Supporting information

A Simple Cyclohexanediamine-derived Primary Amine Thiourea Catalyzed Highly Enantioselective Conjugate Addition of Nitroalkanes to Enones

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1.0 General information

Commercially available enones are dried and purified prior to use (Lancaster, Aldrich, Alfa Aesar, Sinopharm Chemical Reagent Co. Ltd). Flash chromatography is performed on silica gel (200-300 mesh) purchased from by Qingdao Haiyang Chemical Co. Ltd. ^{1}H and ^{13}C NMR spectra are recorded on a Bruker Avance DPX 400 or Bruker Avance DPX 500 spectrometers at ambient temperature and chemical shifts are recorded in ppm (δ) relative to the internal standard TMS, and data for ^{1}H are recorded as follows: chemical shift (ppm), the unit was omitted), and multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet). Enantioselectivity was determined by Agilent 1200 Series HPLC system. Optical rotations were measured on a Perkin-Elmer model 341 polarimeter. Mass spectrometry was performed on a Micromass GCT CA055.

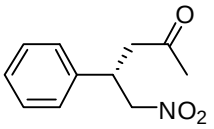
2.0 The synthesis of the screened organocatalysts.

The organocatalysts, **I-II,**[1] and **III-VII**[2] were synthesized by following the known procedures.

3.0 Typical procedure for a Michael reaction

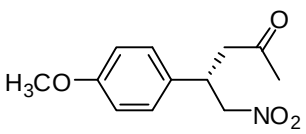
The reaction was carried out with 0.1 mmol α, β-unsaturated enone and 0.1 mL (16 eq) nitromethane in the presence of 15 mol % **VII** in 0.2 mL of ethyl acetate at rt for 5 d. Then the crude product was concentrated and purified by silica gel chromatography without workup using a mixture of EtOAc/hexanes (1/20 up to 1/5) as eluent and fractions were collected and concentrated in vacuo to provide the desired product.

4.0 Characterization data



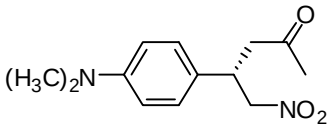
(*S*)-5-Nitro-4-phenylpentan-2-one (3a) (Table 3, entry 1.[3]

White solid, m.p. 114.6-116.1ºC, lit.[4] 120-122 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/8 as eluent in 68% yield and 98% ee; $[\alpha]_D^{20}$ = +2.0 (*c* = 0.87, $CHCl_3$); ^{1}H-NMR (400MHz, $CDCl_3$): δ = 7.28-7.36 (m, 3H), 7.21-7.24 (m, 2H), 4.68-4.70 (m, 1H), 4.62-4.64 (m, 1H), 4.00-4.03 (m, 1H), 2.92-2.94 (m, 2H), 2.13 (s, 3H); ^{13}C-NMR (100 MHz, $CHCl_3$): δ = 205.4, 138.8, 129.1, 127.9, 127.4, 79.5, 46.1, 39.0, 30.4; HRMS (ESI) calcd for $C_{11}H_{13}NO_3$ $[M+H]^+$ 208.0974, obsd 208.0964; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 210 nm, 25 ºC): HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 13.2 min, t_{major} = 9.9 min, ee = 98%.



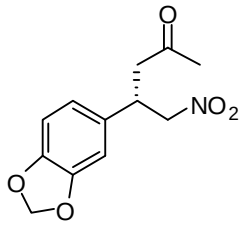
(*S*)-4-(4-Mmethoxyphenyl)-5-nitropentan-2-one (3b) (Table 3, entry 2).[4]

Reaction time: 10 d; white solid, m.p. 90.2-91.7 °C, lit.[4] 93.5-94.5 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 68% yield and 98% ee; $[\alpha]_D^{20}$ = -3.5 (*c* = 0.87, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.14 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 4.54-4.96 (m, 2H), 3.94-3.98 (m, 1H), 3.79 (s, 3H), 2.88-2.90 (m, 2H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.5, 159.1, 130.7, 128.4, 114.4, 79.7, 55.2, 48.3, 38.4, 30.4; HRMS (ESI) calcd for $C_{12}H_{15}NO_4$ $[M+Na]^+$ 260.0899, found 260.0896; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 14.3 min, t_{major} = 26.1 min, ee = 98%.



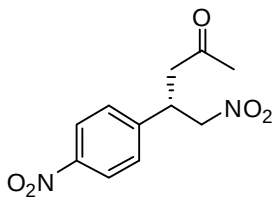
(*S*)-4-(4-(Dimethylamino)phenyl)-5-nitropentan-2-one (3c) (Table 3, entry 3).[5]

Yellow solid, m.p. 128.9-131.7 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 74% yield and 97% ee; $[\alpha]_D^{20}$ = -2.3 (*c* = 0.86, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.08 (d, *J* = 8.8 Hz, 2H), 6.69-6.71 (m, 2H), 4.56-4.64 (m, 2H), 3.89-3.93 (m, 1H), 2.94 (s, 6H), 2.87-2.88(m, 2H), 2.11(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.8, 149.9, 128.1, 112.9, 79.9, 46.4, 40.5, 38.5, 30.4; HRMS (ESI) calcd for $C_{13}H_{18}N_2O_3$ $[M+H]^+$ 251.1396, found 251.1389; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 25.1 min, t_{major} = 14.9 min, ee = 97%.



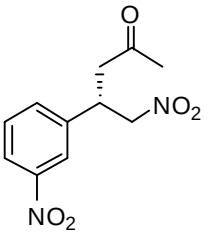
(*S*)-4-(Benzo[d][1,3]dioxol-5-yl)-5-nitropentan-2-one (3d) (Table 3, entry 4).[6]

Pale yellow solid, m.p. 96.7-98.8 °C, lit.[7] 96.5-98.5 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 71% yield and 97% ee; $[\alpha]_D^{20}$ = -3.5 (*c* = 1.11, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 6.68-6.76 (m, 3H), 5.95 (s, 2H), 4.54-4.65(m, 2H), 3.91-3.95 (m, 1H), 2.86-2.89 (m, 2H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.3, 148.1, 147.2, 132.4, 120.7, 108.7, 107.6, 101.2, 79.6, 46.2, 38.8, 30.4; HRMS (ESI) calcd for $C_{12}H_{13}NO_5$ $[M+H]^+$ 252.0872, found 252.0877; HPLC (Chiralpak AS-H, *i*-propanol/hexane =20/80, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 21.1 min, t_{major} = 19.0 min, ee = 97%.



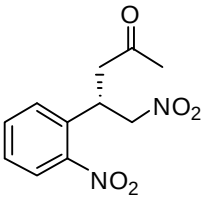
(*S*)-5-Nitro-4-(4-nitrophenyl)pentan-2-one (3e) (Table 3, entry 5).[8]

White solid, m.p. 62.8-65.1 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 88% yield and 92% ee; $[\alpha]_D^{20}$ = +6.9 (*c* = 0.75, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 8.21 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 4.66-4.79 (m, 2H), 4.11-4.19 (m, 1H), 2.96-2.99 (m, 2H), 2.17(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 204.4, 147.5, 146.3, 128.6, 124.2, 78.6, 45.7, 38.6, 30.3; HRMS (ESI) calcd for $C_{11}H_{12}N_2O_5$ $[M+Na]^+$ 275.0644, found 275.0636; HPLC (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 51.8 min, t_{major} = 35.5 min, ee = 92%. .



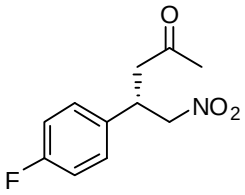
(*S*)-5-Nitro-4-(3-nitrophenyl)pentan-2-one (3f) (Table 3, entry 6).[3]

Pale yellow solid, m.p. 60.2-63.4 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 82 % yield and 95 % yield; $[\alpha]_D^{20}$ = +6.9 (*c* = 0.43, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 8.12-8.13 (m, 2H), 7.52-7.63 (m, 2H), 4.66-4.75 (m, 2H), 4.14-4.18 (m, 1H), 2.98-3.00 (m, 2H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 204.5, 148.6, 141.1, 134.2, 130.1, 123.0, 122.2, 78.7, 45.7, 38.5, 30.3; HRMS (EI) calcd for $C_9H_{11}INO_4$ $[M]^+$ 197.0688, found 197.0680; HPLC (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 11.5 min, t_{major} = 10.1 min, ee = 95%.



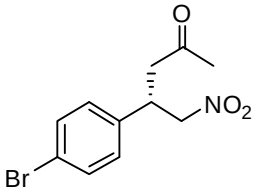
(*S*)-5-Nitro-4-(2-nitrophenyl)pentan-2-one (3g) (Table 3, entry 7).[9]

Yellow oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 70% yield and 95% ee; $[\alpha]_D^{20}$ = -30.9 (*c* = 1.01, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.89 (d, *J* = 8.0 Hz, 1H), 7.57-7.59 (m, 1H), 7.45-7.47 (m, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 4.83-4.85 (m, 2H), 4.50-4.54 (m, 1H), 3.04-3.06 (m, 2H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 204.7, 149.9, 133.5, 133.3, 128.7, 128.5, 125.2, 77.9, 45.3, 33.8, 30.1; HRMS (EI) calcd for $C_{11}H_{12}N_2O_5$ $[M]^+$ 252.0746, found 252.0744; HPLC (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 25.3 min, t_{major} = 23.8 min, ee = 95%.



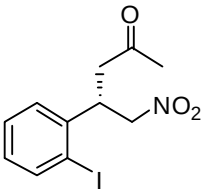
(*S*)-4-(4-Fluorophenyl)-5-nitropentan-2-one (3h) (Table 3, entry 8).

Pale yellow solid, m.p. 102.0-104.9 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/8 as eluent in 87% yield, 99% ee; $[\alpha]_D^{20}$ = -2.5 (*c* = 1.05, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.7.19-7.22 (m, 2H), 7.01-7.05 (m, 2H), 4.58-4.69 (m, 2H), 3.99-4.03 (m, 1H), 2.90-2.92 (m, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.1, 163.4, 160.9, 134.6, 134.5, 129.1, 129.0, 116.1, 115.8, 79.4, 46.1, 38.3, 30.4; HRMS (ESI) calcd for $C_{11}H_{12}FNO_3$ $[M+Na]^+$ 248.0699, found 248.0691; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 15.2 min, t_{major} = 10.4 min, ee = 99%.



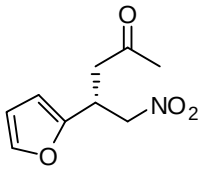
(*S*)-4-(4-Bromophenyl)-5-nitropentan-2-one (3i) (Table 3, entry 9).[9]

Yellow solid, m.p. 103.4-106.5 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/8 as eluent in 89% yield and 99% ee; $[\alpha]_D^{20}$ = +3.0 (*c* = 1.39, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.45-7.47 (m, 2H), 7.10-7.12 (m, 2H), 4.58-4.67 (m, 2H), 3.97-4.00 (m, 1H), 2.89-2.91 (m, 2H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.0, 138.0, 132.3, 129.2, 122.0, 79.2, 46.0, 38.6, 30.5; HRMS (ESI) calcd for $C_{11}H_{12}BrNO_3$ $[M+Na]^+$ 307.9898, found 307.9898; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 15.7 min, t_{major} = 10.3 min, ee = 99%.



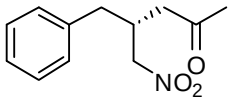
(*S*)-4-(2-Iodophenyl)-5-nitropentan-2-one (3j) (Table 3, entry 10).

Yellow solid, m.p. 76.9-79.8 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/8 as eluent in 76% yield and 96% ee; $[\alpha]_D^{20}$ = +15.2 (*c* = 1.65, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.89 (d, *J* = 8.0 Hz, 1H), 7.31-7.35 (m, 1H), 7.14-7.16 (d, *J* = 8.0 Hz, 1H), 6.96-7.00 (m, 1H), 4.71-4.73 (m, 2H), 4.33-4.37 (m, 1H), 2.94-2.99 (m, 2H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.1, 140.7, 140.5, 129.5, 128.9, 127.0, 101.1, 77.7, 45.1, 42.6, 30.2; HRMS (EI) calcd for $C_{11}H_{12}INO_3$ $[M]^+$ 332.9862, found 332.9862; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 40/60, flow rate 1.0 mL/min, λ = 254 nm, 25 °C): t_{minor} = 13.2 min, t_{major} = 10.4 min, ee = 96%.



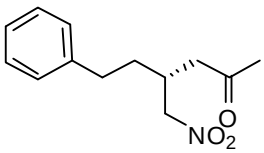
(*R*)-4-(Furan-2-yl)-5-nitropentan-2-one (3k) (Table 3, entry 11).[10]

Pale yellow solid, m.p. 56.8-58.5 ºC, lit.[4] 54.5-56.0 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/8 as eluent in 71% yield and 94% ee; $[\alpha]_D^{20}$ = -9.1 (*c* = 1.04, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.34-7.35 (m, 1H), 6.29-6.30 (m, 1H), 6.14-6.15 (m, 1H), 4.67-4.69 (m, 2H), 4.09-4.12 (m, 1H), 2.92-2.97 (m, 2H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.1, 151.8, 142.3, 110.5, 107.0, 77.1, 43.5, 32.9, 30.1; HPLC (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 27.7 min, t_{major} = 25.6 min, ee = 94%.



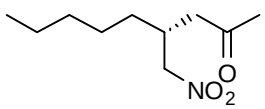
(*R*)-4-Benzyl-5-nitropentan-2-one (3l) (Table 3, entry 12).

Yellow oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 76% yield and 95% ee; $[\alpha]_D^{25}$ = -7.4 (*c* = 1.02, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.31-7.34 (m, 2H), 7.25-7.27 (m, 1H), 7.18-7.20 (m, 2H), 4.43 (d, *J* = 5.6 Hz, 2H), 2.91-2.92 (m, 1H), 2.72-2.74 (d, *J* = 7.2 Hz, 2H), 2.55-2.60 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 206.4, 137.9, 129.1, 128.7, 126.9, 43.8, 37.4, 34.9, 30.5, 29.7; MS (EI, m/z): 222.1, 176.1, 175.1, 161.1, 118.1, 117.1, 91.1, 43.0; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 11.5 min, t_{major} = 12.4 min, ee = 95%.



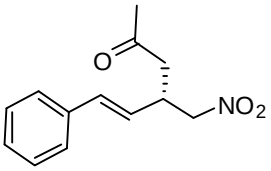
(*R*)-4-(Nitromethyl)-6-phenylhexan-2-one (3m) (Table 3, entry 13).

Yellow oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 82% yield and 93% ee; $[\alpha]_D^{25}$ = +5.6 (*c* = 1.01, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.18-7.23 (m, 2H), 7.11-7.14 (m, 1H), 7.08-7.09 (m, 2H), 4.41-4.43 (m, 2H), 2.60-2.63 (m, 4H), 2.48-2.58 (m, 1H), 2.08 (s, 3H), 1.64-1.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 206.4, 140.8, 128.6, 128.2, 126.3, 78.1 44.5, 33.1, 32.9, 32.7, 30.4; MS (EI, m/z): 236.1, 175.1, 129.1, 118.1, 91.1, 77.0, 43.0; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 11.6 min, t_{major} = 10.3 min, ee = 93%.



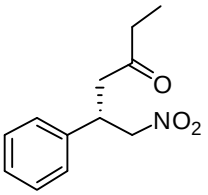
(*R*)-4-(Nitromethyl)nonan-2-one (3n) (Table 3, entry 14).

Reaction time: 10 d; colorless oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/20 as eluent in 83% yield and 95% ee; $[\alpha]_D^{25}$ = -1.9 (*c* = 1.12, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$): 4.37-4.38 (m, 2H), 2.48-2.56 (m, 3H), 2.10 (s, 3H), 1.21-1.24 (m, 8H), 0.81 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 206.6, 78.4, 44.7, 33.1, 31.6, 31.4, 30.5, 26.3, 22.4, 13.9; MS (ESI, m/z): 240.1 ($[M+K]^+$), 224.1 ($[M+Na]^+$), 140,1, 139.1, 128.1; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 10.1 min, t_{major} = 9.6 min, ee = 95%.



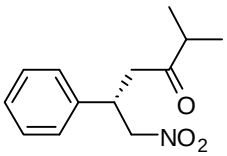
(*S*, *E*)-4-(Nitromethyl)-6-phenylhex-5-en-2-one (3o) (Table 3, entry 15).

White solid, m.p. 108.7-111.3 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 64% yield and 97% ee; $[\alpha]_D^{25}$ = +16.8 (*c* = 0.78, $CHCl_3$); ^1H NMR (500 MHz, $CDCl_3$): δ = 7.22-7.27 (m, 4H), 7.16-7.19 (m, 1H), 6.46 (d, *J* = 15.8 Hz, 1H), 5.98-6.03 (m, 1H), 4.51-4.54 (m, 1H), 4.44-4.48 (m,. 1H), 3.44-3.48 (m, 1H), 2.68-2.69 (m,. 2H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.5, 138.1, 133.4, 128.6, 128.0, 126.4, 126.3, 78.6, 44.9, 37.0, 30.5; MS (EI, m/z): 233.1 (M^+), 187.1, 186.1, 144.1, 143.1, 129.1, 128.1, 91.1, 43.0;. HPLC (Chiralpak AS-H, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 13.2 min, t_{major} = 11.3 min, ee = 97%.



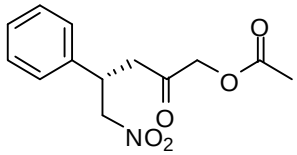
(*S*)-6-Nitro-5-phenylhexan-3-one (3p) (Table 3, entry 16).[4]

White solid, melted < 30 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 61% yield and 97% ee; $[\alpha]_D^{25}$ = +11.4 (*c* = 1.07, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$): δ = 7.31-7.34 (m, 3H), 7.21-7.23 (m, 2H), 4.62-4.70 (m, 2H), 4.01-4.05 (m, 1H), 2.89 (d, *J* = 7.2 Hz, 2H), 2.36-2.40 (m, 2H), 1.01 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 208.2, 138.9, 129.1, 127.9, 127.4, 79.5, 44.9, 39.1, 36.5, 7.6; MS (ESI, m/z): 222.1 ($[M+H]^+$), 175.1, 164.1, 161.1, 105.1, 104.1; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 11.1 min, t_{major} = 9.0 min, 97% ee.



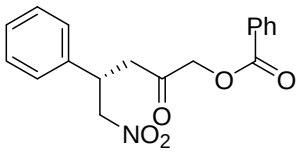
(*S*)-2-Methyl-6-nitro-5-phenylhexan-3-one (3q) (Table 3, entry 17).[11]

Reaction time: 10 d; pale yellow solid, melted < 30 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 38% yield and 96% ee; $[\alpha]_D^{25}$ = +20.6 (*c* = 0.85, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.24-7.27 (m, 2H), 7.19-7.21 (m, 1H), 7.14-7.16 (m, 2H), 4.53-4.66 (m, 2H), 3.94-3.97 (m, 1H), 2.84-2.87 (m, 2H), 2.44-2.47 (m, 1H), 0.98-0.99 (d, *J* = 6.9 Hz, 3H), 0.93-0.94 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 211.4, 139.1, 129.0, 127.8, 127.4, 79.5, 43.1, 41.2, 39.1, 17.9; MS (EI, m/z): 235.1 (M^+), 189.1, 145.1, 132.0, 131.0, 117.1, 104.1, 91.1, 71.0, 43.1; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 8.2 min, t_{major} = 6.3 min, 96% ee.



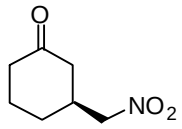
(*S*)-5-Nitro-2-oxo-4-phenylpentyl acetate (3r) (Table 3, entry 18).

Pale yellow oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 58% yield and 94% ee; $[\alpha]_D^{25}$ = +9.2 (*c* = 0.96, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.25-7.28 (m, 2H), 7.19-7.23 (m, 1H), 7.13-7.15 (m, 2H), 4.42-4.65 (m, 4H), 3.94-4.00 (m, 1H), 2.80-2.89 (m, 2H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.2, 170.1, 138.3, 129.2, 128.1, 127.3, 79.2, 68.1, 41.7, 38.7, 20.4; MS (EI, m/z): 266.1, 220.1, 219.1, 218.1, 158.1, 145.1, 104.1, 101.1, 91.1, 43.0; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 50/50, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 23.4 min, t_{major} = 18.8 min, 94% ee.



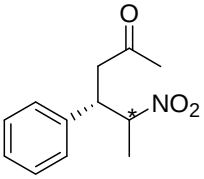
(*S*)-5-Nitro-2-oxo-4-phenylpentyl benzoate (3s) (Table 3, entry 19).

White solid, m.p. 103.6-105.1 ºC; purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/5 as eluent in 73% yield and 98% ee; $[\alpha]_D^{25}$ = +4.3 (*c* = 1.04, $CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.98-8.00 (m, 2H), 7.52-7.55 (m, 1H), 7.38-7.41 (m, 2H), 7.25-7.28 (m, 2H), 7.20-7.23 (m, 1H), 7.14-7.16 (m, 2H), 4.55-4.78 (m, 4H), 3.98-4.04 (m, 1H), 2.88-2.98 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.3, 165.8, 138.4, 133.6, 129.9, 129.2, 128.9, 128.6, 128.1, 127.3, 79.2, 68.5, 41.7, 38.7; MS (EI, m/z): 328.1, 282.1, 281.1, 280.1, 163.0, 158.1, 145.1, 105.0, 91.1, 77.0; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 28.0 min, t_{major} = 19.7 min, 98% ee.



(*S*)-3-(Nitromethyl)cyclohexanone (3t) (Table 3, entry 20).[12]

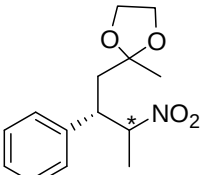
Reaction time: 4 d; colorless oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/20 as eluent in 69% yield and 97% ee; $[\alpha]_D^{20}$ = -9.9 (*c* = 0.83, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.34-4.42 (m, 2H), 2.64-2.65 (m, 1H), 2.43-2.48 (m, 2H), 2.26-2.33 (m, 1H), 2.14-2.21 (m, 2H), 1.97-2.01 (m, 1H), 1.64-1.76 (m, 1H), 1.50-1.53 (m, 1H); ^{13}C-NMR (100 MHz, $CHCl_3$): δ = 208.3, 80.1, 44.6, 40.9, 37.3, 28.3, 24.3; HPLC (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 210 nm, 25 °C): t_{minor} = 15.1 min, t_{major} = 17.8 min, ee = 97%.



(*S*) 5-Nitro-4-phenyl-hexan-2-one (3u) (Less polar, major diastereomer) (Table 3, entry 21)[13]

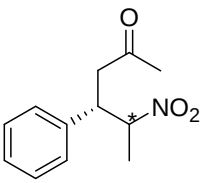
Reaction time: 10 d; colorless oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 43% yield; ^{1}H NMR (400MHz, $CDCl_3$): δ = 7.27-7.36 (m, 3H), 7.19-7.29 (m, 2H), 4.75-4.79 (m, 1H), 3.71-3.72 (m, 1H), 2.94-3.01 (m, 1H), 2.71-2.77 (m, 1H), 2.01 (s, 3H), 1.32-1.33 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 205.0, 138.2, 129.1, 128.2, 127.9, 87.1, 46.2, 45.3, 30.4, 17.8.

Conversion of 3u to 3u-A for chiral HPLC analysis.



3u-A

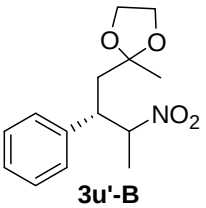
A mixture of compound (**3u**) (17 mg, 0.077 mmol), *p*-TsOH (6 mg) and $HO(CH_2)_2OH$ (20 mg) in dry benzene (5 mL) was heated at reflux for 1h. Then the crude product was concentrated and purified by silica gel chromatography directly using CH_2Cl_2 as eluent and fractions were collected and concentrated in vacuo to provide the desired product by purification via silica gel chromatography using a mixture of CH_2Cl_2 as eluent in 91% yield. $[\alpha]_D^{20}$ = -4.4 (*c* = 0.94, $CHCl_3$); ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.27-7.33 (m, 3H), 7.15-7.17 (m, 2H), 4.75-4.79 (m, 1H), 3.81-3.86 (m, 3H), 3.71-3.74 (m, 1H), 3.48-3.49 (m, 1H), 2.18-2.24 (m, 1H), 1.96-2.01 (m, 1H), 1.26-1.28 (d, *J* = 6.4 Hz, 3H), 1.14 (s, 3H); ^{13}C-NMR (100 MHz, $CDHCl_3$): δ = 139.4, 128.7, 128.5, 127.4, 106.9, 87.7, 64.4, 64.3, 45.8, 40.8, 24.5, 16.8; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 1/99, flow rate 0.5 mL/min, λ = 254 nm, 25 ºC): t_{minor} = 21.3 min, t_{major} = 18.4 min, ee = 94%.



(*S*) 5-Nitro-4-phenyl-hexan-2-one (3u') (More polar, minor diastereomer) (Table 3, entry 21)[13]

Colorless oil, purified by silica gel chromatography using a mixture of EtOAc/hexane = 1/10 as eluent in 39% yield; ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.27-7.31 (m, 3H), 7.14-7.16 (m, 2H), 4.87-4.90 (m, 1H), 3.73-3.75 (m, 1H), 3.03-3.08 (m, 1H), 2.87-2.94 (m, 1H), 2.12 (s, 3H), 1.48-1.49 (d, *J* = 6.8 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 205.8, 137.8, 128.7, 128.1, 127.9, 85.8, 44.8, 44.6, 30.6, 16.8.

Conversion of 3u' to 3u'-B for chiral HPLC analysis.



3u'-B

A mixture of compound (**3u'**) (15 mg, 0.068 mmol), *p*-TsOH (5 mg) and $HO(CH_2)_2OH$ (18 mg,) in dry benzene (5 mL) was heated at reflux for 6 h. Then the crude product was concentrated and purified by silica gel chromatography directly using CH_2Cl_2 as eluent and fractions were collected and concentrated in vacuo to provide the desired product by purification via silica gel chromatography using a mixture of CH_2Cl_2 as eluent in 89% yield. $[\alpha]_D^{20}$ = -9.5 (*c* = 0.91, $CHCl_3$); ^{1}H-NMR (400MHz, $CDCl_3$): δ = 7.28-7.32 (m, 2H), 7.18-7.24 (m, 3H), 4.74-4.77 (m, 1H), 3.85-3.89 (m, 3H), 3.71-3.72 (m, 1H), 3.41-3.45 (m, 1H), 2.13-2.22 (m, 2H), 1.54-1.55 (m, 3H), 1.15 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$): δ = 139.9, 128.5, 128.3, 127.4, 109.2, 87.9, 64.5, 64.4, 45.8, 39.2, 24.6, 16.5; HPLC (Chiralpak AS-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm, 25 ºC): t_{minor} = 8.8 min, t_{major} = 6.7 min, ee = 94%.

5.0 Preparation of racemic samples

Racemic samples of the products were prepared using racemic catalyst **VII**.

6.0 References

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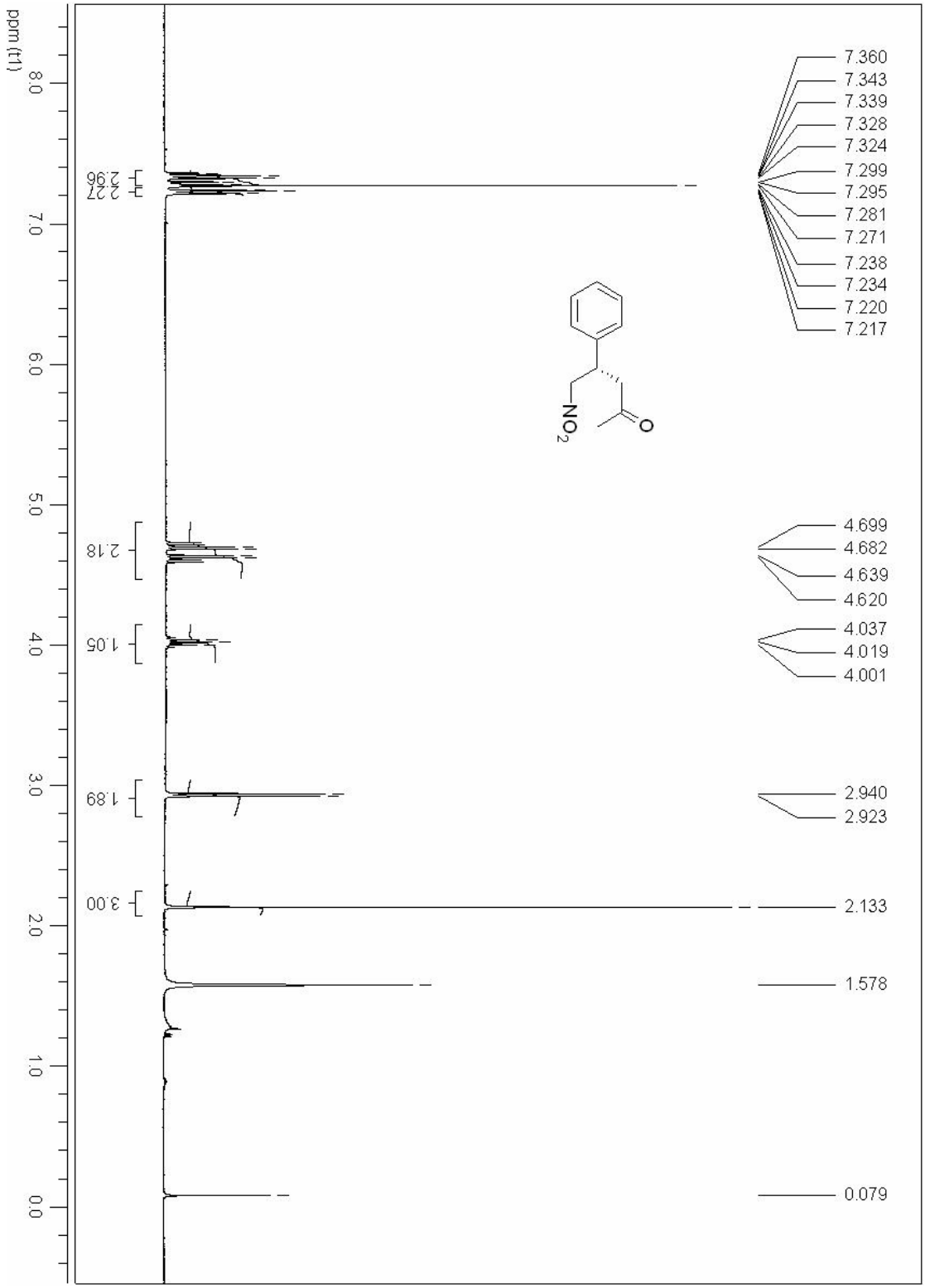
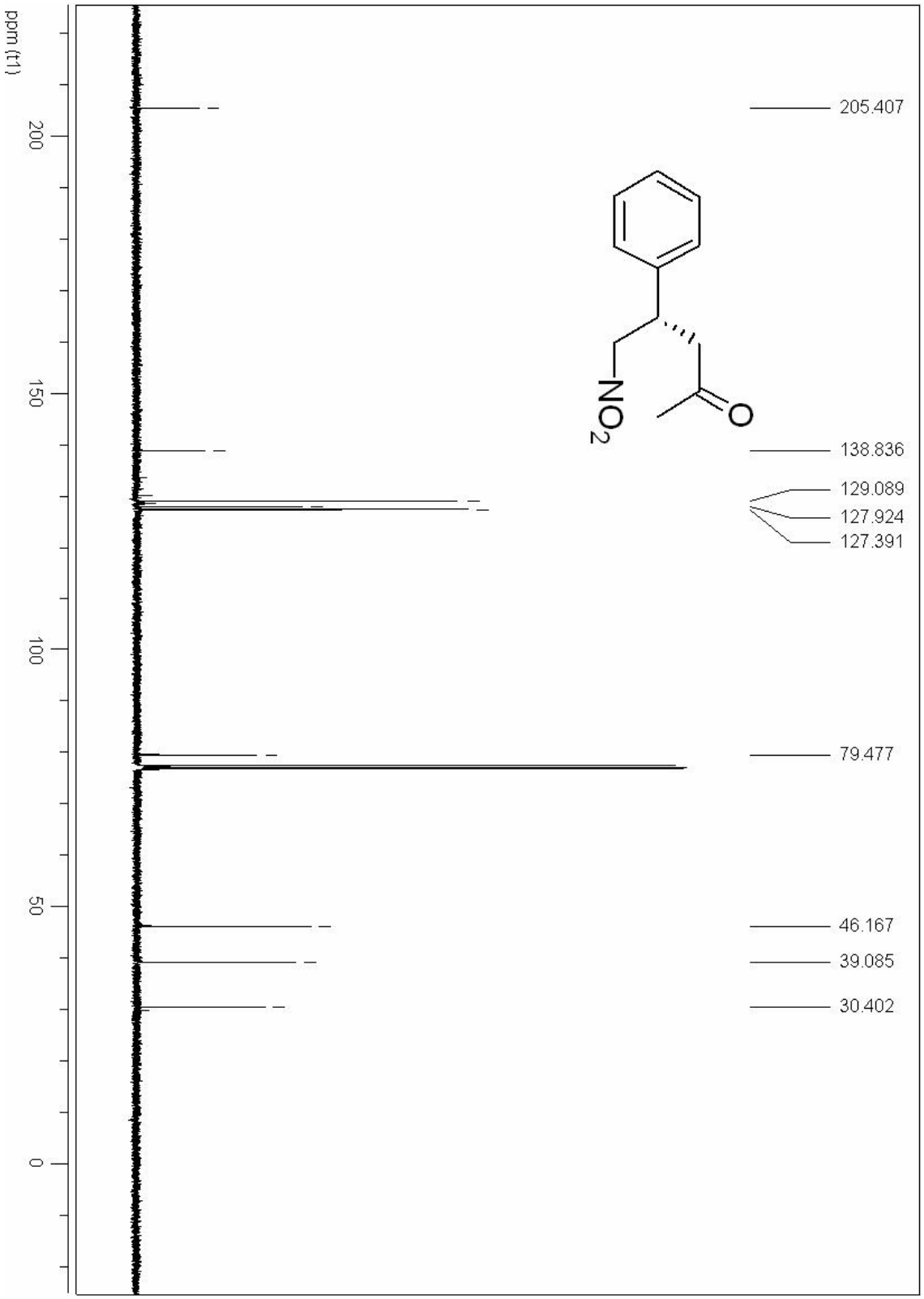
7.0 NMR spectra

