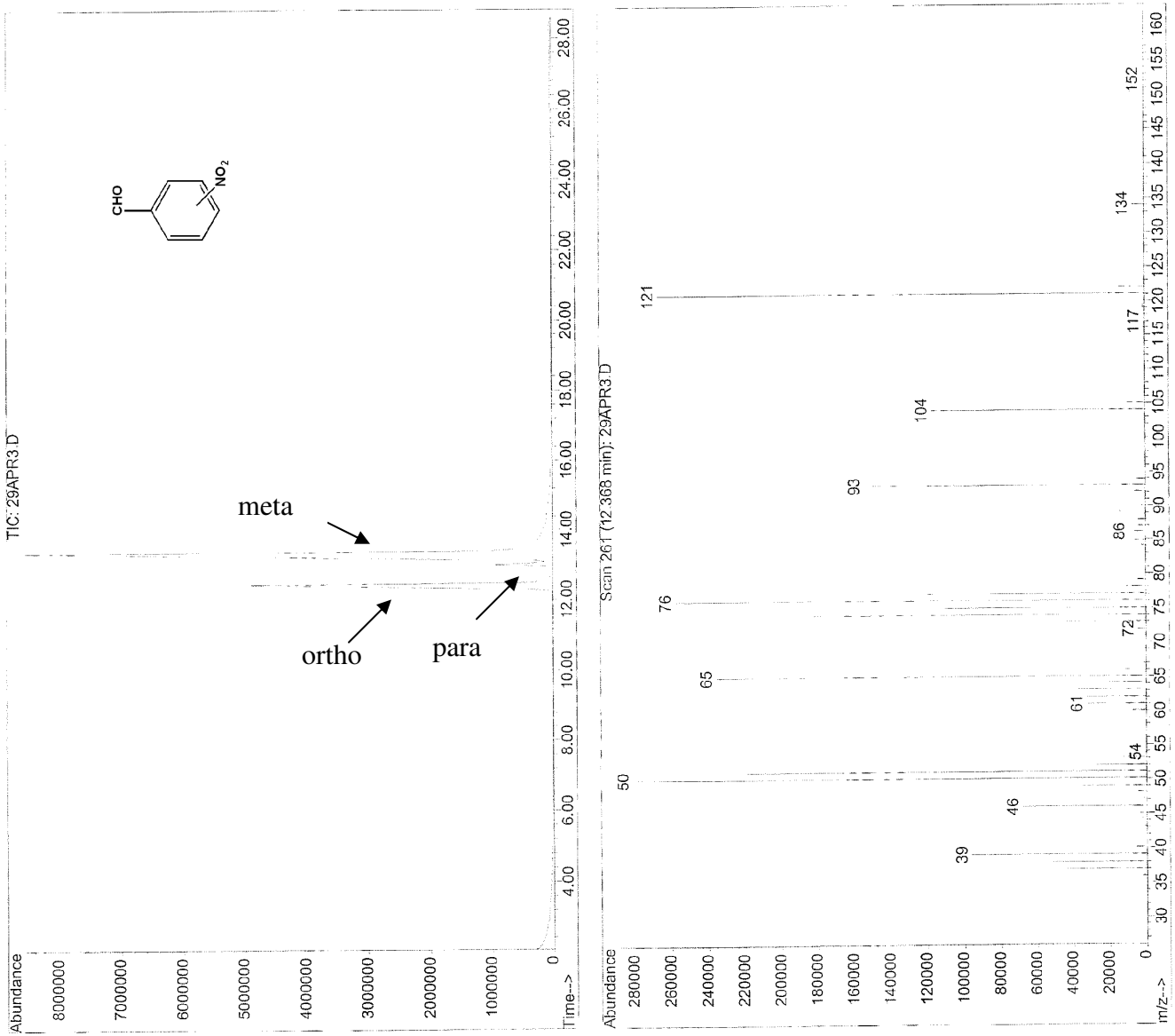

TIC: 10FEB5.D
Abundance
Time-->
meta
ortho
Acetophenone
COCH3
NO2
Scan 145 (7.765 min): 10FEB5.D
Abundance
m/z-->

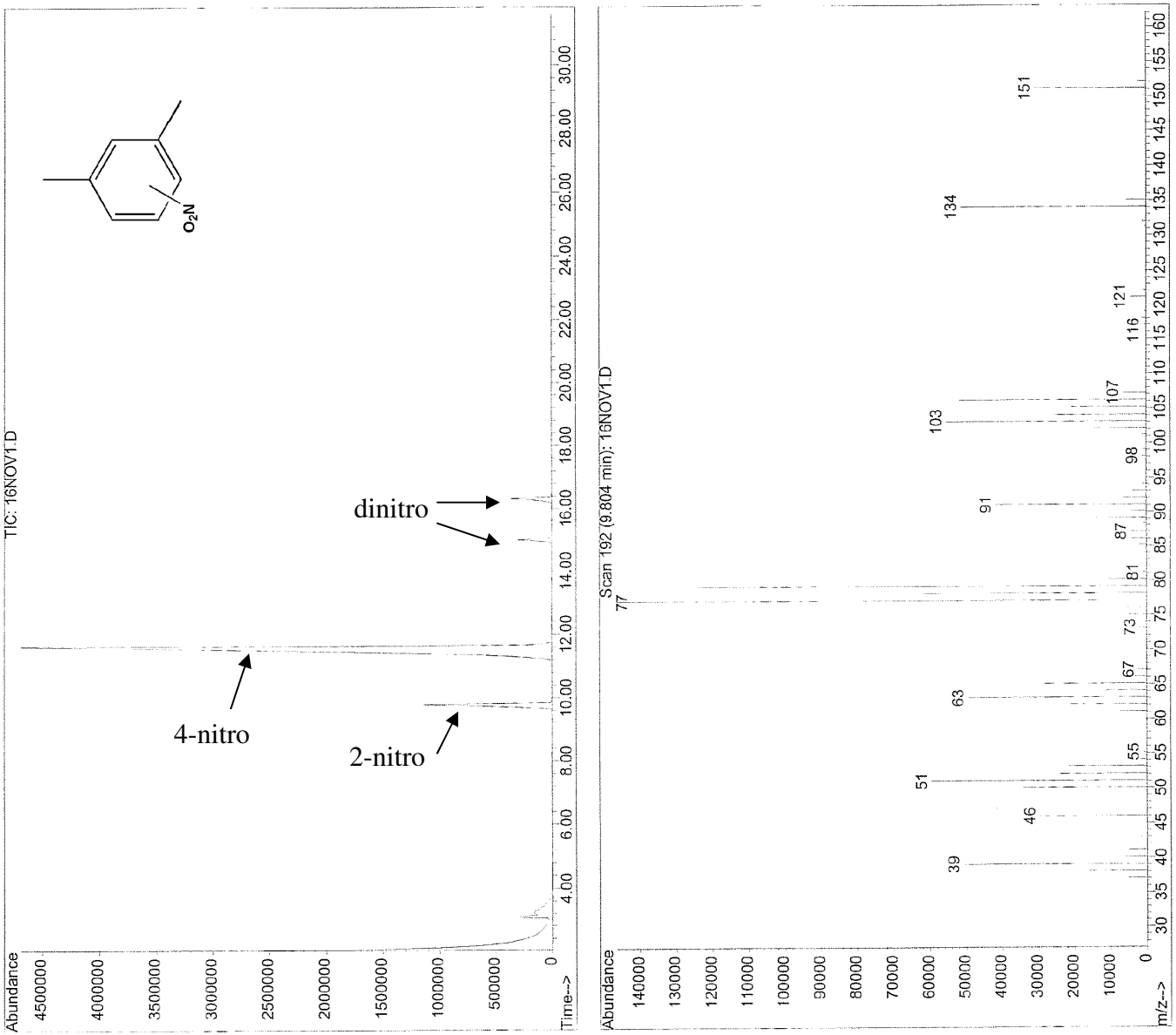

COCH3
NO2
8.726
8.722
8.719
8.393
8.391
8.389
8.377
8.375
8.372
8.272
8.270
8.267
8.257
8.254
8.252
7.687
7.671
7.655
2.667
9
8
7
6
5
4
3
2
ppm
0.85
0.88
0.95
1.00
2.66
io
10.0
cr
9.46
is
3286.6
delta

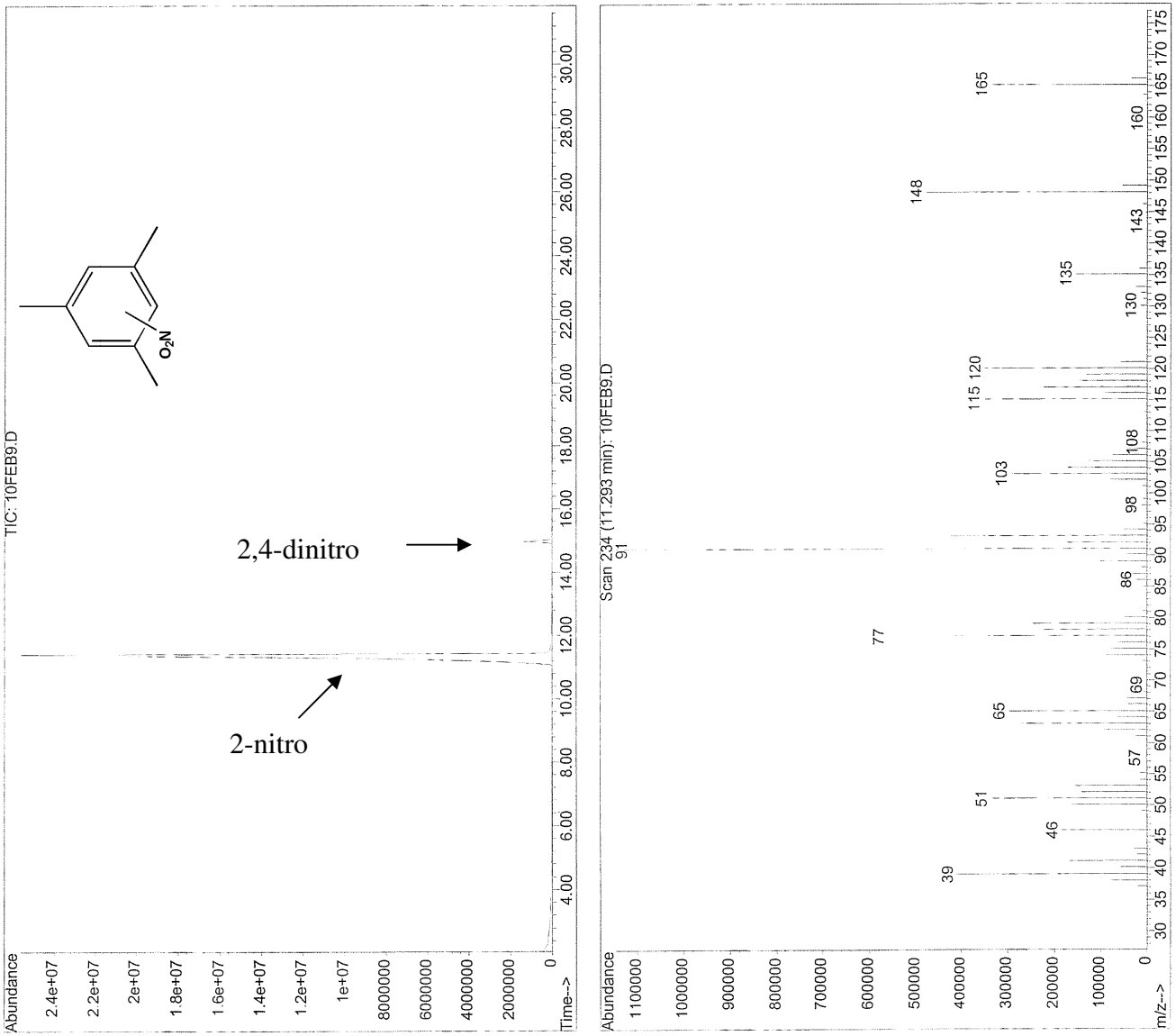

COCH3
NO2
195.759
148.496
138.307
133.879
130.007
127.452
123.239
77.419
77.160
76.908
26.787
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
80.51
vs
16254.6
delta

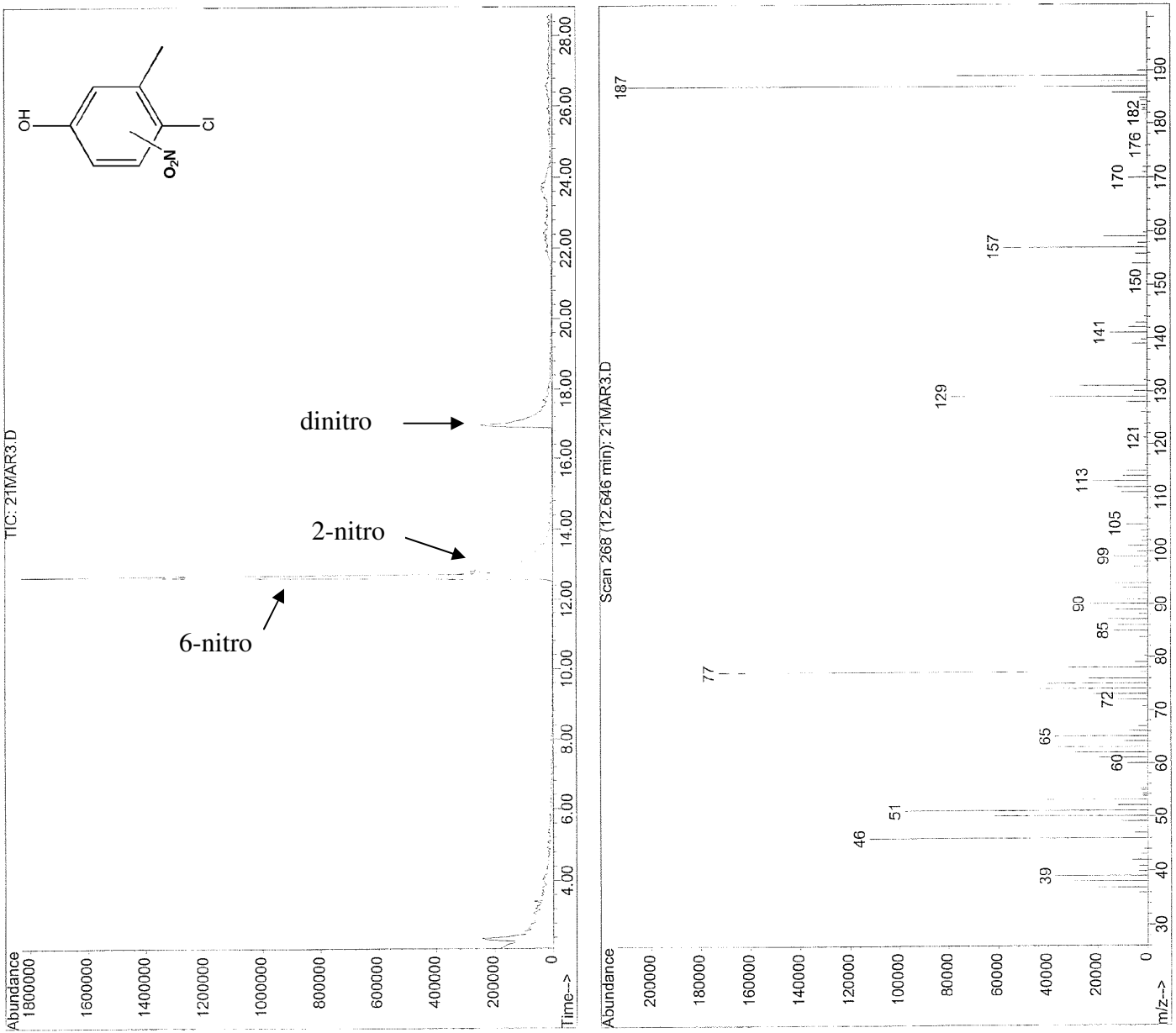

10.368
10.139
10.101
8.671
8.464
8.461
8.448
8.445
8.365
8.348
8.226
8.211
8.091
8.089
8.076
8.074
8.068
8.051
7.920
7.917
7.905
7.902
7.805
7.791
7.790
7.778
7.770
7.766
7.762
7.755
7.751
7.746
7.740
7.737
7.260
CHO
NO2
10
9
8
7
6
5
4
3
2
ppm
0.36 1.00
0.05
0.97 0.11 0.30 0.37
0.98 1.00 1.12 1.79
io
10.0
cr
10.58
is
1466.1
delta

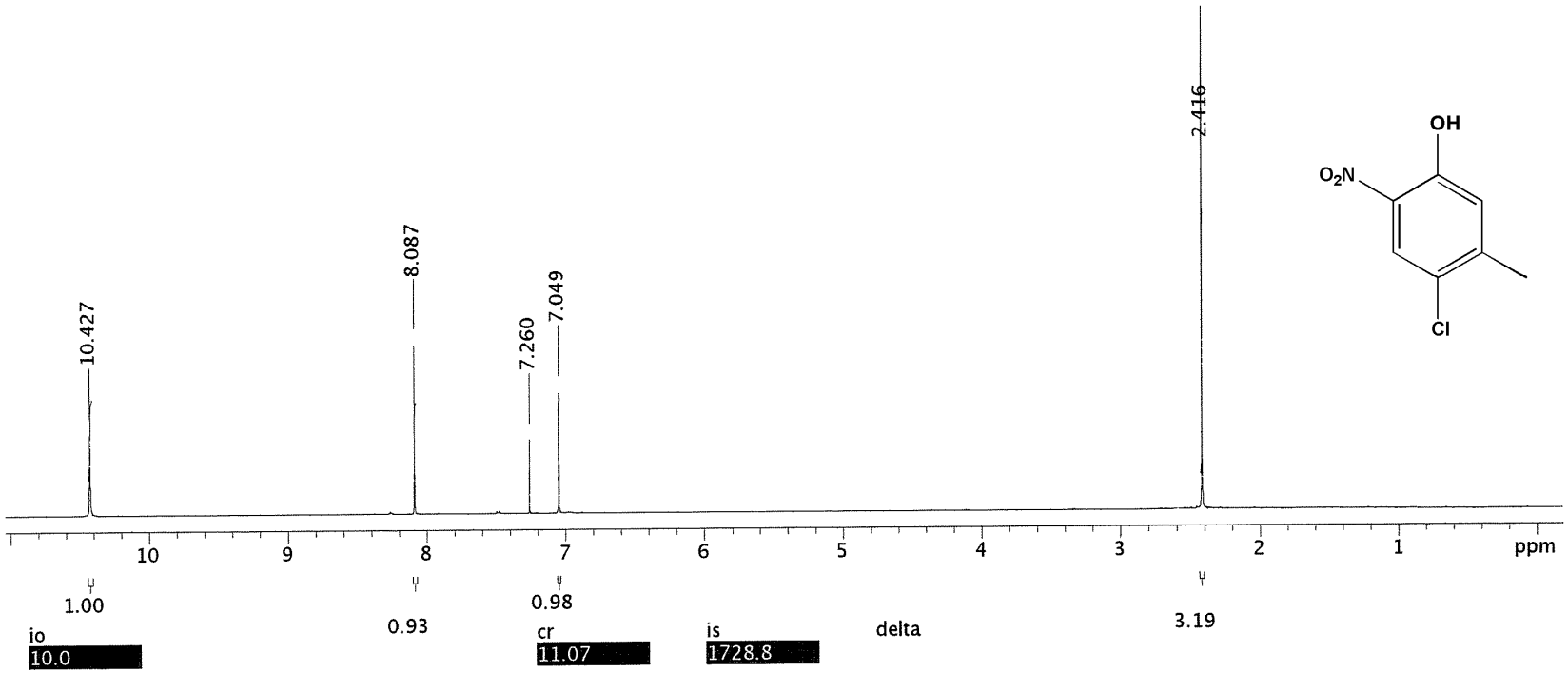

189.887
190.458
188.236
148.785
137.426
134.812
134.161
133.805
131.347
130.540
130.480
129.666
128.607
124.520
124.379
124.327
77.412
77.160
76.901
CHO
NO2
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
197.33
vs
18872.8