Compound **3a**



Compound **3a**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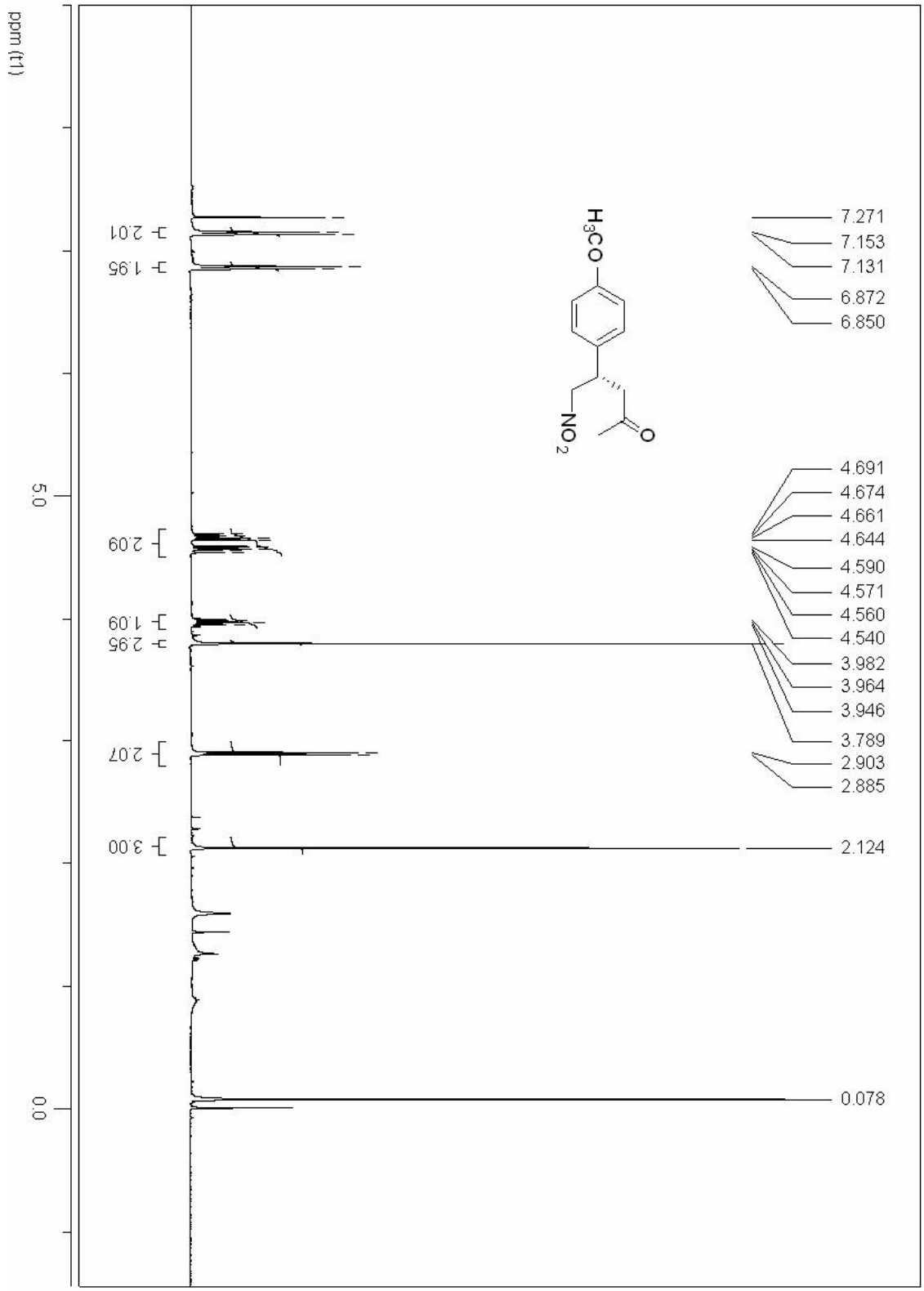
O

Compound **3b**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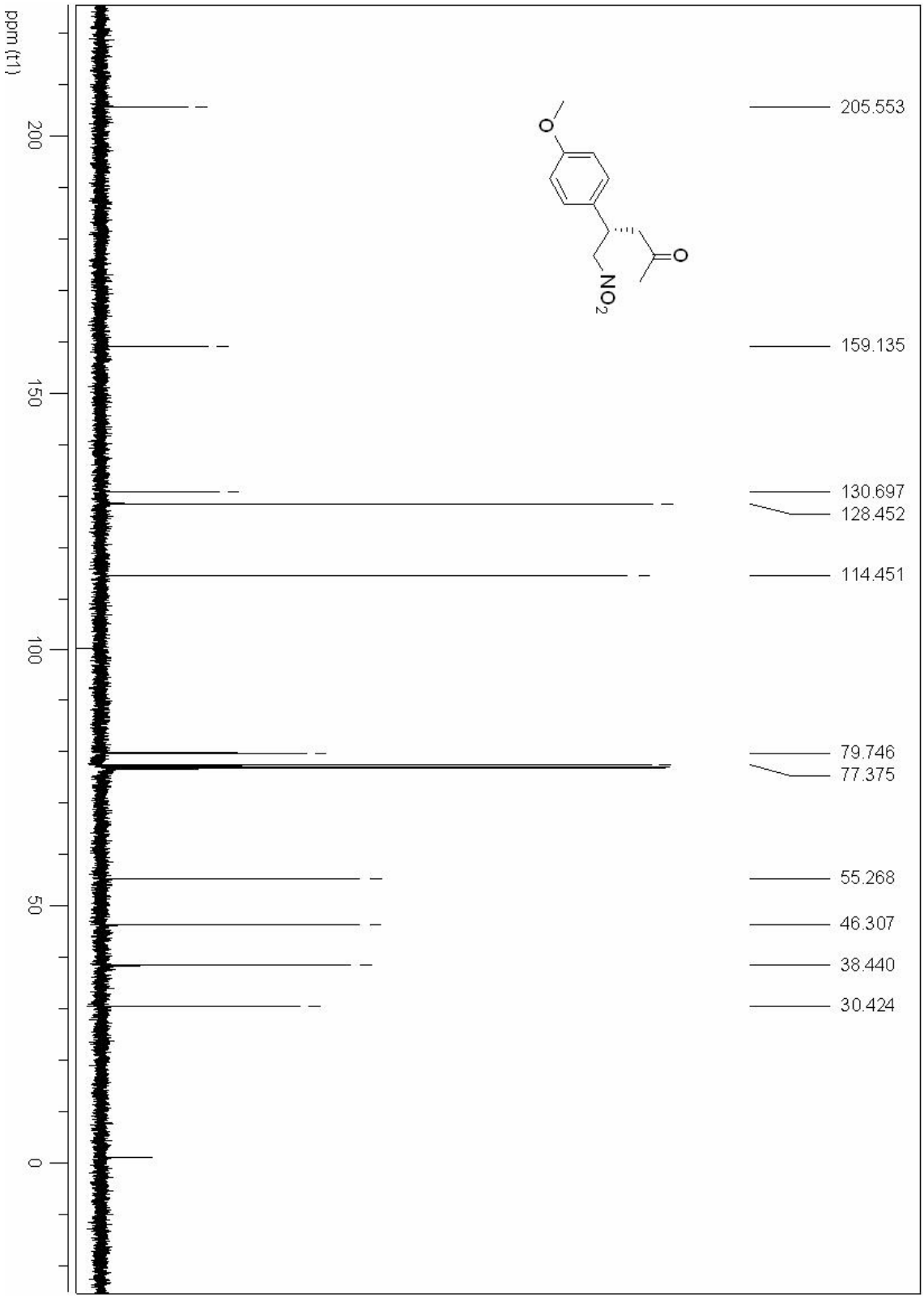
O

Compound **3b**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O
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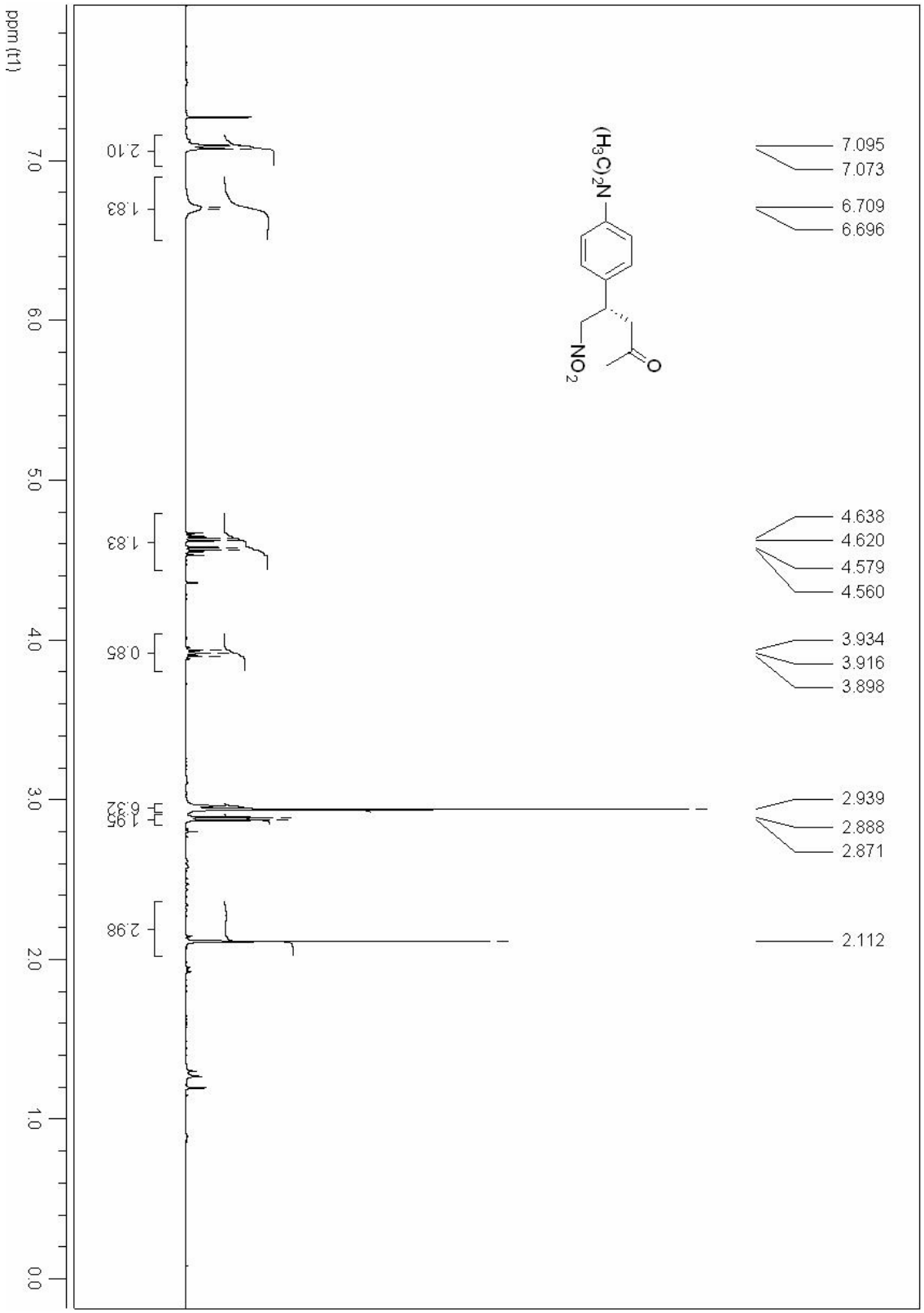
Compound **3c**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O
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7.073
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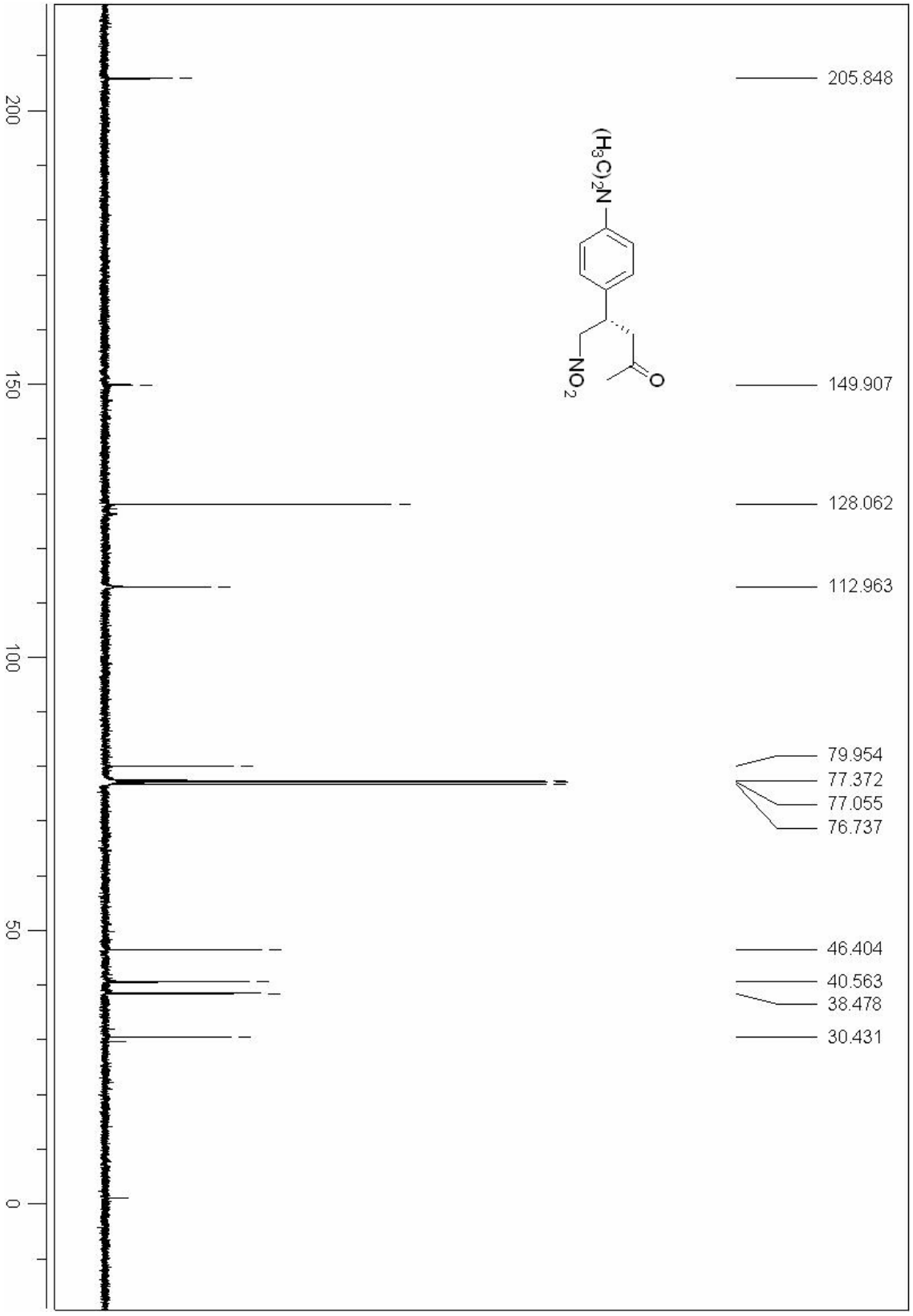
2.112

Compound **3c**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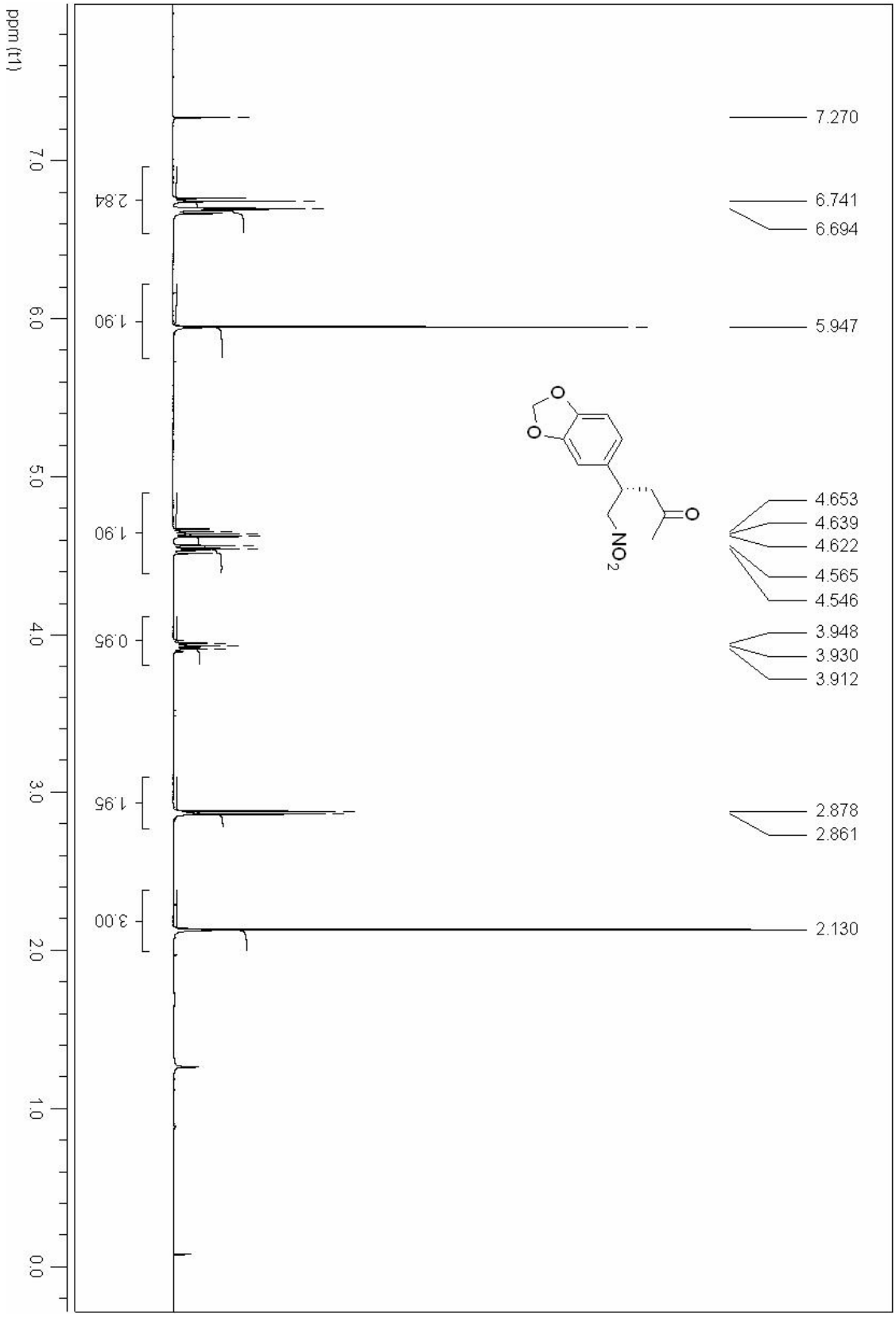
NO2
O

Compound **3d**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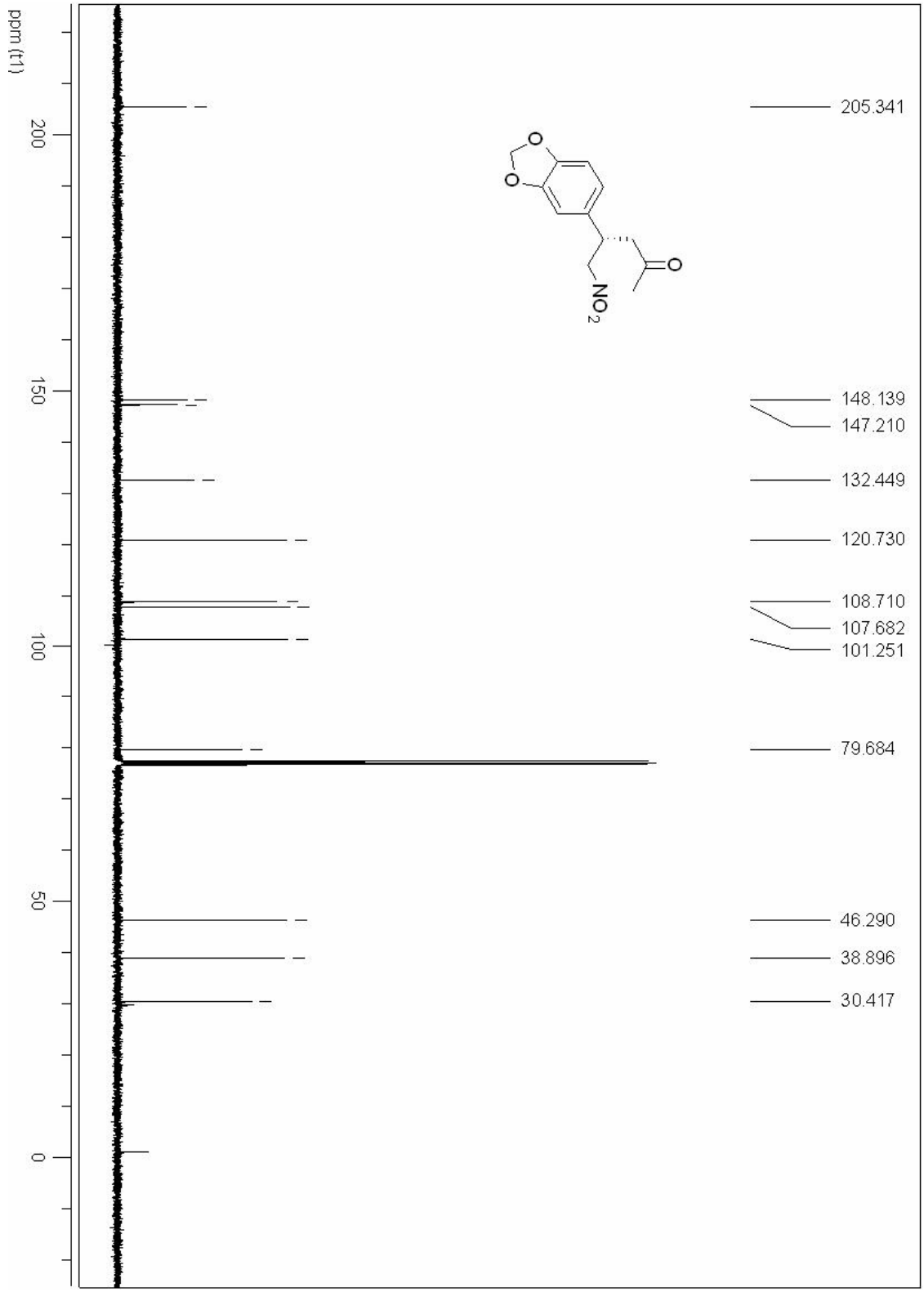
O
O
NO2

Compound **3d**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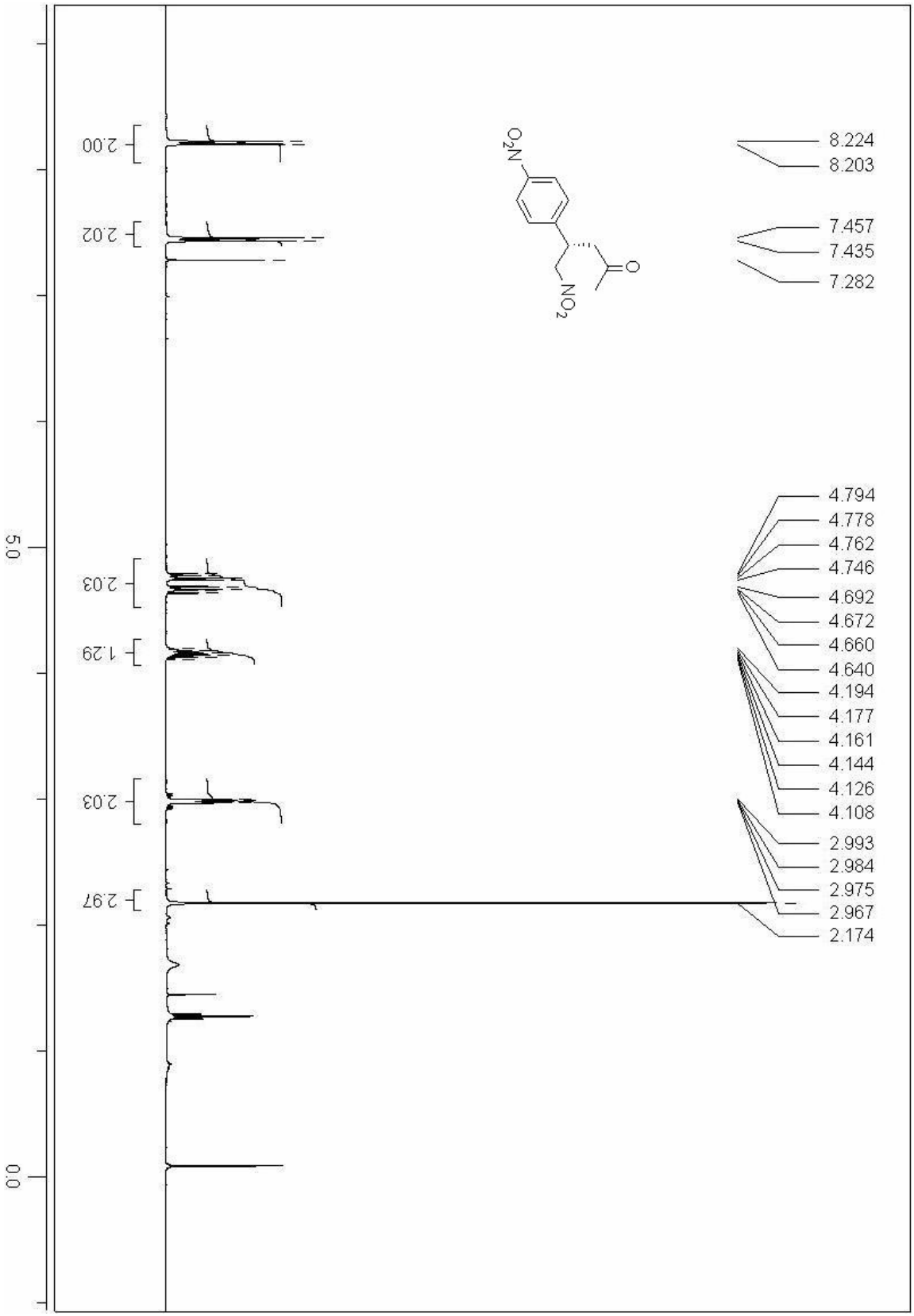
O
O
O
NO2

Compound **3e**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4.640
4.194
4.177
4.161
4.144
4.126
4.108
2.993
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2.97
5.0
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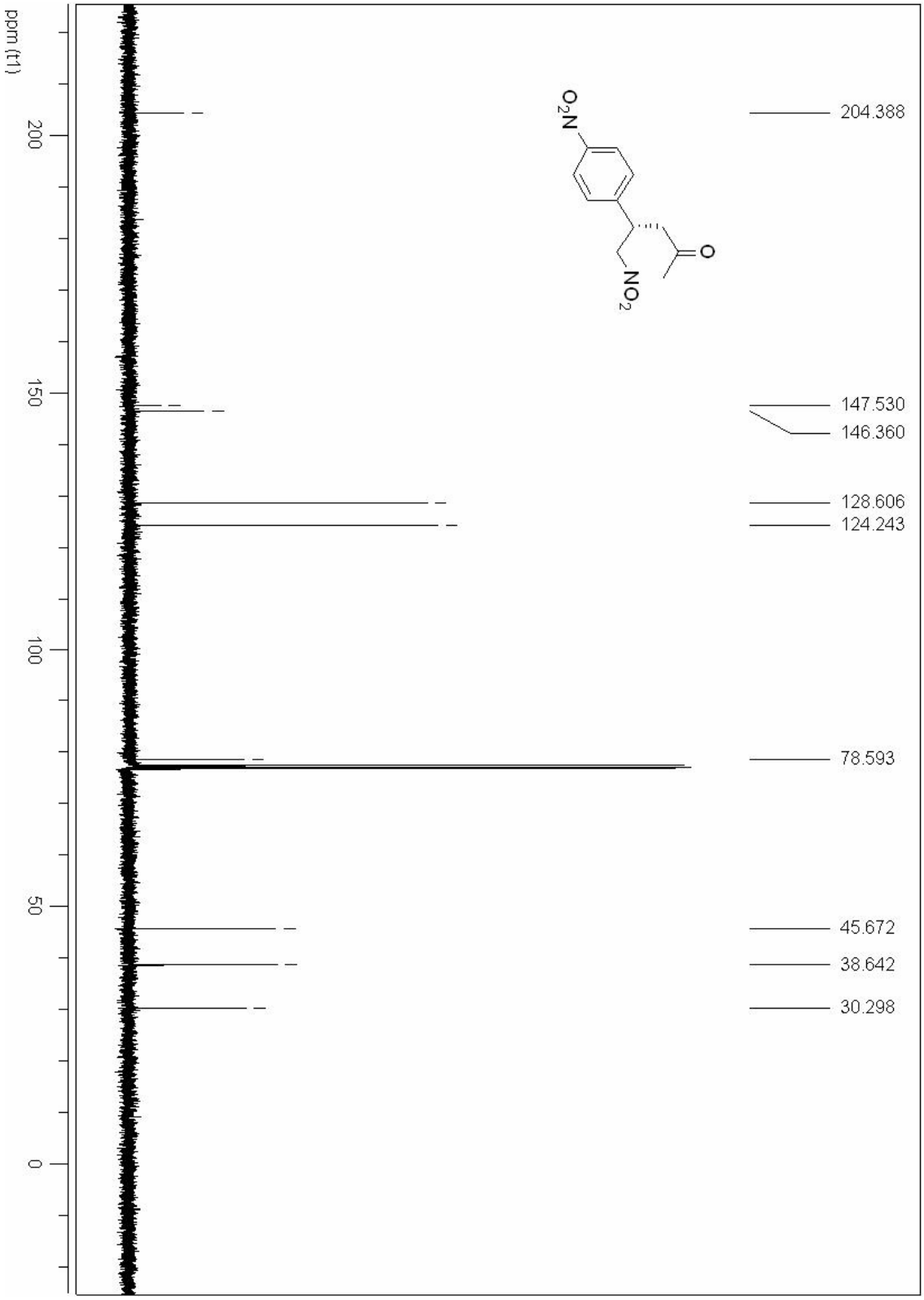
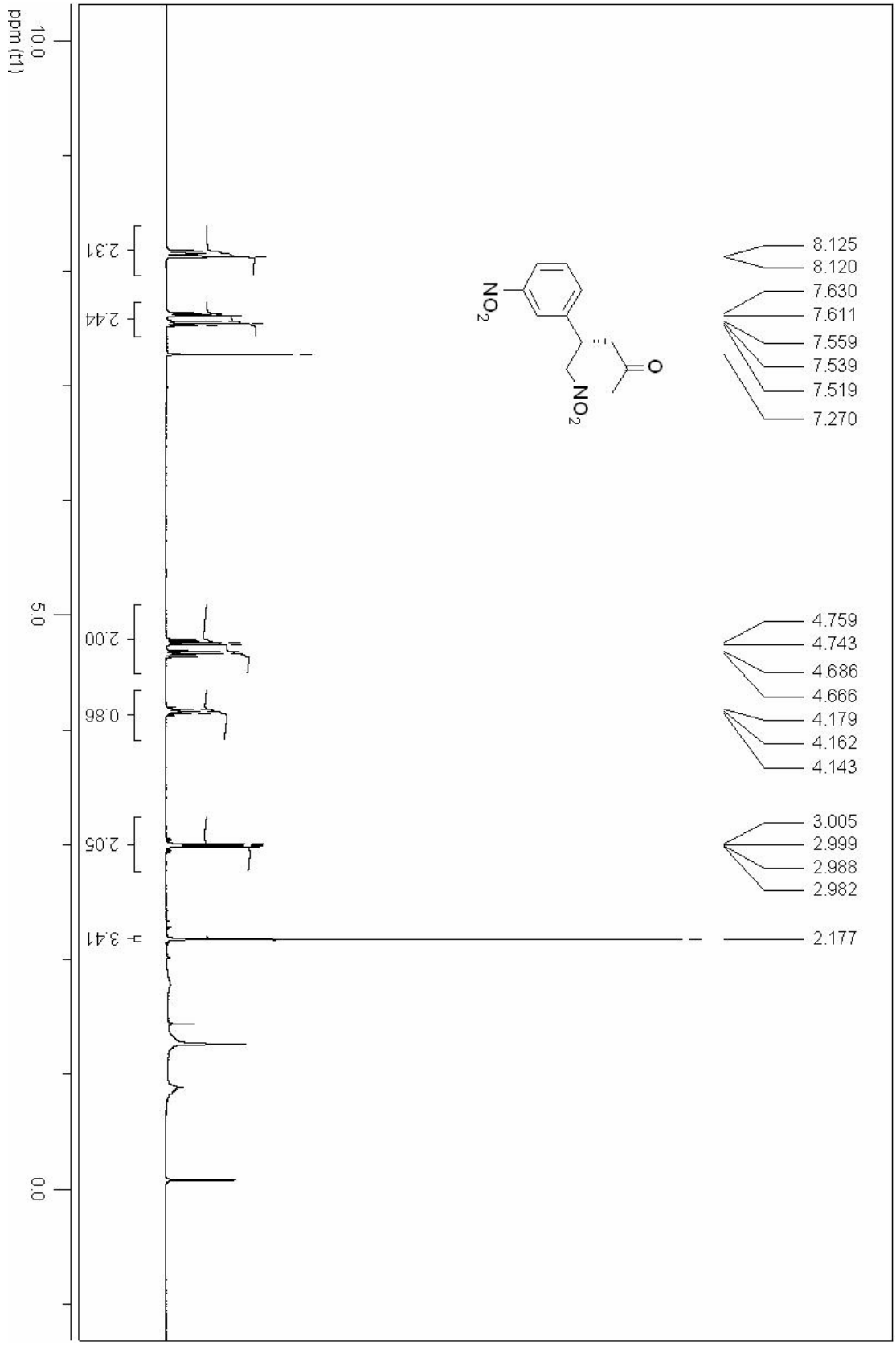
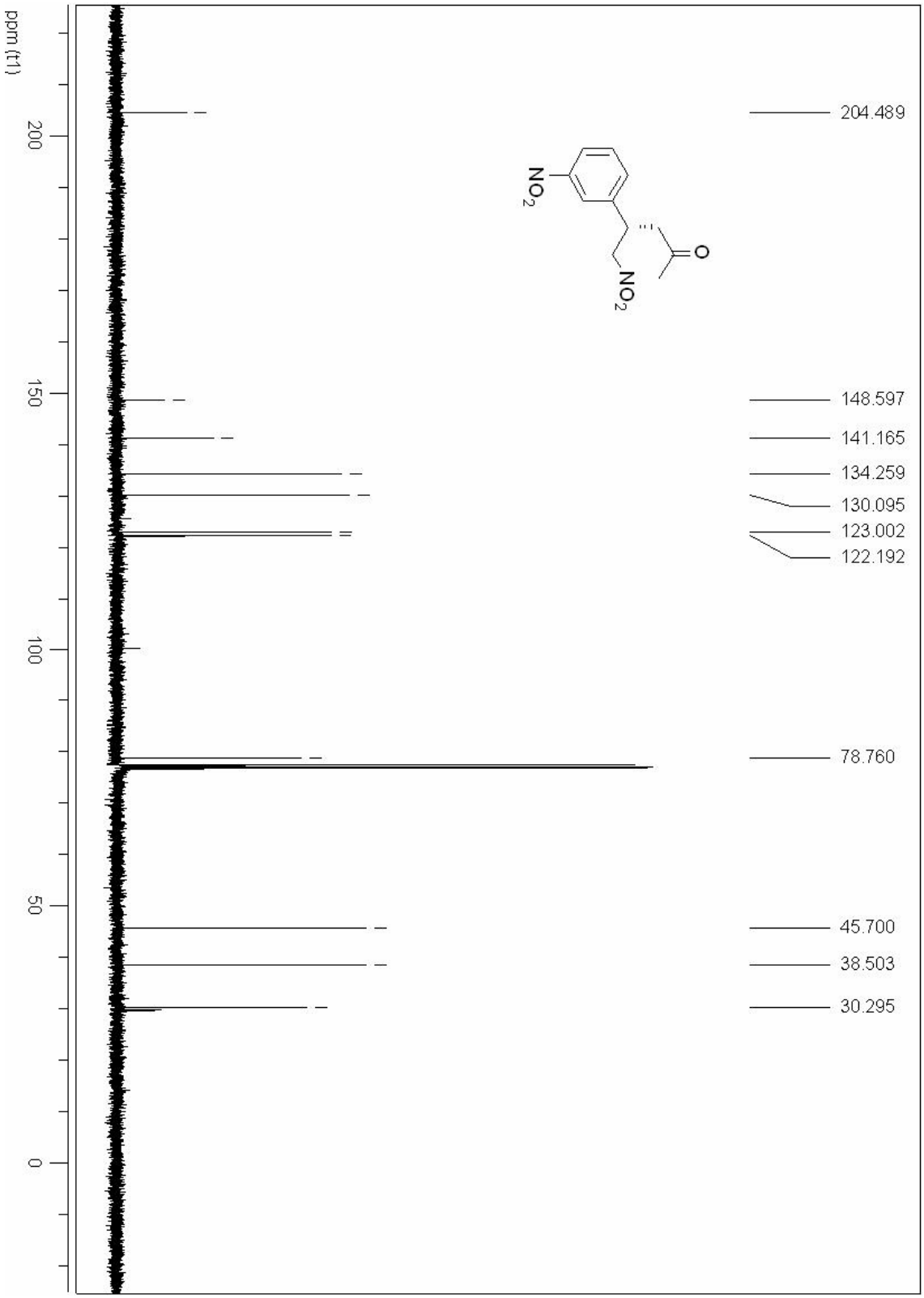
Compound **3e**


ppm (t1)
200
150
100
50
0
204.388
147.530
146.360
128.606
124.243
78.593
45.672
38.642
30.298

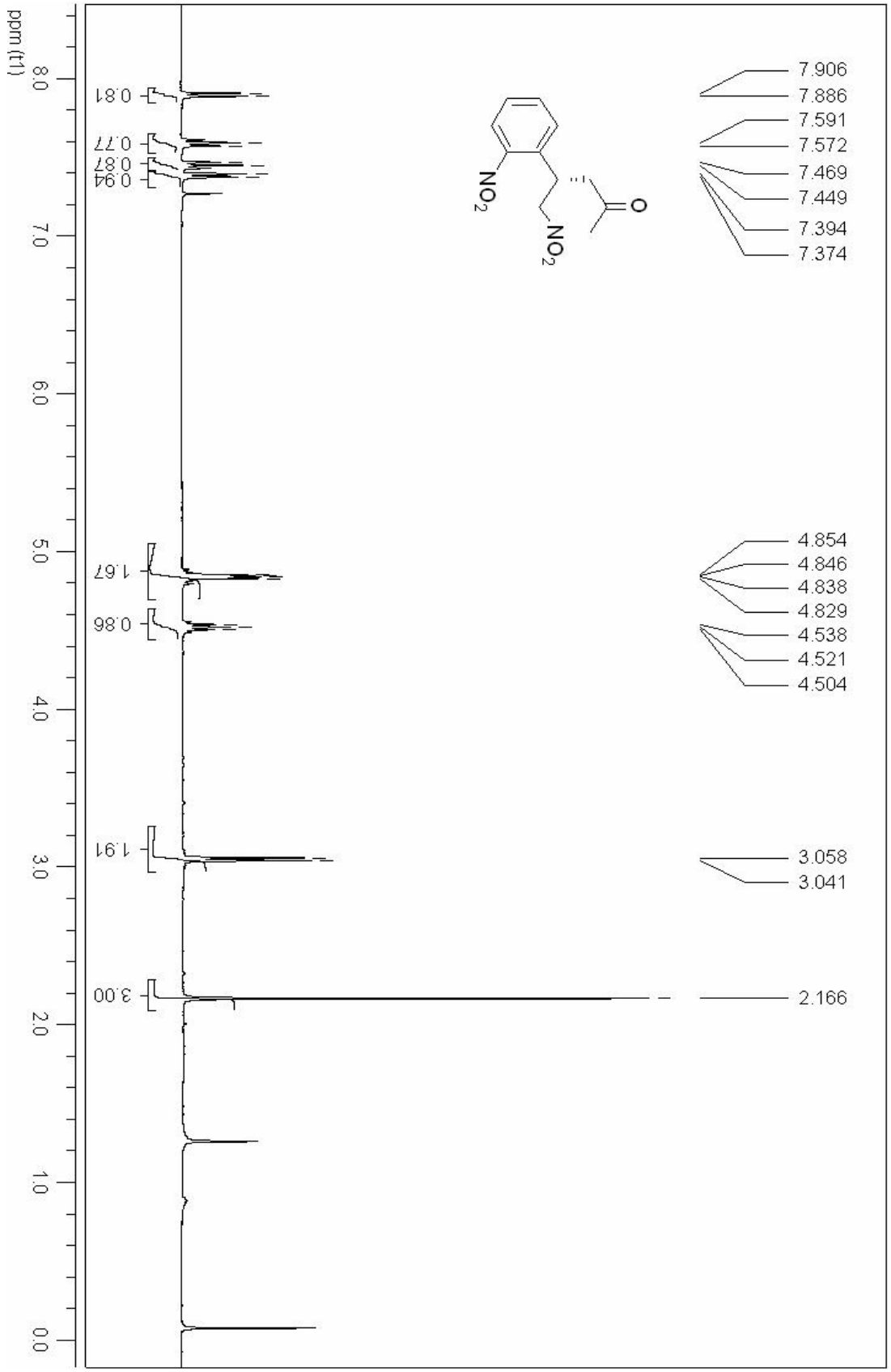
Compound **3f**


10.0
ppm (t1)
5.0
0.0
2.31
2.44
3.41
2.00
0.86
2.05
8.125
8.120
7.630
7.611
7.559
7.539
7.519
7.270
4.759
4.743
4.686
4.666
4.179
4.162
4.143
3.005
2.999
2.988
2.982
2.177
O2N
NO2
O

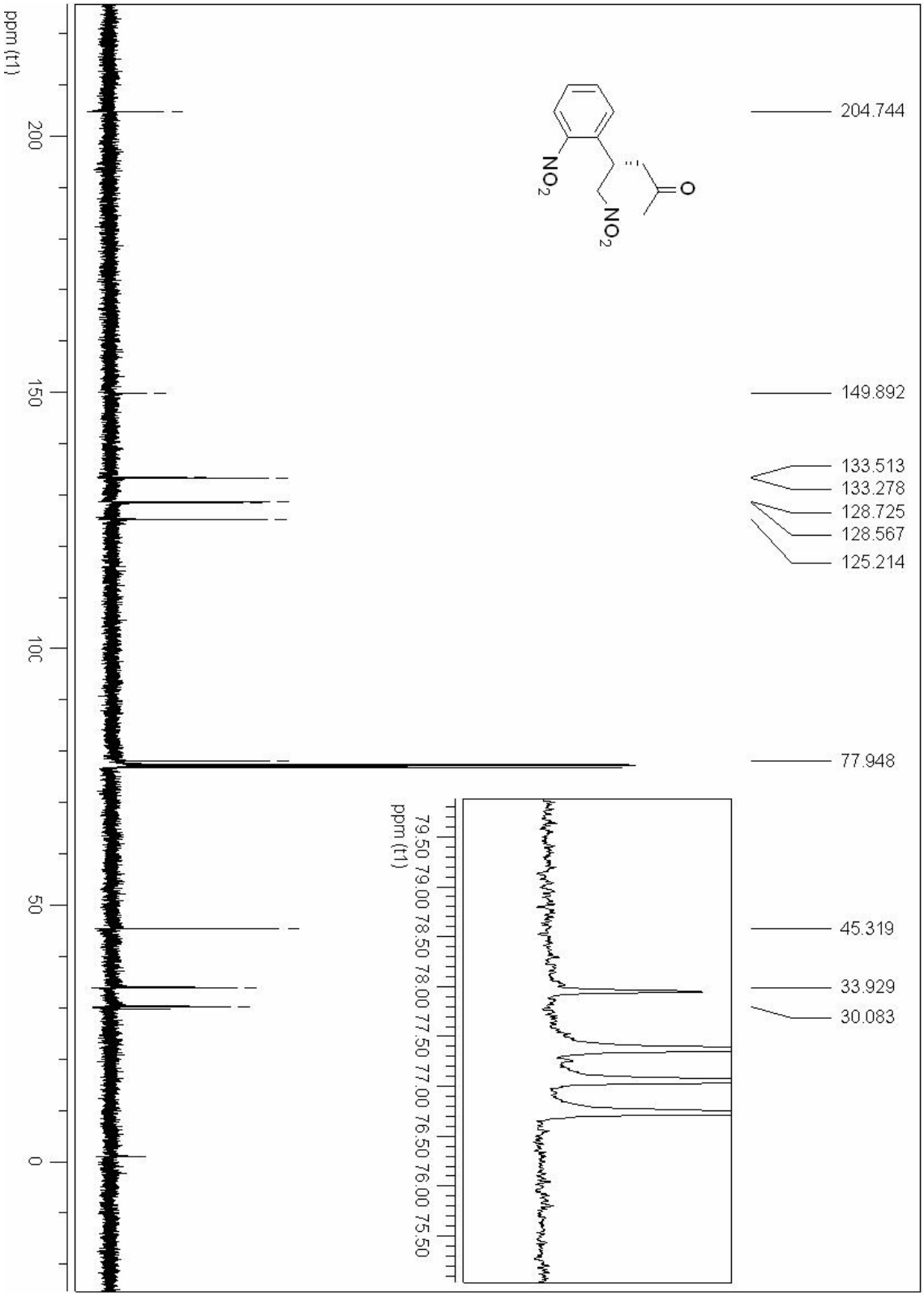
Compound **3f**


ppm (t1)
200
150
100
50
0
204.489
148.597
141.165
134.259
130.095
123.002
122.192
78.760
45.700
38.503
30.295
NO2
NO2
O

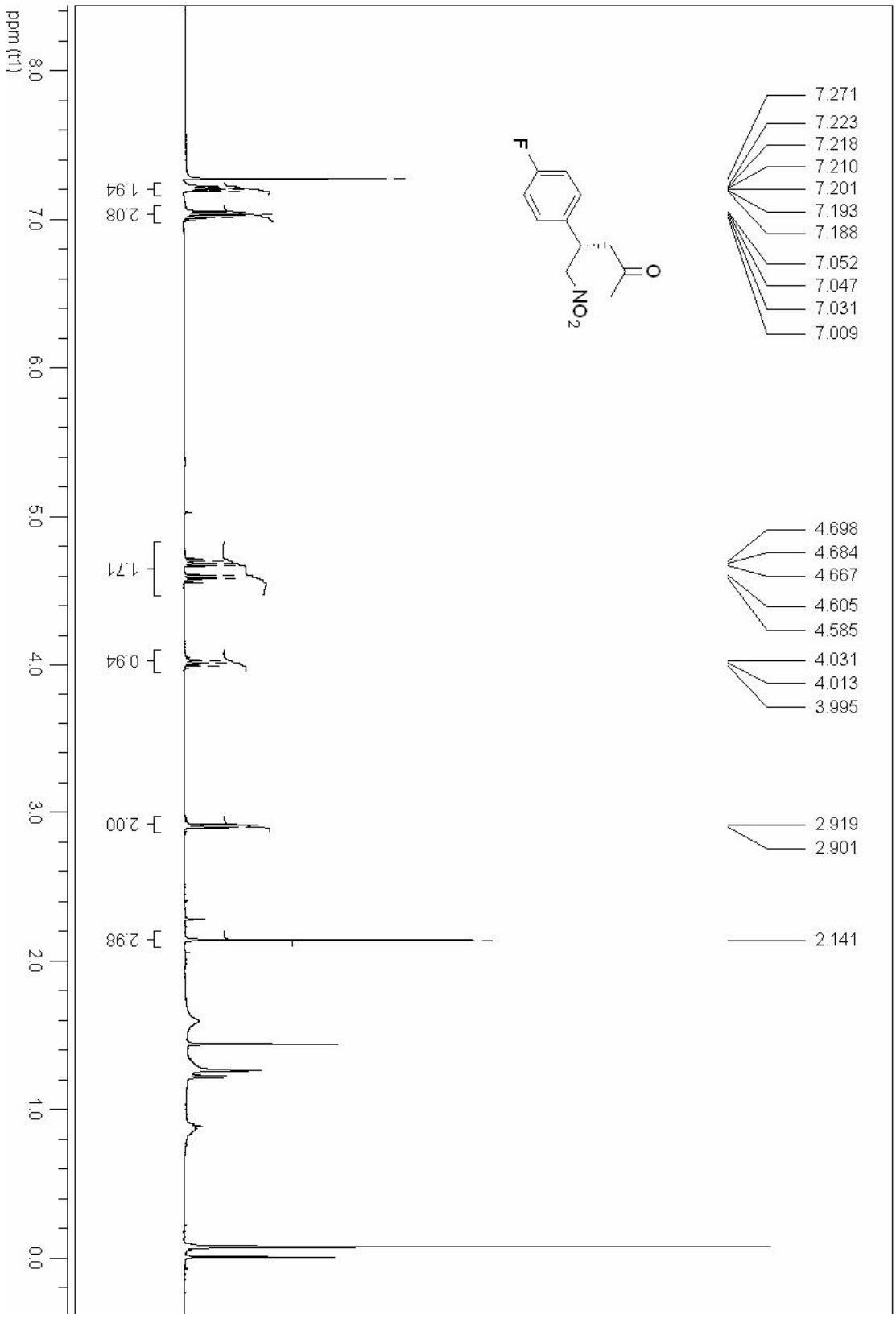
Compound **3g**


ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.81
0.77
0.87
0.94
1.67
0.86
1.91
3.00
7.906
7.886
7.591
7.572
7.469
7.449
7.394
7.374
4.854
4.846
4.838
4.829
4.538
4.521
4.504
3.058
3.041
2.166
NO2
NO2
O

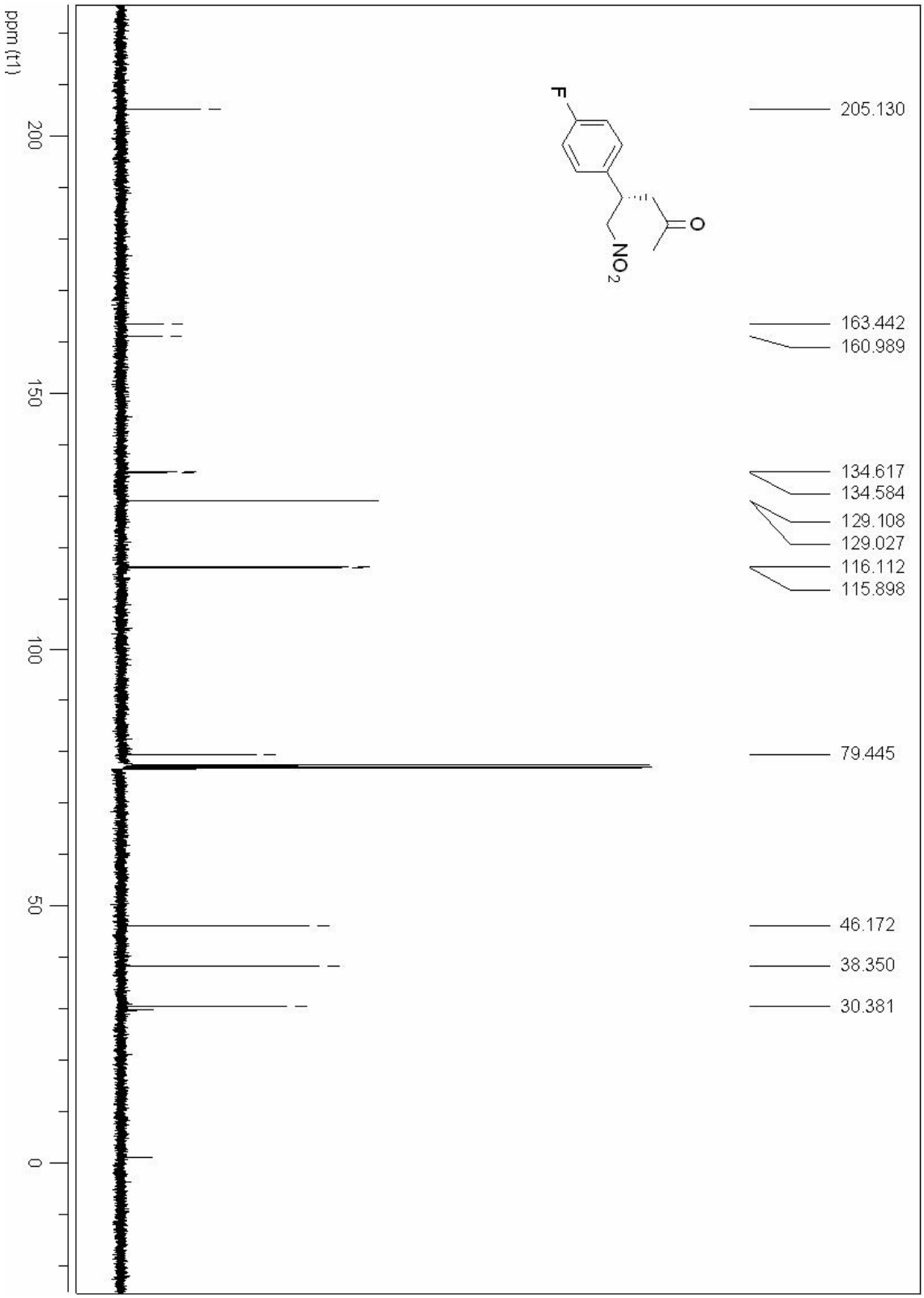
Compound **3g**


ppm (t1)
200
150
100
50
0
204.744
149.892
133.513
133.278
128.725
128.567
125.214
77.948
45.319
33.929
30.083
NO2
NO2
O
79.50 79.00 78.50 78.00 77.50 77.00 76.50 76.00 75.50
ppm (t1)

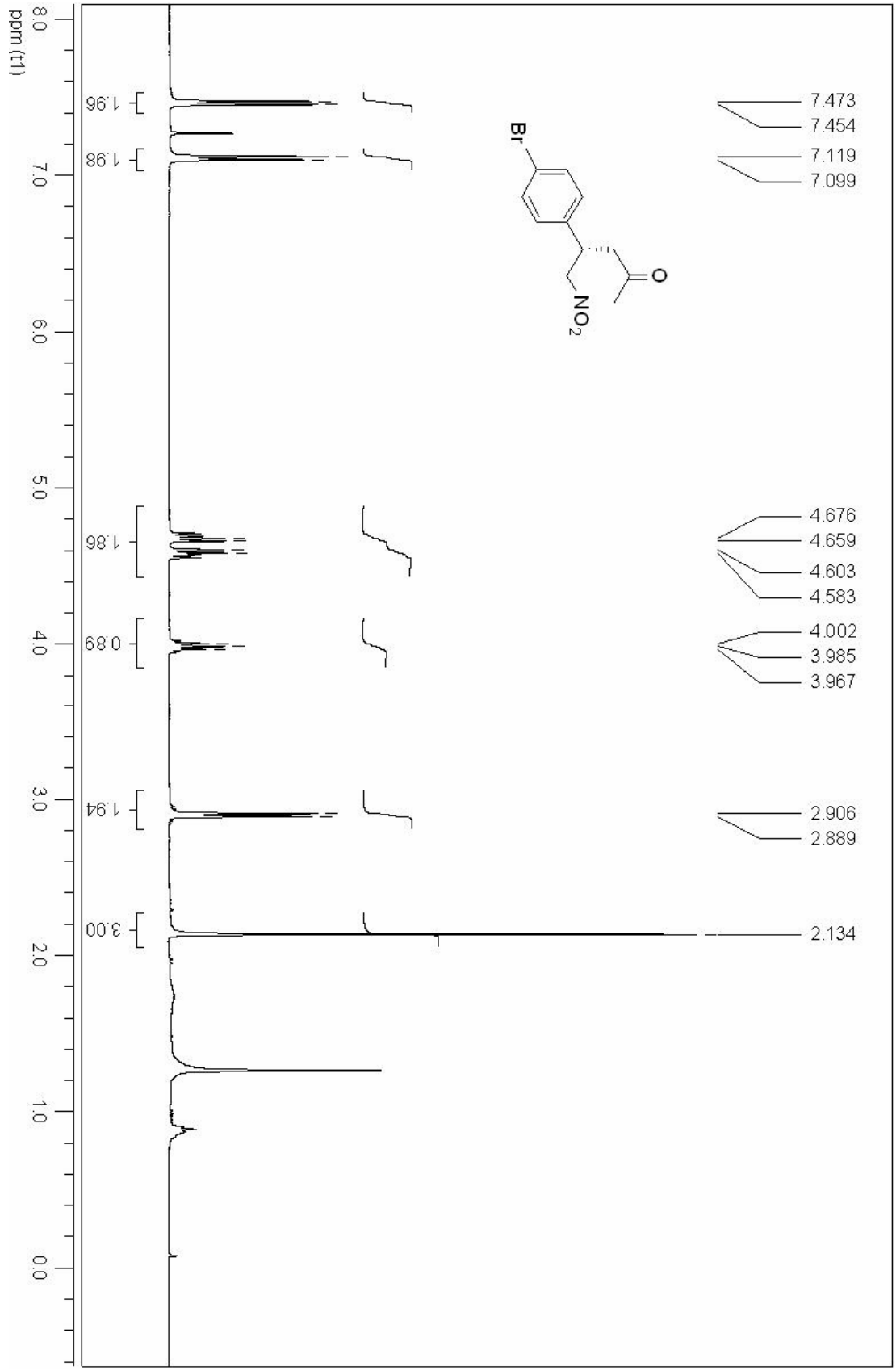
Compound **3h**


ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.94
2.08
1.71
0.94
2.00
2.98
F
O
NO2
7.271
7.223
7.218
7.210
7.201
7.193
7.188
7.052
7.047
7.031
7.009
4.698
4.684
4.667
4.605
4.585
4.031
4.013
3.995
2.919
2.901
2.141

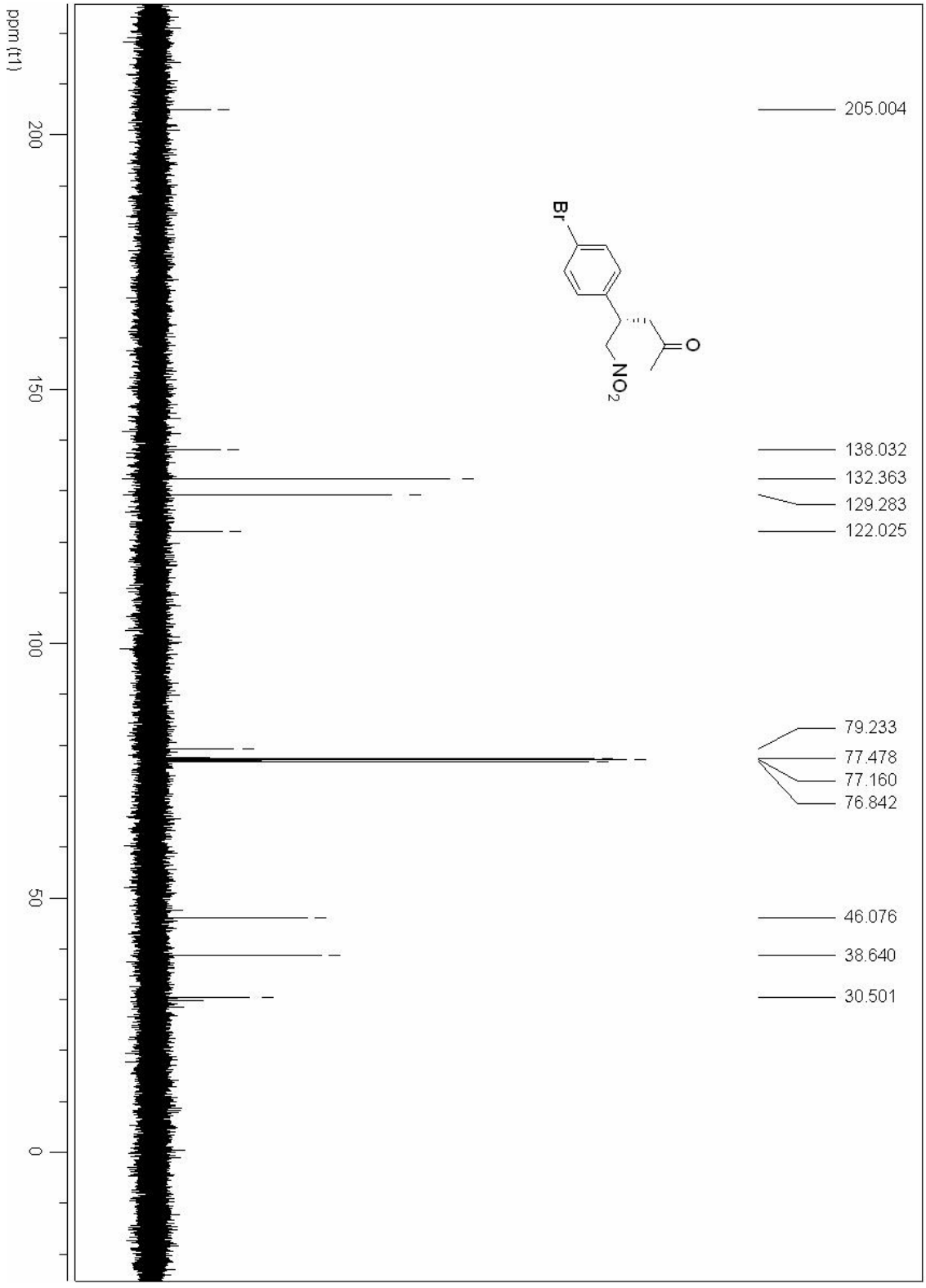
Compound **3h**


ppm (t1)
200
150
100
50
0
F
O
NO2
205.130
163.442
160.989
134.617
134.584
129.108
129.027
116.112
115.898
79.445
46.172
38.350
30.381

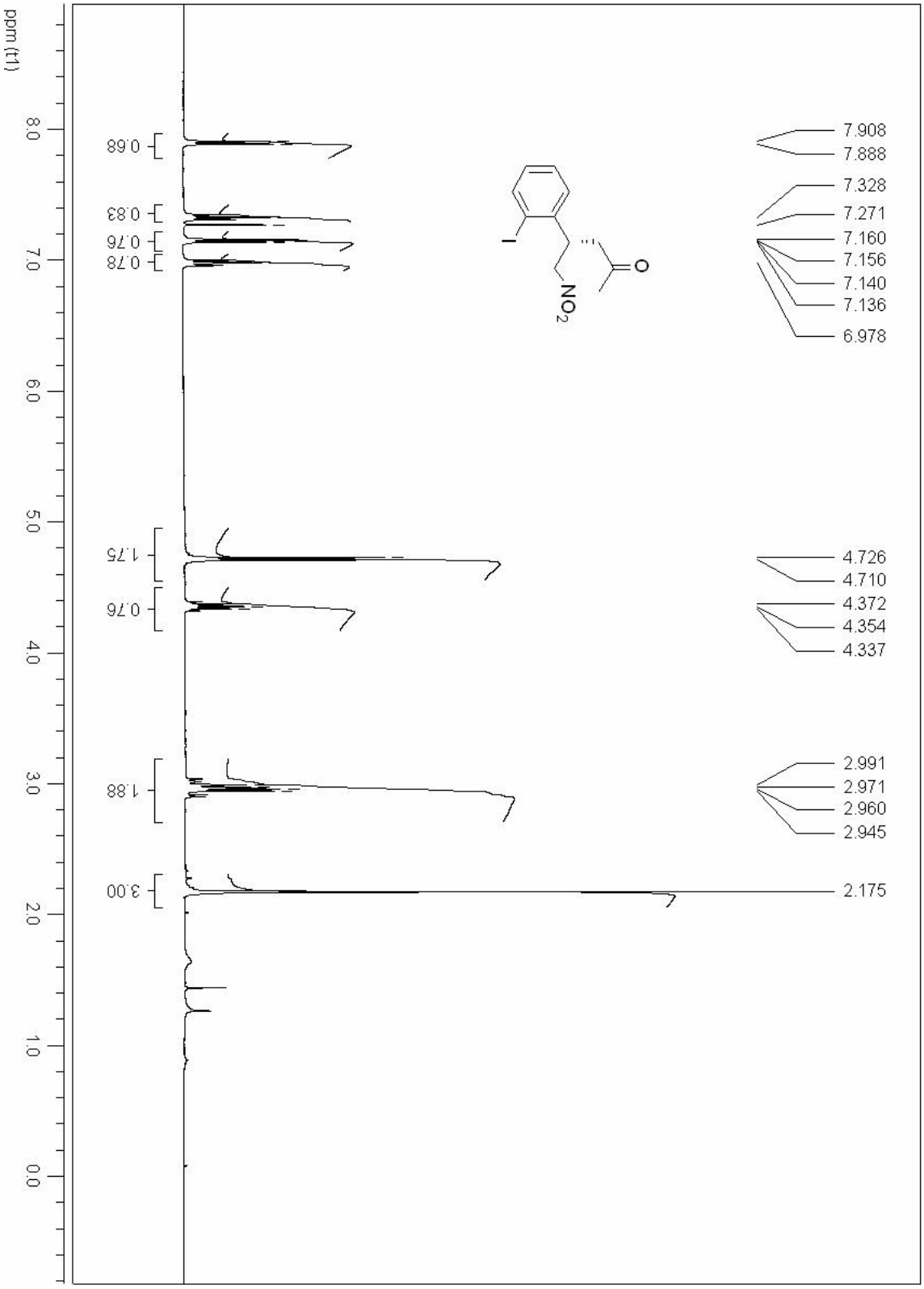
Compound **3i**


ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.96
1.98
1.86
0.89
1.94
3.00
7.473
7.454
7.119
7.099
4.676
4.659
4.603
4.583
4.002
3.985
3.967
2.906
2.889
2.134
Br
O
NO2