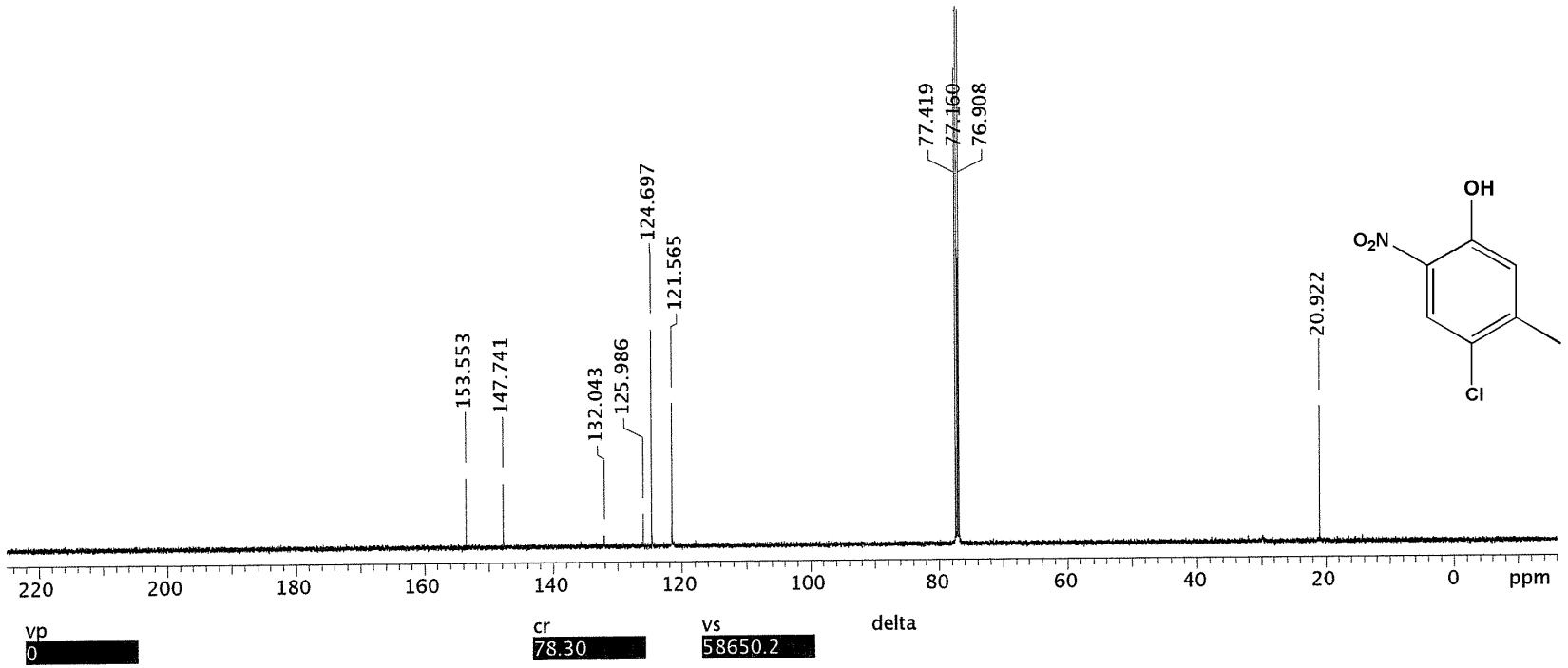

TIC: 29APR3.D
Abundance
Time-->
meta
ortho
para
CHO
NO2
Scan 261 (12.368 min): 29APR3.D
Abundance
m/z-->

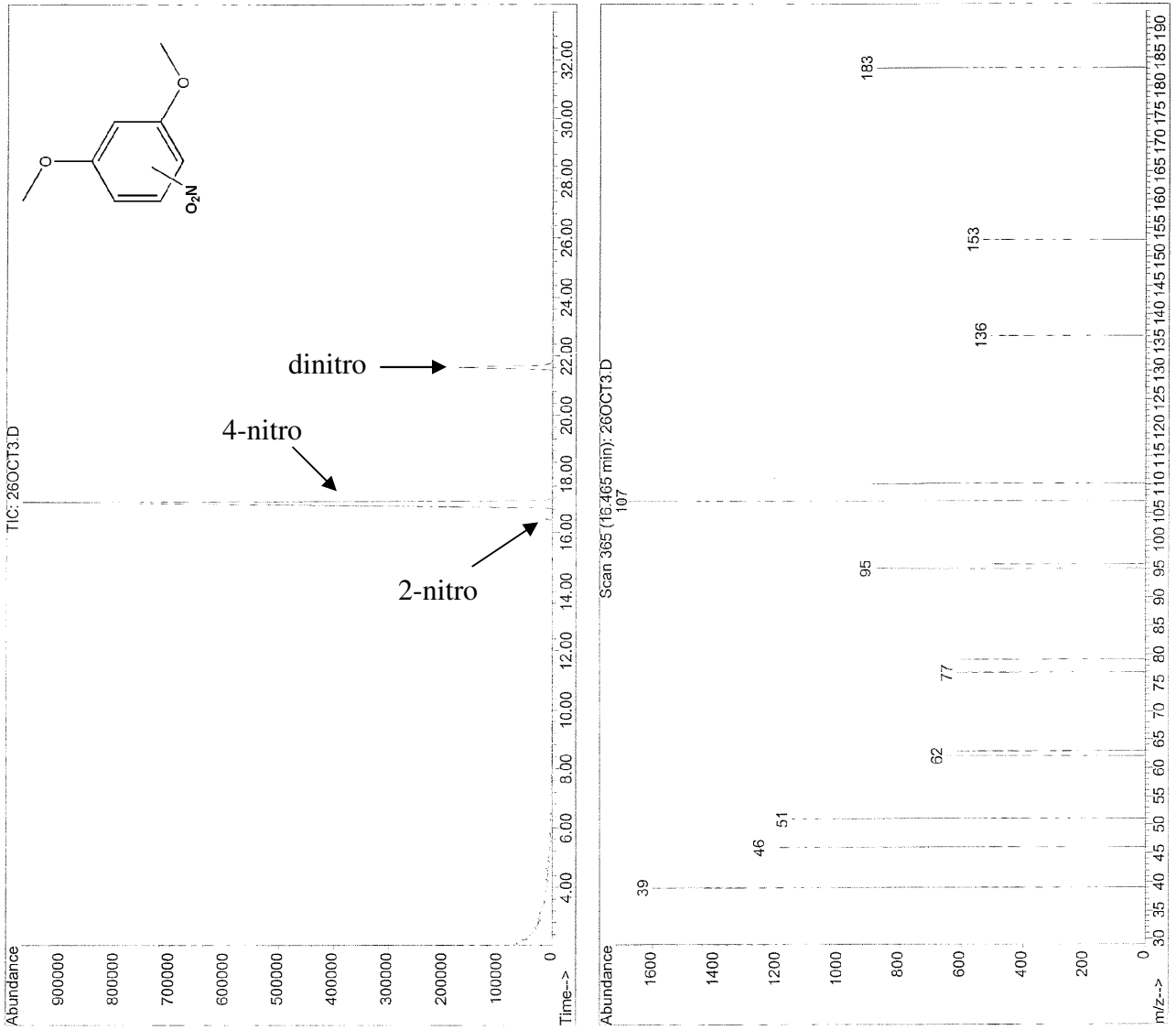

TIC: 16NOV1.D
Abundance
Time-->
4-nitro
2-nitro
dinitro
O_2N
Scan 192 (9.804 min): 16NOV1.D
Abundance
m/z-->

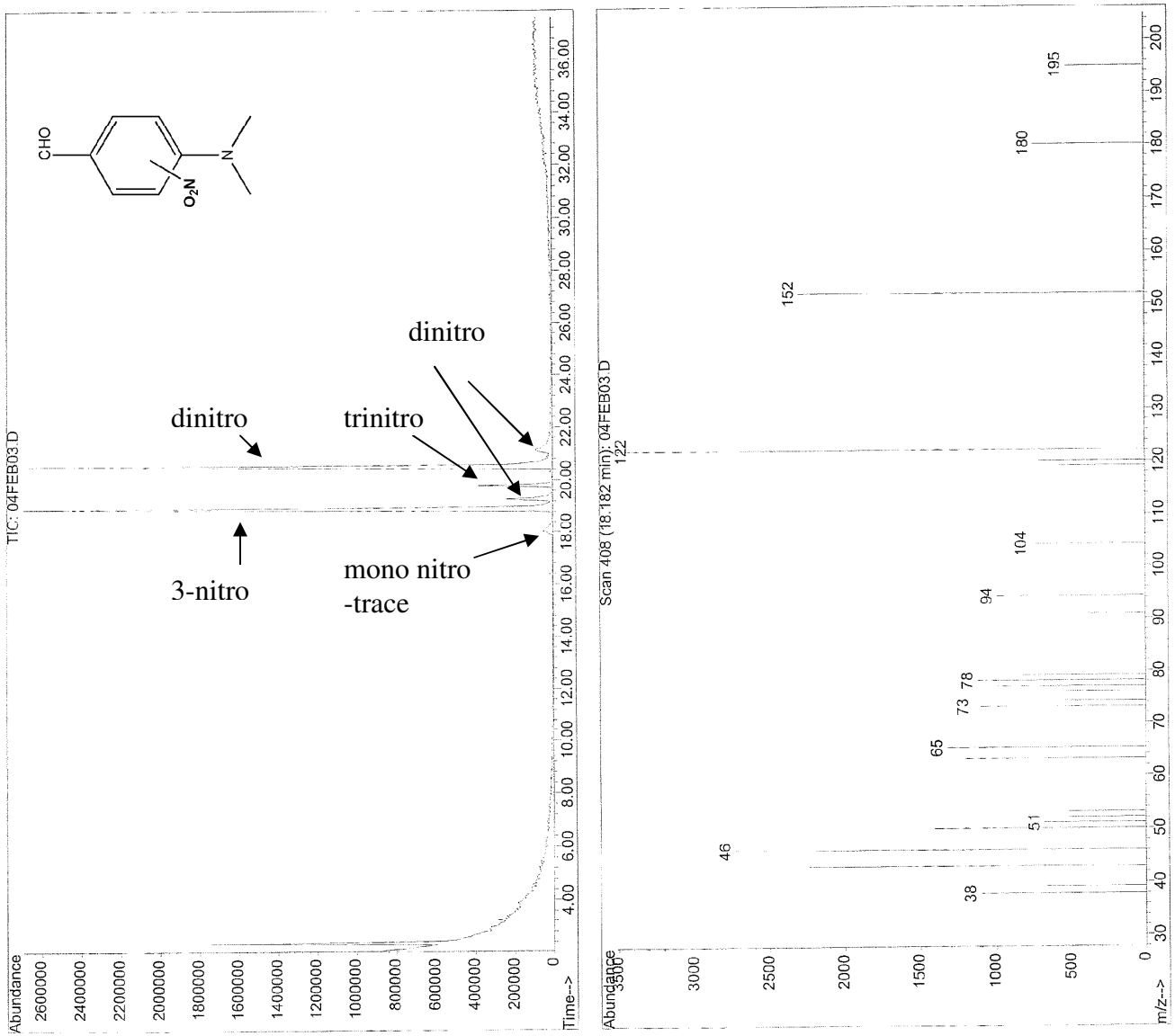

TIC: 10FEB9.D
Abundance
Time-->
2,4-dinitro
2-nitro
Scan 234 (11.293 min): 10FEB9.D
Abundance
m/z-->

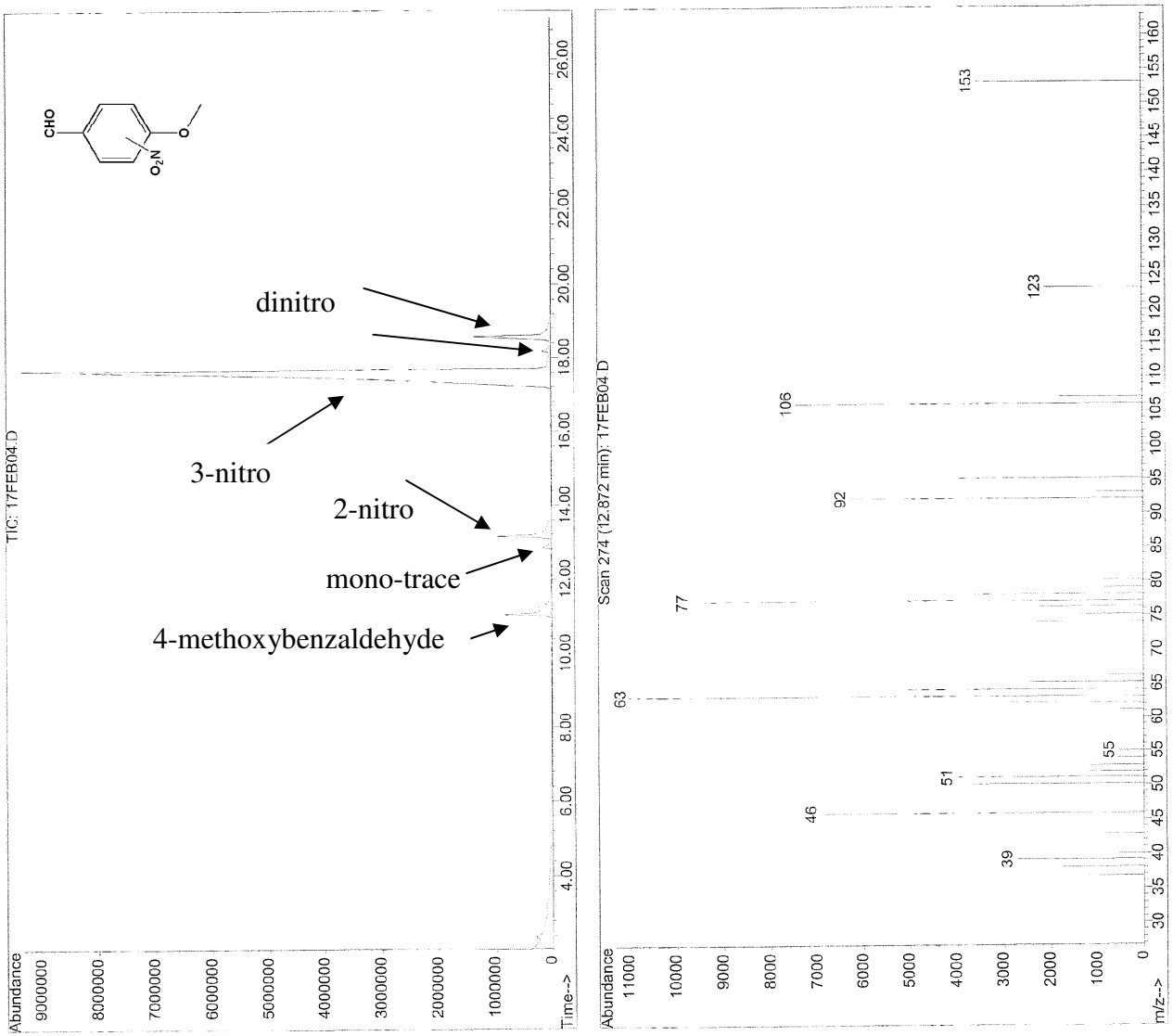

TIC: 21MAR3.D
Abundance
Time-->
dinitro
2-nitro
6-nitro
OH
Cl
O2N
Scan 268 (12.646 min): 21MAR3.D
m/z-->

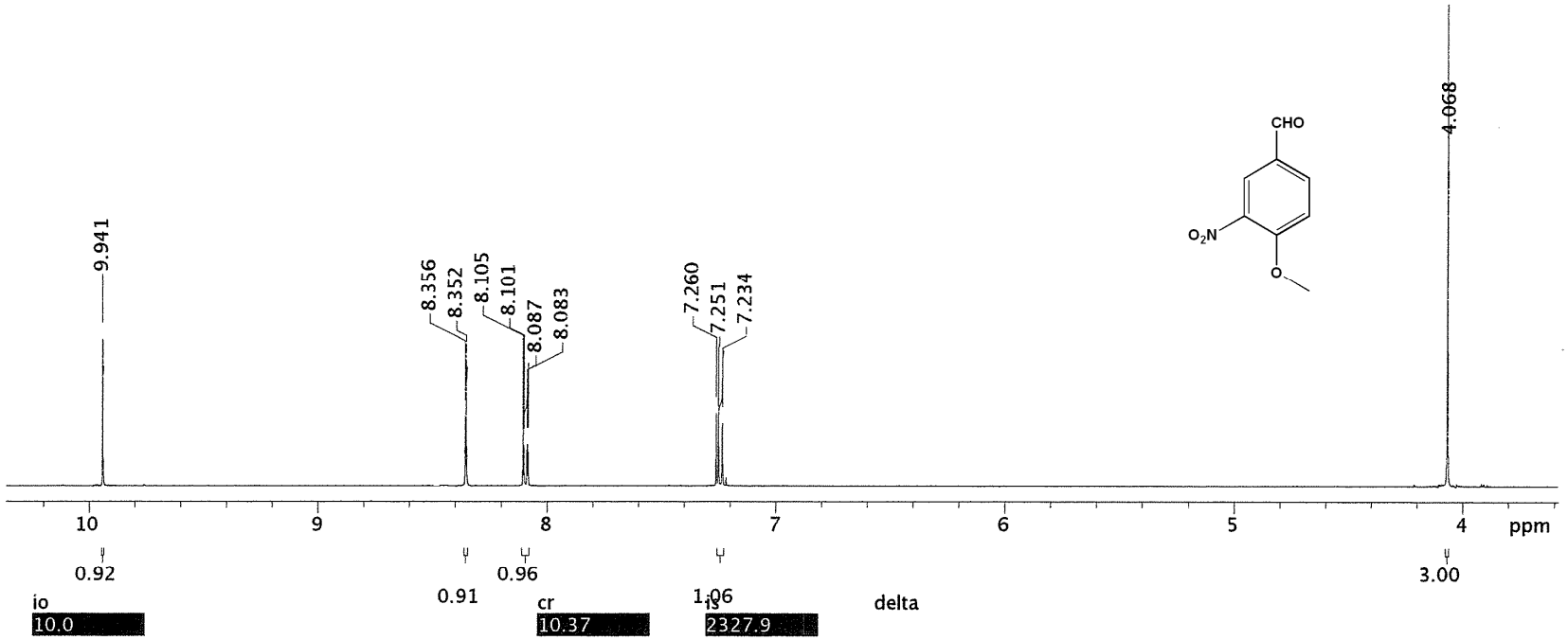

10.427
8.087
7.260
7.049
2.416
OH
O2N
Cl
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.93
0.98
3.19
io
10.0
cr
11.07
is
1728.8
delta

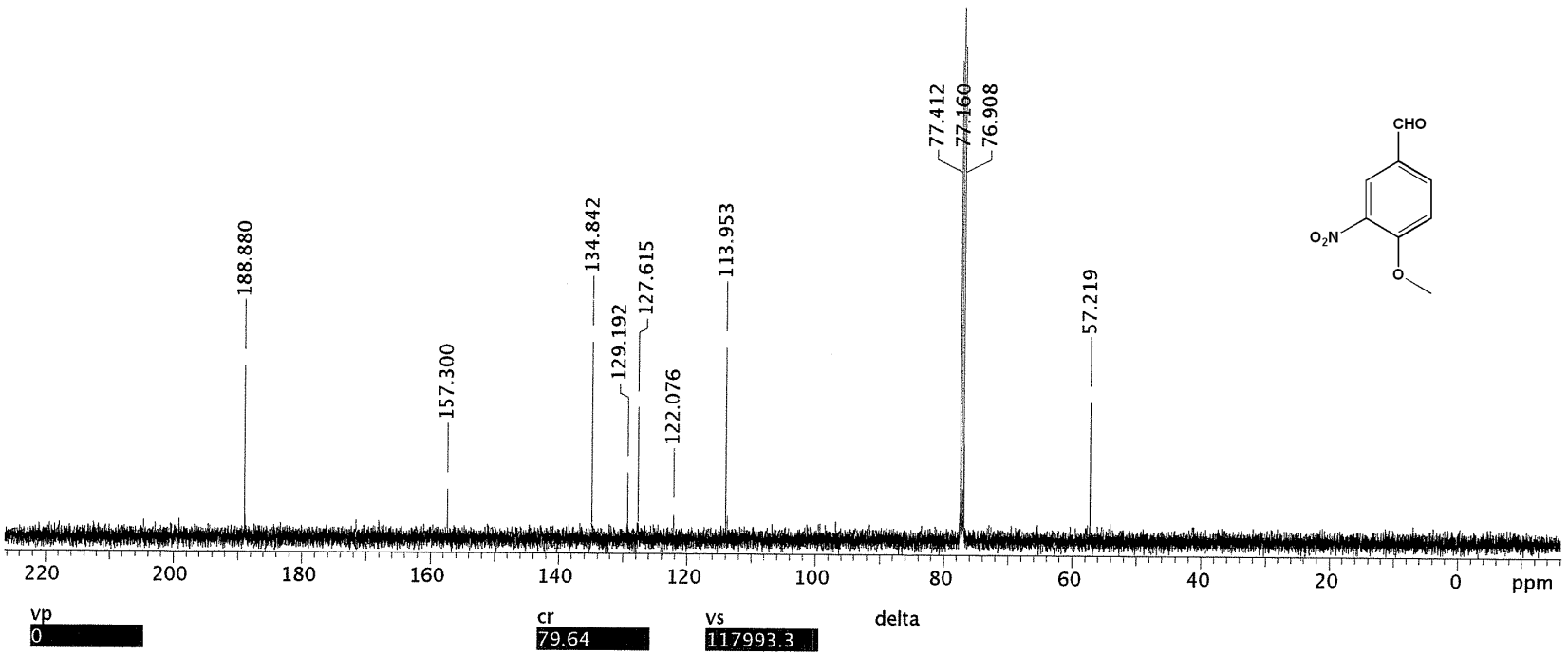

153.553
147.741
132.043
125.986
124.697
121.565
77.419
77.160
76.908
20.922
OH
O2N
Cl
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
78.30
vs
58650.2

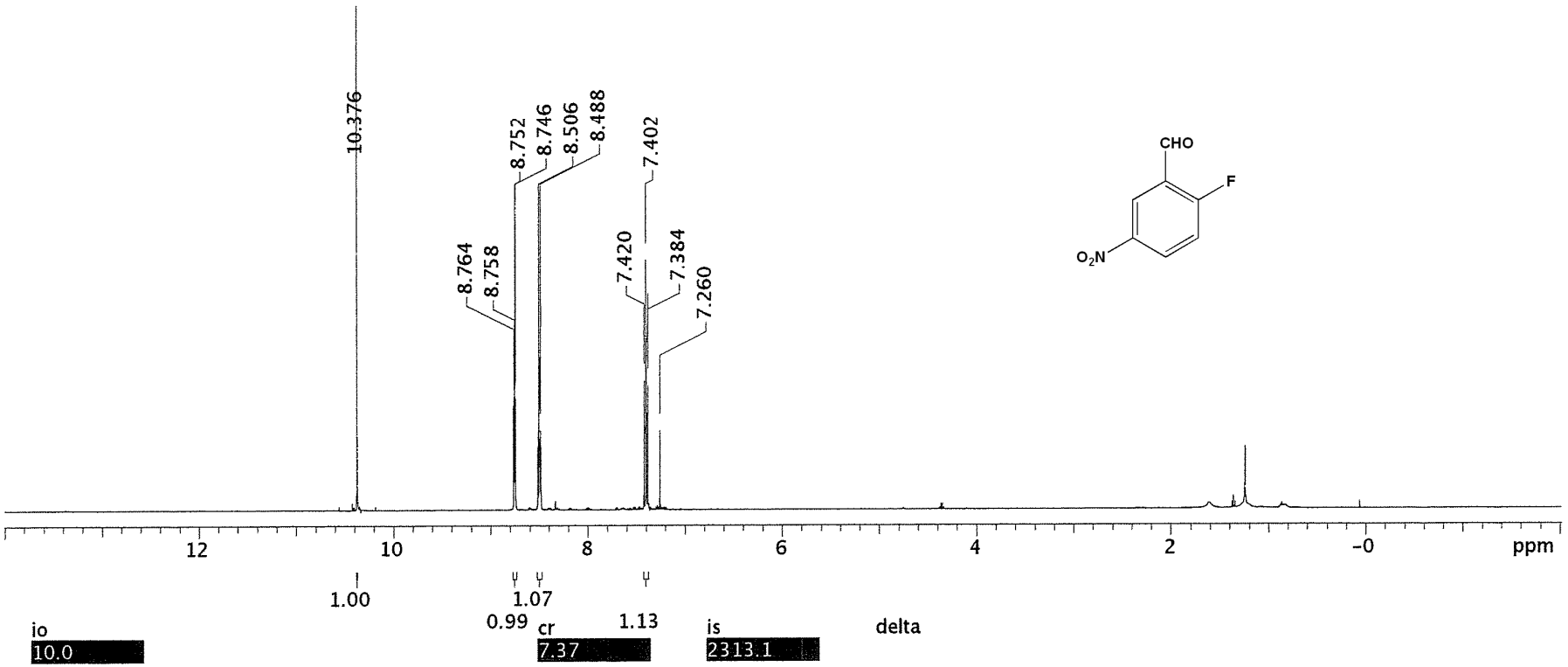

TIC: 26OCT3.D
Abundance
Time-->
dinitro
4-nitro
2-nitro
Scan 365 (16.465 min): 26OCT3.D
m/z-->

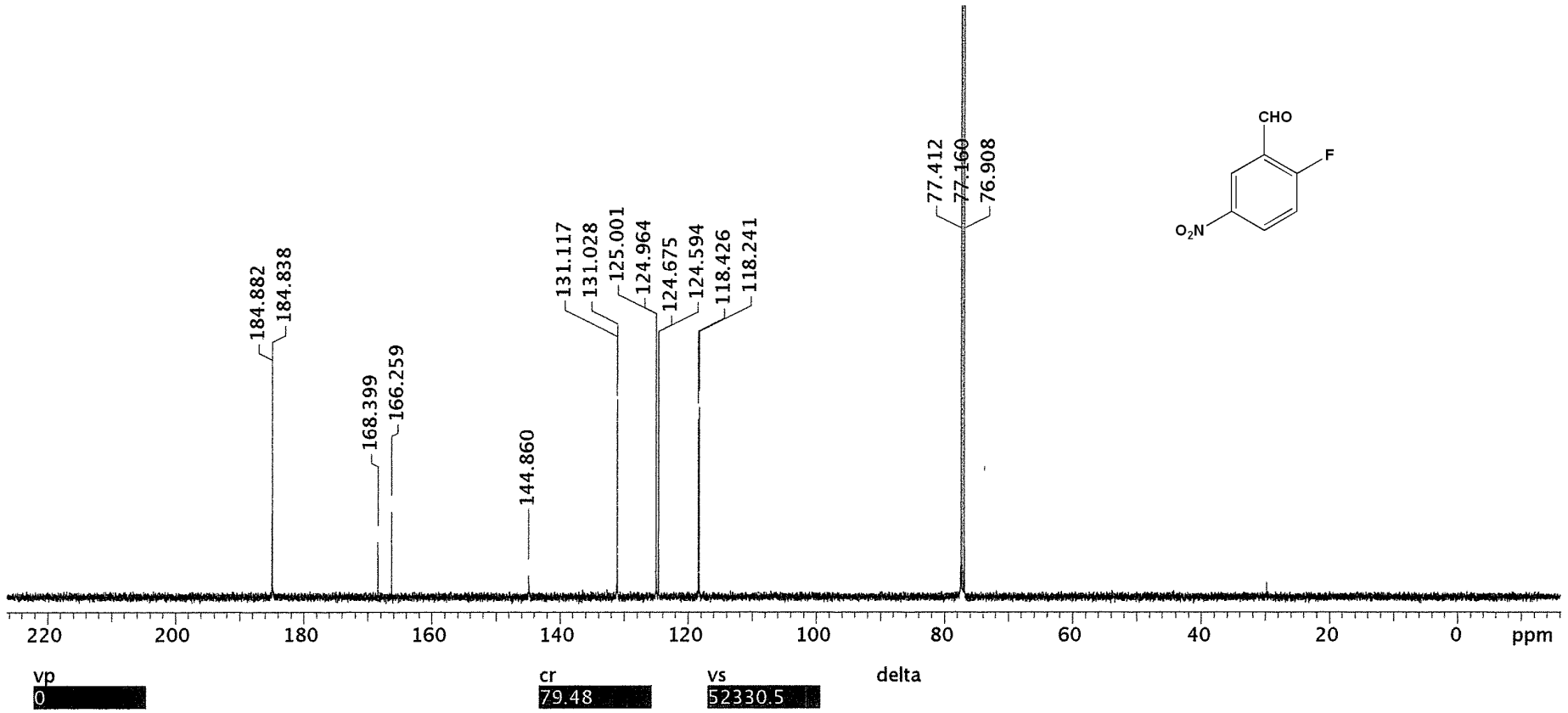

TIC: 04FEB03.D
Abundance
Time-->
dinitro
trinitro
dinitro
3-nitro
mono nitro
-trace
CHO
O2N
N
Scan 408 (18.182 min): 04FEB03.D
Abundance
m/z-->

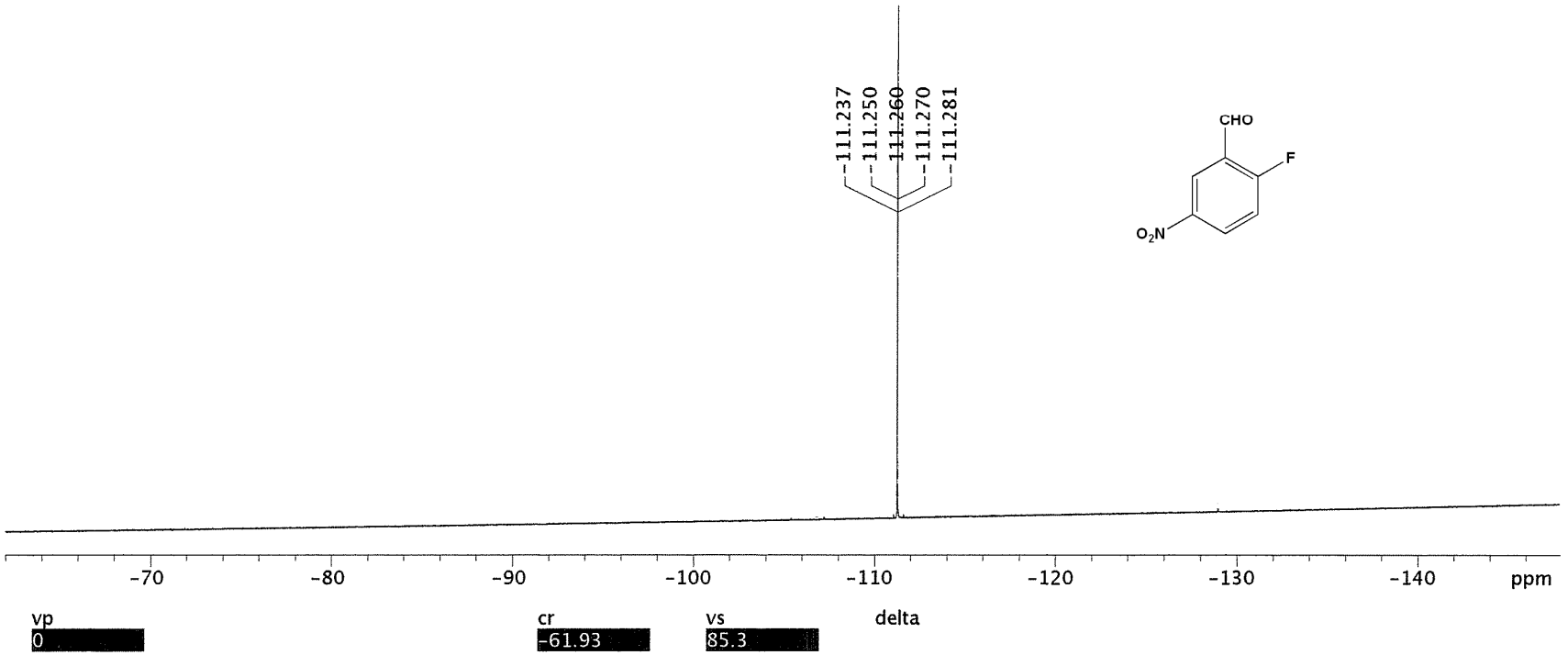

TIC: 17FEB04.D
Abundance
Time-->
dinitro
3-nitro
2-nitro
mono-trace
4-methoxybenzaldehyde
CHO
O2N
O
Scan 274 (12.872 min): 17FEB04.D
m/z-->

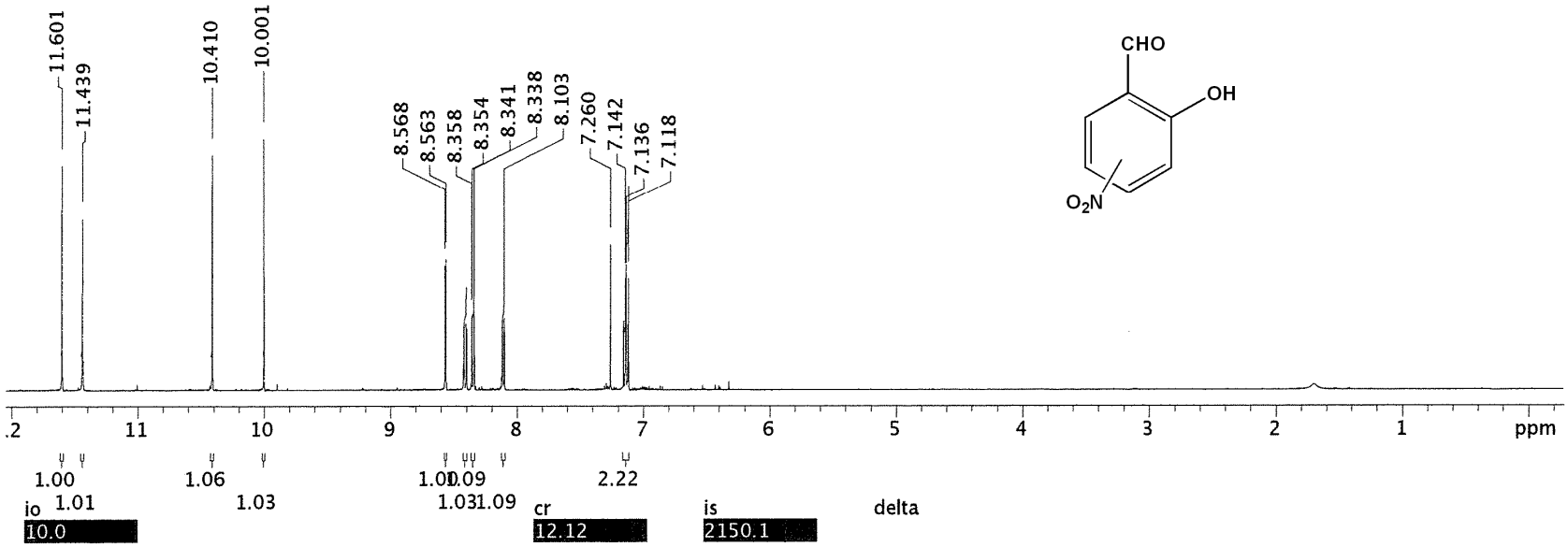

9.941
8.356
8.352
8.105
8.101
8.087
8.083
7.260
7.251
7.234
4.068
CHO
O2N
O
10
9
8
7
6
5
4
ppm
0.92
0.91
0.96
1.06
3.00
io
10.0
cr
10.37
is
2327.9
delta

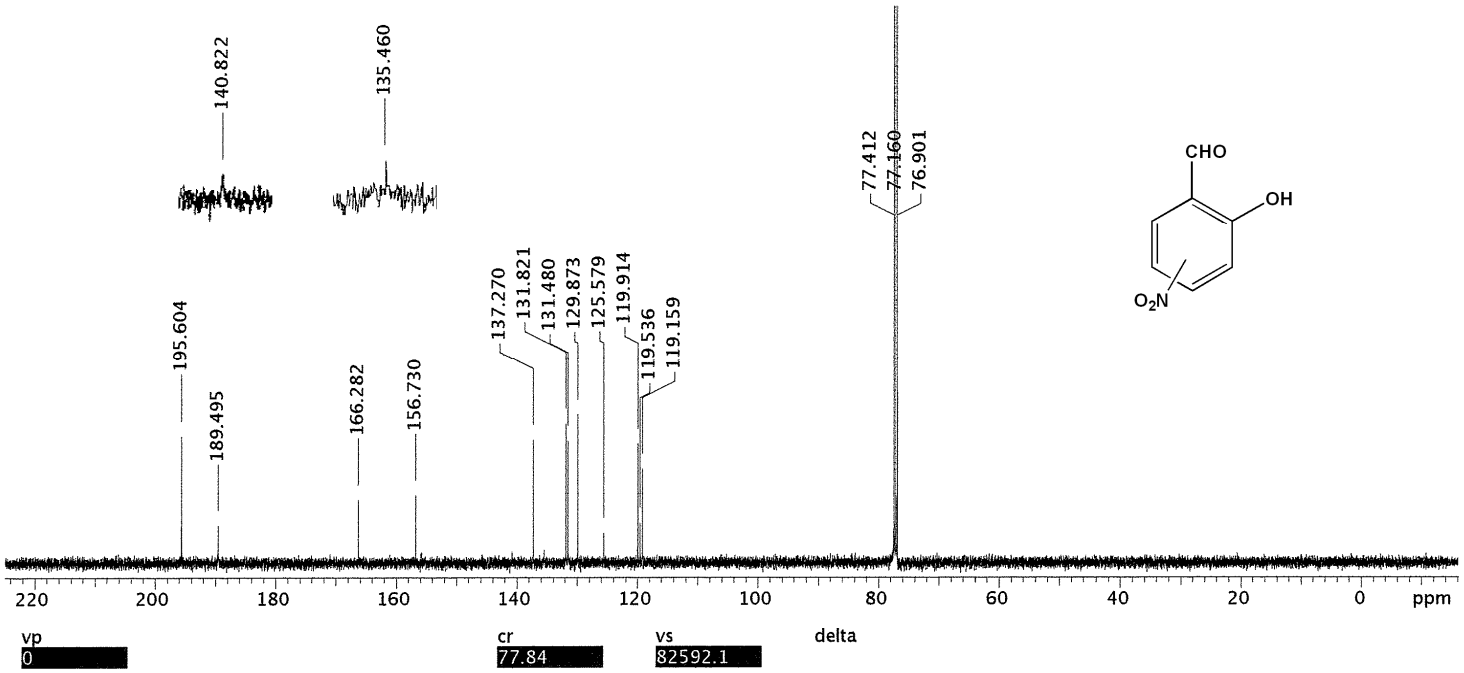

188.880
157.300
134.842
129.192
127.615
122.076
113.953
77.412
77.160
76.908
57.219
CHO
O2N
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
79.64
vs
117993.3
delta

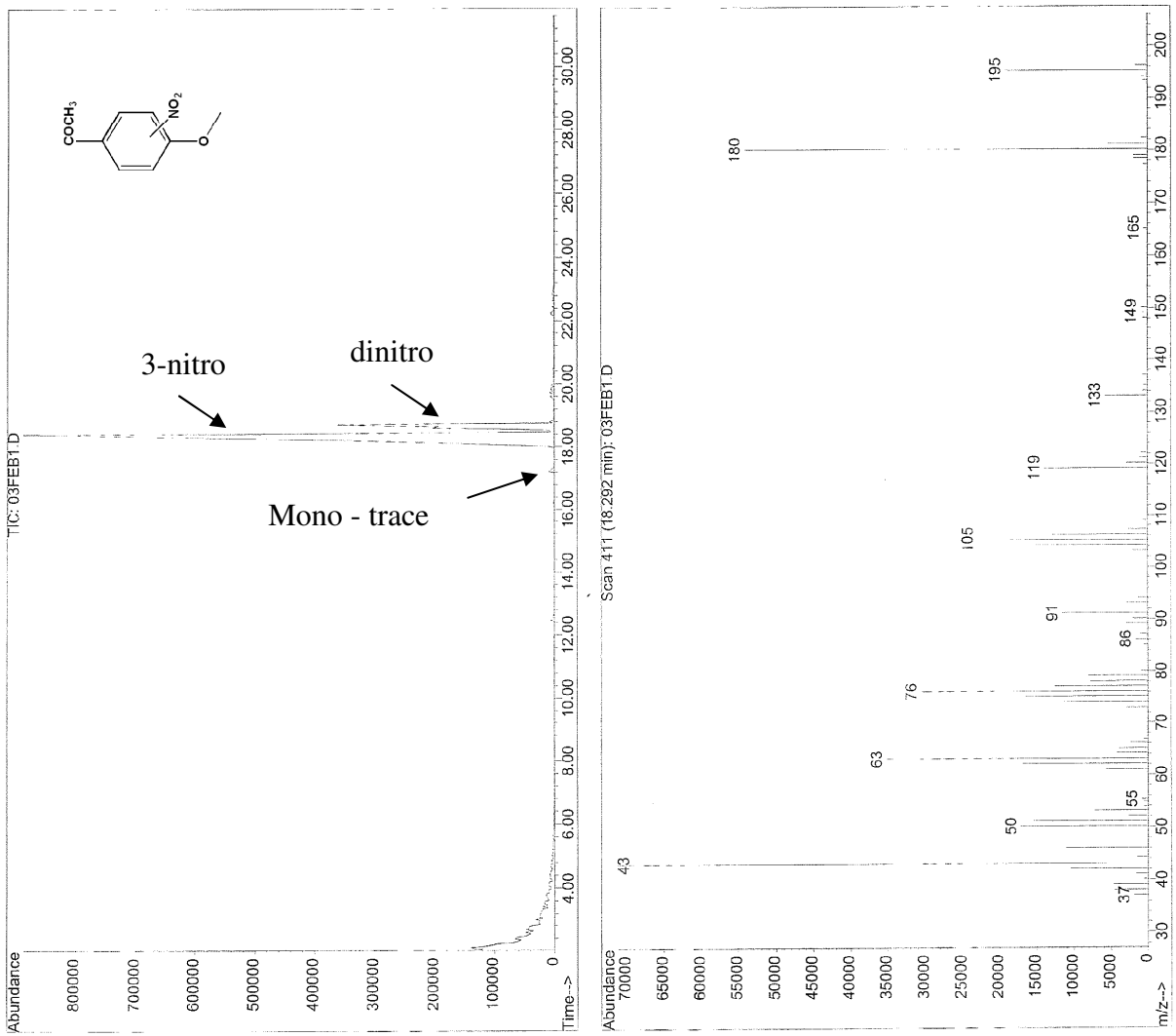

10.376
8.764
8.758
8.752
8.746
8.506
8.488
7.420
7.402
7.384
7.260
CHO
F
O2N
12
10
8
6
4
2
-0
ppm
1.00
1.07
0.99
1.13
io
10.0
cr
7.37
is
2313.1
delta