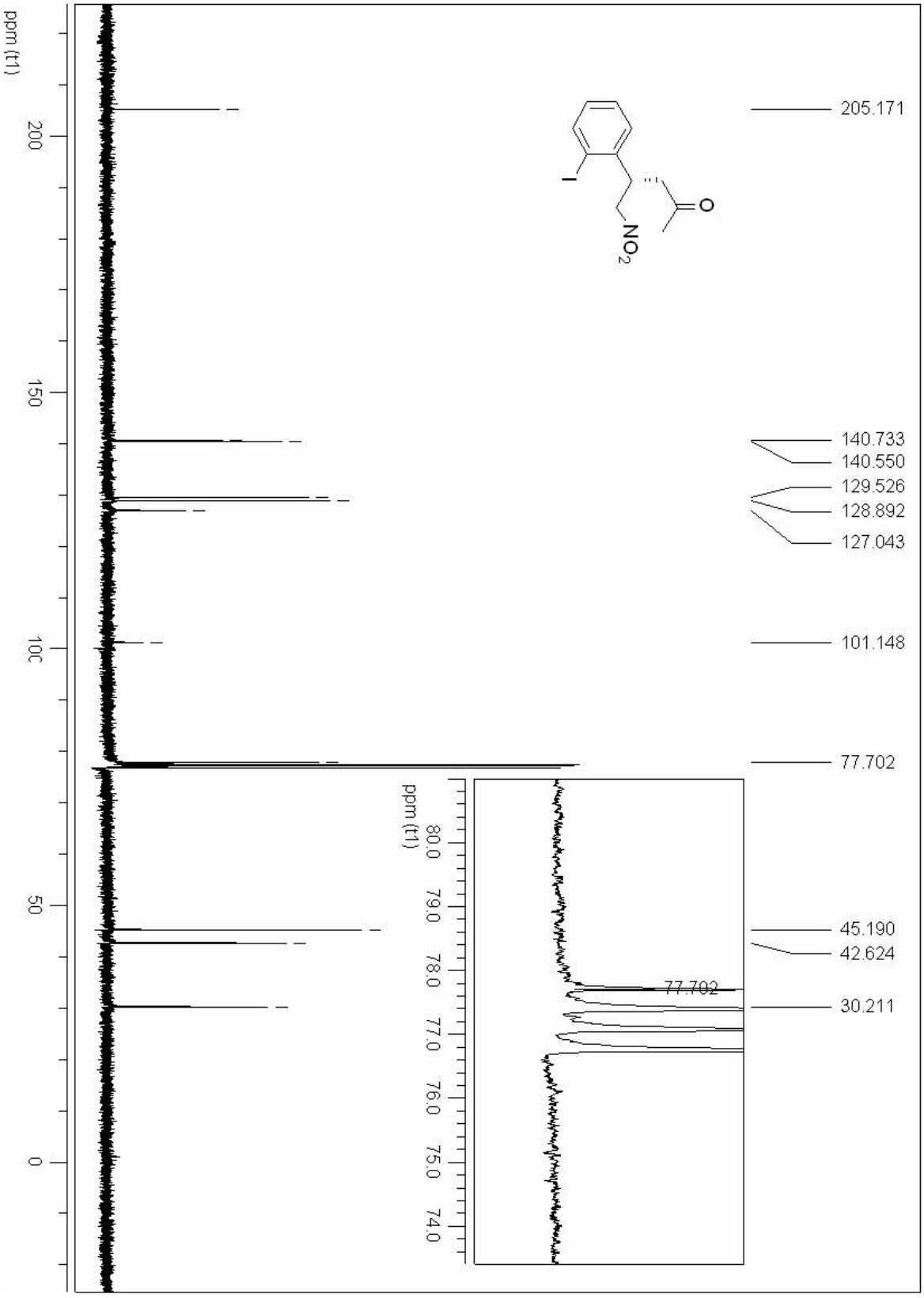
Compound **3i**


ppm (t1)
200
150
100
50
0
205.004
138.032
132.363
129.283
122.025
79.233
77.478
77.160
76.842
46.076
38.640
30.501
Br
O
NO2

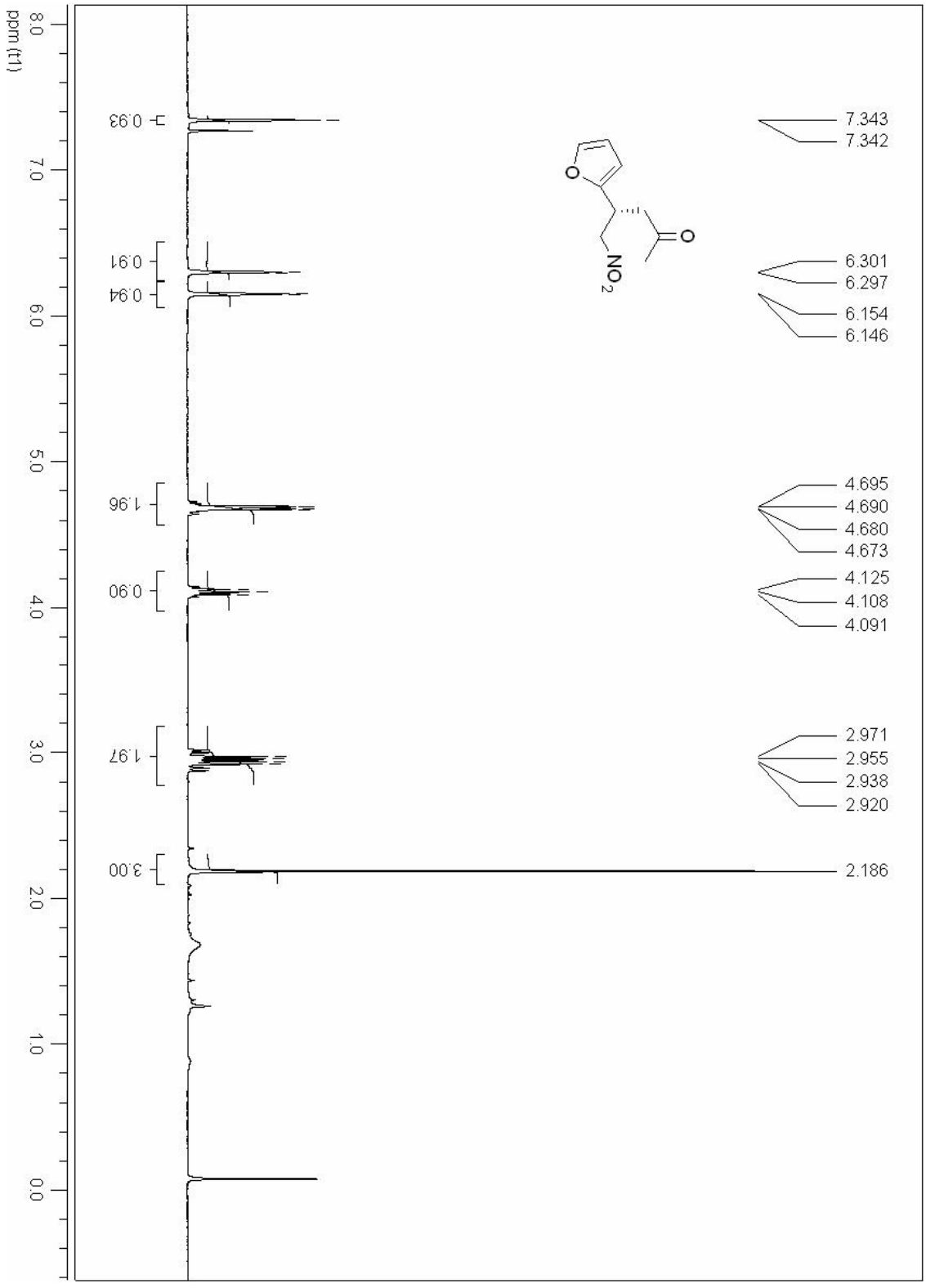
Compound **3j**


ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.68
0.83
0.76
0.78
1.75
0.76
1.88
3.00
I
O
NO2
7.908
7.888
7.328
7.271
7.160
7.156
7.140
7.136
6.978
4.726
4.710
4.372
4.354
4.337
2.991
2.971
2.960
2.945
2.175

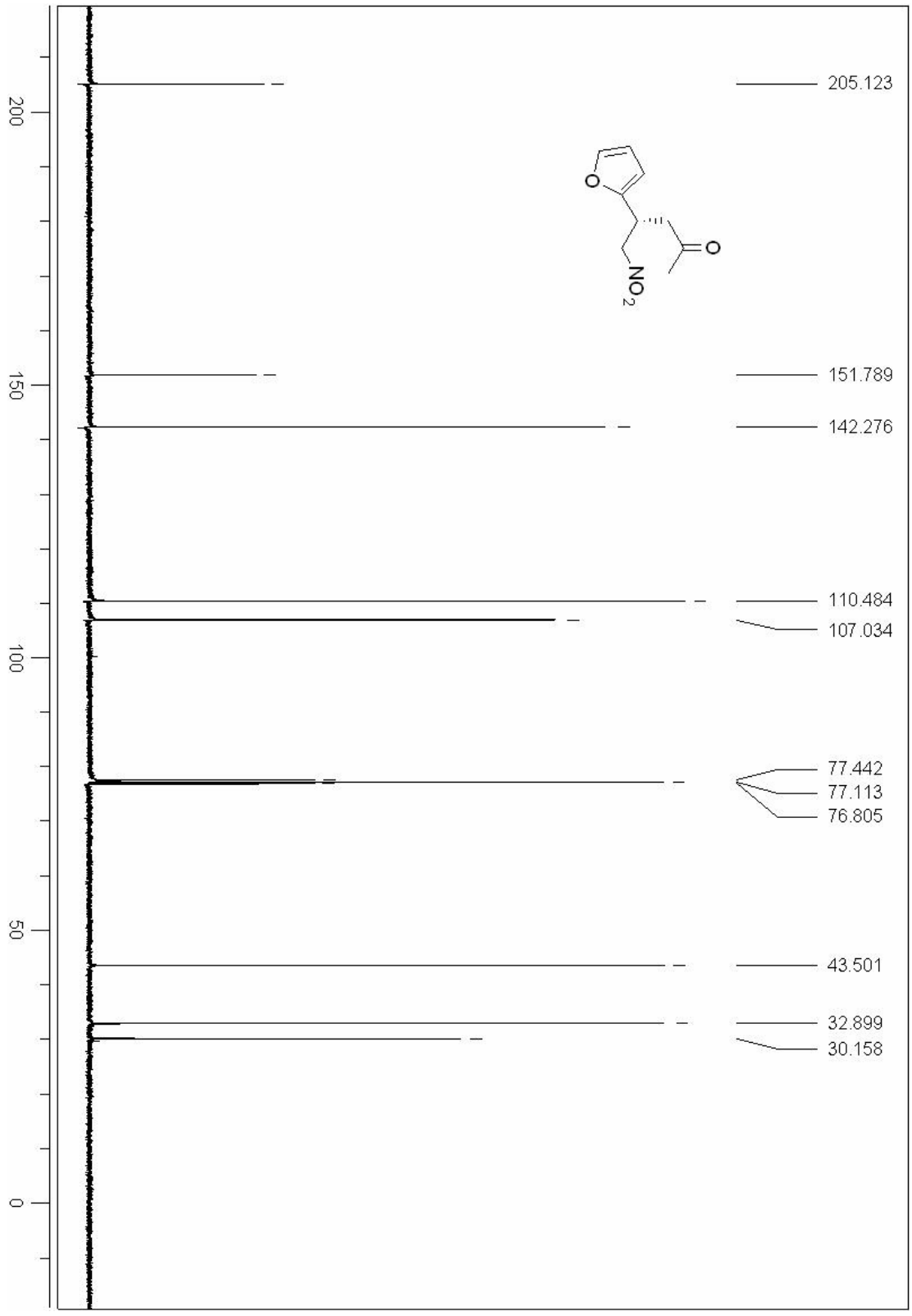
Compound **3j**


ppm (t1)
200
150
100
50
0
205.171
140.733
140.550
129.526
128.892
127.043
101.148
77.702
45.190
42.624
30.211
77.702
ppm (t1)
80.0
79.0
78.0
77.0
76.0
75.0
74.0
I
O
NO2

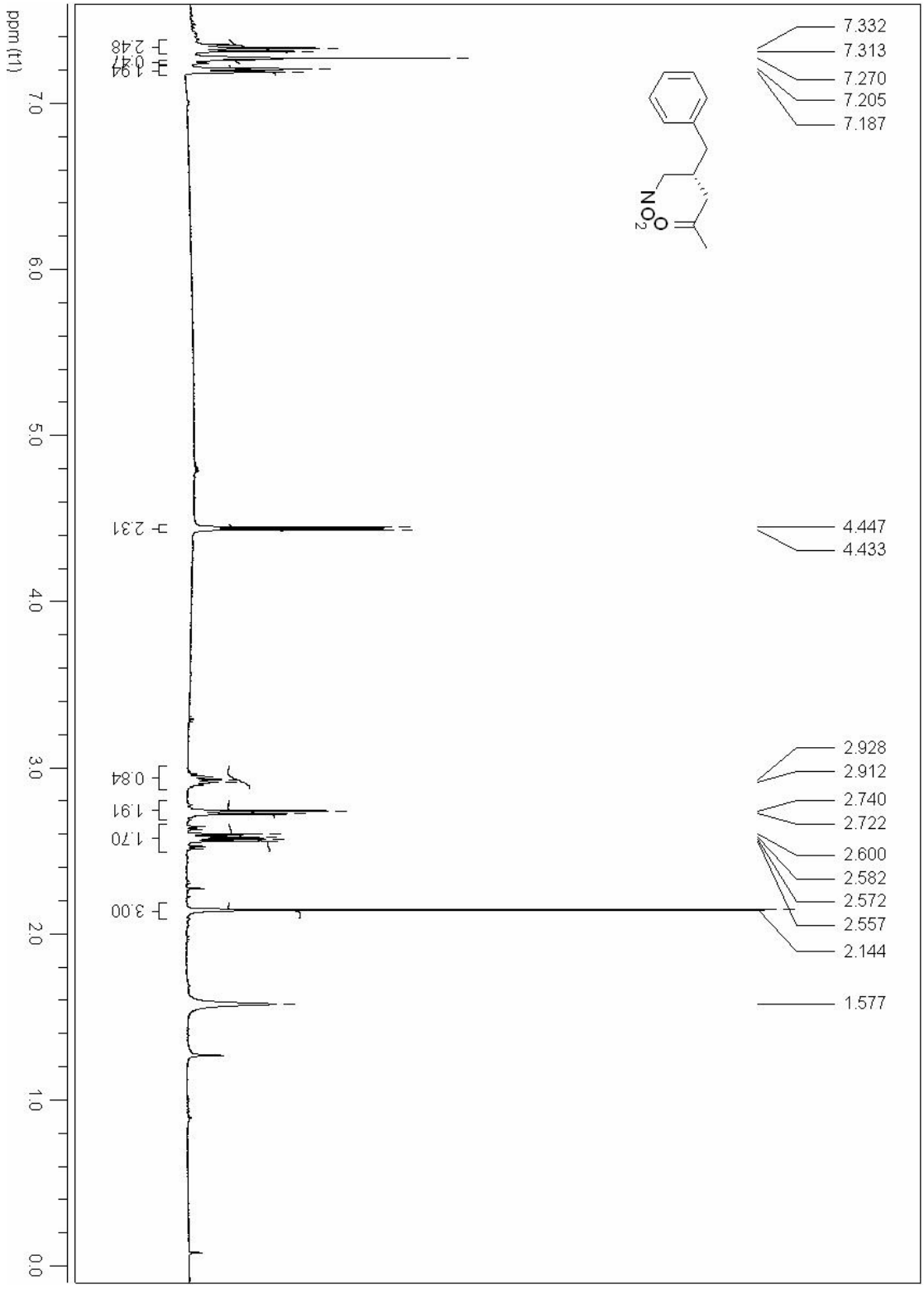
Compound **3k**


ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.93
0.91
0.94
1.96
0.90
1.97
3.00
7.343
7.342
6.301
6.297
6.154
6.146
4.695
4.690
4.680
4.673
4.125
4.108
4.091
2.971
2.955
2.938
2.920
2.186
O
O
NO2

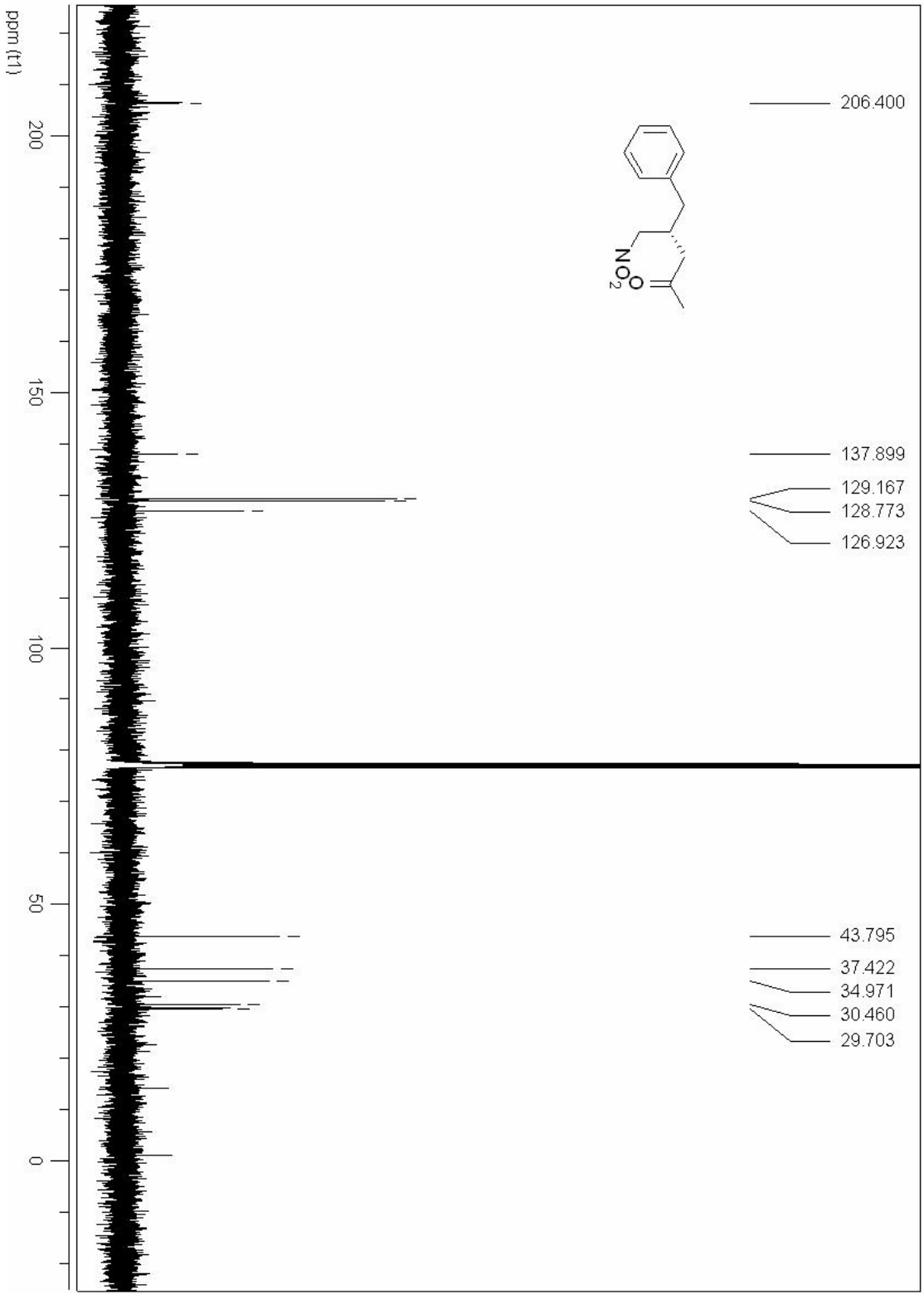
Compound **3k**


205.123
151.789
142.276
110.484
107.034
77.442
77.113
76.805
43.501
32.899
30.158
200
150
100
50
0
O
O
NO2

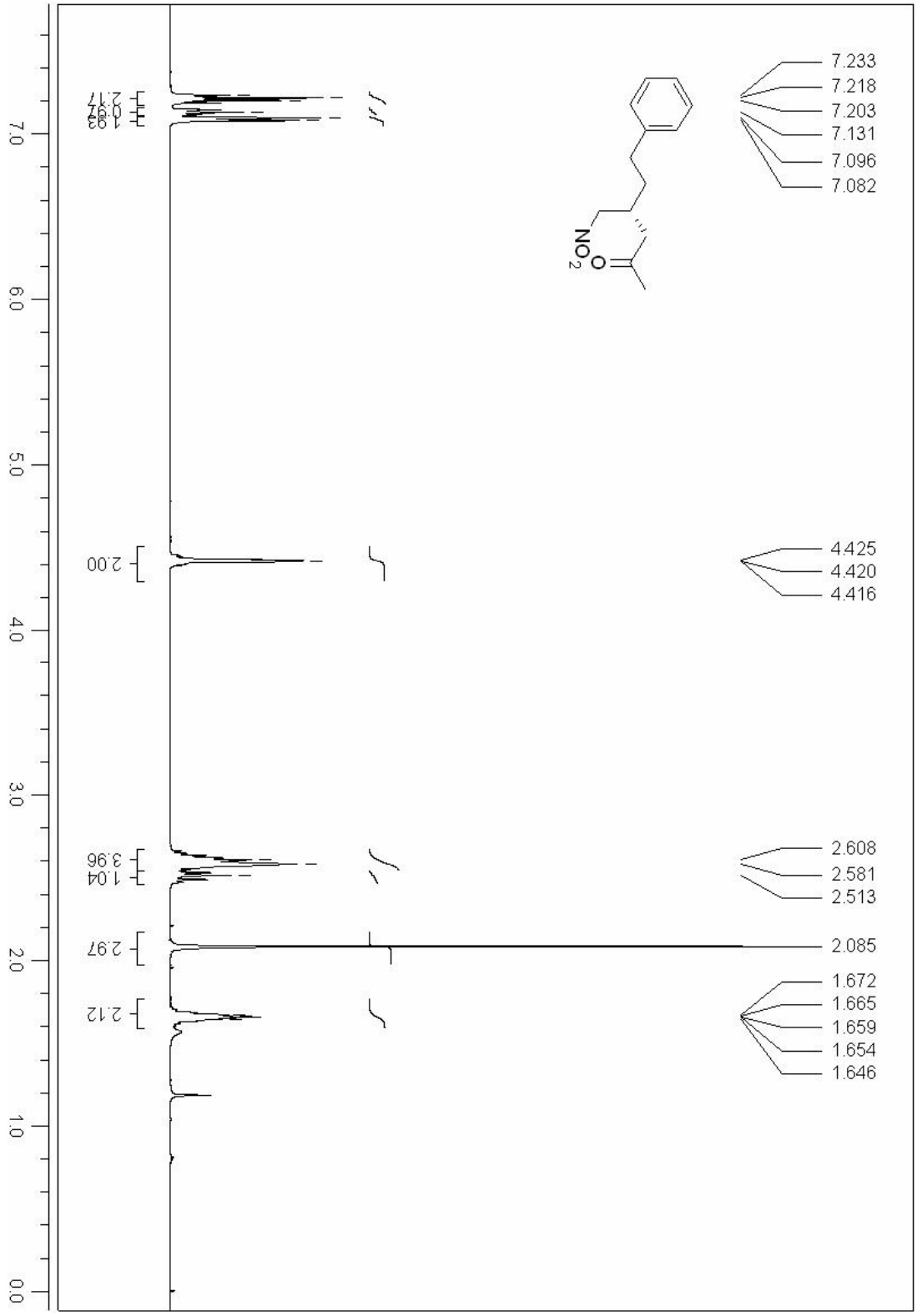
Compound **3l**


ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.48
0.47
1.94
2.31
0.84
1.91
1.70
3.00
7.332
7.313
7.270
7.205
7.187
4.447
4.433
2.928
2.912
2.740
2.722
2.600
2.582
2.572
2.557
2.144
1.577

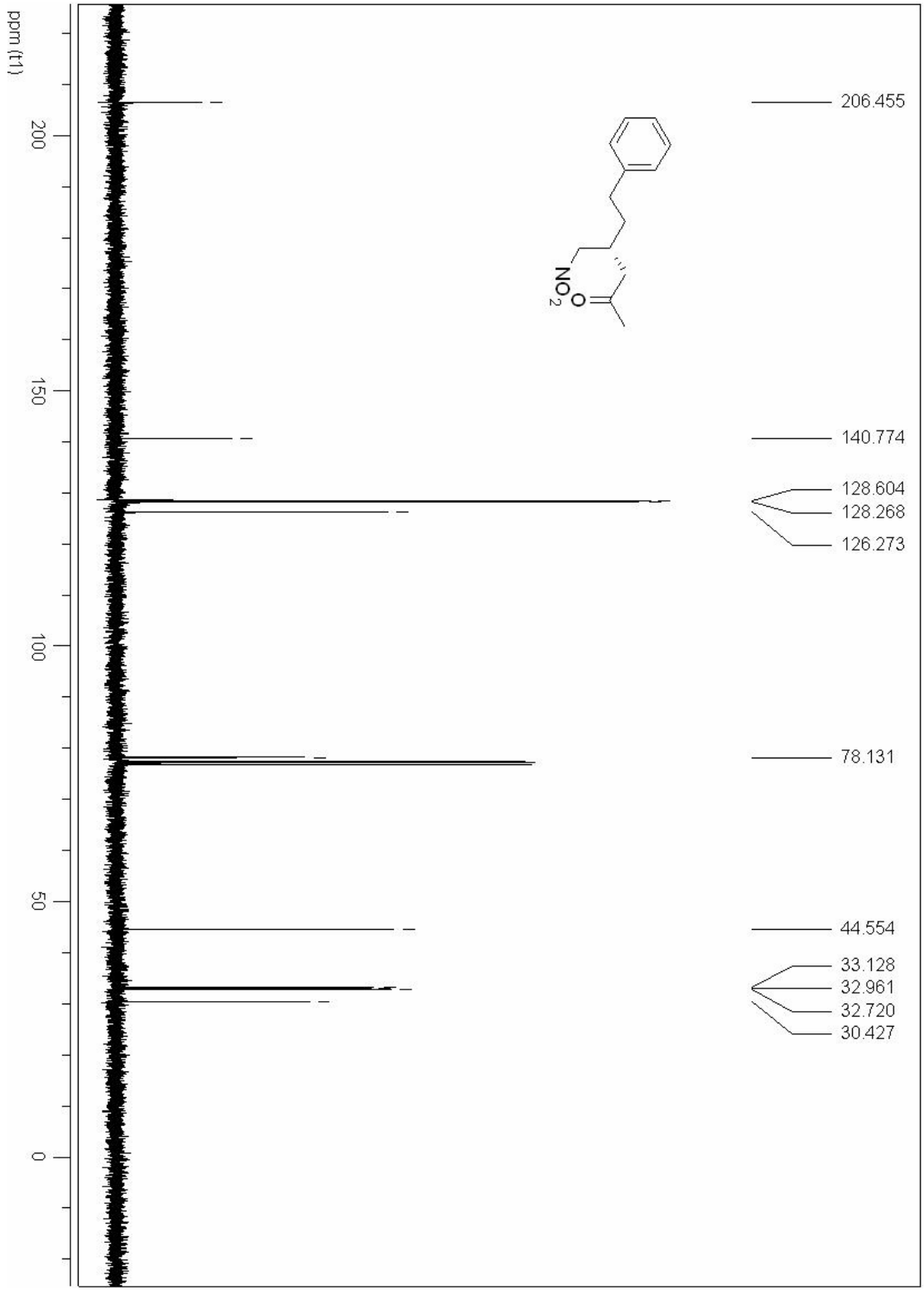
Compound **3l**


ppm (t1)
200
150
100
50
0
206.400
137.899
129.167
128.773
126.923
43.795
37.422
34.971
30.460
29.703
NO2

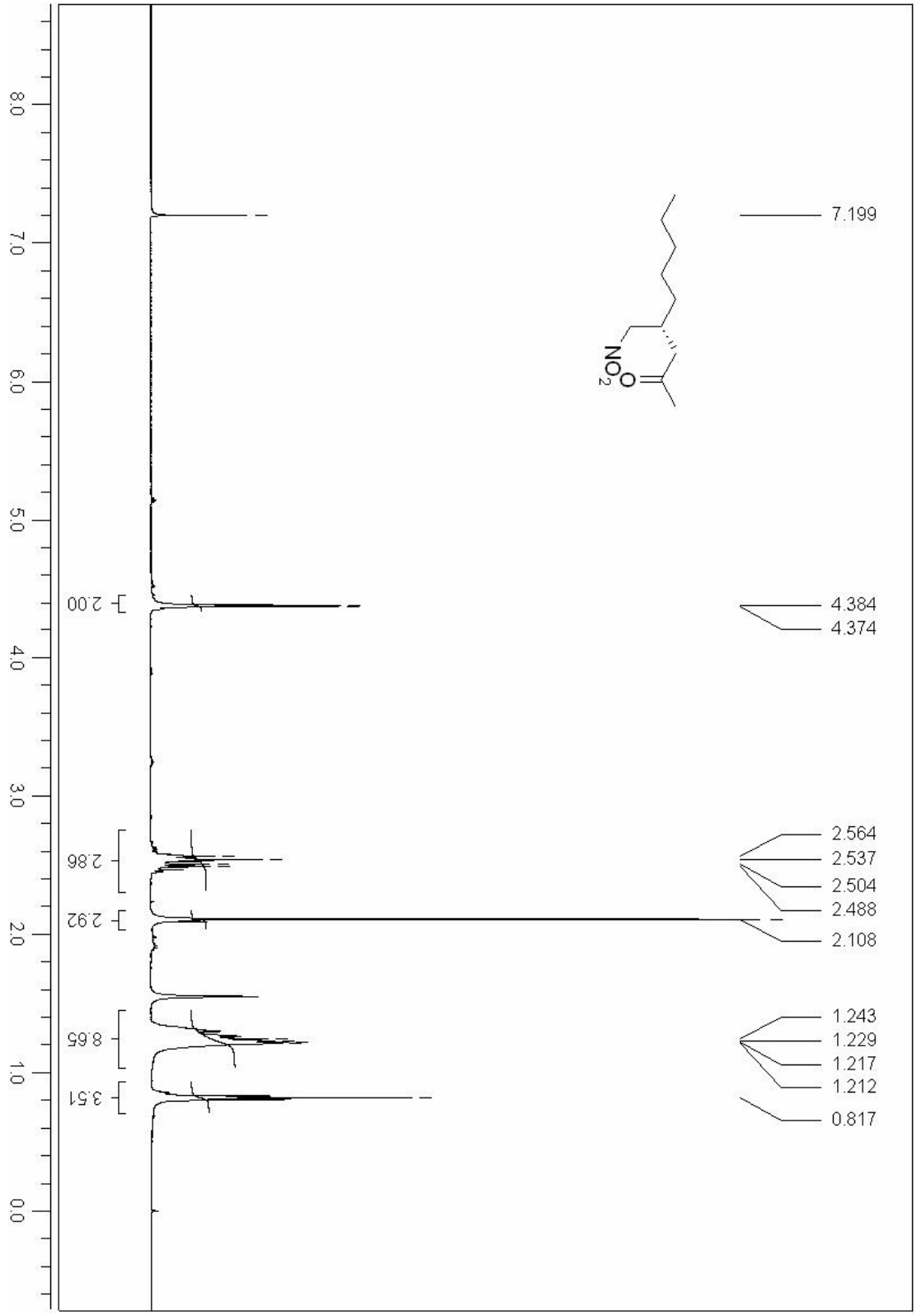
Compound **3m**


7.233
7.218
7.203
7.131
7.096
7.082
4.425
4.420
4.416
2.608
2.581
2.513
2.085
1.672
1.665
1.659
1.654
1.646
2.17
1.93
0.97
2.00
3.96
1.04
2.97
2.12
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

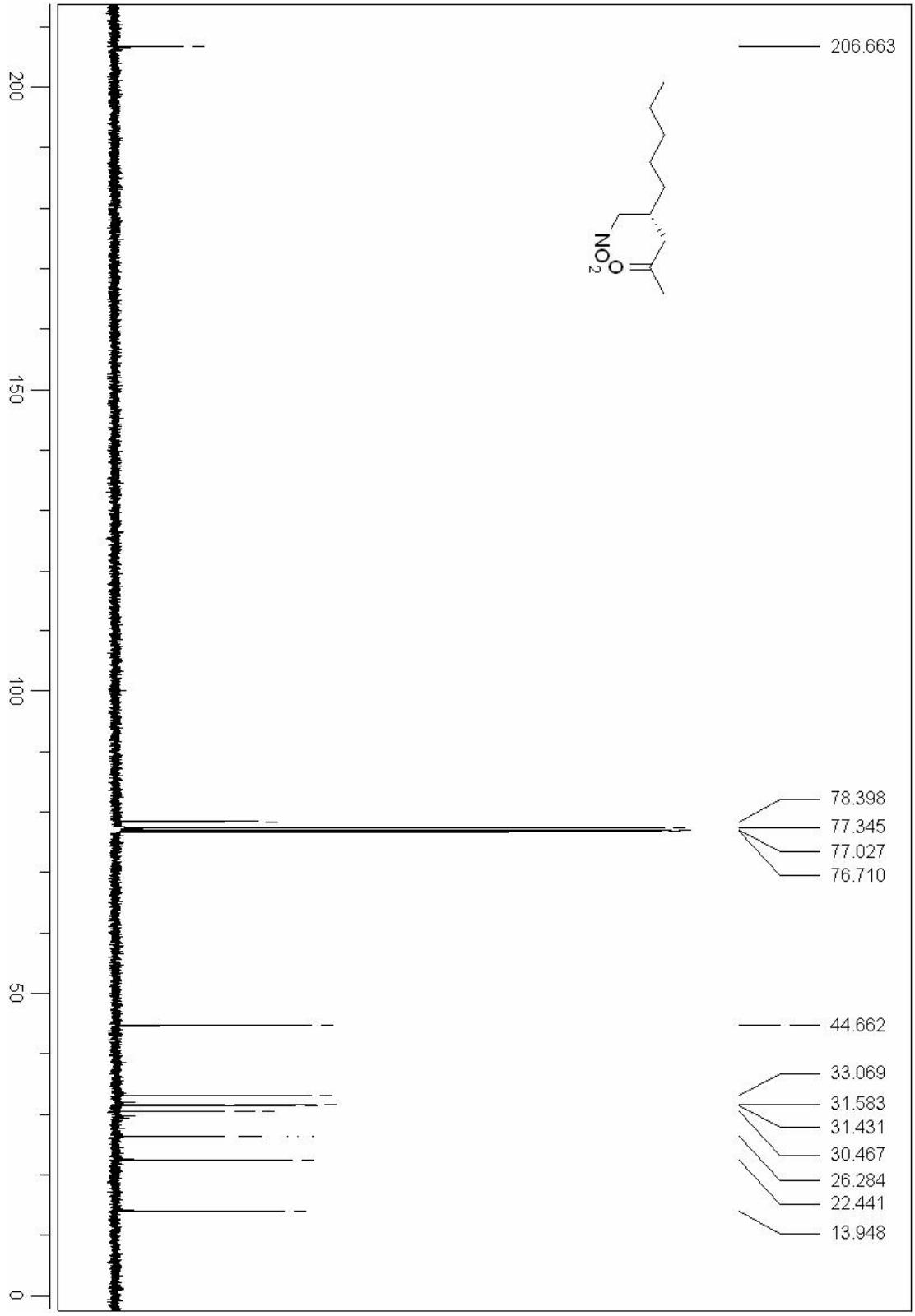
Compound **3m**


ppm (t1)
200
150
100
50
0
206.455
140.774
128.604
128.268
126.273
78.131
44.554
33.128
32.961
32.720
30.427
NO2
O

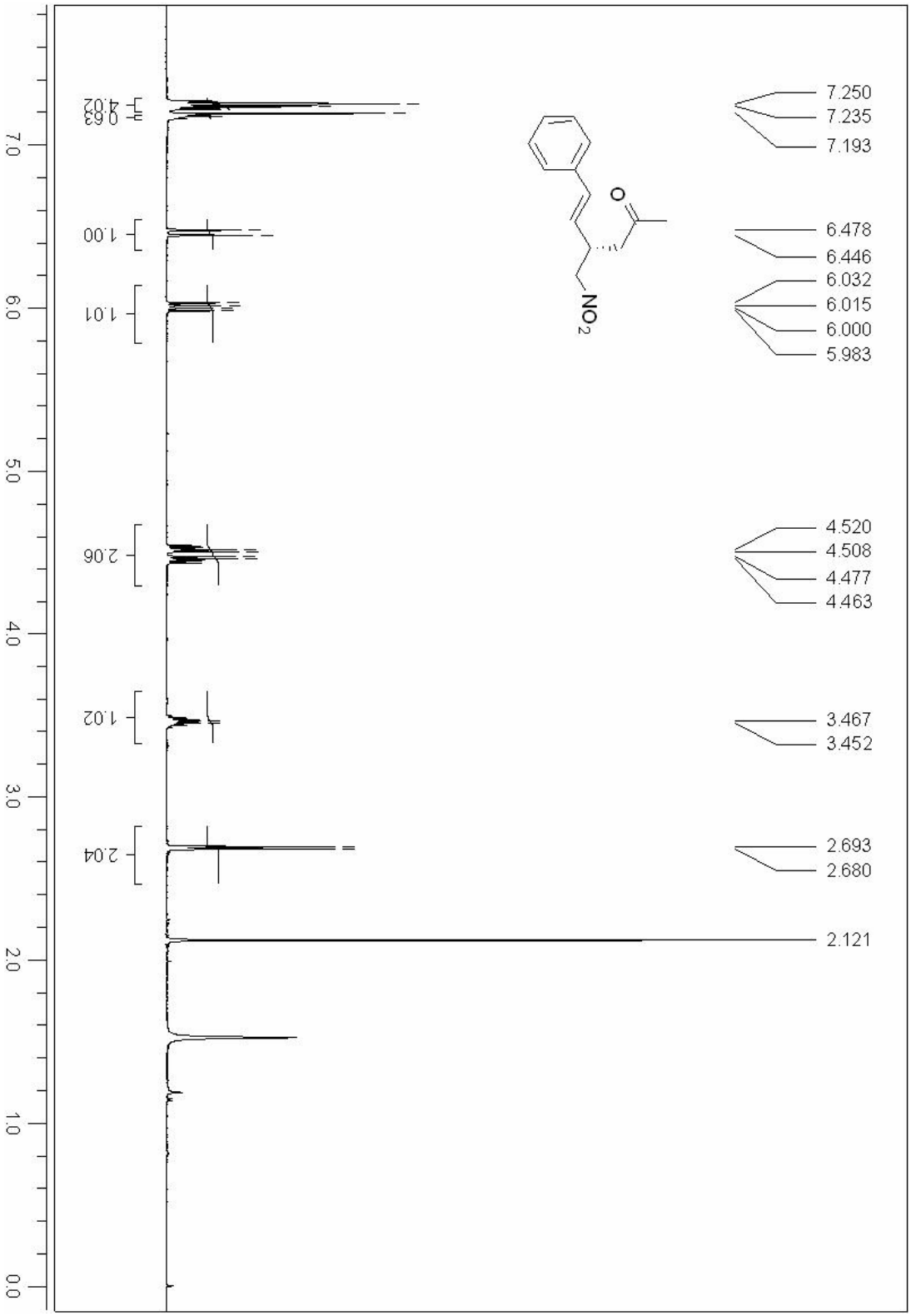
Compound **3n**


7.199
4.384
4.374
2.564
2.537
2.504
2.488
2.108
1.243
1.229
1.217
1.212
0.817
2.00
2.86
2.92
8.65
3.51
NO2
O
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

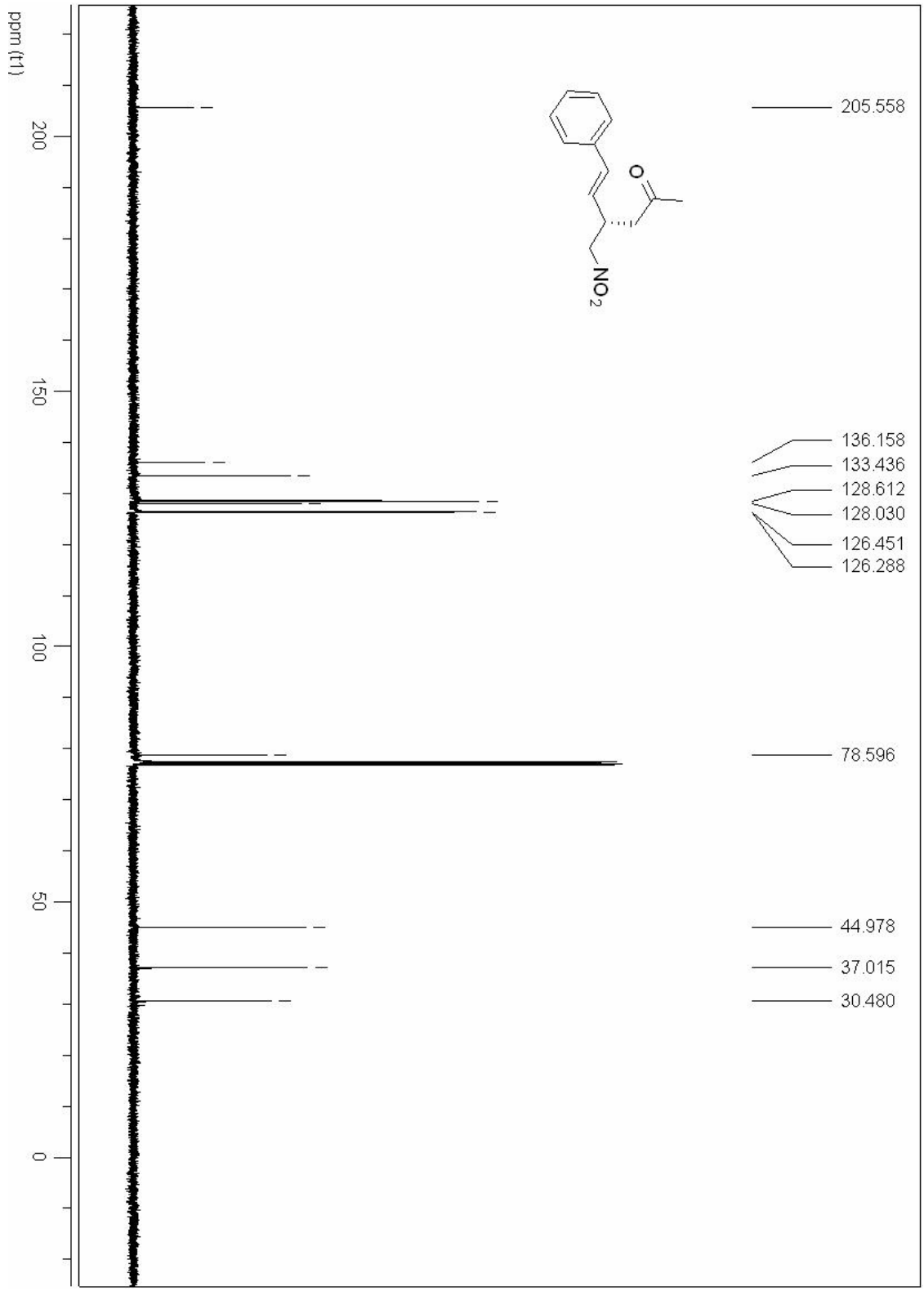
Compound **3n**


206.663
78.398
77.345
77.027
76.710
44.662
33.069
31.583
31.431
30.467
26.284
22.441
13.948
200
150
100
50
0
NO2
O

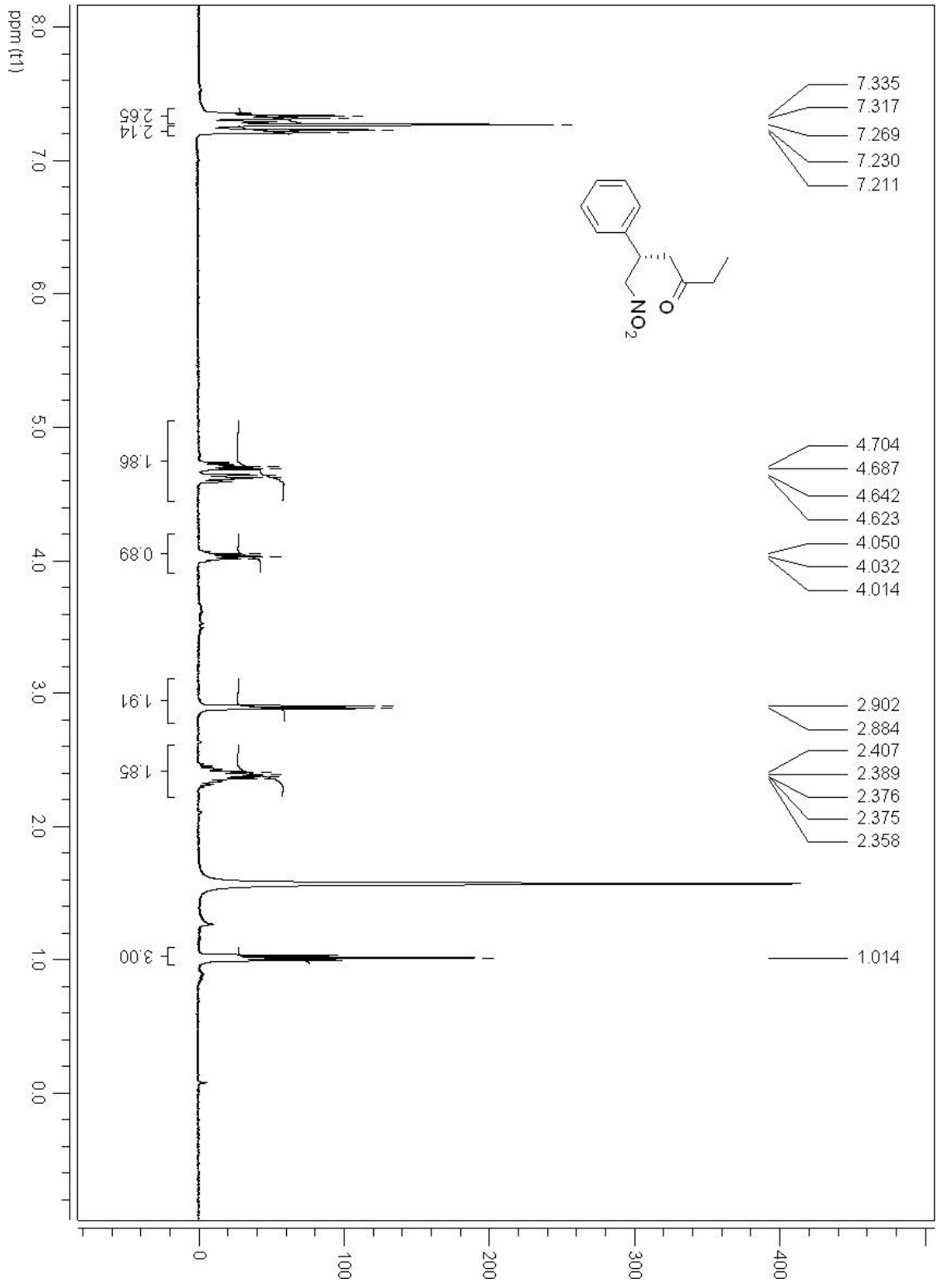
Compound **3o**


7.250
7.235
7.193
6.478
6.446
6.032
6.015
6.000
5.983
4.520
4.508
4.477
4.463
3.467
3.452
2.693
2.680
2.121
4.02
0.63
1.00
1.01
2.06
1.02
2.04
O
NO2
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

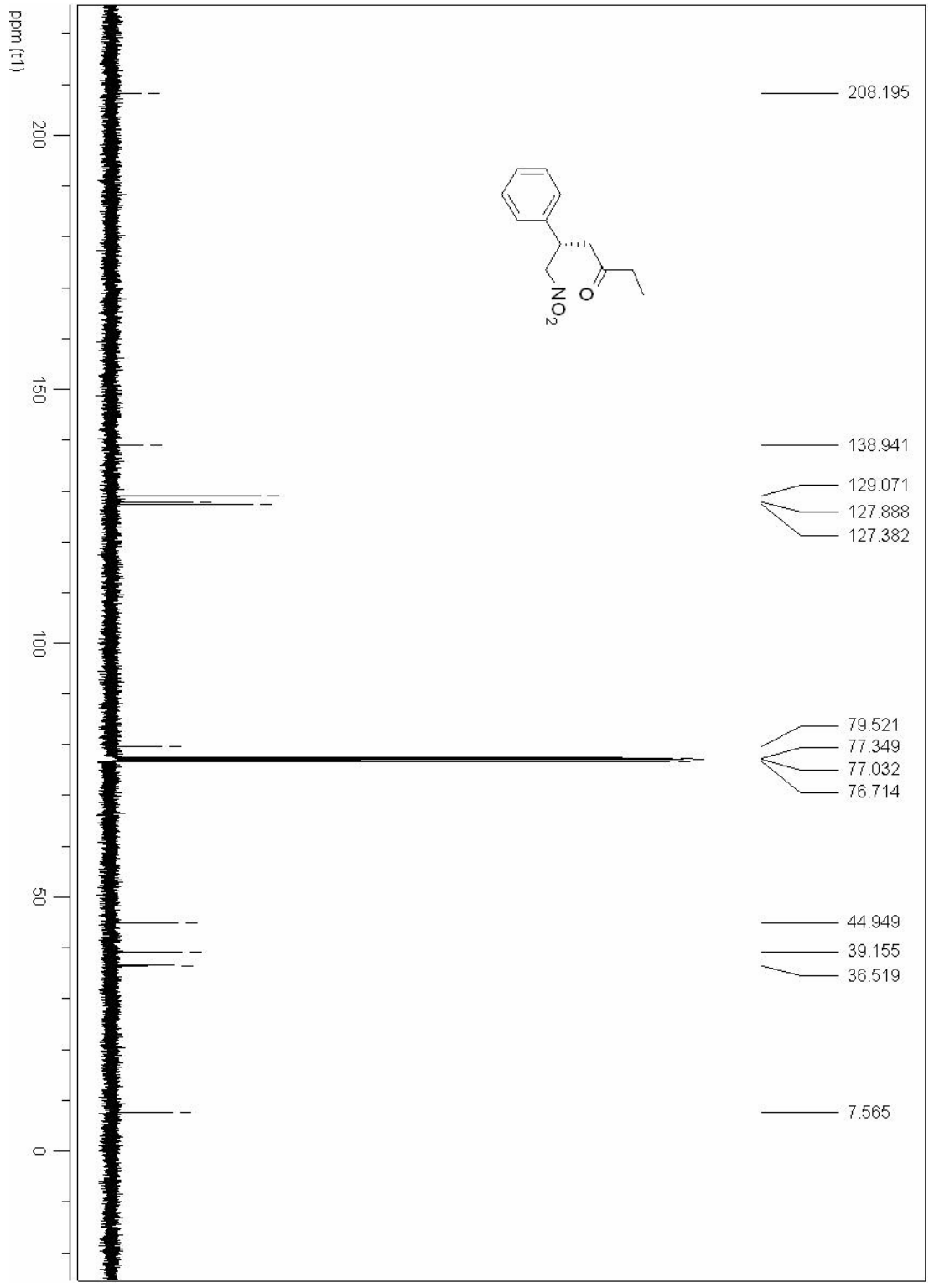
Compound **3o**


ppm (t1)
200
150
100
50
0
205.558
136.158
133.436
128.612
128.030
126.451
126.288
78.596
44.978
37.015
30.480
O
NO2

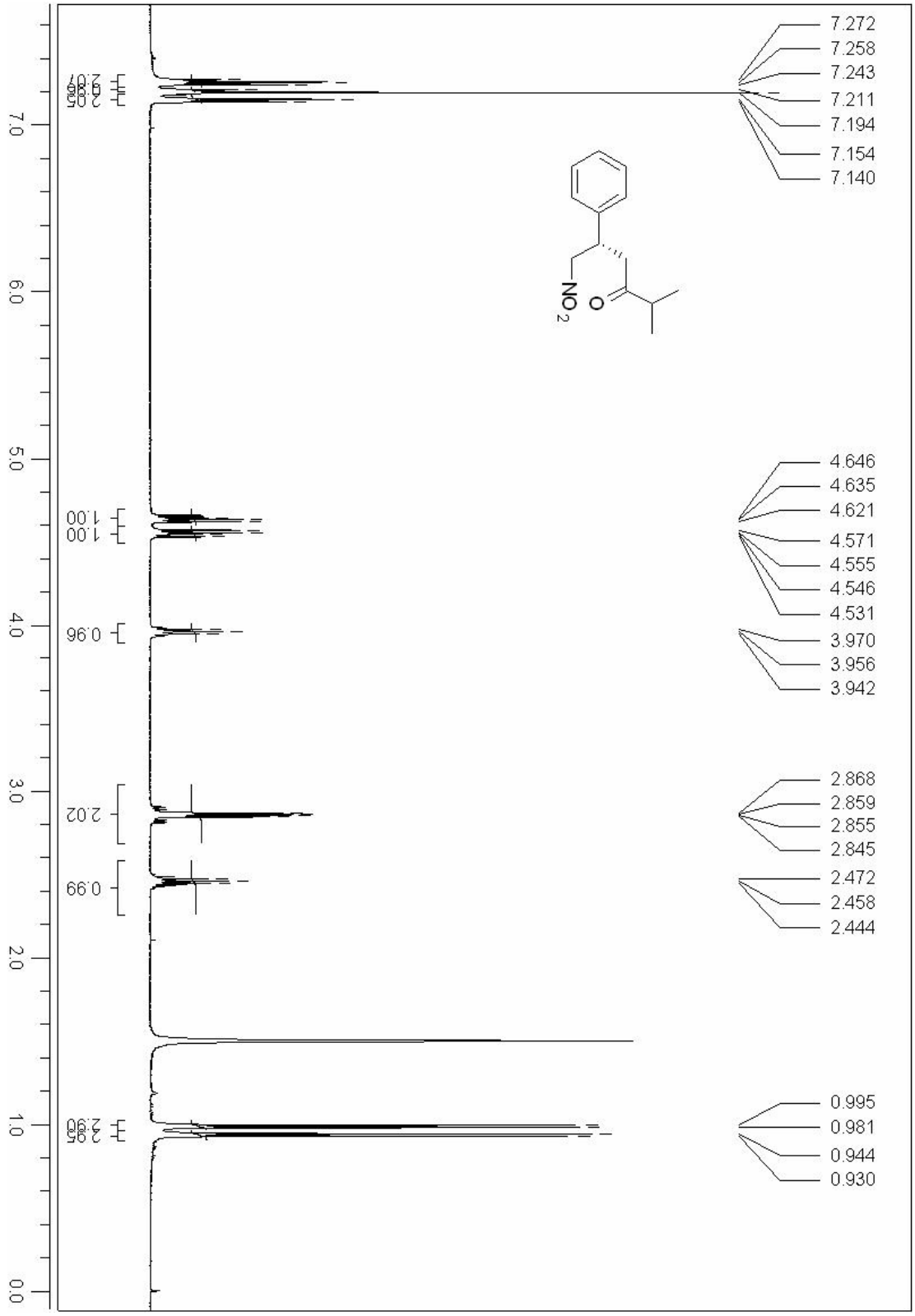
Compound **3p**


7.335
7.317
7.269
7.230
7.211
4.704
4.687
4.642
4.623
4.050
4.032
4.014
2.902
2.884
2.407
2.389
2.376
2.375
2.358
1.014
2.65
2.14
1.86
0.89
1.91
1.85
3.00
NO2
O
ppm (t1)

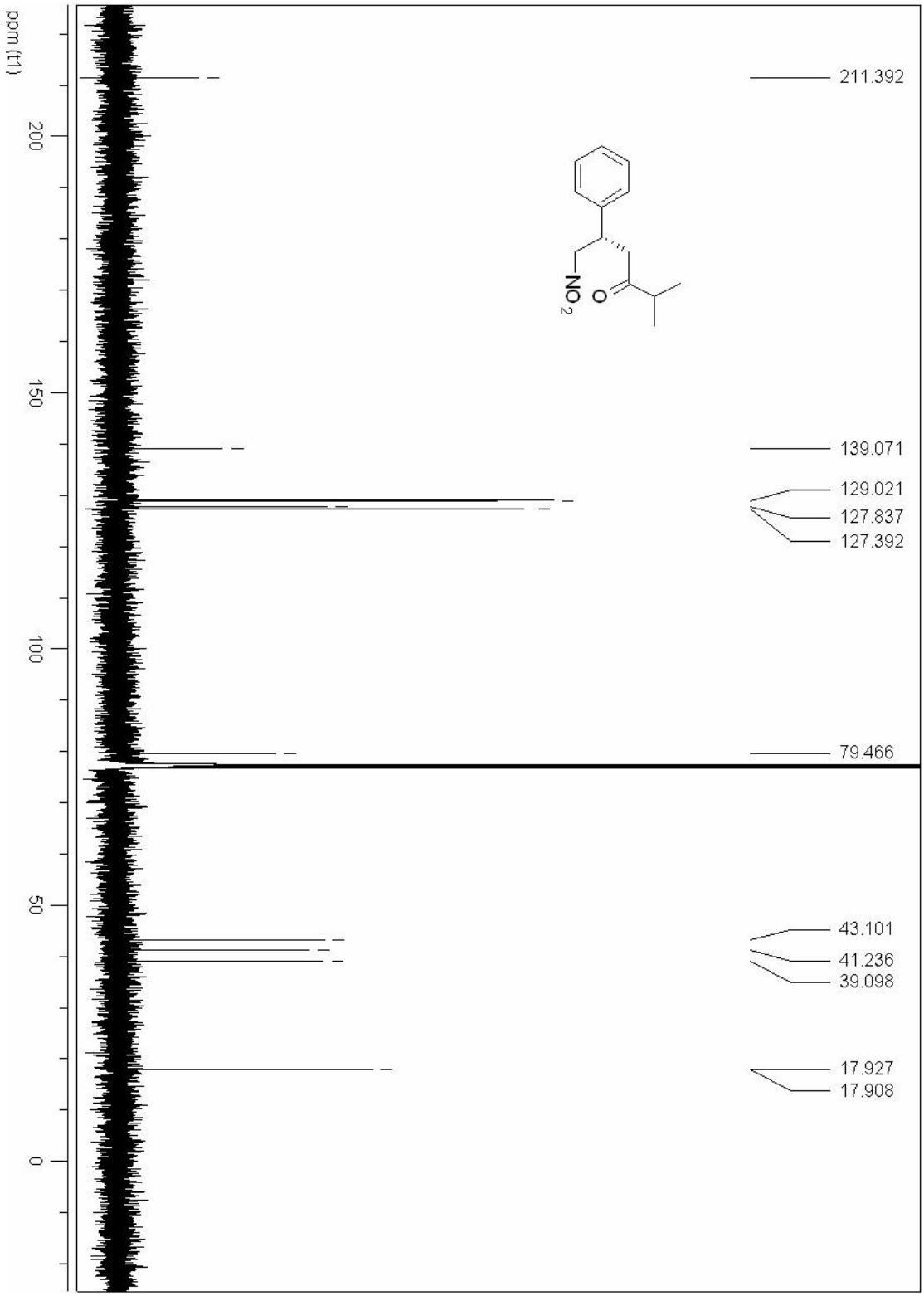
Compound **3p**


ppm (t1)
200
150
100
50
0
208.195
138.941
129.071
127.888
127.382
79.521
77.349
77.032
76.714
44.949
39.155
36.519
7.565
NO2
O

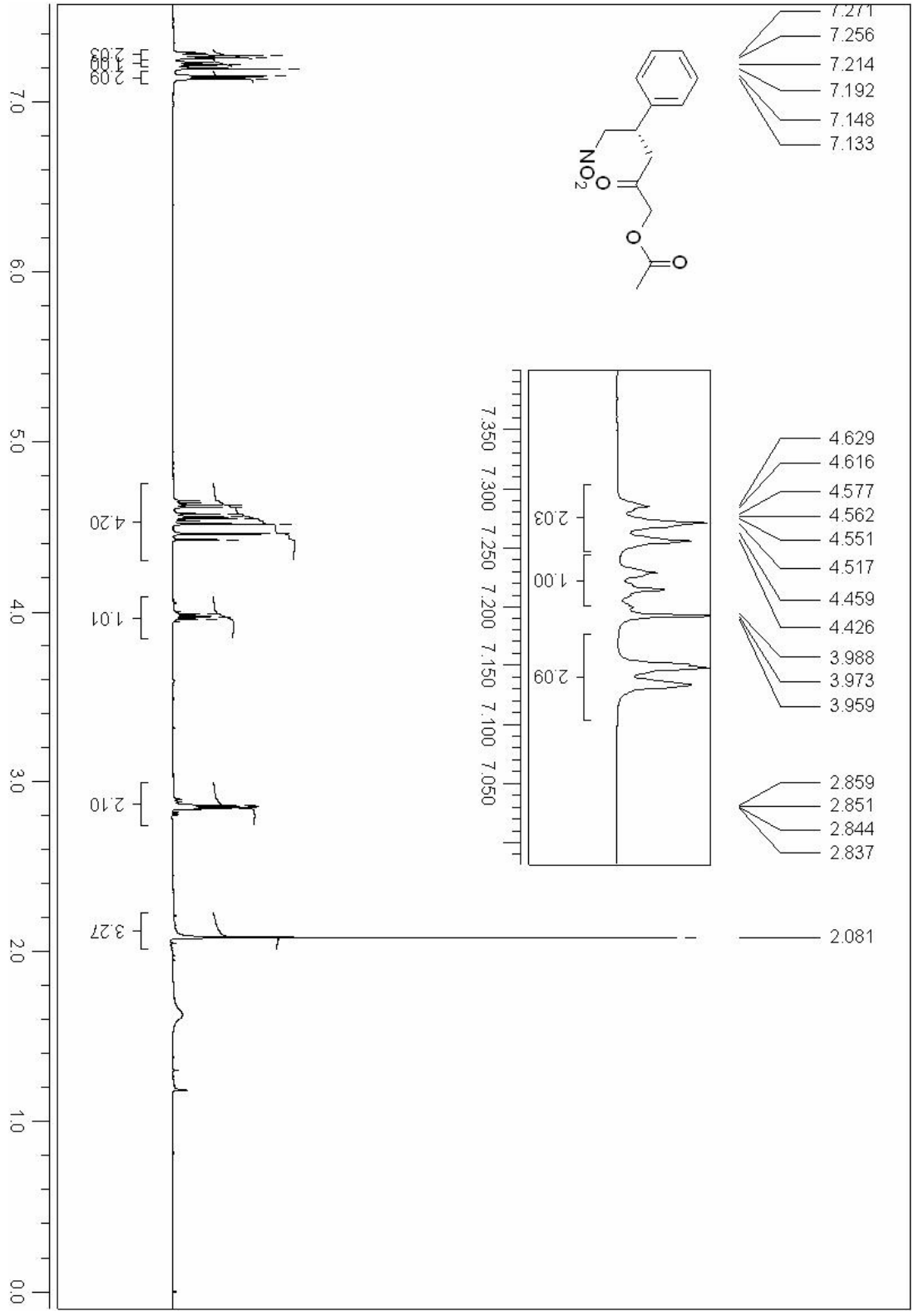
Compound **3q**


7.272
7.258
7.243
7.211
7.194
7.154
7.140
4.646
4.635
4.621
4.571
4.555
4.546
4.531
3.970
3.956
3.942
2.868
2.859
2.855
2.845
2.472
2.458
2.444
0.995
0.981
0.944
0.930
NO2
O
2.07
1.00
1.00
0.96
2.02
0.99
2.90