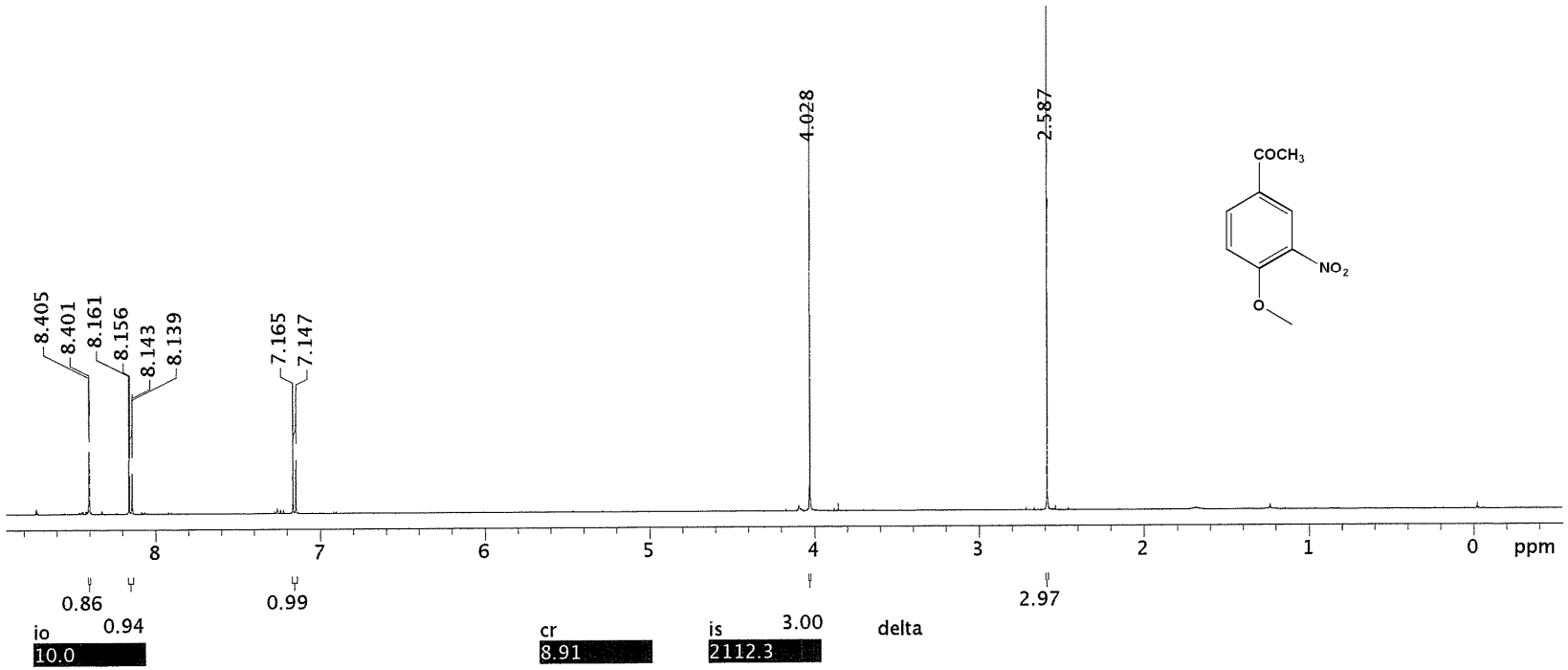

184.882
184.838
168.399
166.259
144.860
131.117
131.028
125.001
124.964
124.675
124.594
118.426
118.241
77.412
77.160
76.908
CHO
F
O2N
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
79.48
vs
52330.5
delta

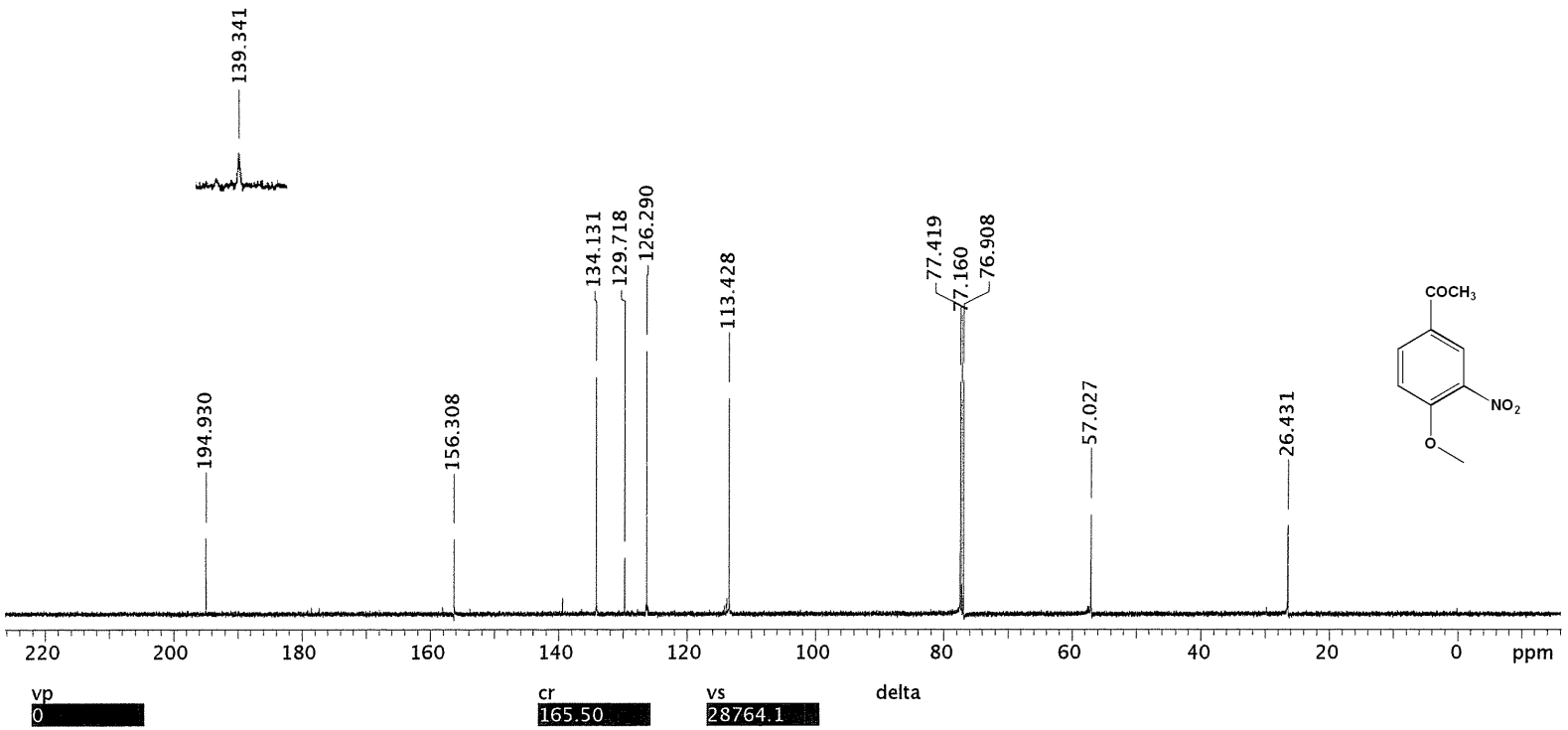

-111.237
-111.250
-111.260
-111.270
-111.281
CHO
F
O2N
-70
-80
-90
-100
-110
-120
-130
-140
ppm
vp
0
cr
-61.93
vs
85.3
delta

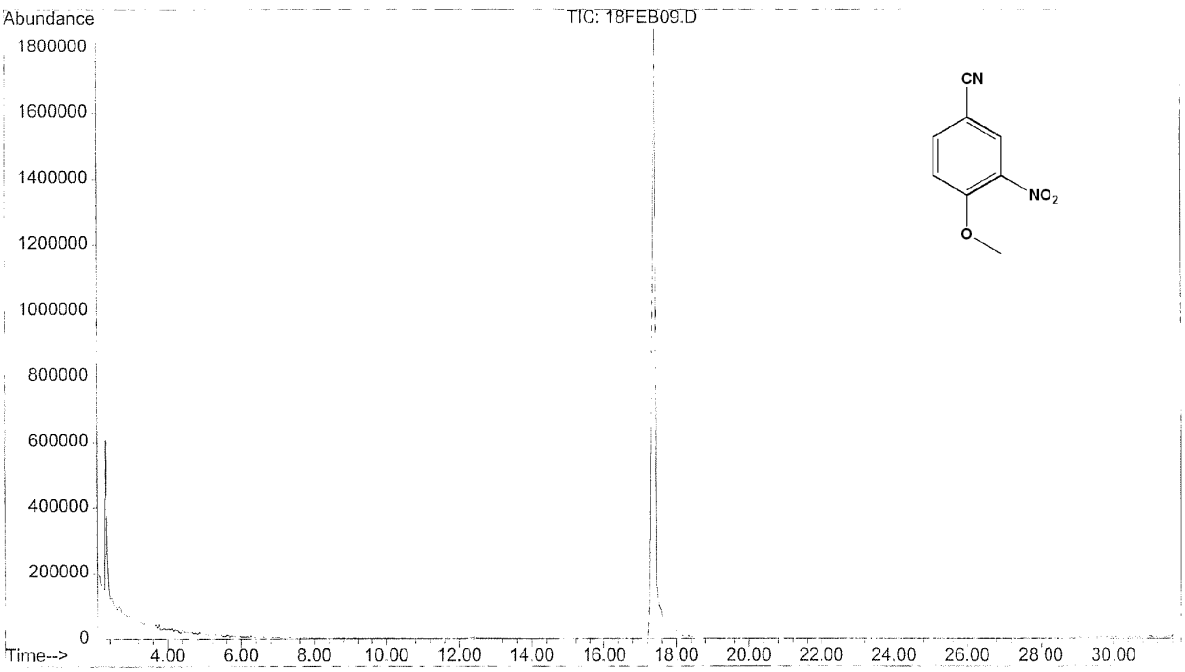

11.601
11.439
10.410
10.001
8.568
8.563
8.358
8.354
8.341
8.338
8.103
7.260
7.142
7.136
7.118
CHO
OH
O2N
ppm
1.00
1.01
1.06
1.03
1.03
1.09
2.22
io
10.0
cr
12.12
is
2150.1
delta

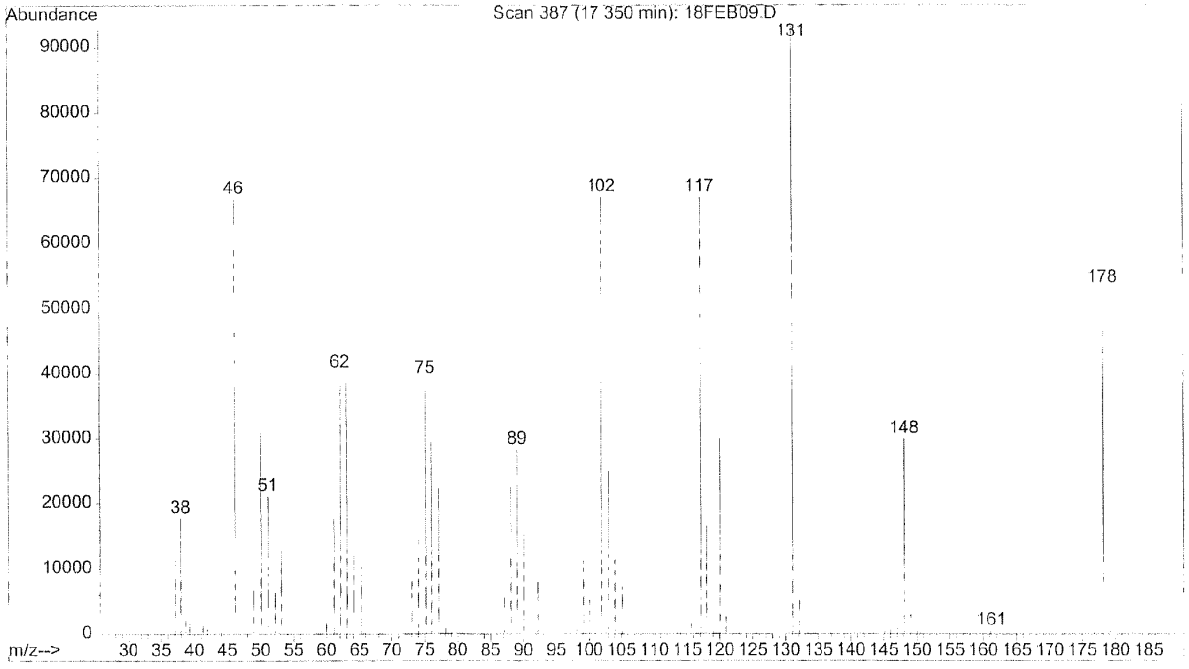

140.822
135.460
77.412
77.160
76.901
195.604
189.495
166.282
156.730
137.270
131.821
131.480
129.873
125.579
119.914
119.536
119.159
CHO
OH
O2N
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
77.84
vs
82592.1
delta

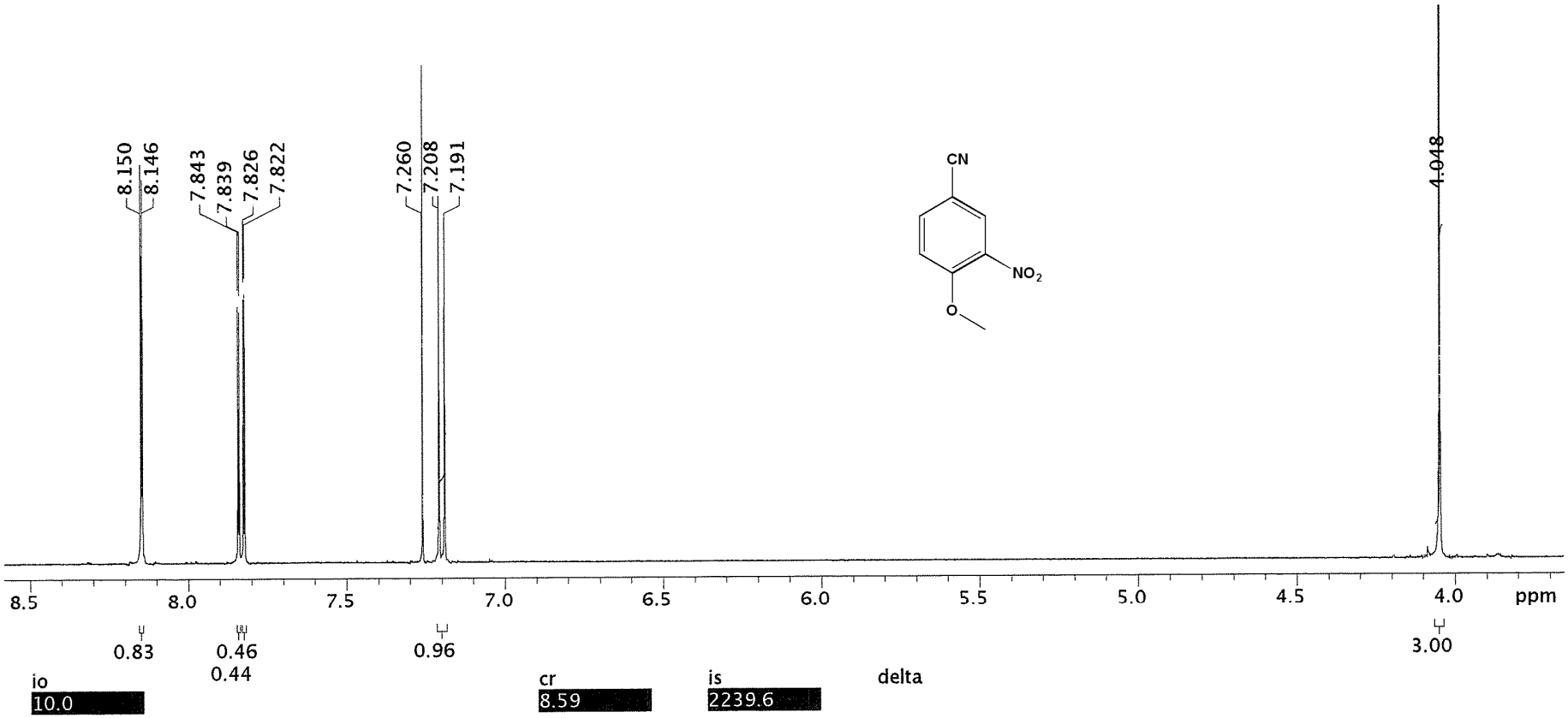

TIC: 03FEB1.D
Abundance
Time-->
3-nitro
dinitro
Mono - trace
Scan 411 (18.292 min): 03FEB1.D
Abundance
m/z-->

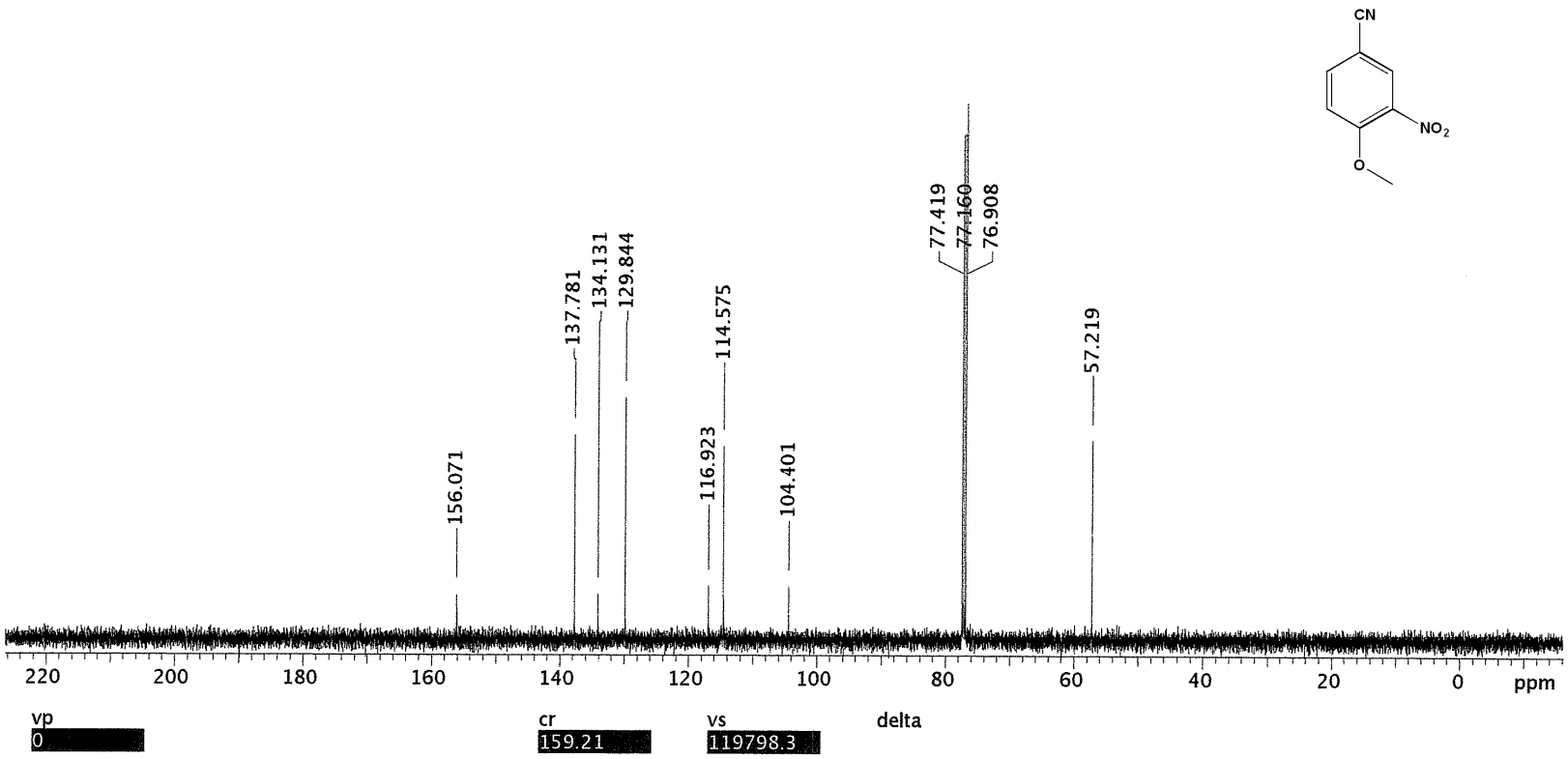

8.405
8.401
8.161
8.156
8.143
8.139
7.165
7.147
4.028
2.587
COCH3
NO2
O
8
7
6
5
4
3
2
1
0
ppm
0.86
0.94
0.99
3.00
2.97
io
10.0
cr
8.91
is
2112.3
delta

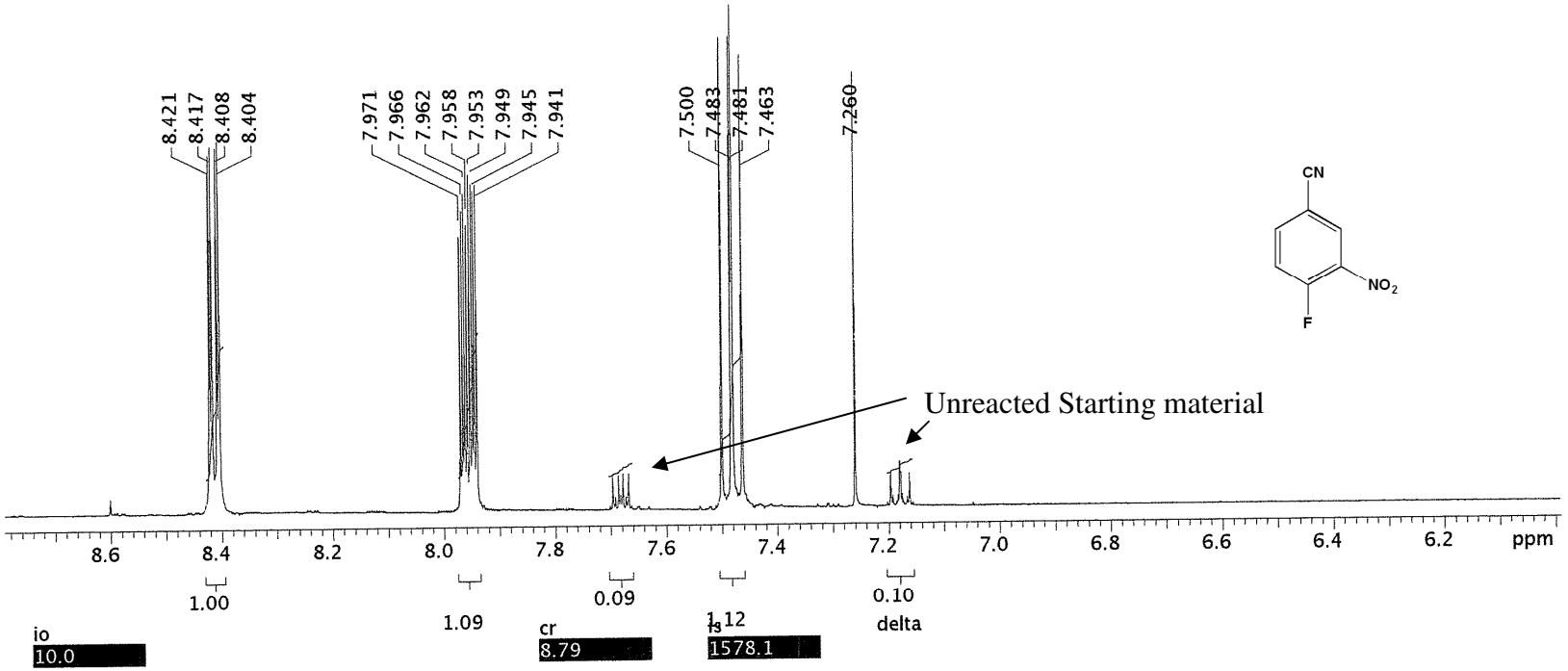

139.341
194.930
156.308
134.131
129.718
126.290
113.428
77.419
77.160
76.908
57.027
26.431
COCH3
NO2
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
165.50
vs
28764.1
delta

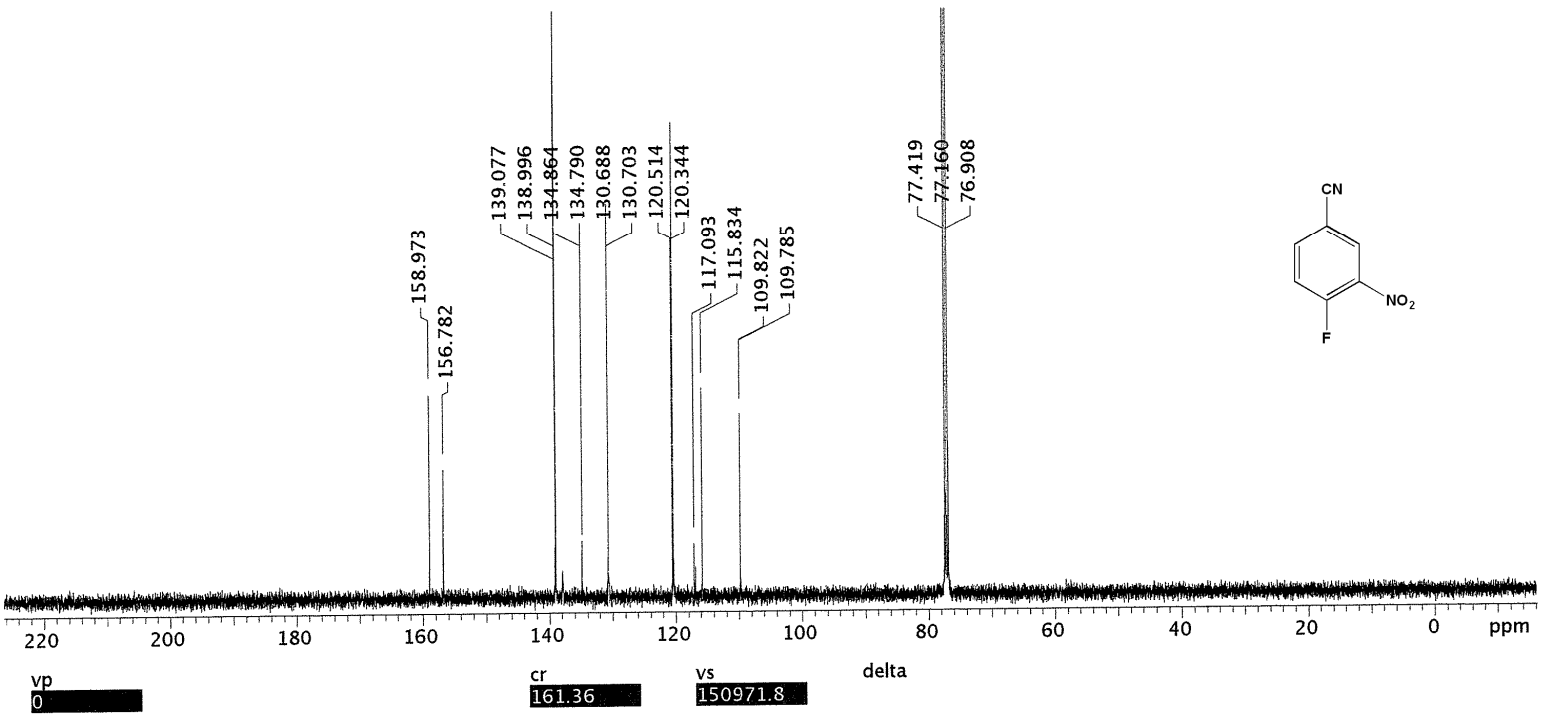

Abundance
TIC: 18FEB09.D
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
30.00
CN
NO2
O

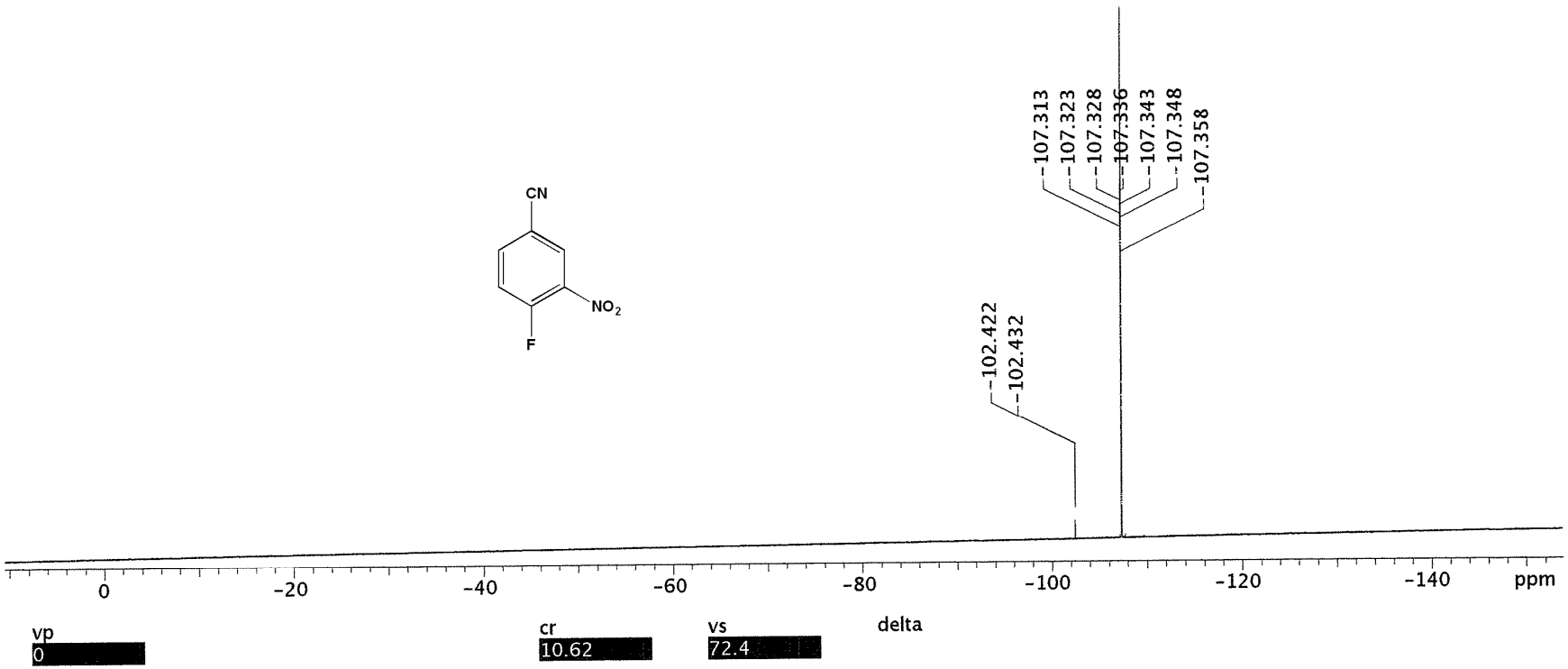

Abundance
Scan 387 (17.350 min): 18FEB09.D
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
m/z-->
30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 170 175 180 185
38
46
51
62
75
89
102
117
131
148
161
178

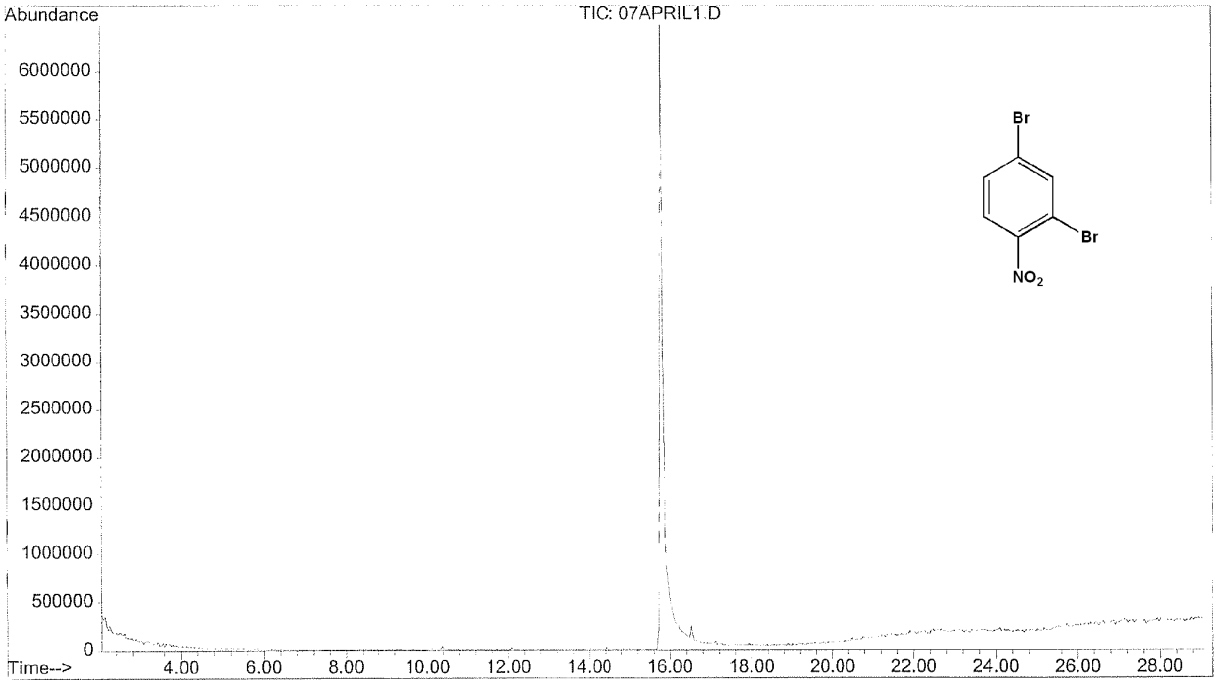

8.150
8.146
7.843
7.839
7.826
7.822
7.260
7.208
7.191
4.048
CN
NO2
O
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
0.83
0.46
0.44
0.96
3.00
io
10.0
cr
8.59
is
2239.6
delta

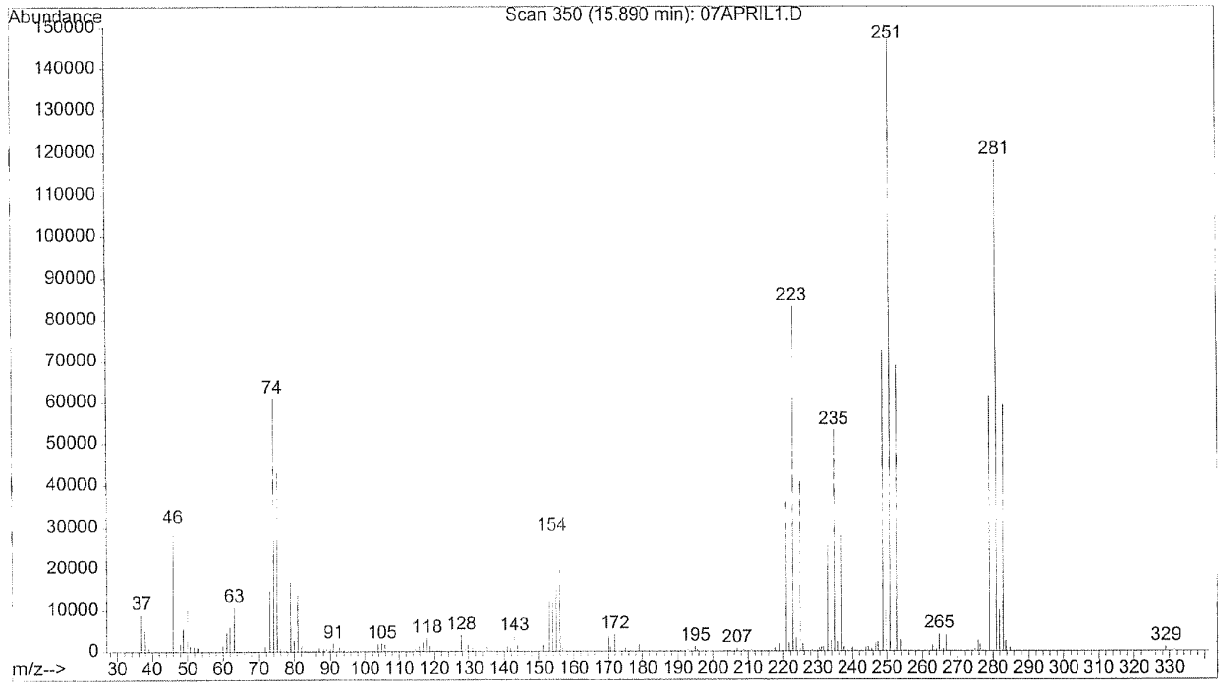

CN
NO2
O
156.071
137.781
134.131
129.844
116.923
114.575
104.401
77.419
77.160
76.908
57.219
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
159.21
vs
119798.3
delta

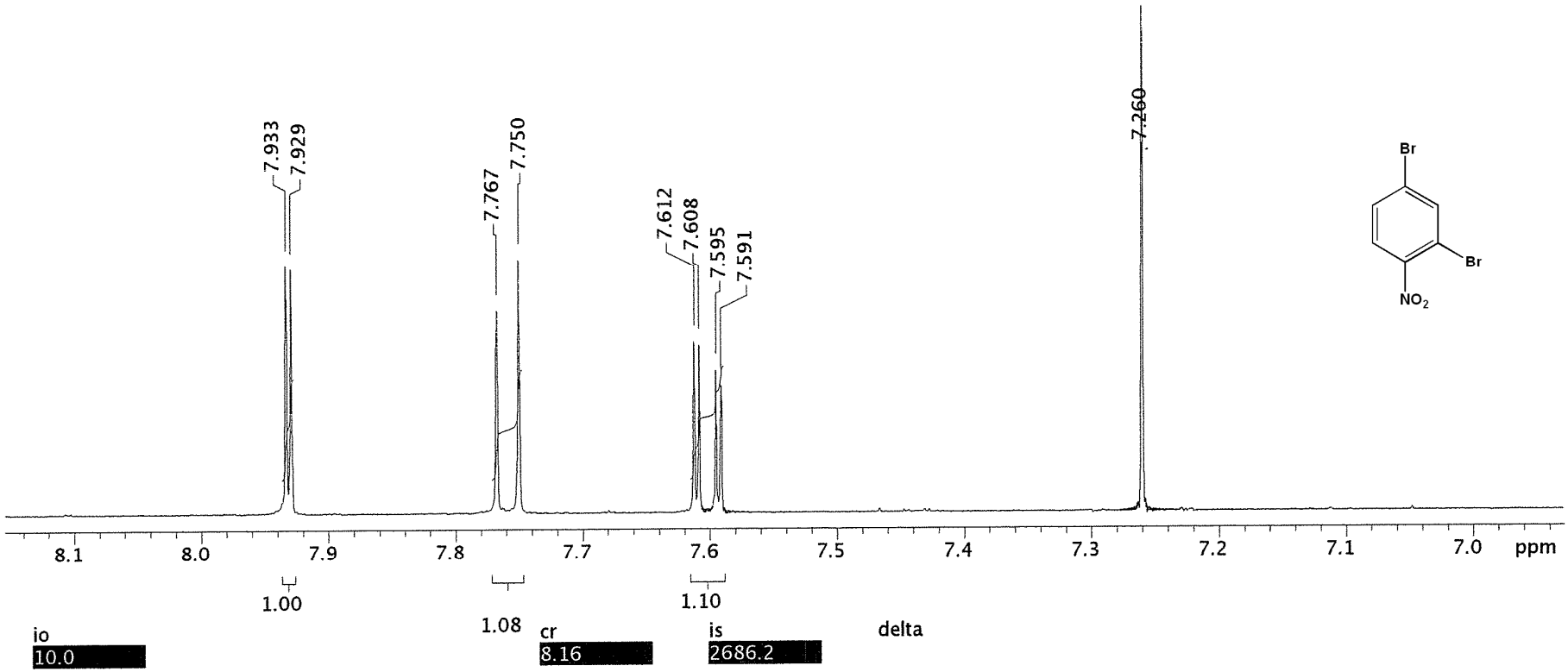

8.421
8.417
8.408
8.404
7.971
7.966
7.962
7.958
7.953
7.949
7.945
7.941
7.500
7.483
7.481
7.463
7.260
CN
NO2
F
Unreacted Starting material
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
ppm
1.00
1.09
0.09
1.12
0.10
delta
io
10.0
cr
8.79
1578.1

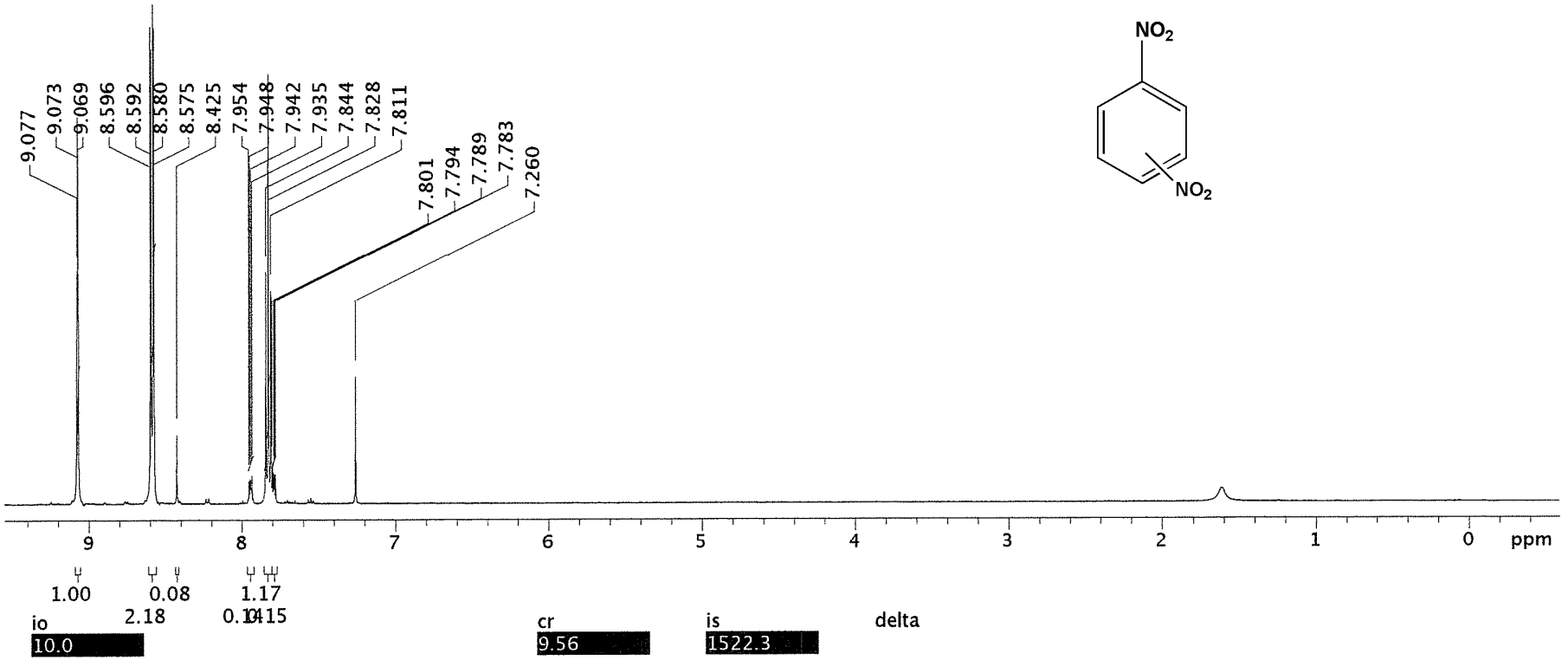

158.973
156.782
139.077
138.996
134.864
134.790
130.688
130.703
120.514
120.344
117.093
115.834
109.822
109.785
77.419
77.160
76.908
CN
NO2
F
220
200
180
160
140
120
100
80
60
40
20
0
ppm
delta
vp
0
cr
161.36
vs
150971.8