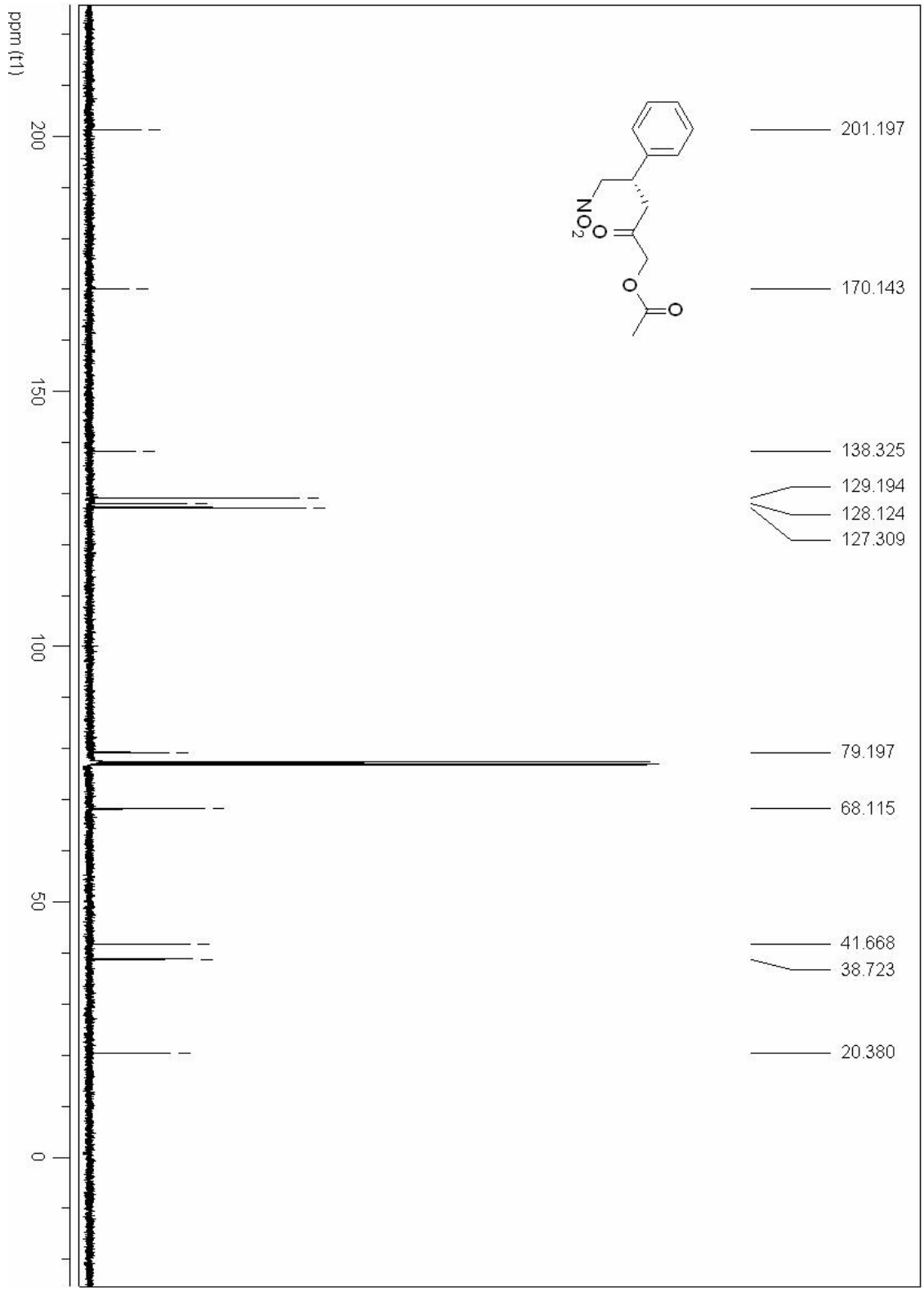
Compound **3q**



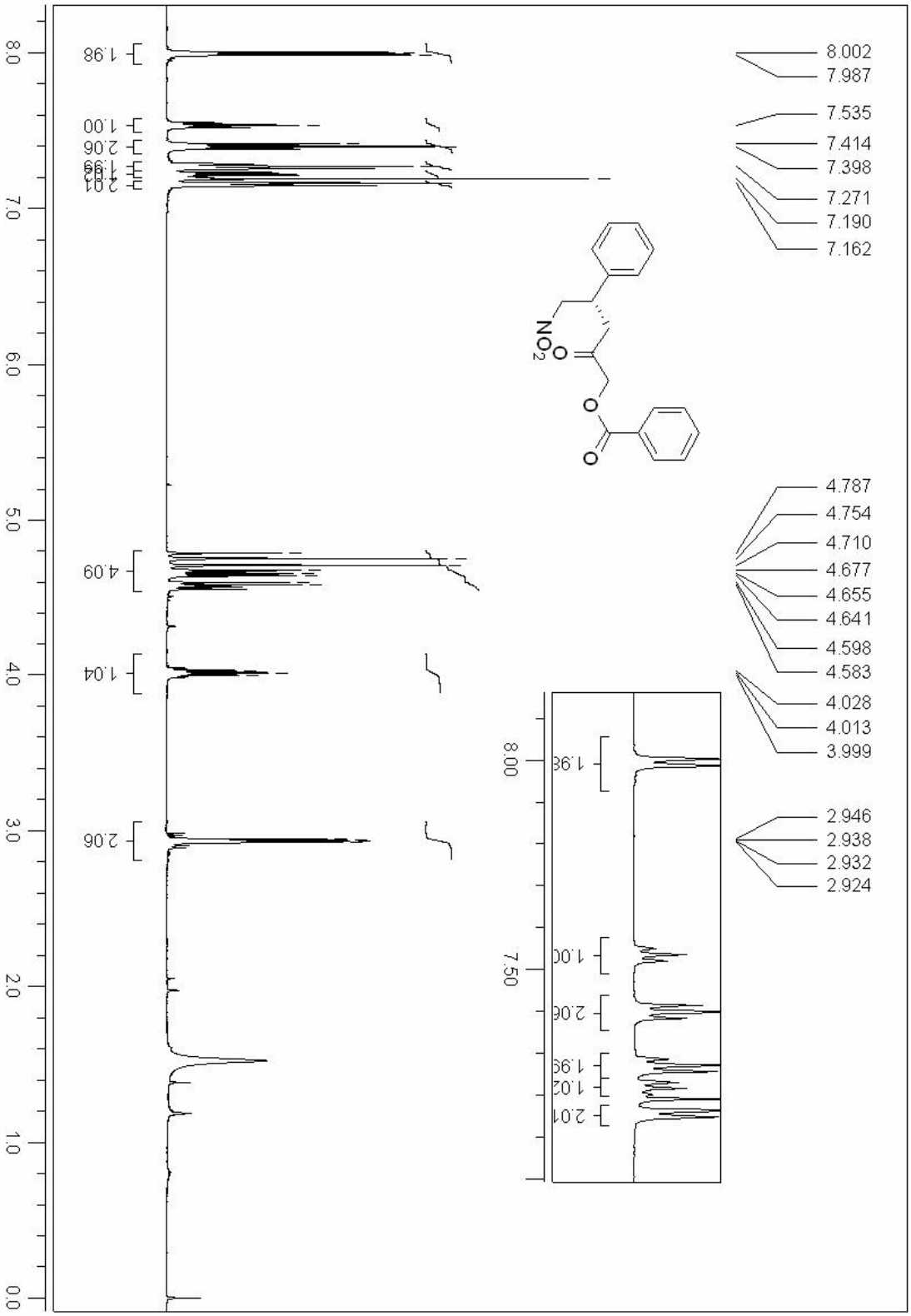
Compound **3r**


7.271
7.256
7.214
7.192
7.148
7.133
4.629
4.616
4.577
4.562
4.551
4.517
4.459
4.426
3.988
3.973
3.959
2.859
2.851
2.844
2.837
2.081
4.20
1.01
2.10
3.27
2.03
1.00
2.09
7.350 7.300 7.250 7.200 7.150 7.100 7.050
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

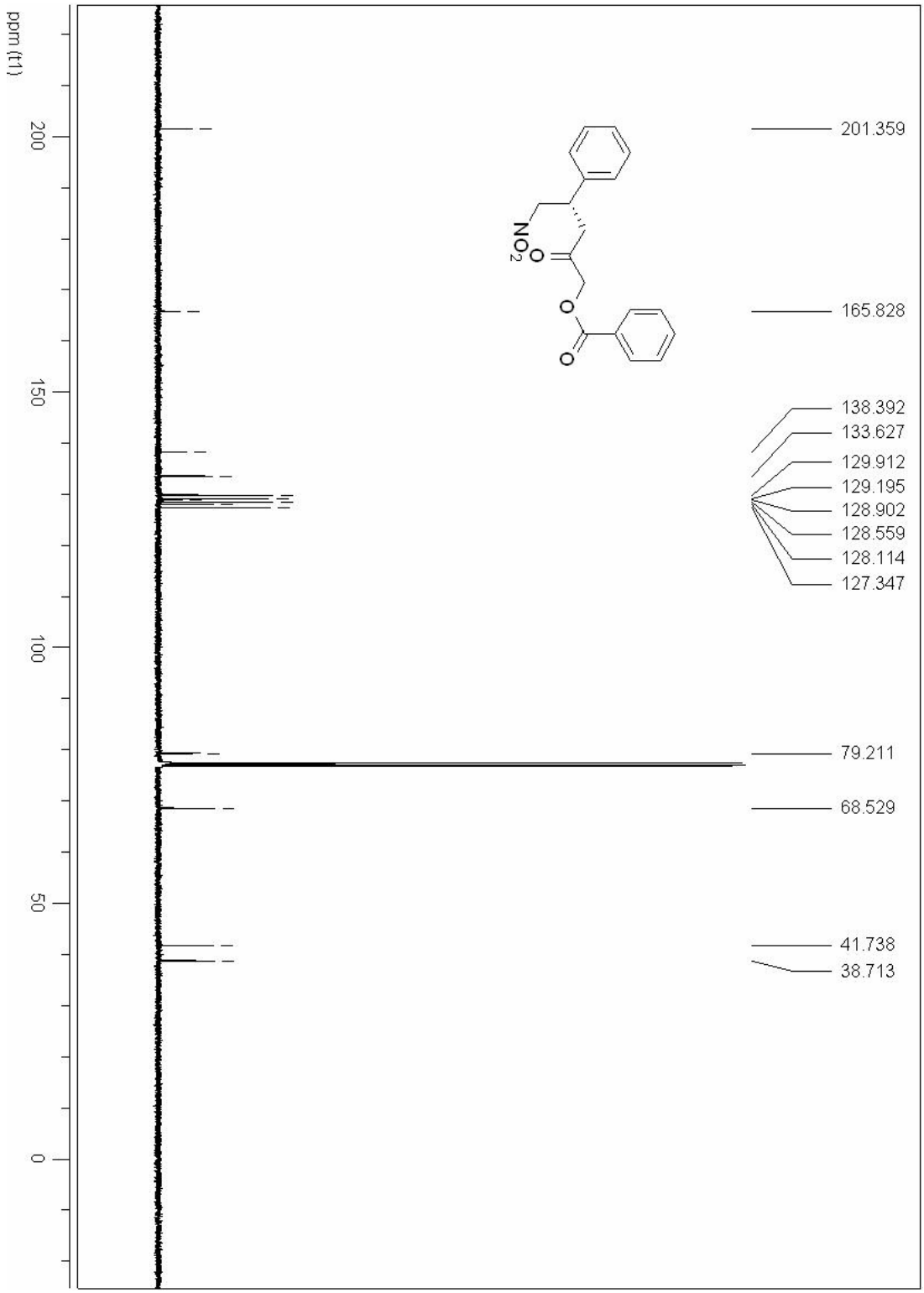
Compound **3r**


ppm (t1)
200
150
100
50
0
201.197
170.143
138.325
129.194
128.124
127.309
79.197
68.115
41.668
38.723
20.380
NO2
O
O
O

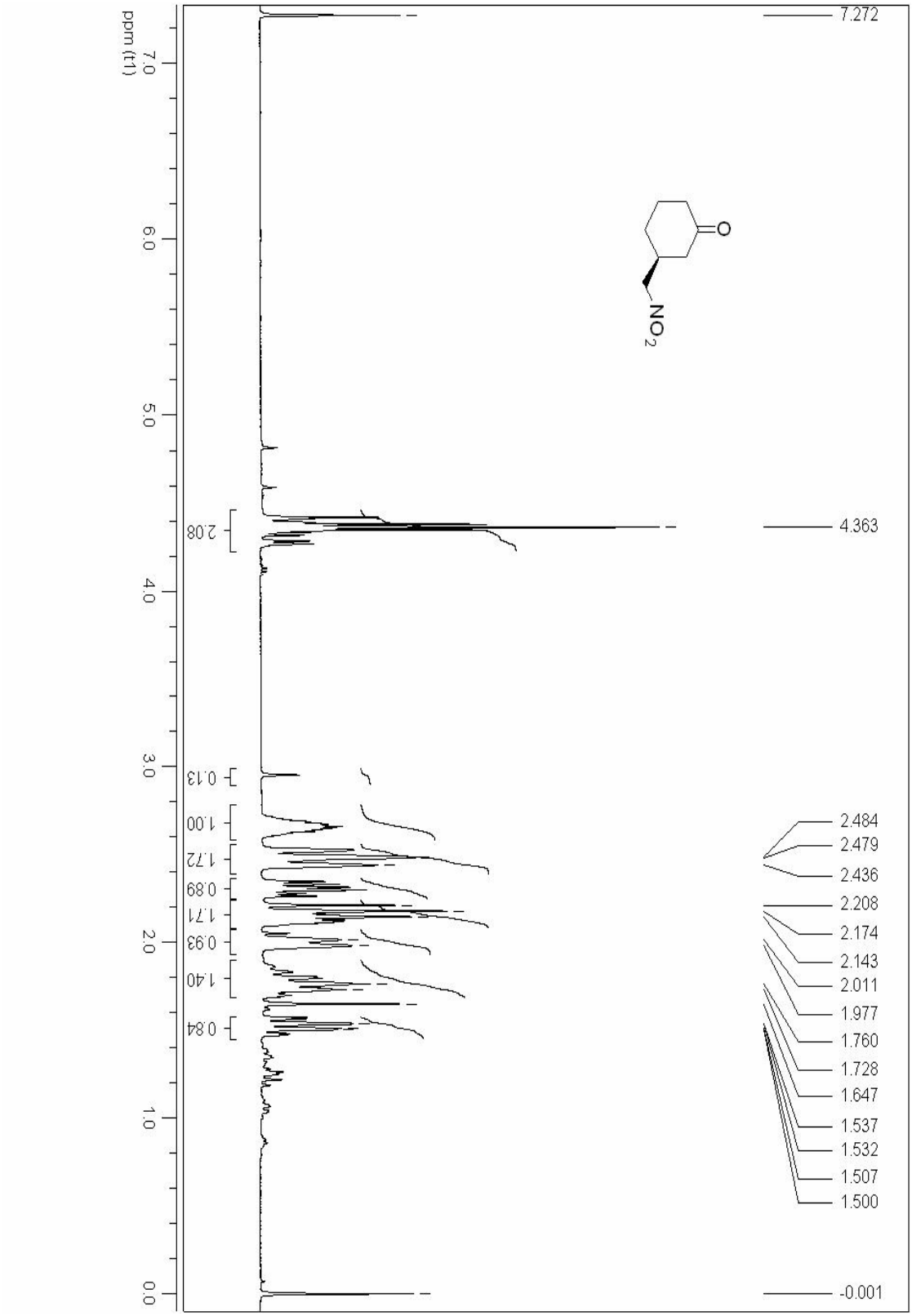
Compound **3s**


8.002
7.987
7.535
7.414
7.398
7.271
7.190
7.162
4.787
4.754
4.710
4.677
4.655
4.641
4.598
4.583
4.028
4.013
3.999
2.946
2.938
2.932
2.924
1.98
4.09
1.04
2.06
1.00
2.01
8.00
7.50

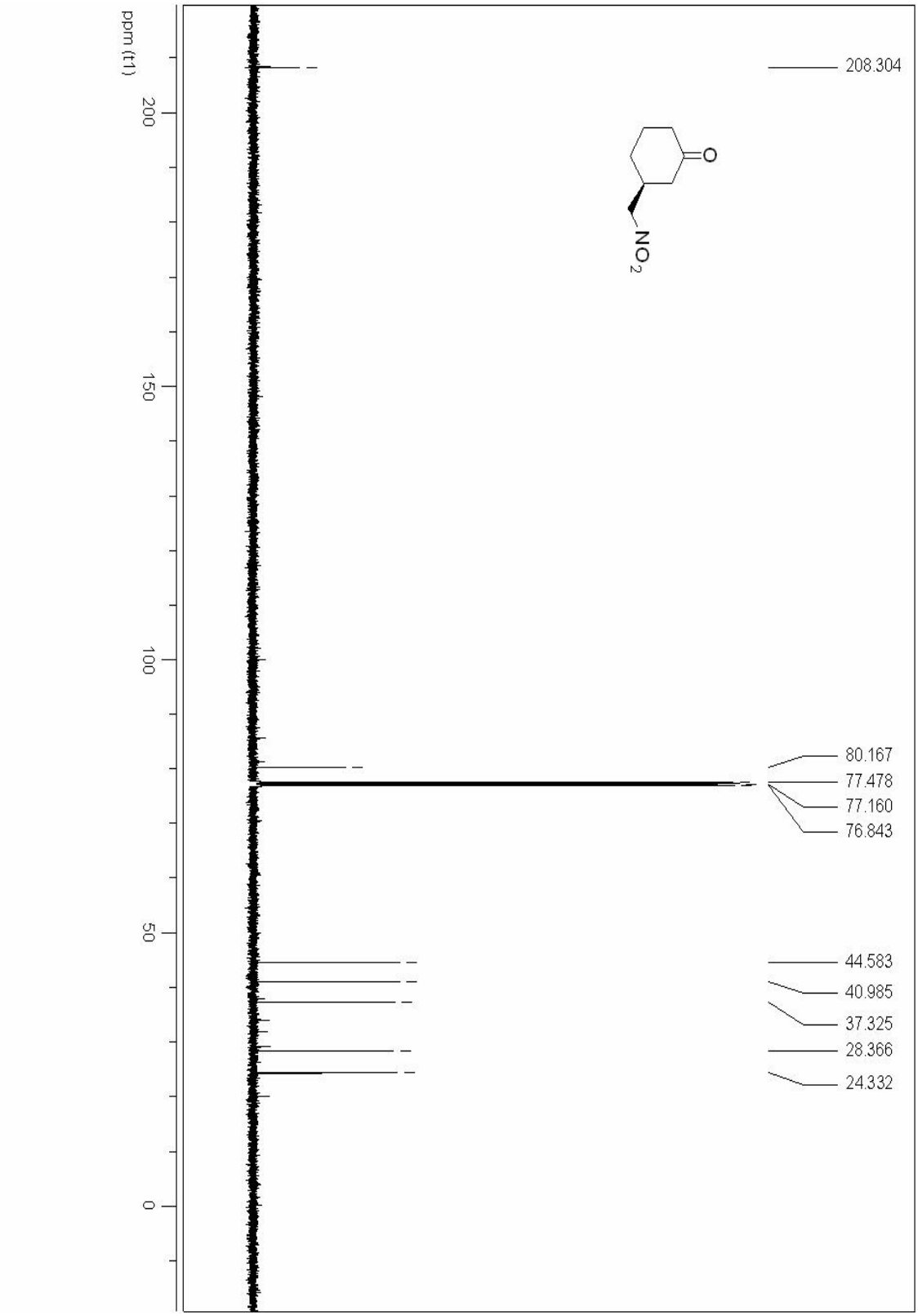
Compound **3s**


ppm (t1)
200
150
100
50
0
201.359
165.828
138.392
133.627
129.912
129.195
128.902
128.559
128.114
127.347
79.211
68.529
41.738
38.713
NO2
O
O
O

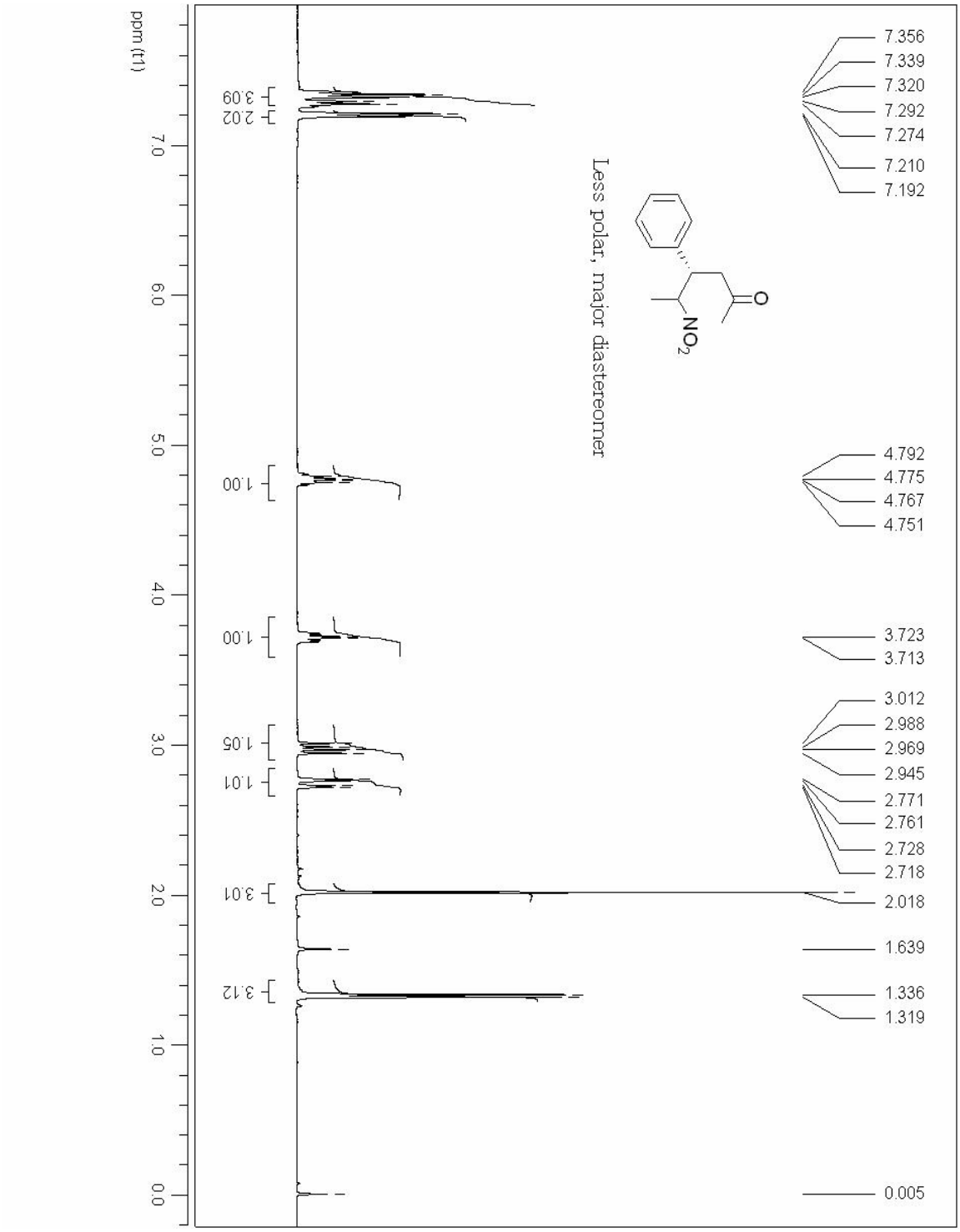
Compound **3t**


ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.08
0.13
1.00
1.72
0.89
1.71
0.93
1.40
0.84
7.272
4.363
2.484
2.479
2.436
2.208
2.174
2.143
2.011
1.977
1.760
1.728
1.647
1.537
1.532
1.507
1.500
-0.001
O
NO2

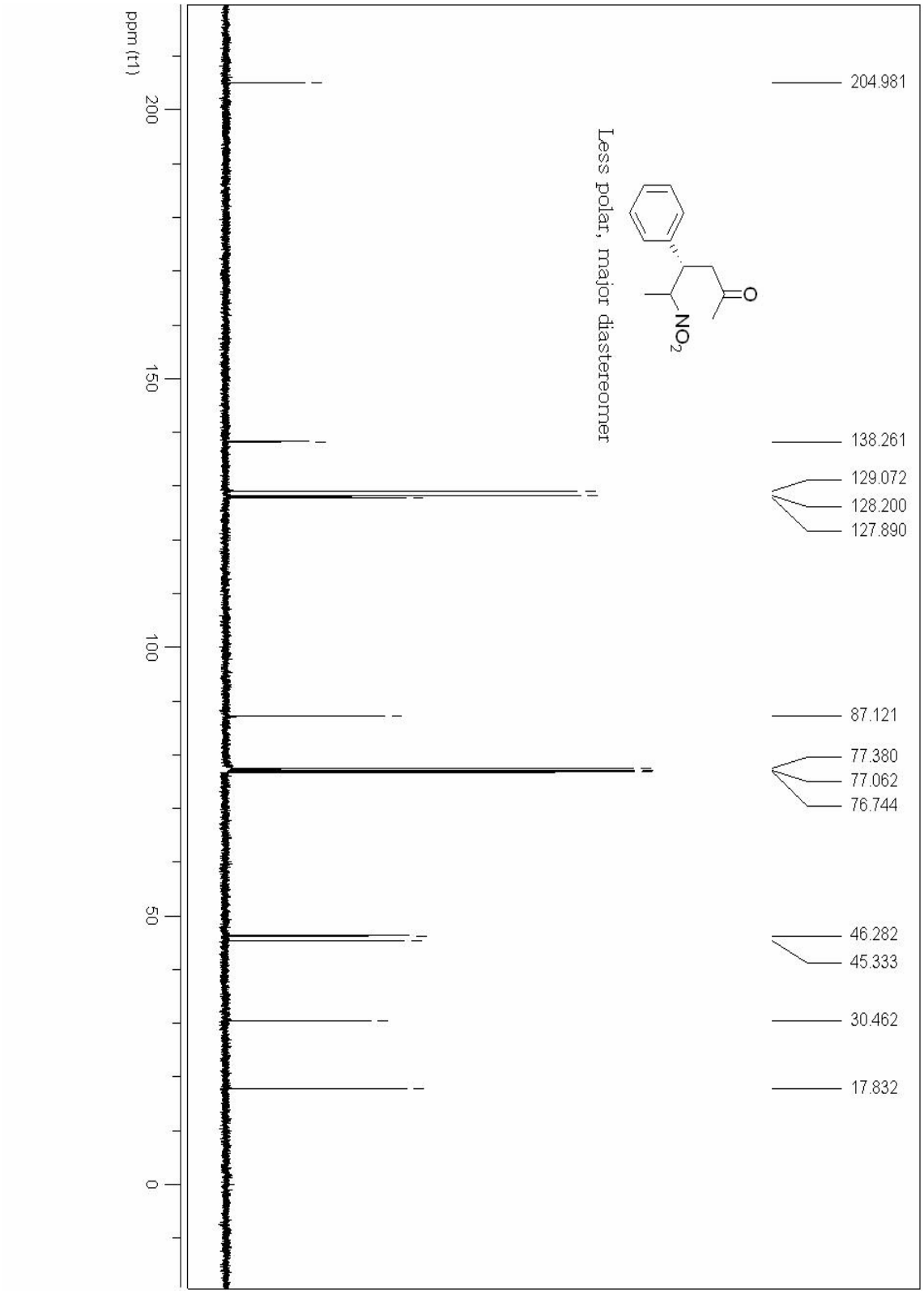
Compound **3t**


ppm (t1)
200
150
100
50
0
208.304
O
NO2
80.167
77.478
77.160
76.843
44.583
40.985
37.325
28.366
24.332

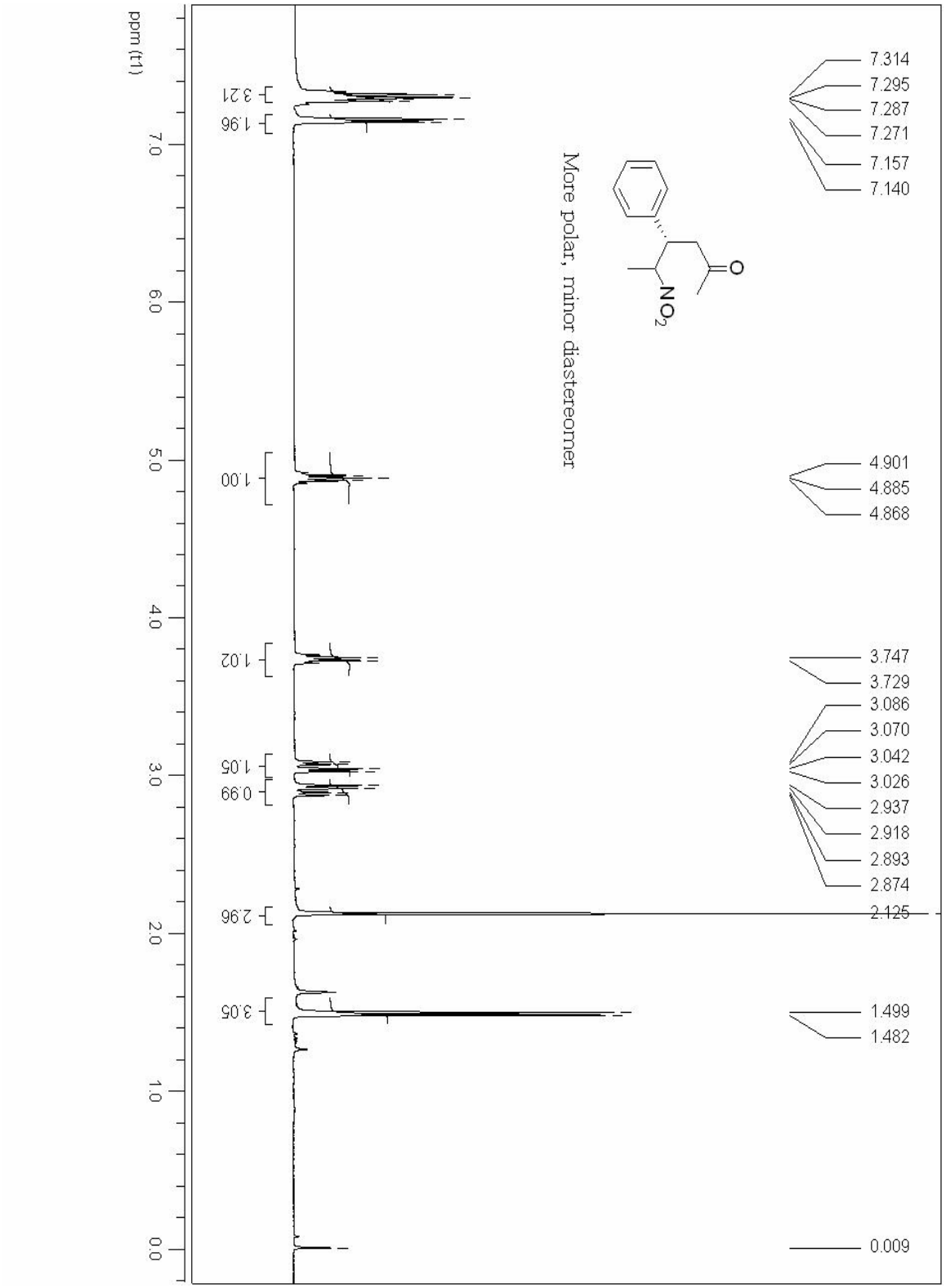
Compound **3u**


ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
3.09
2.02
1.00
1.00
1.05
1.01
3.01
3.12
Less polar, major diastereomer
O
NO2
7.356
7.339
7.320
7.292
7.274
7.210
7.192
4.792
4.775
4.767
4.751
3.723
3.713
3.012
2.988
2.969
2.945
2.771
2.761
2.728
2.718
2.018
1.639
1.336
1.319
0.005