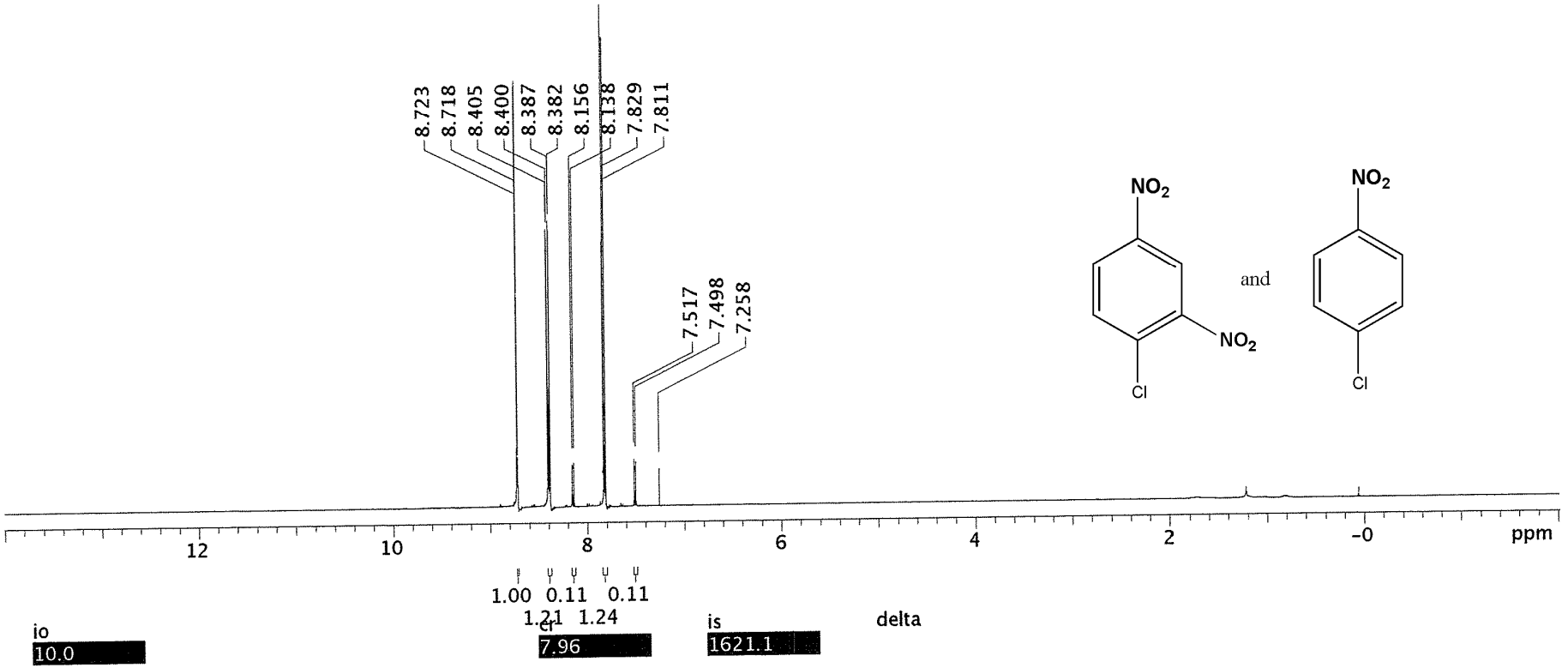

CN
NO2
F
107.313
107.323
107.328
107.336
107.343
107.348
107.358
102.422
102.432
0
-20
-40
-60
-80
-100
-120
-140
ppm
vp
0
cr
10.62
vs
72.4
delta

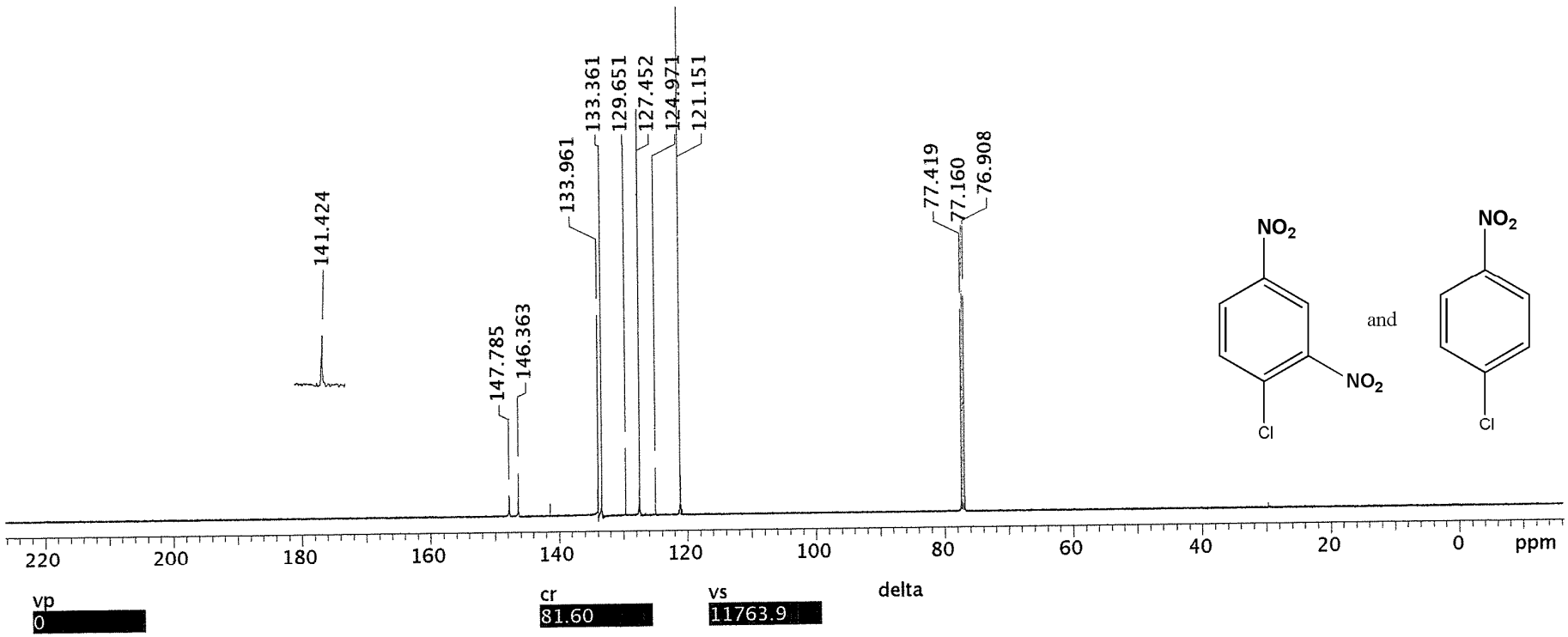

Abundance
TIC: 07APRIL1.D
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
Br
Br
NO2

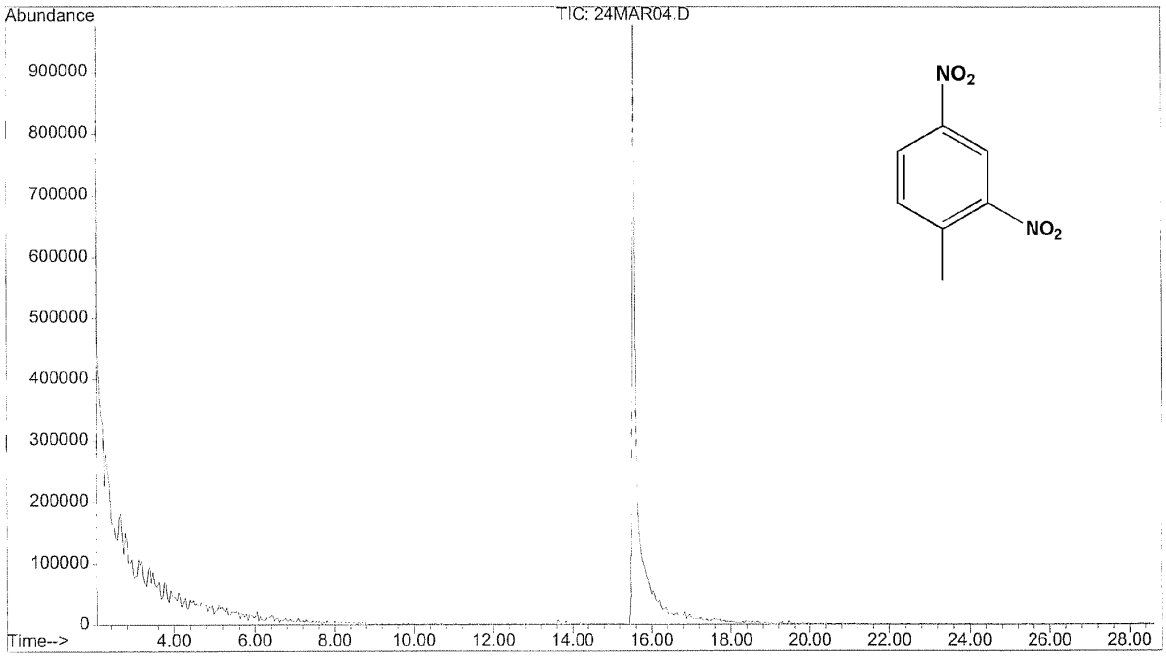

Abundance
Scan 350 (15.890 min): 07APRIL1.D
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
m/z-->
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330
37
46
63
74
91
105
118
128
143
154
172
195
207
223
235
251
265
281
329

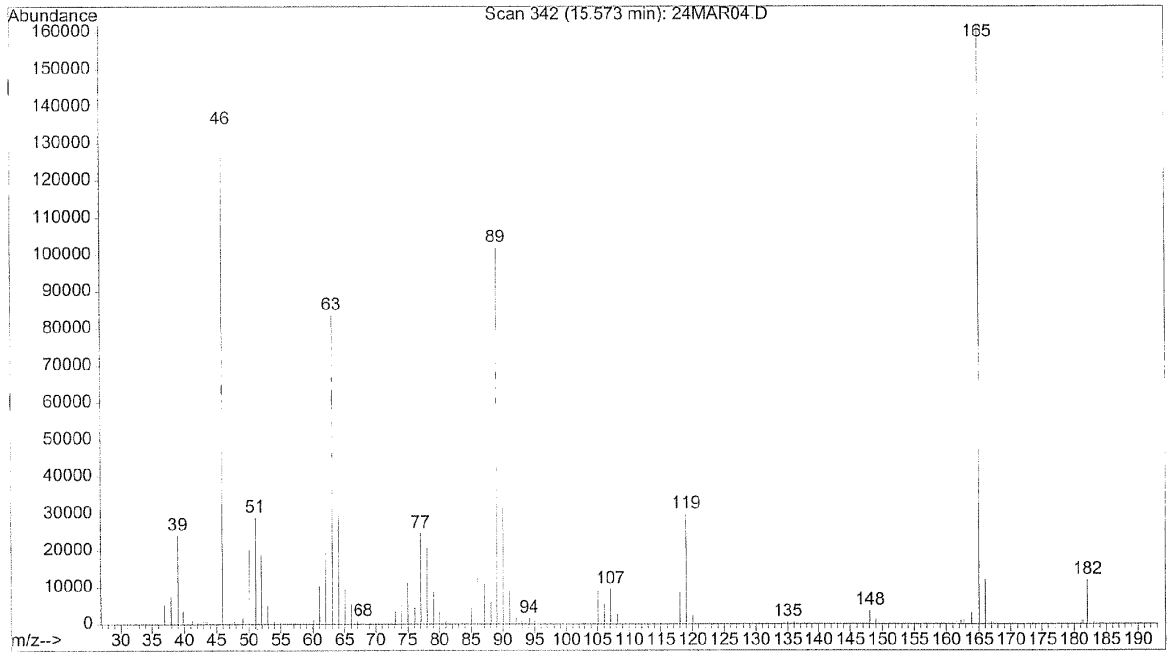

7.933
7.929
7.767
7.750
7.612
7.608
7.595
7.591
7.260
Br
Br
NO2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
1.00
1.08
1.10
io
10.0
cr
8.16
is
2686.2
delta

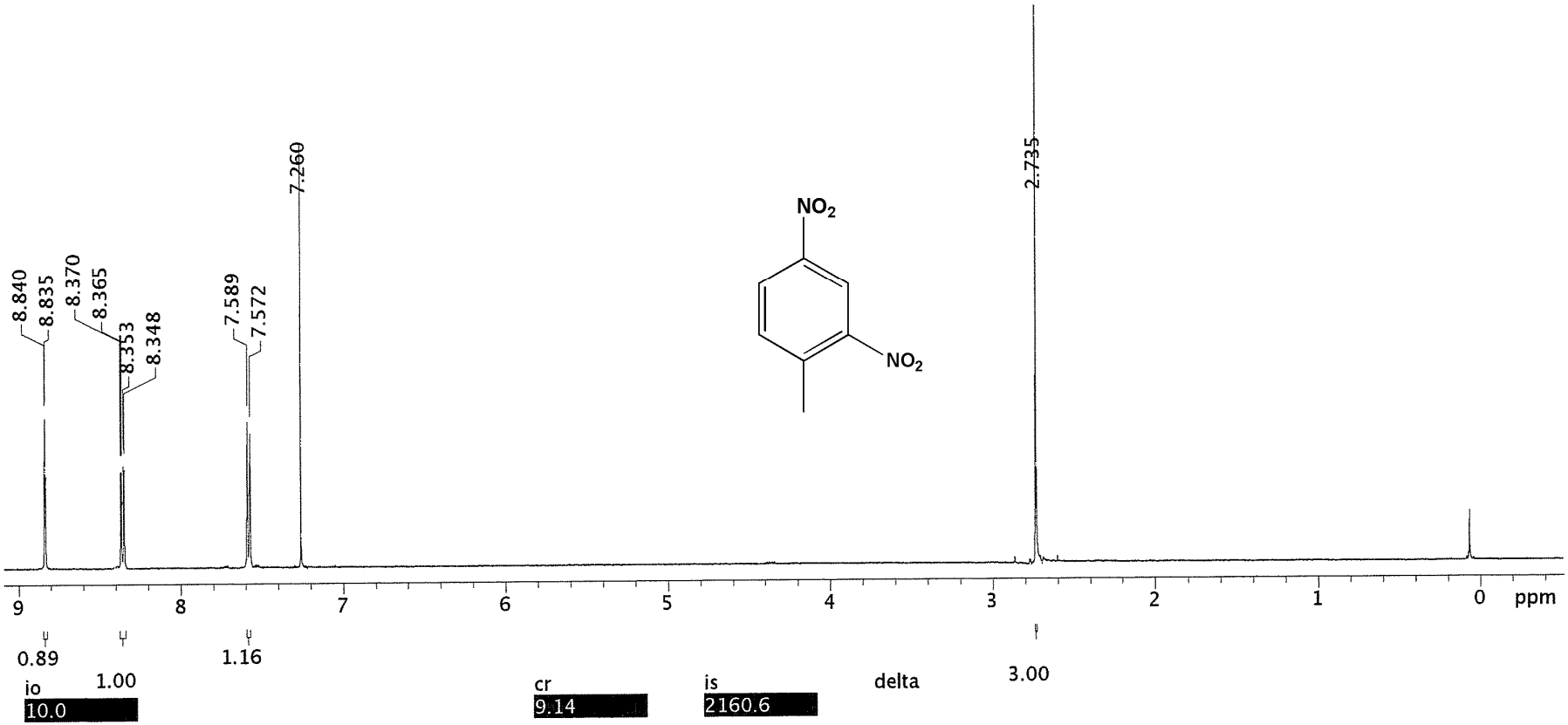

9.077
9.073
9.069
8.596
8.592
8.580
8.575
8.425
7.954
7.948
7.942
7.935
7.844
7.828
7.811
7.801
7.794
7.789
7.783
7.260
NO2
NO2
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.08
1.17
2.18
io
10.0
cr
9.56
is
1522.3
delta

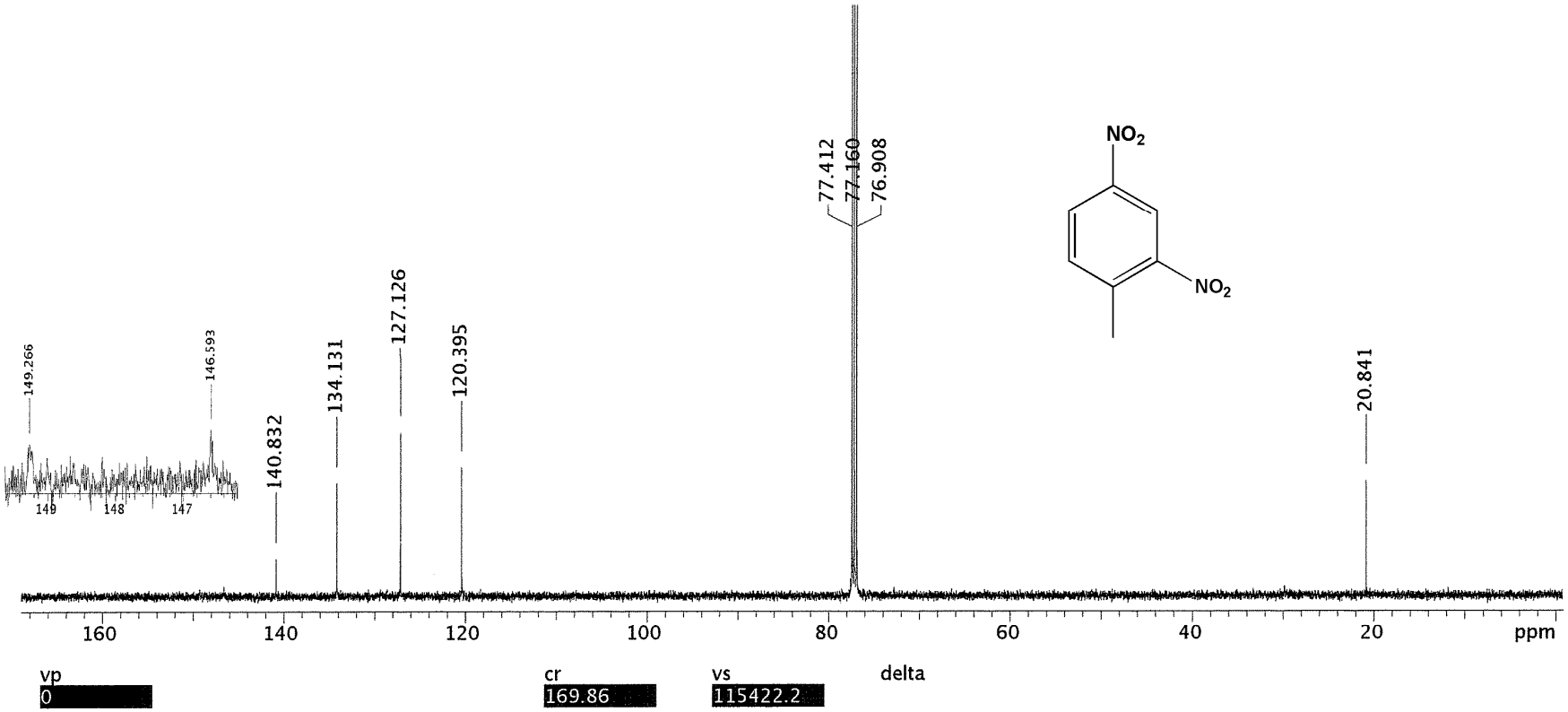

8.723
8.718
8.405
8.400
8.387
8.382
8.156
8.138
7.829
7.811
7.517
7.498
7.258
12
10
8
6
4
2
-0
ppm
1.00
0.11
0.11
1.21
1.24
io
10.0
cr
7.96
is
1621.1
delta
NO2
NO2
Cl
and
NO2
Cl

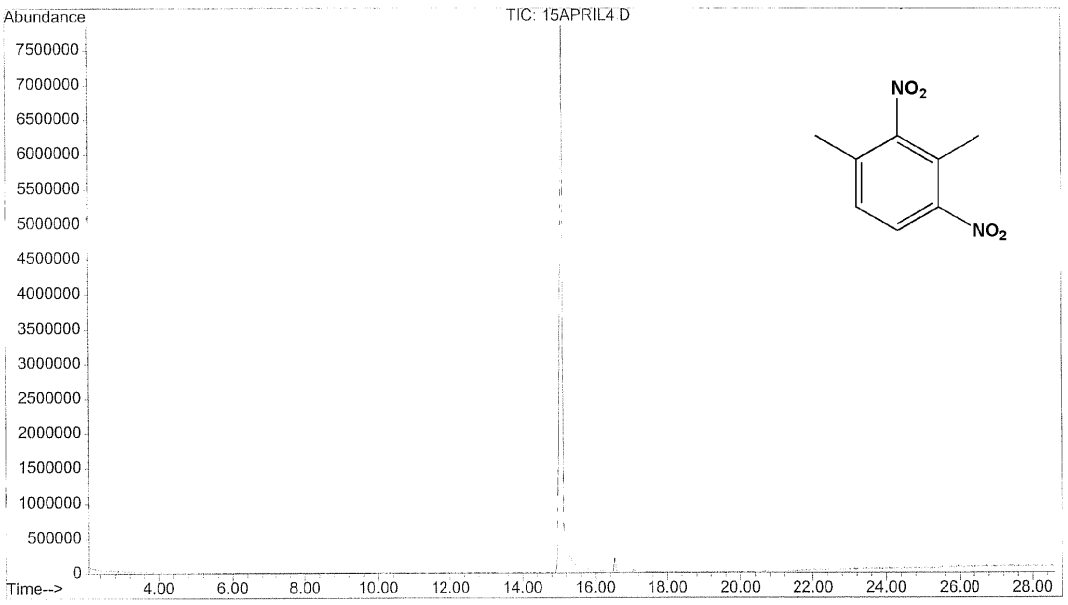

141.424
147.785
146.363
133.961
133.361
129.651
127.452
124.971
121.151
77.419
77.160
76.908
NO2
NO2
Cl
and
NO2
Cl
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
81.60
vs
11763.9
delta

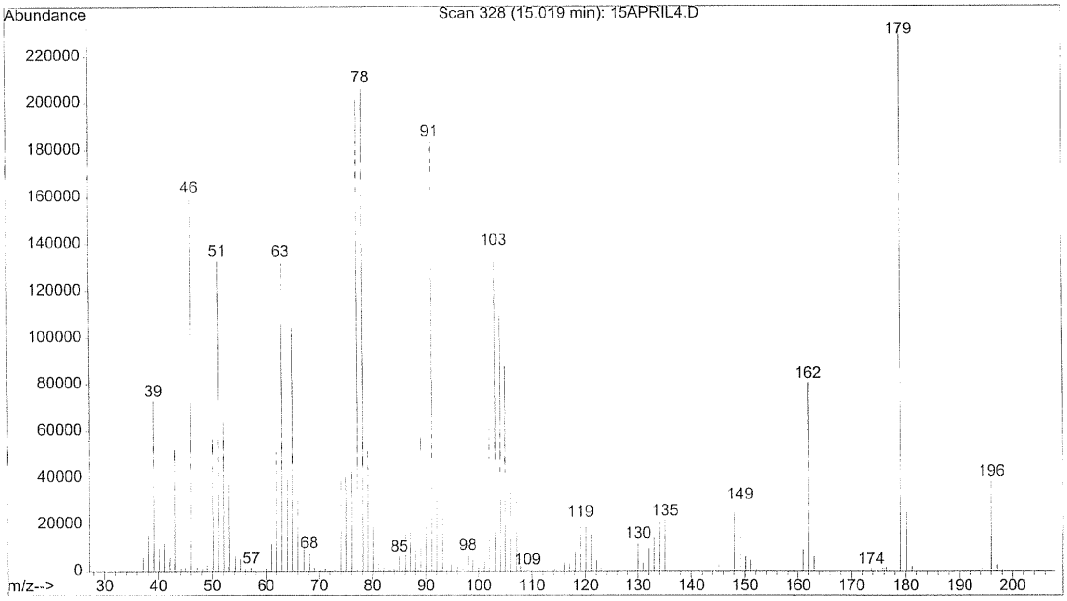

Abundance
TIC: 24MAR04.D
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
NO2
NO2

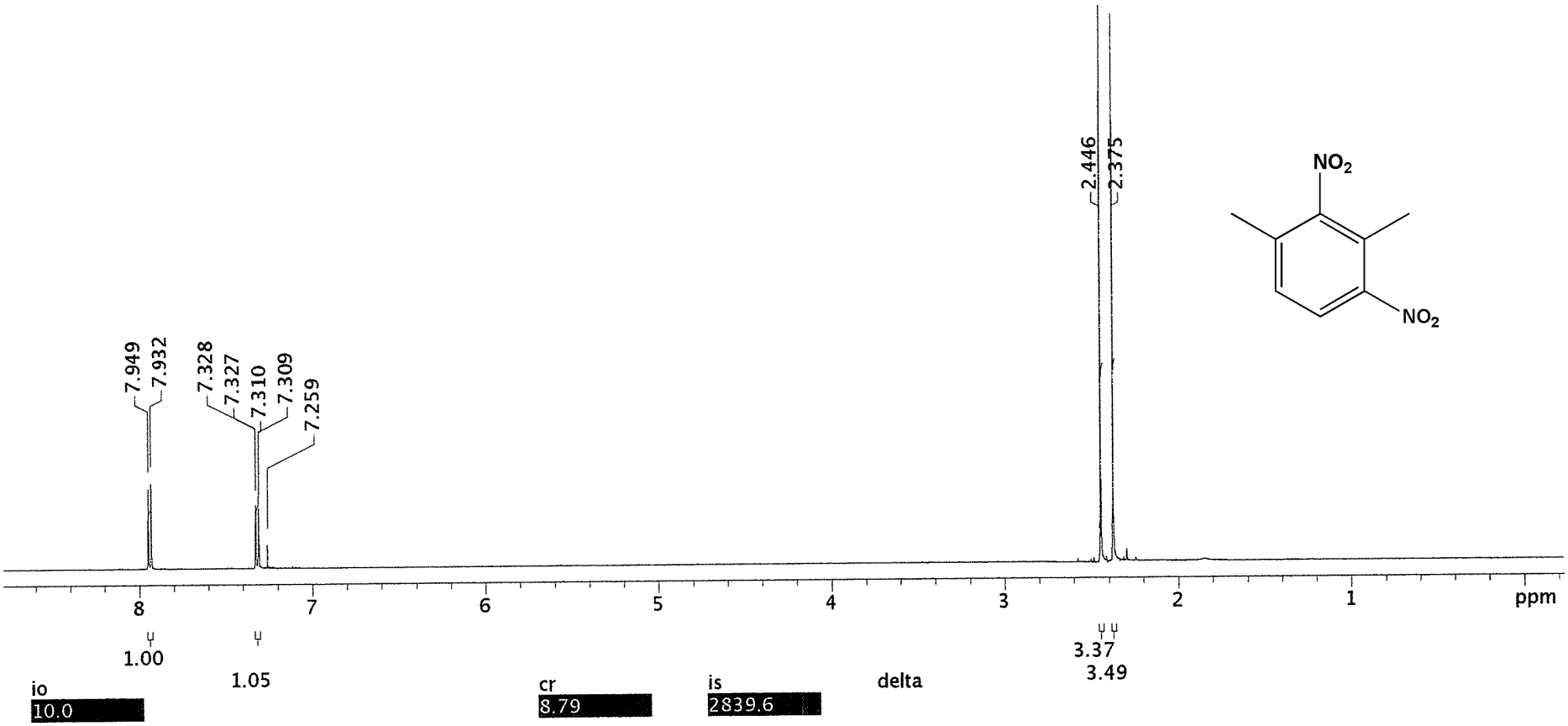

Abundance
Scan 342 (15.573 min): 24MAR04.D
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
m/z-->
30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165 170 175 180 185 190
165
46
89
63
51
39
77
119
107
182
68
94
135
148

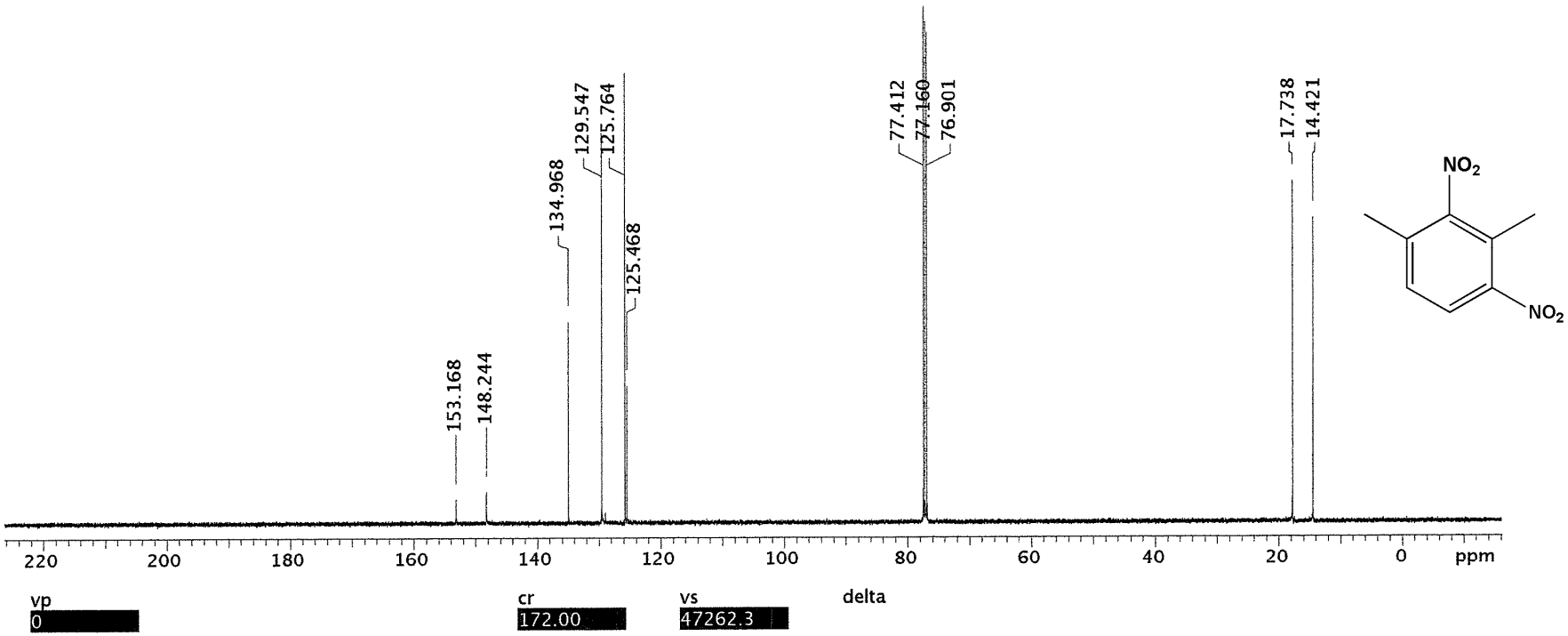

8.840
8.835
8.370
8.365
8.353
8.348
7.589
7.572
7.260
2.735
NO2
NO2
9
8
7
6
5
4
3
2
1
0
ppm
0.89
1.00
1.16
3.00
io
10.0
cr
9.14
is
2160.6
delta

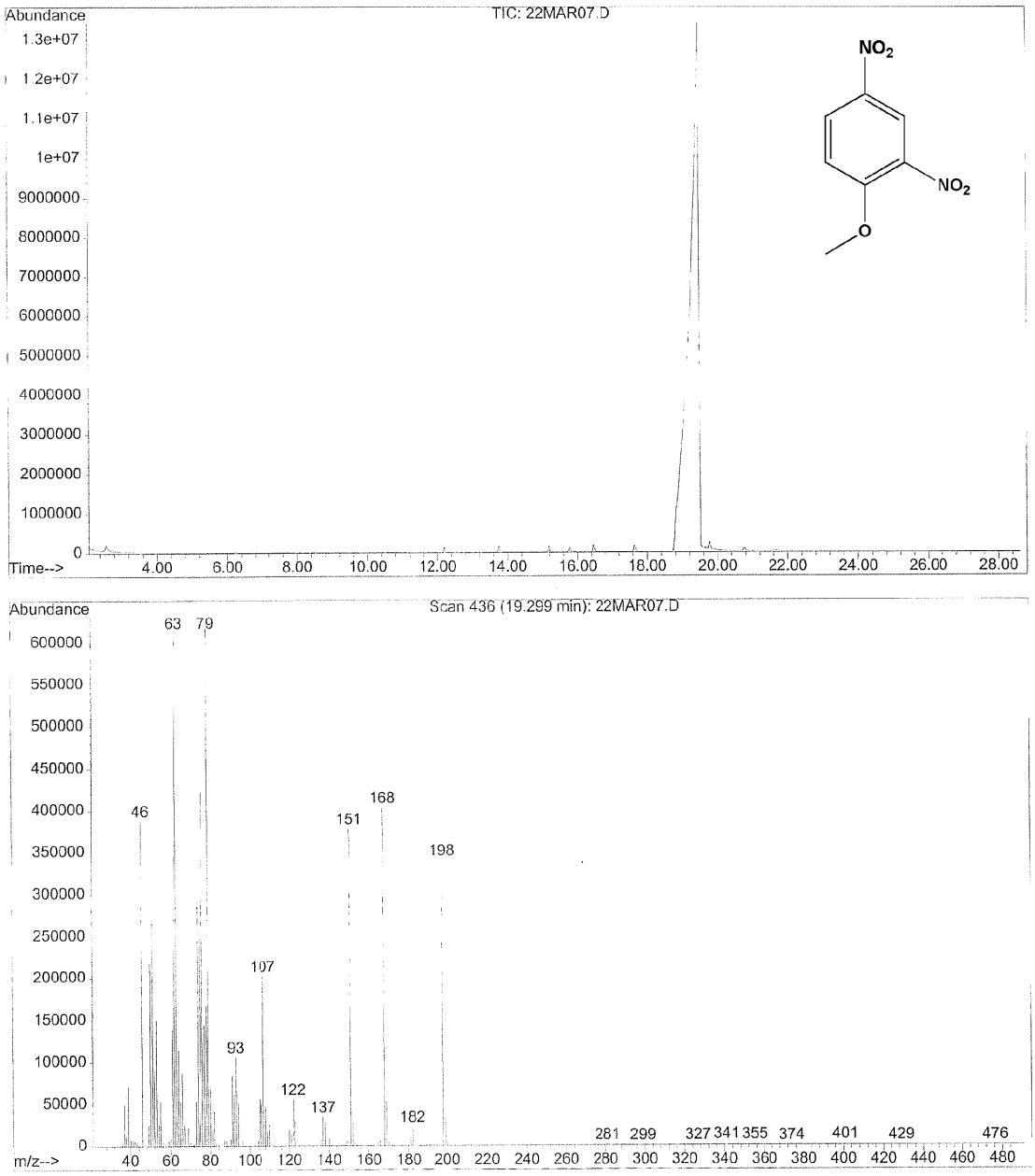

149.266
146.593
140.832
134.131
127.126
120.395
77.412
77.160
76.908
20.841
NO2
NO2
149
148
147
160
140
120
100
80
60
40
20
ppm
vp
0
cr
169.86
vs
115422.2
delta

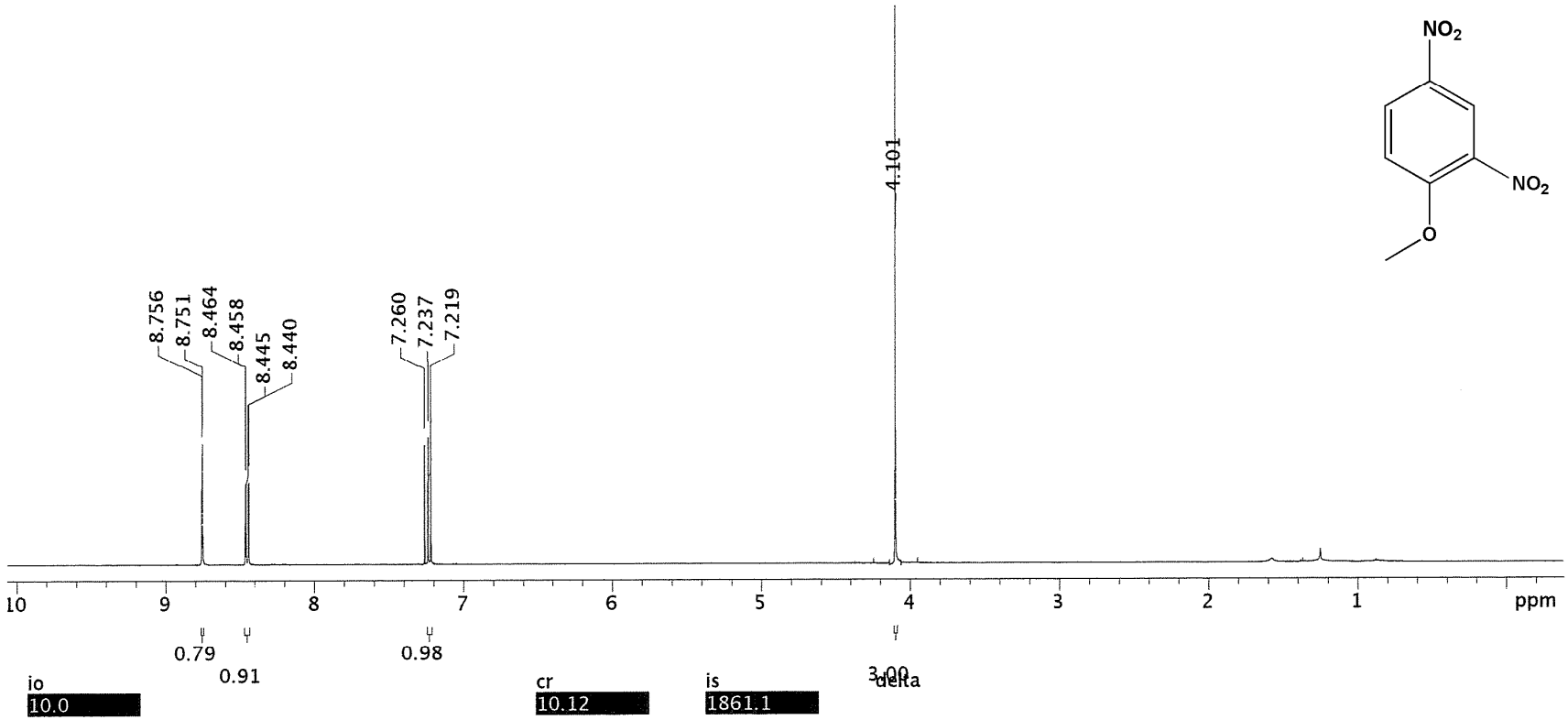

TIC: 15APRIL4.D
Abundance
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
NO2
NO2

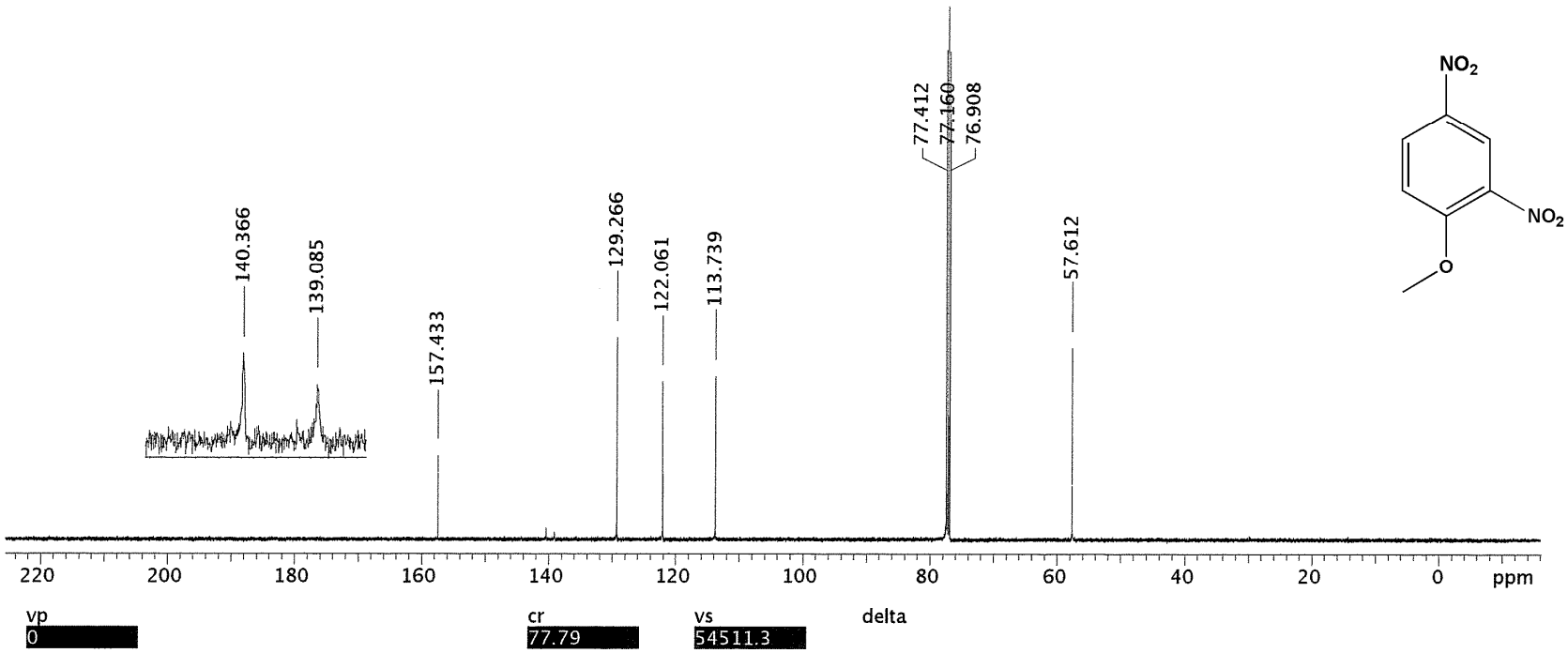

Abundance
Scan 328 (15.019 min): 15APRIL4.D
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
m/z-->
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
179
78
91
46
51
63
103
39
162
196
149
119
135
130
57
68
85
98
109
174