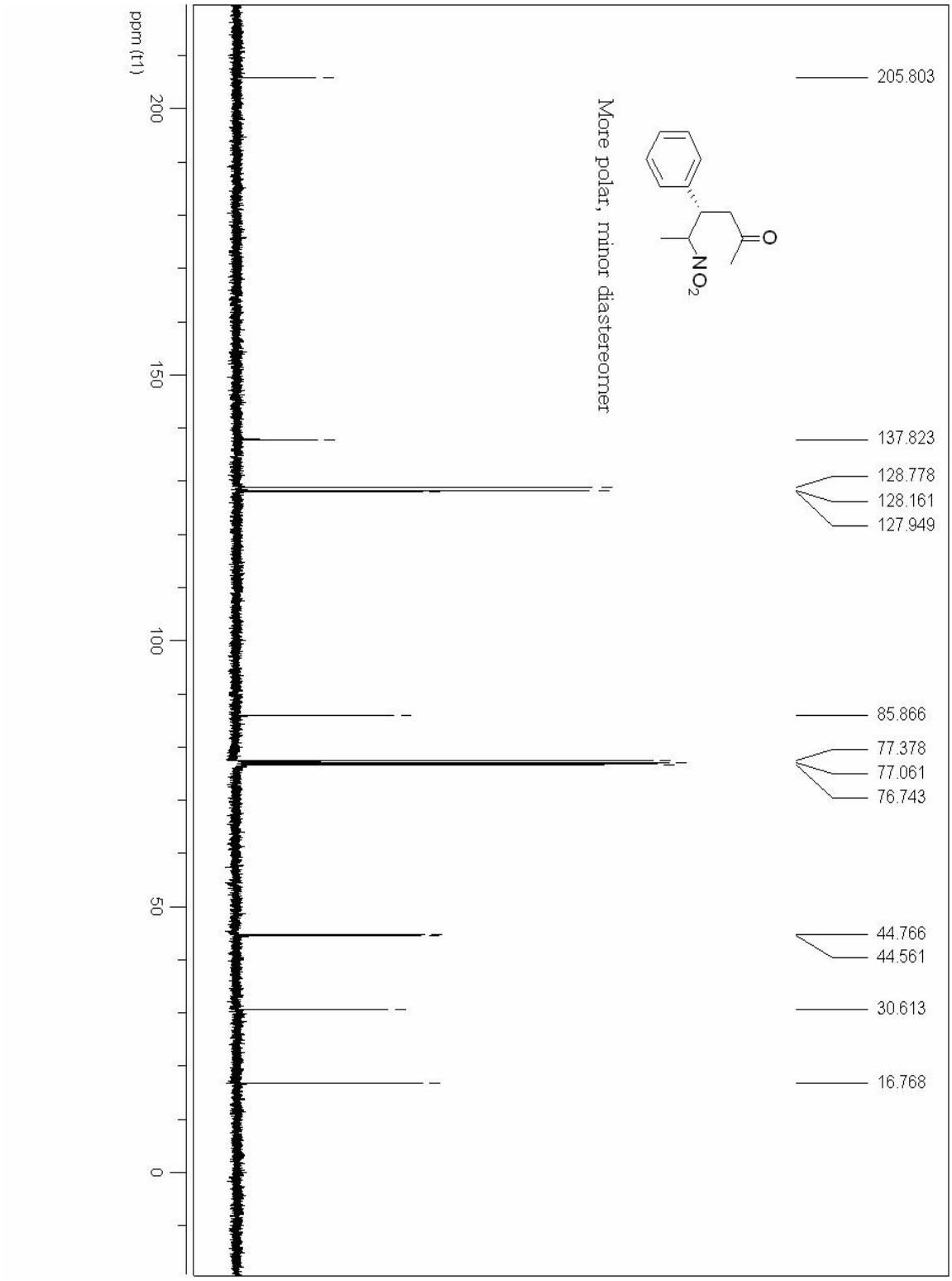
Compound **3u**


ppm (t1)
200
150
100
50
0
Less polar, major diastereomer
O
NO2
204.981
138.261
129.072
128.200
127.890
87.121
77.380
77.062
76.744
46.282
45.333
30.462
17.832

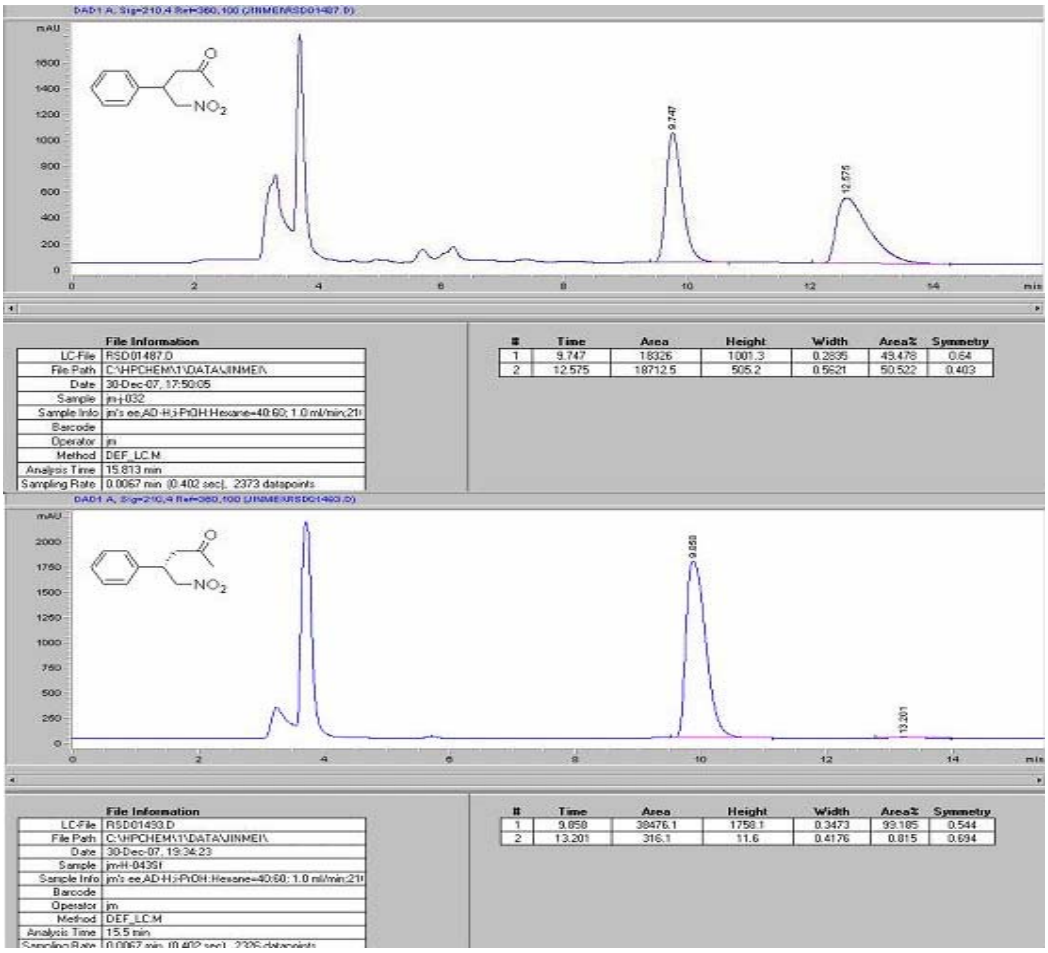
Compound **3u'**

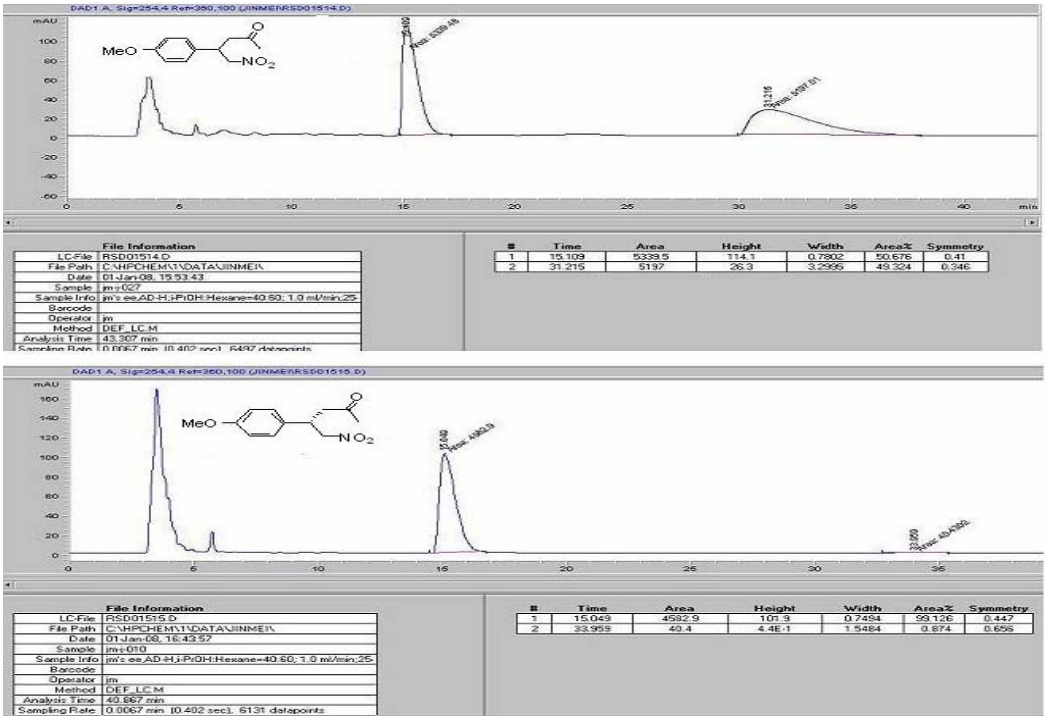

ppm (t1)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
3.21
1.96
1.00
1.02
1.05
0.99
2.96
3.05
More polar, minor diastereomer
NO2
O
7.314
7.295
7.287
7.271
7.157
7.140
4.901
4.885
4.868
3.747
3.729
3.086
3.070
3.042
3.026
2.937
2.918
2.893
2.874
2.125
1.499
1.482
0.009

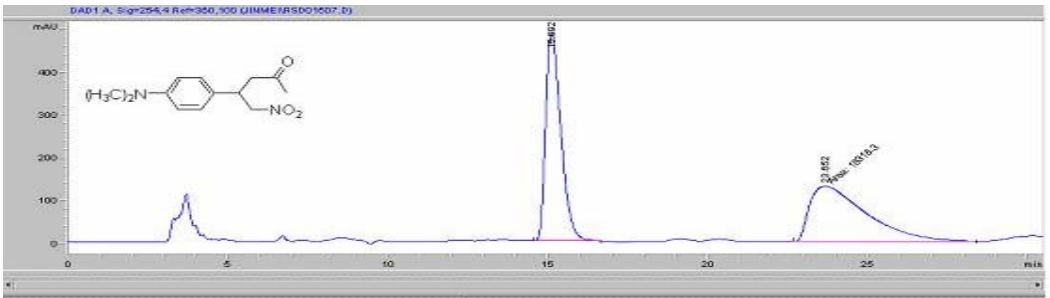
Compound **3u'**


ppm (t1)
200
150
100
50
0
More polar, minor diastereomer
O
NO2
205.803
137.823
128.778
128.161
127.949
85.866
77.378
77.061
76.743
44.766
44.561
30.613
16.768

8.0 HPLC traces



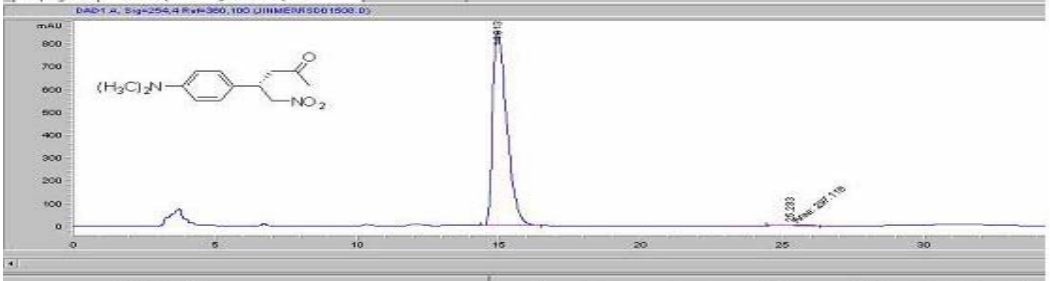




File Information

LC-File	RSD01507.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	31-Dec-07, 20:13:29
Sample	jm-j-024
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=30:70; 1.0 ml/min;25
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	30.513 min
Sampling Rate	0.0067 min (0.402 sec), 4579 datapoints

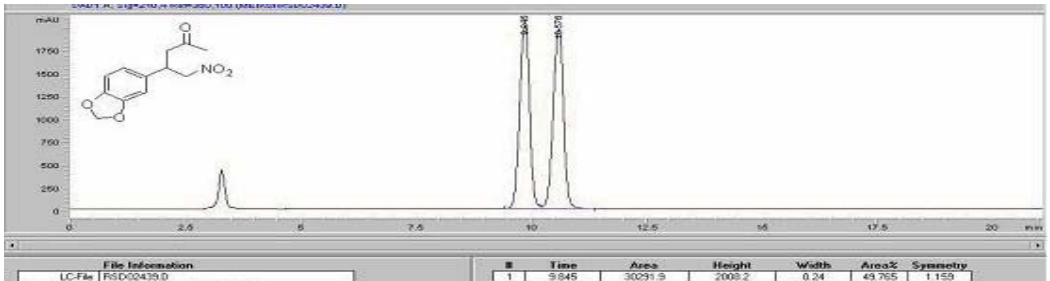
#	Time	Area	Height	Width	Area%	Symmetry
1	15.092	16055.2	487.4	0.5083	49.594	0.57
2	23.652	16318.3	130.4	2.0851	50.406	0.356



File Information

LC-File	RSD01508.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	31-Dec-07, 20:51:21
Sample	jm-j-025
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=30:70; 1.0 ml/min;25-
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	35.867 min
Sampling Rate	0.0067 min (0.402 sec), 5381 datapoints

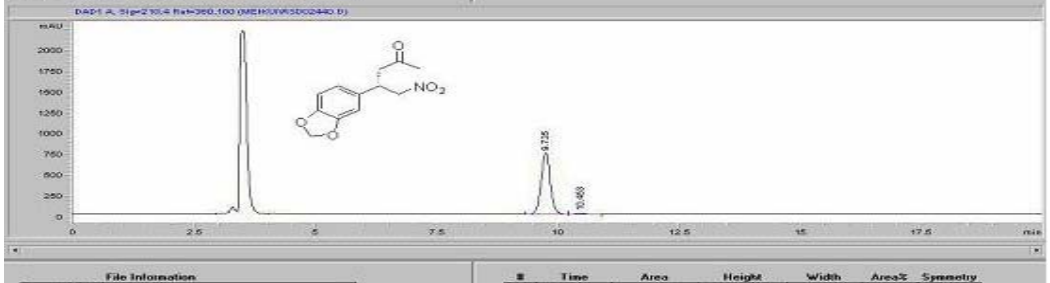
#	Time	Area	Height	Width	Area%	Symmetry
1	14.913	29238.1	852.6	0.5309	98.596	0.503
2	25.233	297.1	3.4	1.4515	1.004	0.522



File Information

LC-File	RSD02439.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	13-Jul-08, 23:40:07
Sample	mk-k-74-02-sac
Sample Info	AD-H,Hexi-PrOH=80:20;1ml/min
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	21.127 min
Sampling Rate	0.0067 min (0.402 sec), 3170 datapoints

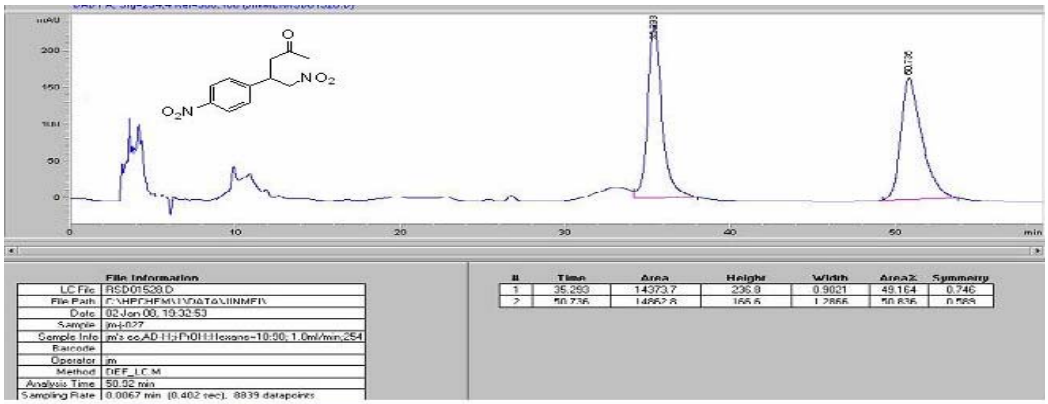
#	Time	Area	Height	Width	Area%	Symmetry
1	9.845	30291.9	2068.2	0.24	49.765	1.159
2	10.576	30578.2	1955.9	0.2484	50.235	1.138



File Information

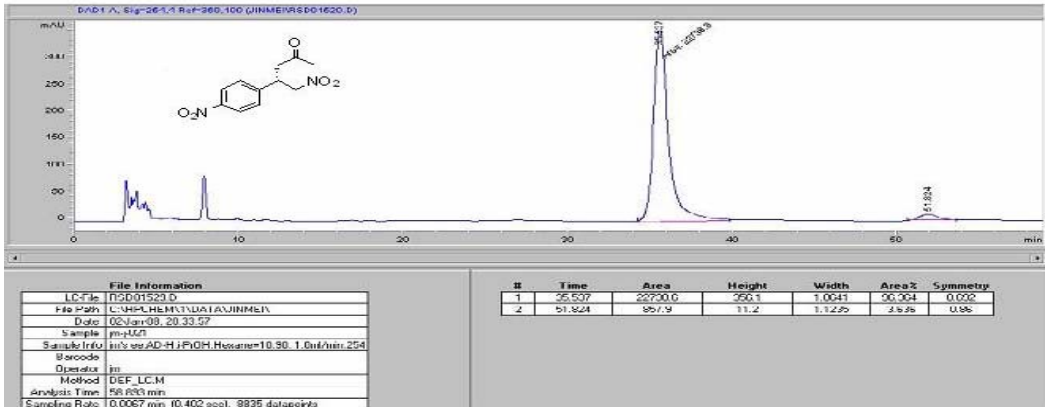
LC-File	RSD02440.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	14-Jul-08, 00:04:58
Sample	mk-k-74-01
Sample Info	AD-H,Hexi-PrOH=80:20;1ml/min
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	20.027 min
Sampling Rate	0.0067 min (0.402 sec), 3005 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	9.735	9676.1	737.3	0.2031	98.229	0.993
2	10.453	174.5	12.3	0.2155	1.771	1.036



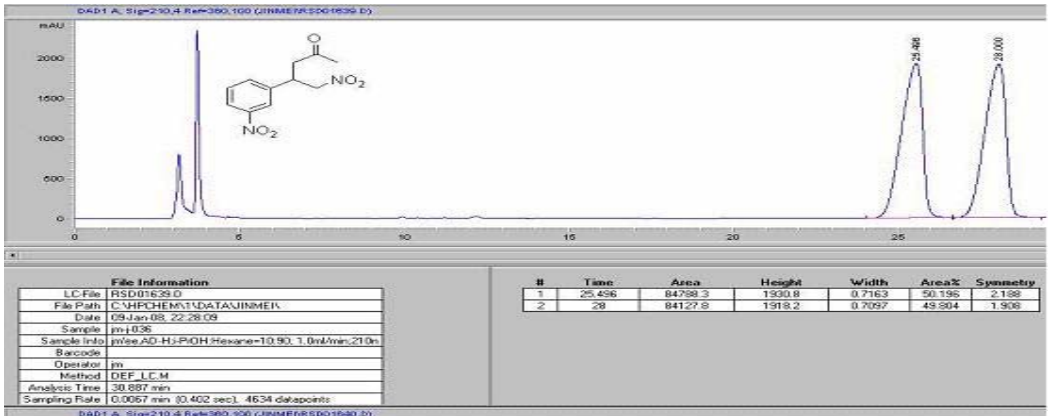
File Information	
LC File	RSD01528.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-00, 19:32:53
Sample	jm-j-027
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	50.92 min
Sampling Rate	0.0067 min (0.402 sec), 8839 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	35.293	14373.7	236.8	0.9021	49.164	0.746
2	50.736	14862.8	166.6	1.2866	50.836	0.589



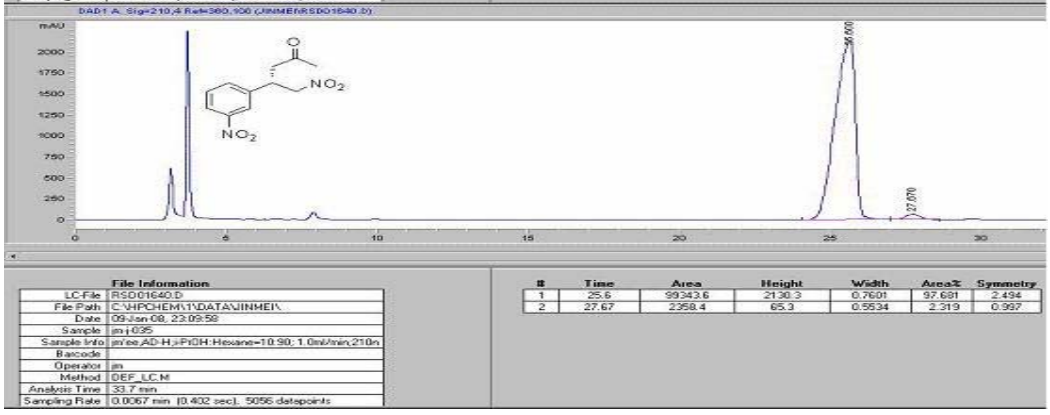
File Information	
LC File	RSD01529.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-08, 20:33:57
Sample	jm-j-027
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	58.899 min
Sampling Rate	0.0067 min (0.402 sec), 8835 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	35.537	22700.0	350.1	1.0041	96.004	0.932
2	51.824	957.9	11.2	1.1265	3.936	0.96



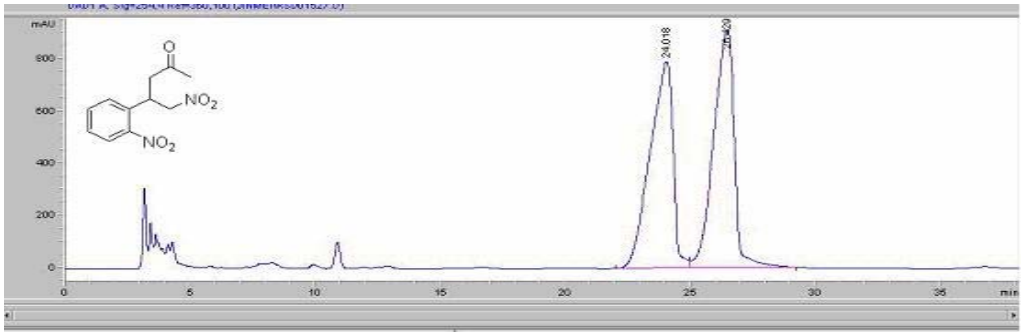
File Information	
LC File	RSD01639.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	09-Jan-08, 22:28:09
Sample	jm-j-036
Sample Info	jm'ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;210n
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	38.887 min
Sampling Rate	0.0067 min (0.402 sec), 4634 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	25.496	84798.3	1930.8	0.7163	50.196	2.168
2	28	84127.8	1918.2	0.7097	49.804	1.908



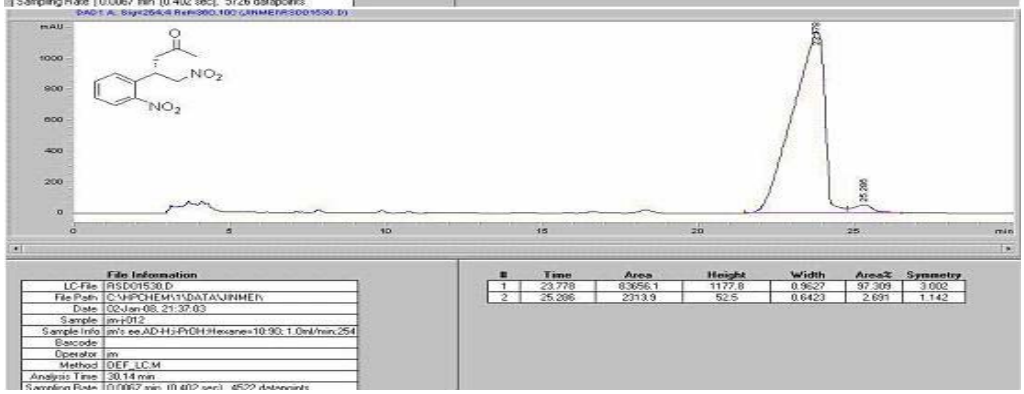
File Information	
LC File	RSD01640.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	09-Jan-08, 23:09:58
Sample	jm-j-035
Sample Info	jm'ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;210n
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	33.7 min
Sampling Rate	0.0067 min (0.402 sec), 5056 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	25.6	99343.6	2130.3	0.7601	97.681	2.494
2	27.67	2358.4	65.3	0.5534	2.319	0.997



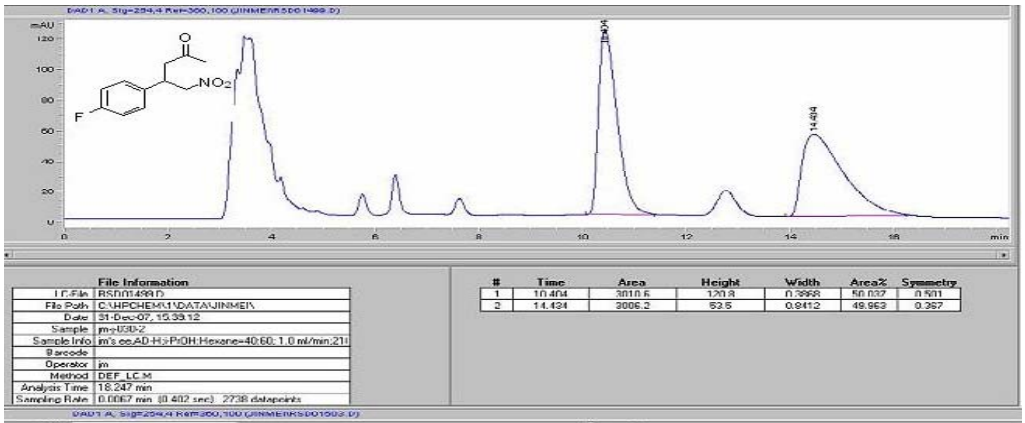
File Information	
LC-File	RSD01527.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-08, 18:49:38
Sample	jm-j028
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	38.167 min
Sampling Rate	0.0067 min (0.402 sec), 5726 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	24.018	51076.1	791.4	0.931	49.168	2.445
2	26.429	52805.3	910.1	0.9409	50.832	1.627



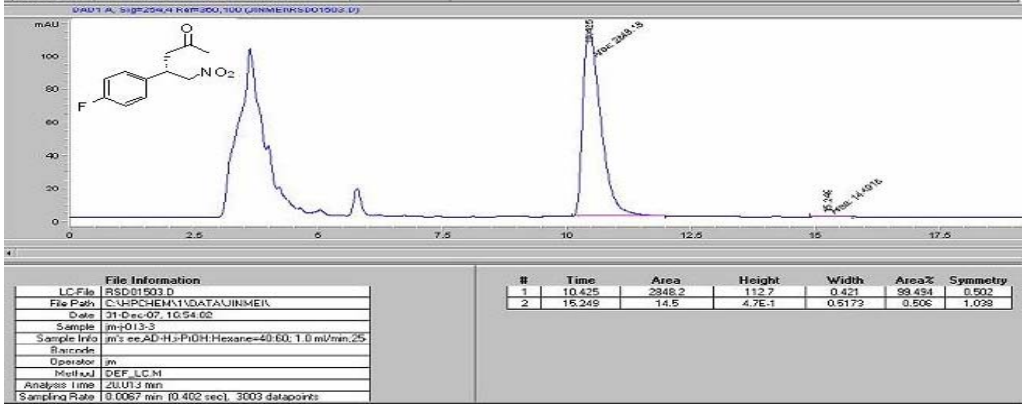
File Information	
LC-File	RSD01530.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-08, 21:37:03
Sample	jm-j012
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	30.14 min
Sampling Rate	0.0067 min (0.402 sec), 4522 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	23.778	83656.1	1177.8	0.9627	97.309	3.002
2	25.286	2313.9	52.5	0.6423	2.691	1.142



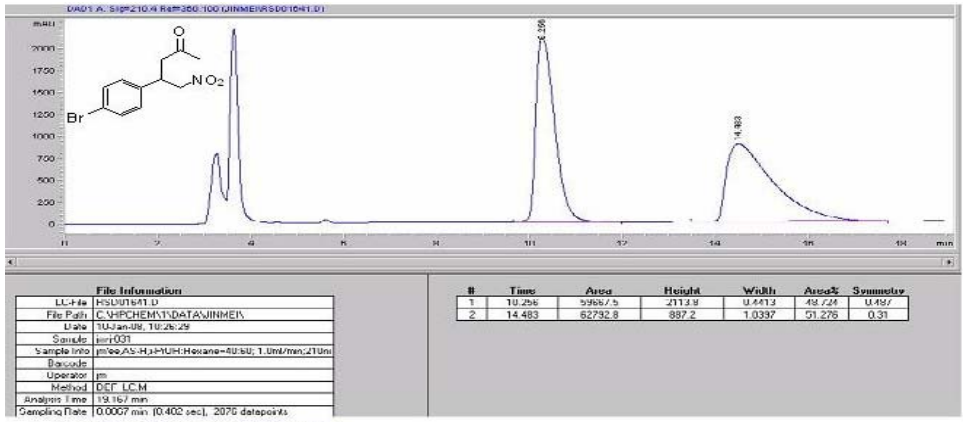
File Information	
LC-File	RSD01499.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	31-Dec-07, 15:39:12
Sample	jm-j036-2
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=40:60; 1.0 ml/min;21
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	18.247 min
Sampling Rate	0.0067 min (0.402 sec), 2738 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.404	3010.6	120.8	0.3968	50.037	0.501
2	14.434	3006.2	53.5	0.9412	49.963	0.367



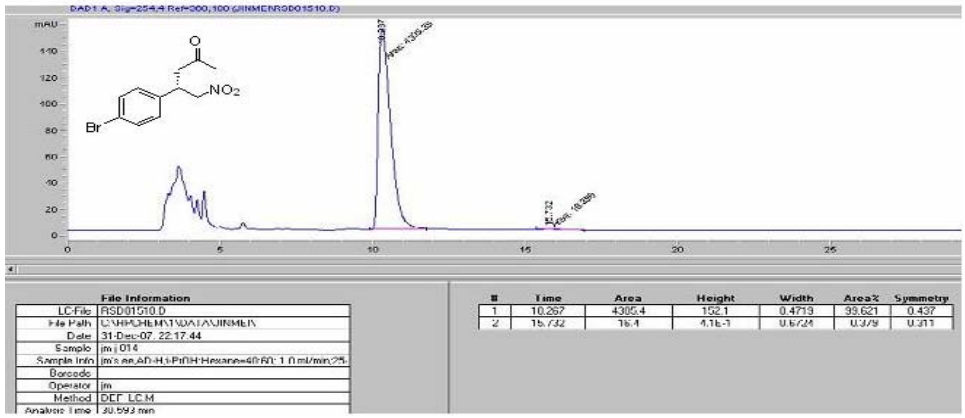
File Information	
LC-File	RSD01503.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	31-Dec-07, 16:54:02
Sample	jm-j013-3
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=40:60; 1.0 ml/min;25
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	20.013 min
Sampling Rate	0.0067 min (0.402 sec), 3003 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.425	2848.2	112.7	0.421	99.494	0.502
2	15.249	14.5	4.7E-1	0.5173	0.506	1.039



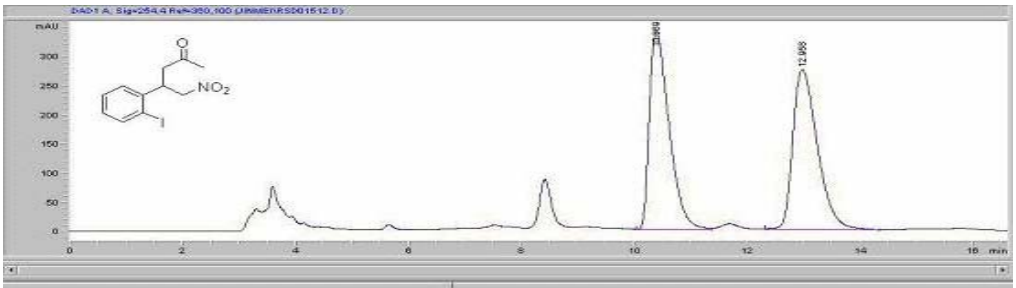
File Information	
LC-File	RSD01641.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	10-Jan-08, 10:26:29
Sample	jin1001
Sample Info	jm'ee,AS-H,i-PrOH:Hexane=40:60; 1.0ml/min;210nm
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	19.167 min
Sampling Rate	0.0067 min (0.402 sec), 2870 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.256	59667.5	2113.8	0.4413	48.724	0.497
2	14.483	62732.8	887.2	1.0337	51.276	0.31



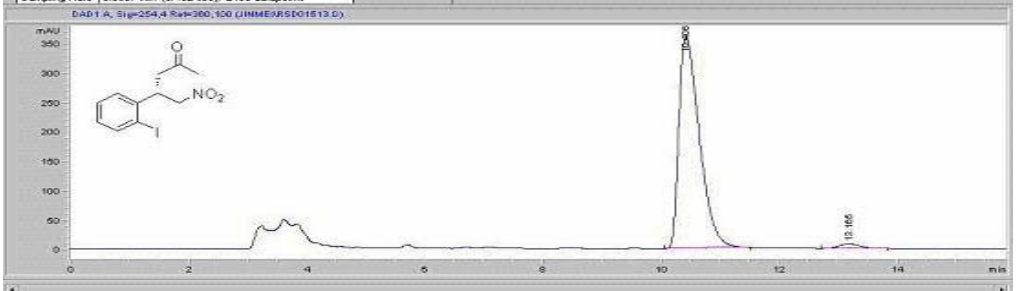
File Information	
LC-File	RSD01510.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	31-Dec-07, 22:17:44
Sample	jin j-014
Sample Info	jin's ee,AD-H,i-PrOH:Hexane=40:60; 1.0 ml/min;25
Barcode	
Operator	jin
Method	DEF_LC.M
Analysis Time	30.593 min