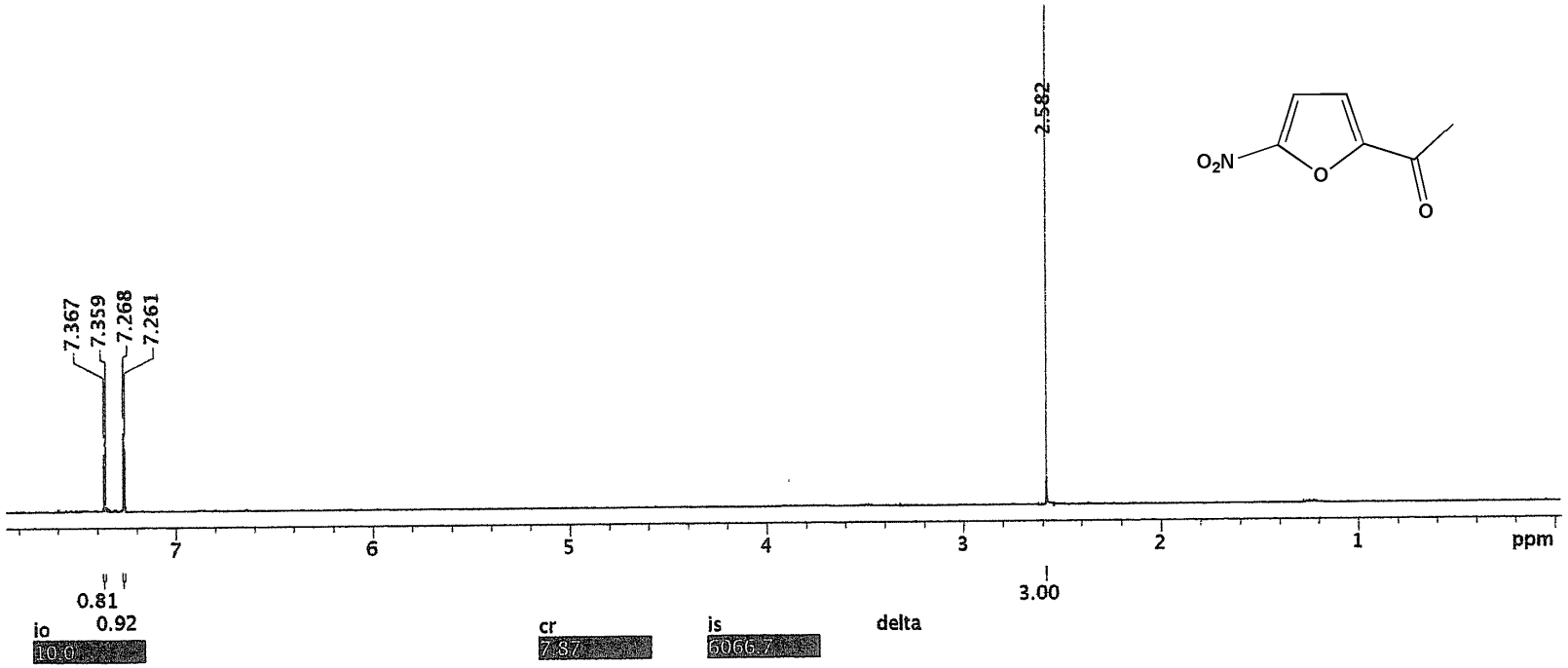

7.949
7.932
7.328
7.327
7.310
7.309
7.259
2.446
2.375
NO2
NO2
8
7
6
5
4
3
2
1
ppm
1.00
1.05
3.37
3.49
io
10.0
cr
8.79
is
2839.6
delta

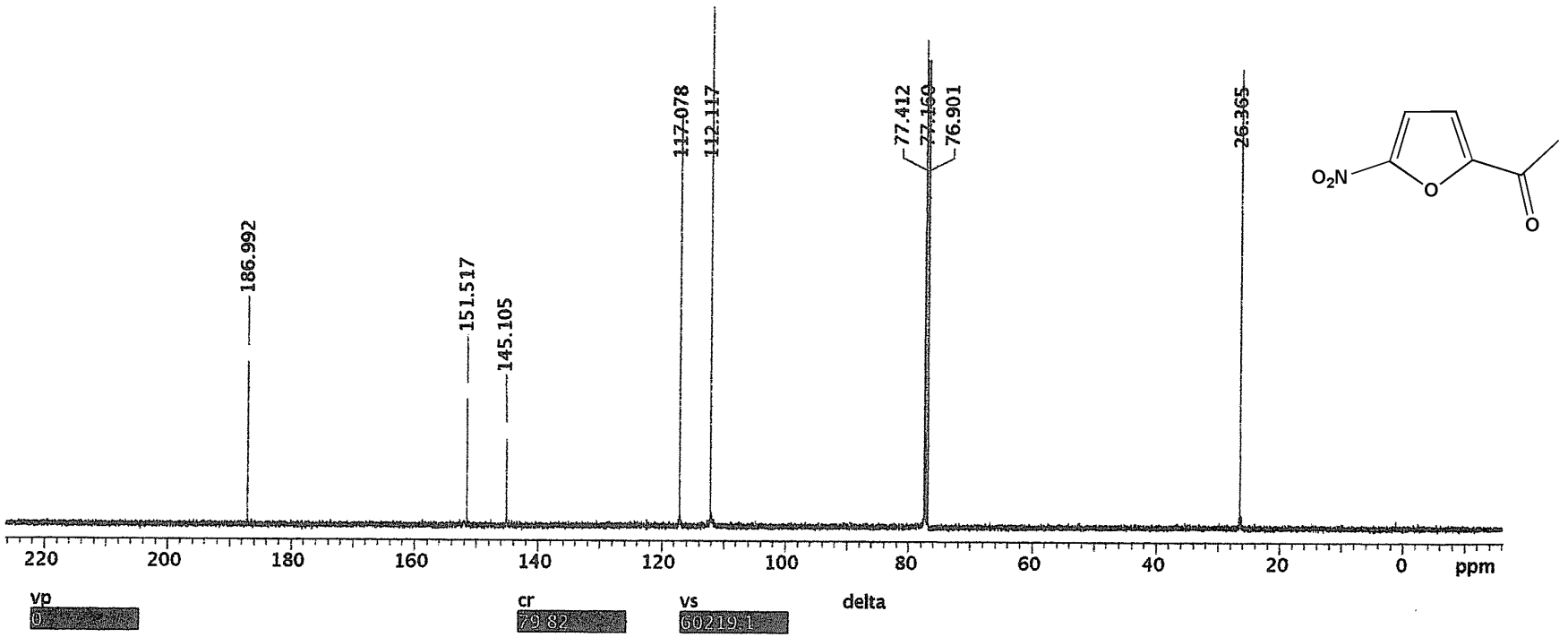

153.168
148.244
134.968
129.547
125.764
125.468
77.412
77.160
76.901
17.738
14.421
NO2
NO2
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
172.00
vs
47262.3
delta

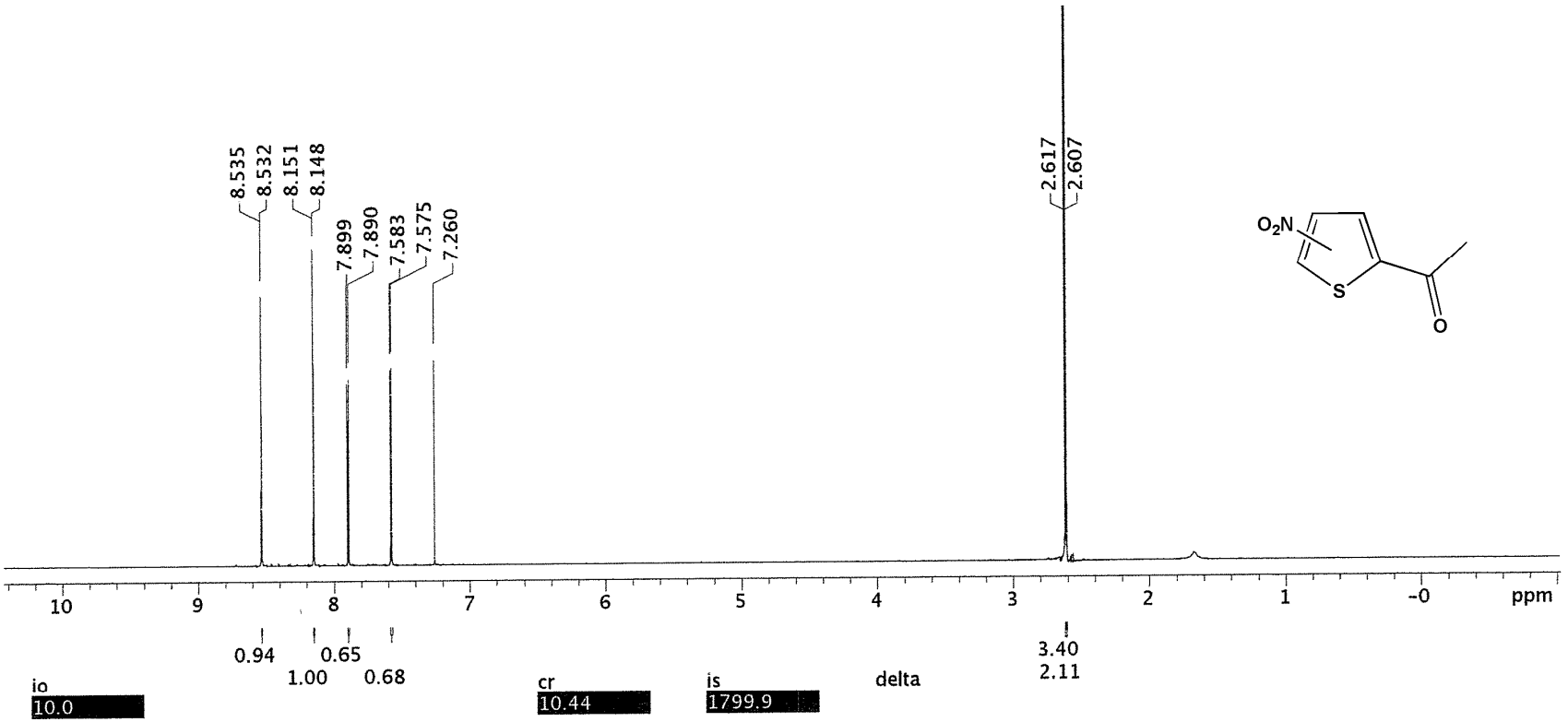

TIC: 22MAR07.D
Abundance
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
Time-->
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
24.00
26.00
28.00
NO2
NO2
O
Scan 436 (19.299 min): 22MAR07.D
Abundance
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
m/z-->
63
79
46
168
151
198
107
93
122
137
182
281
299
327
341
355
374
401
429
476
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480

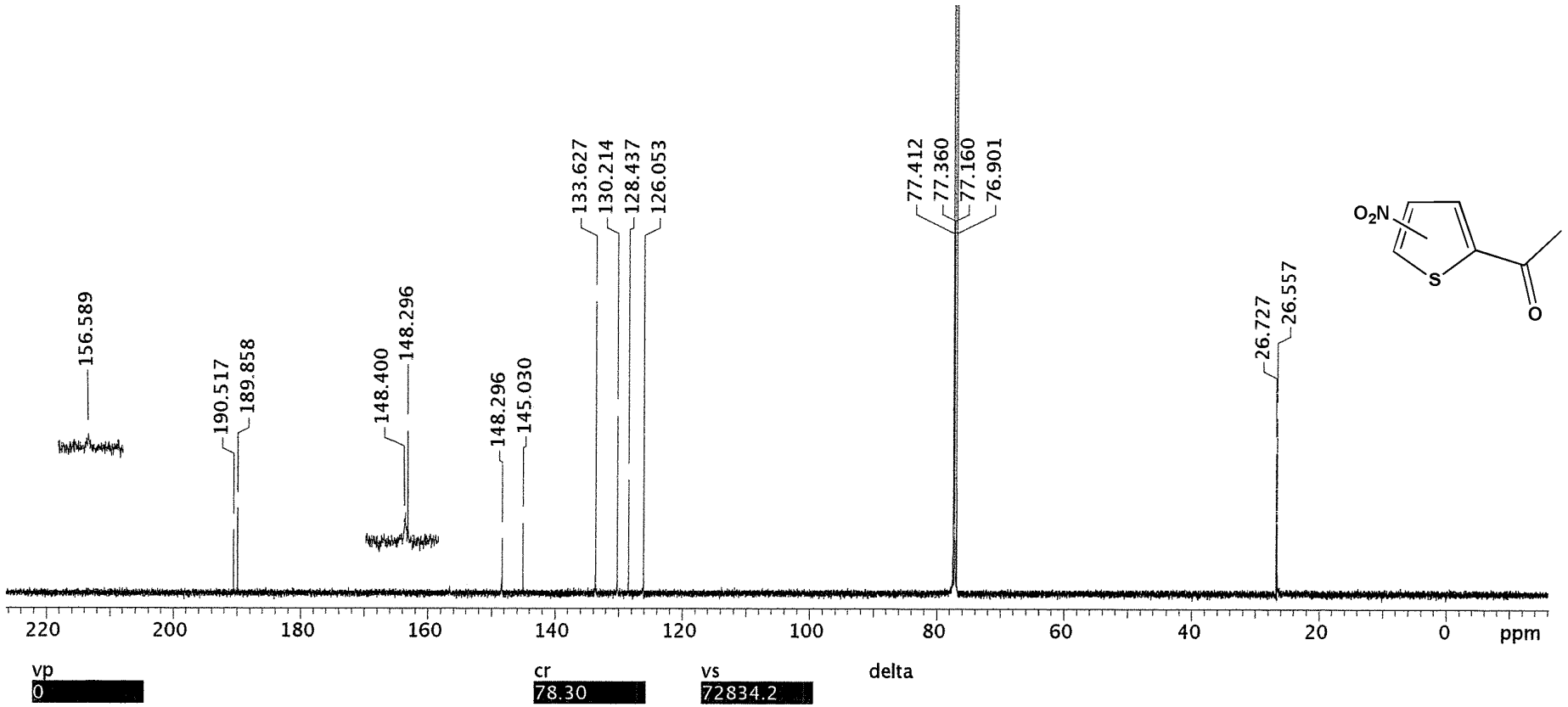

NO2
NO2
O
8.756
8.751
8.464
8.458
8.445
8.440
7.260
7.237
7.219
4.101
10
9
8
7
6
5
4
3
2
1
ppm
0.79
0.91
0.98
3.00
delta
io
10.0
cr
10.12
is
1861.1

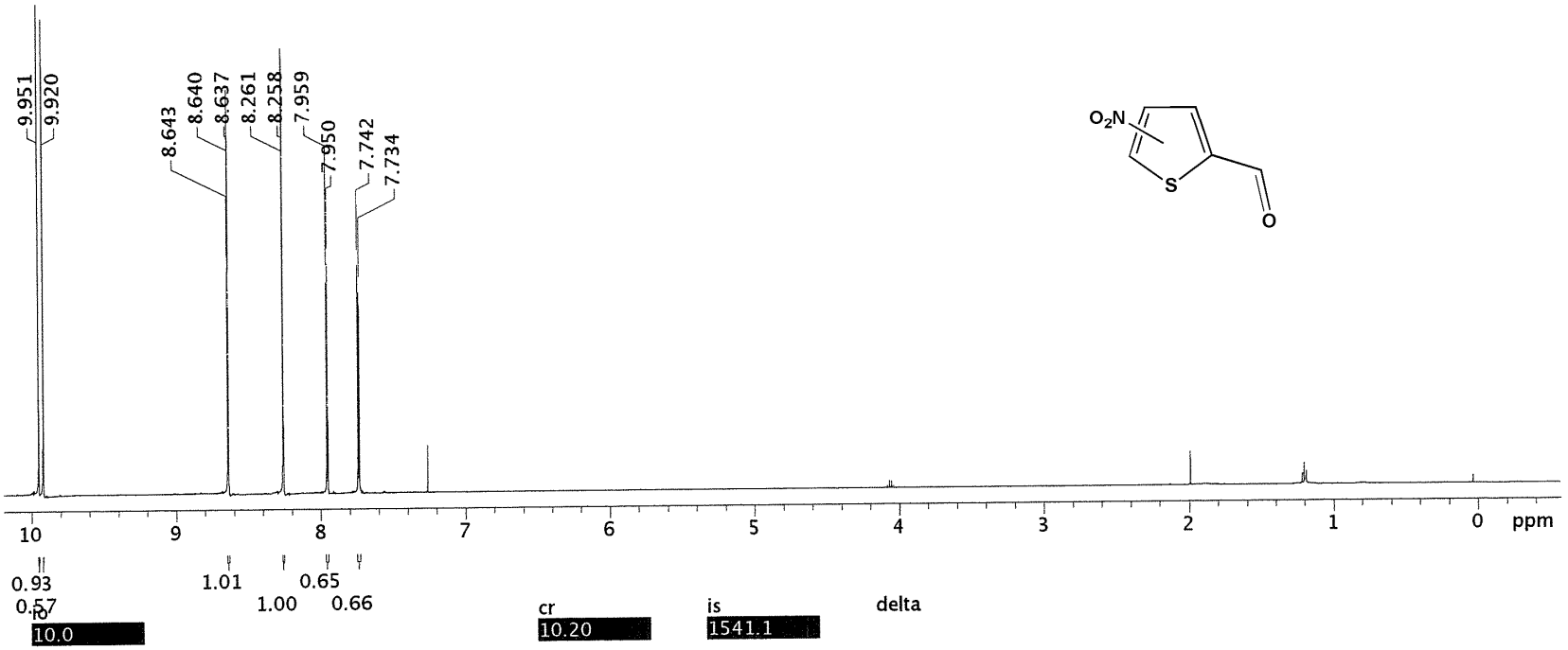

140.366
139.085
157.433
129.266
122.061
113.739
77.412
77.160
76.908
57.612
NO2
NO2
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
77.79
vs
54511.3
delta

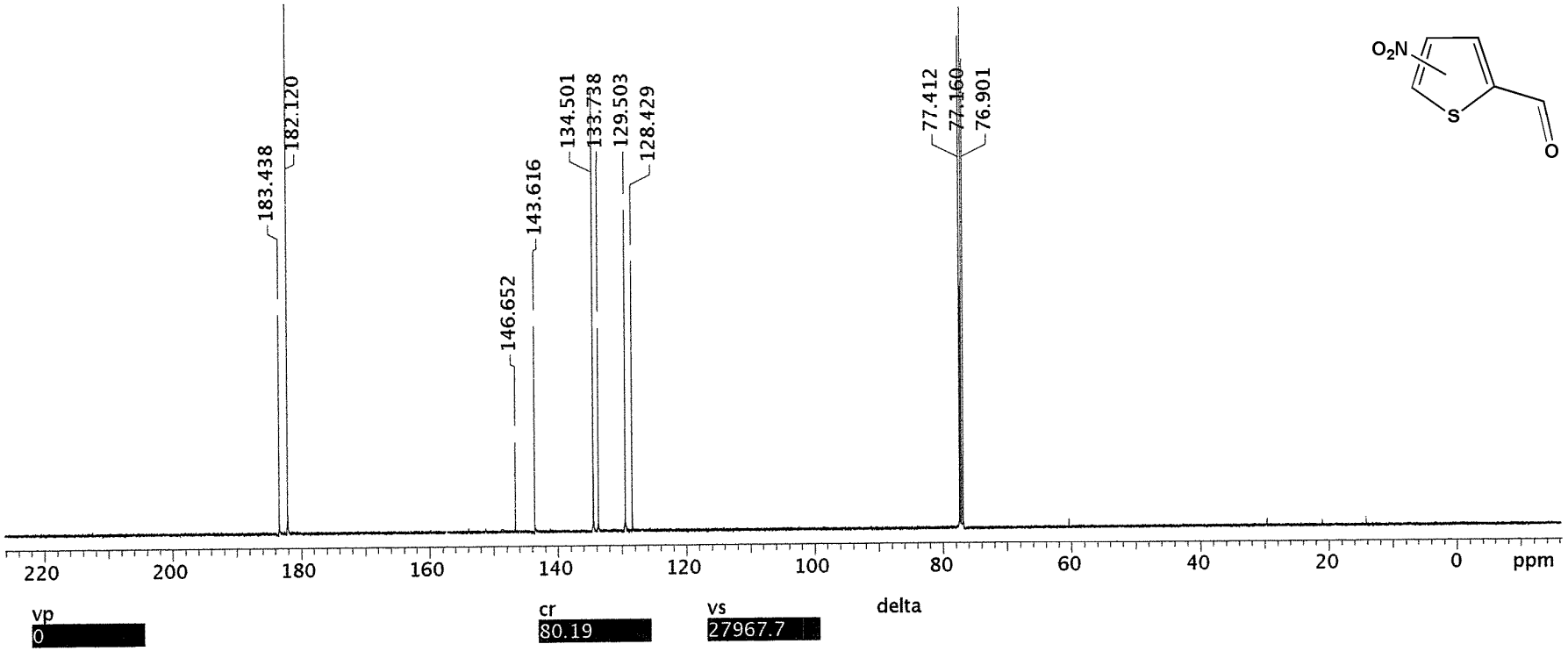

7.367
7.359
7.268
7.261
2.582
O_2N
O
O
7
6
5
4
3
2
1
ppm
0.81
0.92
3.00
ia
cr
is
delta
10.0
7.87
6066.7


186.992
151.517
145.105
117.078
112.117
77.412
77.160
76.901
26.365
O2N
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
cr
vs
delta


8.535
8.532
8.151
8.148
7.899
7.890
7.583
7.575
7.260
2.617
2.607
O2N
S
O
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.94
1.00
0.65
0.68
3.40
2.11
io
10.0
cr
10.44
is
1799.9
delta


156.589
190.517
189.858
148.400
148.296
148.296
145.030
133.627
130.214
128.437
126.053
77.412
77.360
77.160
76.901
26.727
26.557
O2N
S
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
78.30
vs
72834.2
delta


9.951
9.920
8.643
8.640
8.637
8.261
8.258
7.959
7.950
7.742
7.734
O2N
S
O
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.57
1.01
1.00
0.65
0.66
ro
10.0
cr
10.20
is
1541.1
delta


183.438
182.120
146.652
143.616
134.501
133.738
129.503
128.429
77.412
77.160
76.901
O2N
S
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
vp
0
cr
80.19
vs
27967.7
delta