#	Time	Area	Height	Width	Area%	Symmetry
1	10.267	4305.4	152.1	0.4719	39.621	0.437
2	15.732	16.4	4.1E-1	0.6724	0.379	0.311



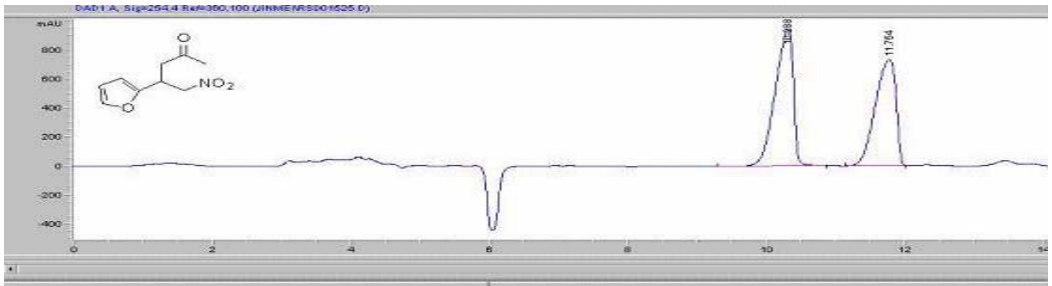
File Information	
LC-File	RSD01512.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	01-Jan-08, 15:05:16
Sample	jin j-024
Sample Info	jin's ee,AD-H,i-PrOH:Hexane=40:60; 1.0 ml/min;25
Barcode	
Operator	jin
Method	DEF_LC.M
Analysis Time	16.647 min
Sampling Rate	0.0067 min (0.402 sec), 2498 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.369	8267.7	340	0.3737	49.724	0.49
2	12.958	8359.6	274.8	0.4709	50.276	0.595



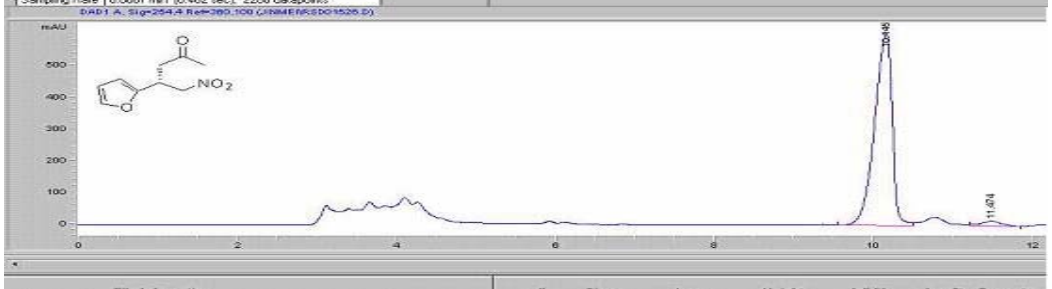
File Information	
LC-File	RSD01513.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	01-Jan-08, 15:31:46
Sample	jin j-018
Sample Info	jin's ee,AD-H,i-PrOH:Hexane=40:60; 1.0 ml/min;25
Barcode	
Operator	jin
Method	DEF_LC.M
Analysis Time	15.887 min
Sampling Rate	0.0067 min (0.402 sec), 2384 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.406	8715.4	360.7	0.372	97.847	0.49
2	13.165	191.9	7.7	0.3836	2.153	0.609



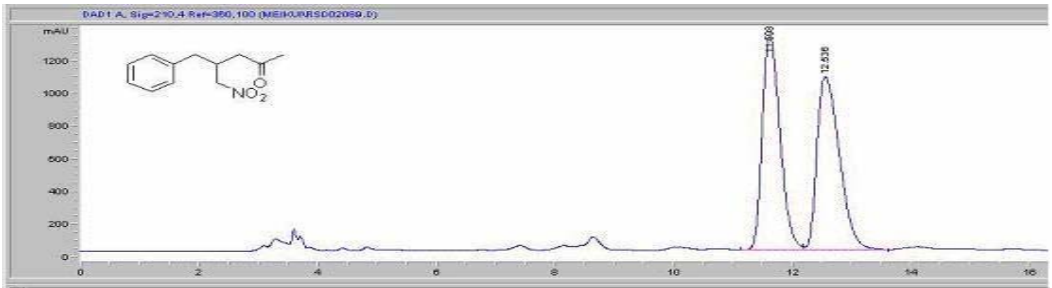
File Information	
LC-File	RSD01525.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-08, 18:00:21
Sample	jm-j-026-3
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	14.7 min
Sampling Rate	0.0067 min (0.402 sec), 2206 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.288	17228.7	947.2	0.2922	53.212	2.204
2	11.754	15148.9	737.1	0.3398	46.788	2.109



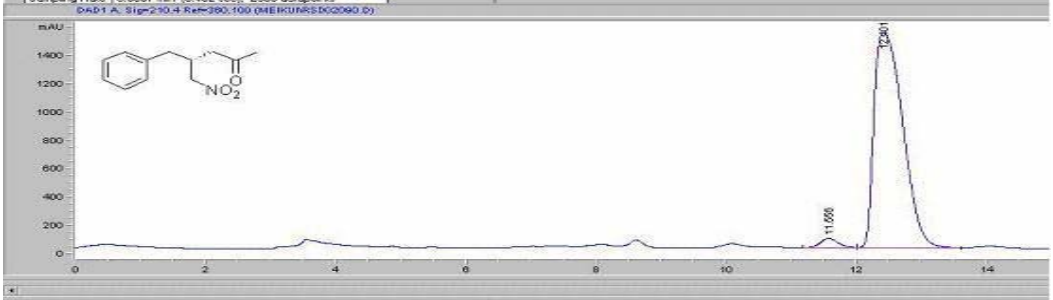
File Information	
LC-File	RSD01526.D
File Path	C:\HPCHEM\1\DATA\JINMEI\
Date	02-Jan-08, 18:28:44
Sample	jm-j-020
Sample Info	jm's ee,AD-H,i-PrOH:Hexane=10:90; 1.0ml/min;254
Barcode	
Operator	jm
Method	DEF_LC.M
Analysis Time	12.807 min
Sampling Rate	0.0067 min (0.402 sec), 1922 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.145	9365.4	611.5	0.2407	96.873	1.741
2	11.474	302.3	15.8	0.2795	3.127	1.055



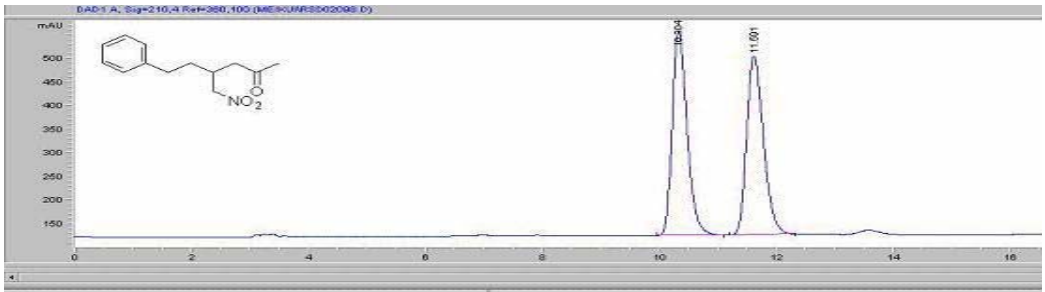
File Information	
LC-File	RSD02089.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	20-May-08, 16:33:48
Sample	mk-k-23-2-rac
Sample Info	AS-H,hexi-PrOH=80:20;1.0ml/min; 210nm, 25 deg
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	17.1 min
Sampling Rate	0.0067 min (0.402 sec), 2566 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	11.598	27328.1	1386	0.3281	49.346	0.688
2	12.536	28052.9	1060.2	0.4187	50.654	0.557



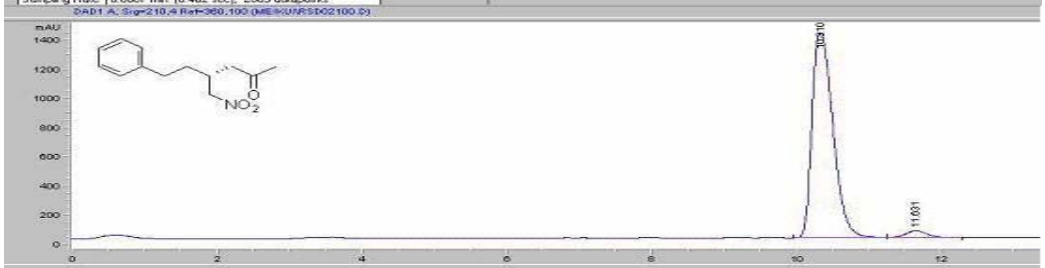
File Information	
LC-File	RSD02090.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	20-May-08, 16:58:34
Sample	mk-k-23-1
Sample Info	AS-H,hexi-PrOH=80:20;1.0ml/min; 210nm, 25 deg
Barcode	
Operator	mk

#	Time	Area	Height	Width	Area%	Symmetry
1	11.556	1288.5	67.2	0.2957	2.677	0.825
2	12.401	46840.1	1521.6	0.5011	97.323	0.479



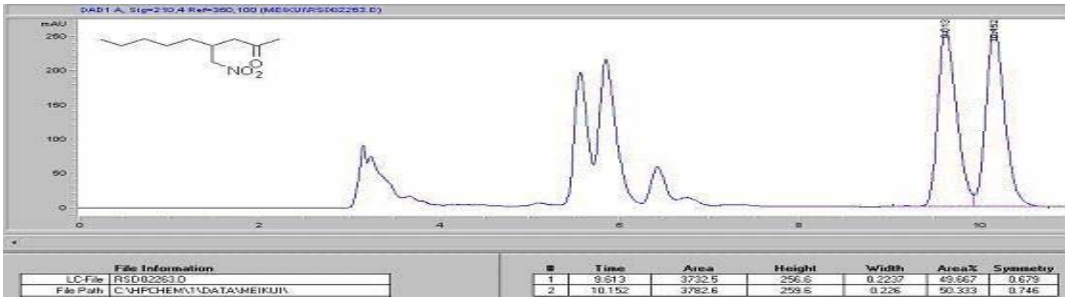
File Information	
LC File	RSD02098.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	23-May-08, 10:39:25
Sample	mk-k-24-2-rac
Sample Info	AS-H,Hexi-PrOH=80:20,1.0ml/min; 210nm, 25 deg
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	17.36 min
Sampling Rate	0.0067 min (0.402 sec), 2605 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	10.304	7607.4	432.9	0.271	50.253	0.717
2	11.591	7530.8	377.5	0.3087	49.747	0.721



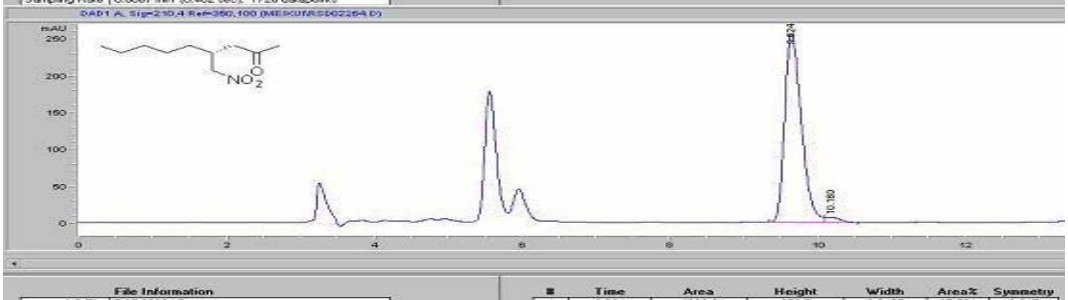
File Information	
LC File	RSD02100.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	23-May-08, 14:45:29
Sample	mk-k-24-1
Sample Info	AS-H,Hexi-PrOH=80:20,1.0ml/min; 210nm, 25 deg
Barcode	
Operator	mk

#	Time	Area	Height	Width	Area%	Symmetry
1	10.31	28167.7	1403.3	0.3182	96.668	0.682
2	11.631	970.8	47.1	0.3147	3.332	0.905



File Information	
LC File	RSD02263.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	16-Jun-08, 13:32:31
Sample	mk-k-29-2-2-rac
Sample Info	AS-H,Hexi-PrOH=95:5,1ml/min, 29 c
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	11.5 min
Sampling Rate	0.0067 min (0.402 sec), 1726 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	9.613	3732.5	256.6	0.2237	49.667	0.679
2	10.152	3782.6	259.6	0.226	50.333	0.746

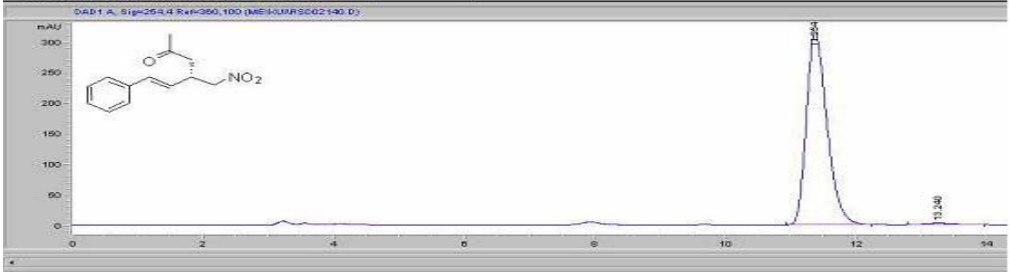


File Information	
LC File	RSD02264.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	16-Jun-08, 13:54:27
Sample	mk-k-39-2-1
Sample Info	AS-H,Hexi-PrOH=95:5,1ml/min, 29 c
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	14 min
Sampling Rate	0.0067 min (0.402 sec), 2101 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	9.624	4038.3	256.5	0.2437	97.591	0.645
2	10.16	99.7	7.3	0.2033	2.409	0.458

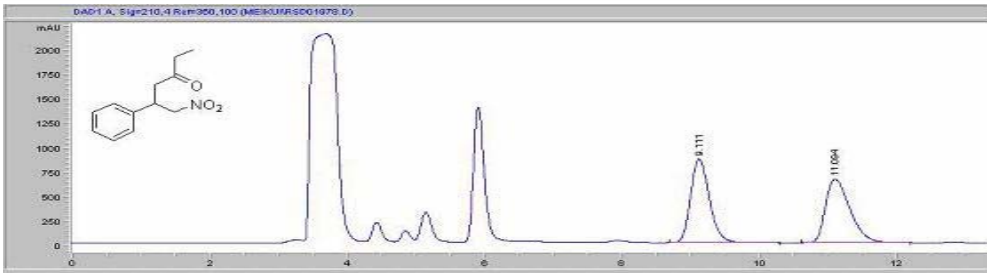
File Information	
LC File	RSD02141.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-Jun-08, 11:36:34
Sample	mk-38-2-rac
Sample Info	AS-H,hexi-PrOH=30:70,1ml/min; 25degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	15 min
Sampling Rate	0.0067 min (0.402 sec), 2251 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	11.232	4489.2	214.4	0.3223	50.445	0.723
2	12.728	4409.9	111.8	0.6043	49.555	0.447



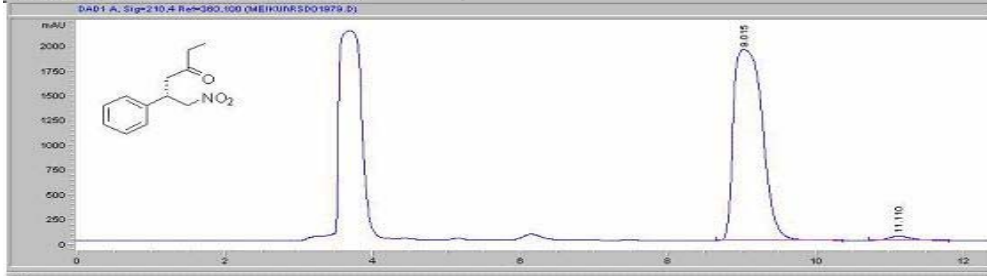
File Information	
LC File	RSD02140.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-Jun-08, 11:19:01
Sample	mk-38-1
Sample Info	AS-H,hexi-PrOH=30:70,1ml/min; 25degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	14.993 min
Sampling Rate	0.0067 min (0.402 sec), 2250 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	11.354	6894.7	315.3	0.3371	98.751	0.693
2	13.24	87.2	2.6	0.4896	1.249	0.745



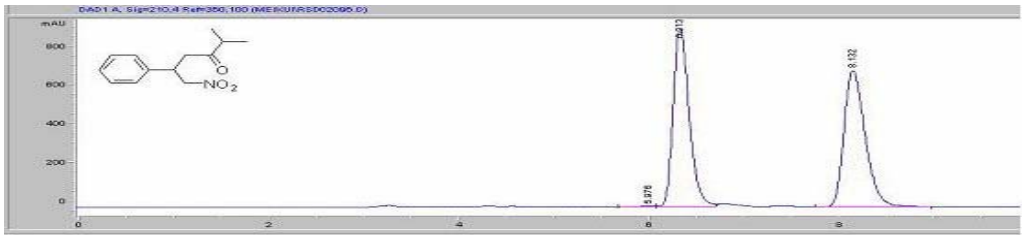
File Information	
LC File	RSD01978.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-May-08, 19:40:12
Sample	mk-jm-k-10-2-rac
Sample Info	AS-H,hexi-PrOH=70:30,1ml/min,210nm
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	13.98 min
Sampling Rate	0.0067 min (0.402 sec), 2098 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	9.111	16203.5	852.4	0.2938	50.417	0.762
2	11.094	15935.4	648.1	0.3809	49.583	0.606



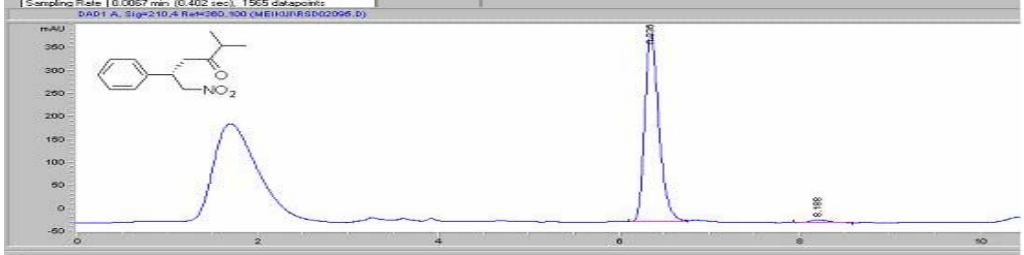
File Information	
LC File	RSD01979.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-May-08, 19:56:37
Sample	mk-jm-k-10-1
Sample Info	AS-H,hexi-PrOH=70:30,1ml/min,210nm
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	12.987 min
Sampling Rate	0.0067 min (0.402 sec), 1949 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	9.015	51896.9	1924.2	0.4367	98.310	0.549
2	11.11	892.2	41.4	0.3297	1.690	0.746



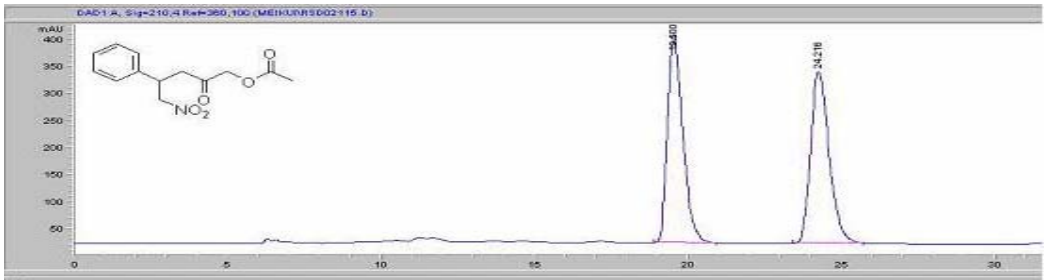
File Information	
LC File	RSD02096.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	22-May-08, 21:31:21
Sample	mk-k-18-2-rac
Sample Info	AS-H,hexi-PrOH=70:30;1.0ml/min; 210nm, 25 degi
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	10.427 min
Sampling Rate	0.0067 min (0.402 sec), 1565 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	5.976	62.9	5	0.1889	0.288	1.529
2	6.313	10827.8	923.6	0.1808	49.559	0.711
3	8.132	10957.7	704.4	0.2415	50.153	0.679



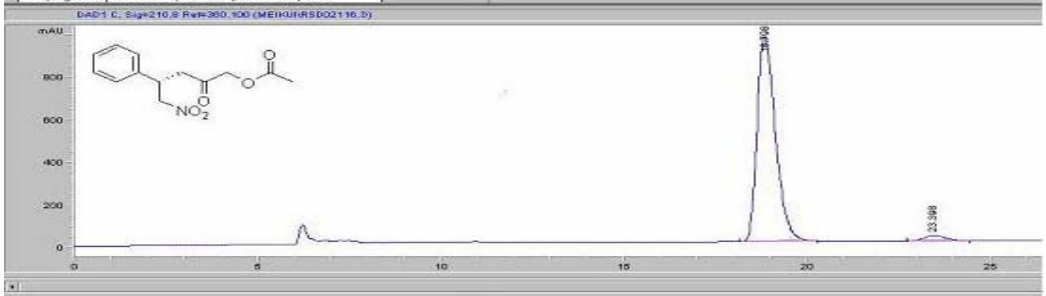
File Information	
LC File	RSD02095.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	22-May-08, 21:07:03
Sample	mk-k-19-1
Sample Info	AS-H,hexi-PrOH=70:30;1.0ml/min; 210nm, 25 deg
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	10.967 min
Sampling Rate	0.0067 min (0.402 sec), 1646 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	6.336	4502.5	409.4	0.1663	98.257	0.712
2	8.188	79.9	5.9	0.2135	1.743	0.79



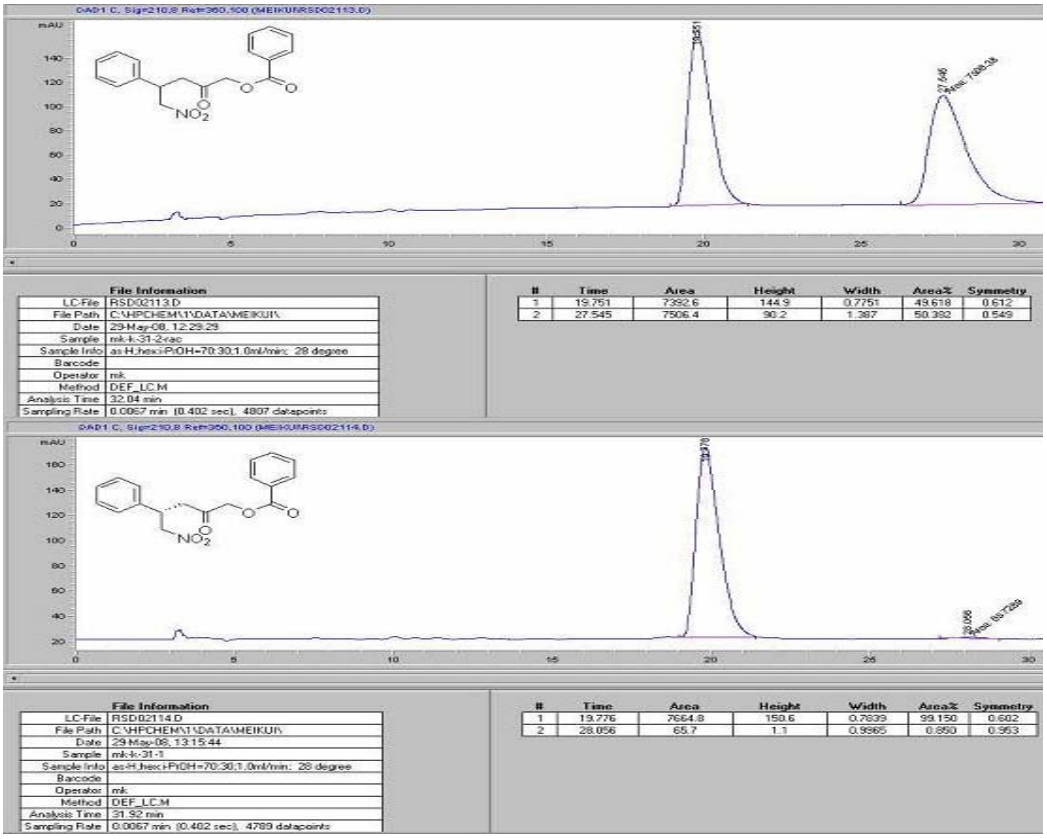
File Information	
LC File	RSD02115.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	29-May-08, 14:25:28
Sample	mk-k-33-2-rac
Sample Info	as-H,hexi-PrOH=50:50;0.5ml/min; 28 degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	33.073 min
Sampling Rate	0.0067 min (0.402 sec), 4962 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	19.5	13297.4	384.3	0.5297	50.110	0.663
2	24.216	13239.1	316.5	0.644	49.890	0.717



File Information	
LC File	RSD02116.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	29-May-08, 21:49:05
Sample	mk-k-33-1
Sample Info	as-H,hexi-PrOH=50:50;0.5ml/min; 28 degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	27.66 min
Sampling Rate	0.0067 min (0.402 sec), 4150 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	18.798	33364.7	962.1	0.5406	97.062	0.649
2	23.398	1010.1	25.7	0.5985	2.938	0.79

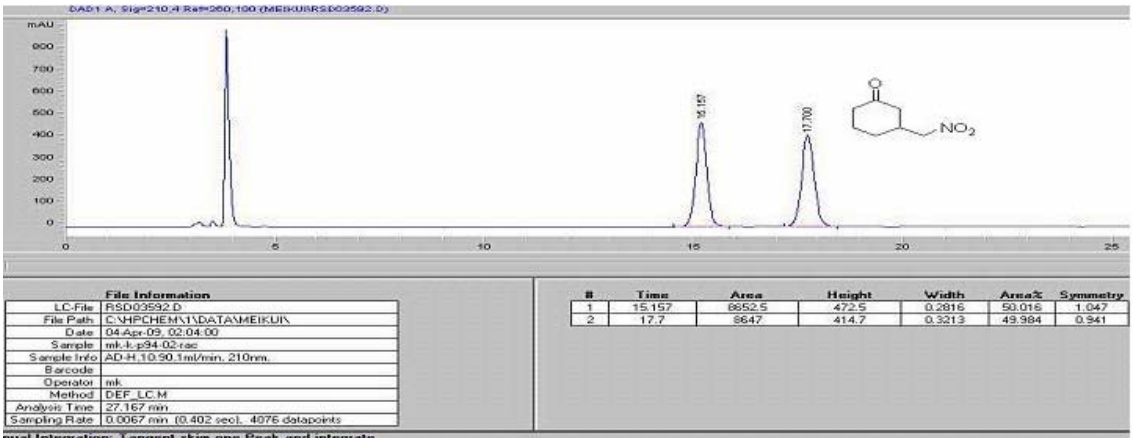


File Information	
LC-File	RSD02113.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	29-May-08, 12:29:29
Sample	mk-k-31-2-rac
Sample Info	as-H,hexi-PrOH=70:30,1.0ml/min; 28 degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	32.04 min
Sampling Rate	0.0067 min (0.402 sec), 4807 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	19.751	7392.6	144.9	0.7751	49.618	0.612
2	27.545	7506.4	90.2	1.397	50.382	0.549

File Information	
LC-File	RSD02114.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	29-May-08, 13:15:44
Sample	mk-k-31-1
Sample Info	as-H,hexi-PrOH=70:30,1.0ml/min; 28 degree
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	31.92 min
Sampling Rate	0.0067 min (0.402 sec), 4789 datapoints

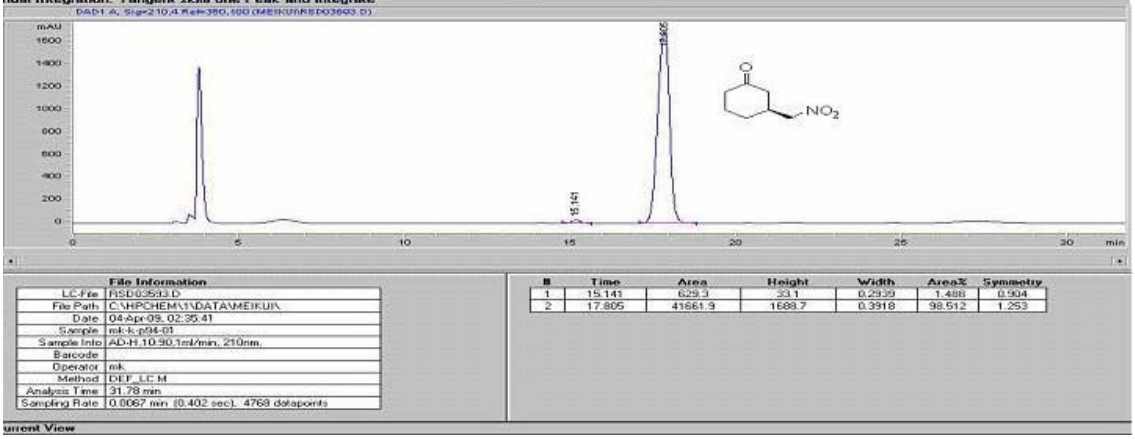
#	Time	Area	Height	Width	Area%	Symmetry
1	19.776	7664.8	150.6	0.7639	99.150	0.602
2	28.056	65.7	1.1	0.9965	0.850	0.963



File Information	
LC-File	RSD03592.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-Apr-09, 02:04:00
Sample	mk-k-p34-02-rac
Sample Info	AD-H,10:90,1ml/min, 210nm.
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	27.167 min
Sampling Rate	0.0067 min (0.402 sec), 4076 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	15.157	8852.5	472.5	0.2816	50.016	1.047
2	17.7	8847	414.7	0.3213	49.984	0.941

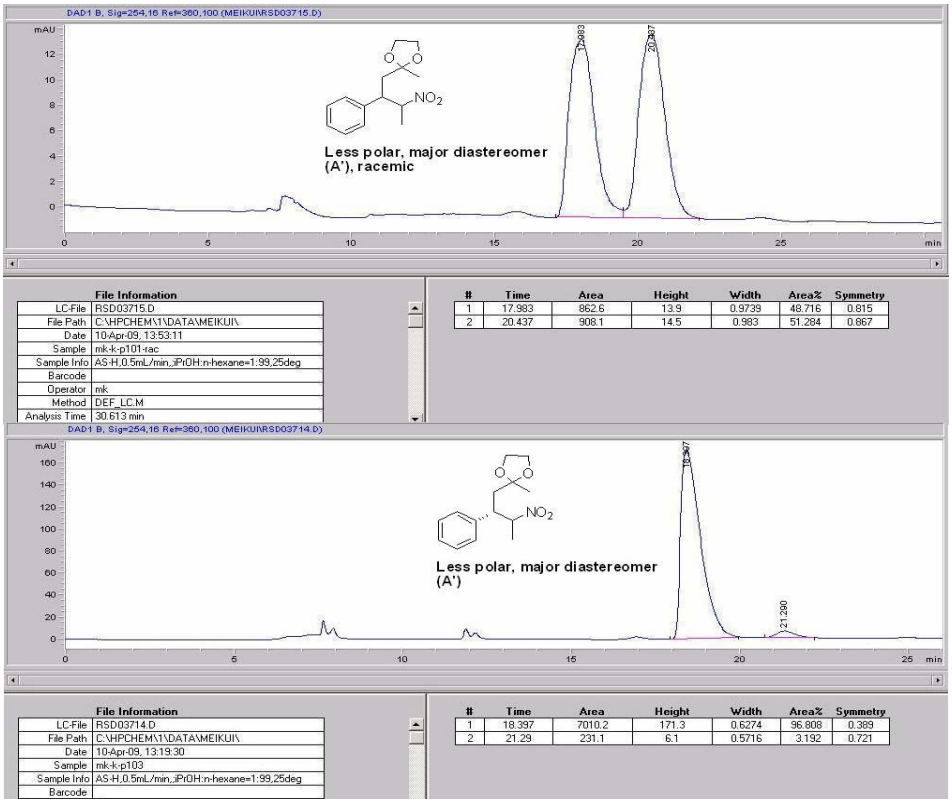
nual Integration: Tangent skim one Peak and integrate



File Information	
LC-File	RSD03593.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	04-Apr-09, 02:35:41
Sample	mk-k-p34-01
Sample Info	AD-H,10:90,1ml/min, 210nm.
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	31.78 min
Sampling Rate	0.0067 min (0.402 sec), 4768 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	15.141	629.3	33.1	0.2939	1.488	0.904
2	17.805	41661.9	1688.7	0.3918	98.512	1.253

urrent View

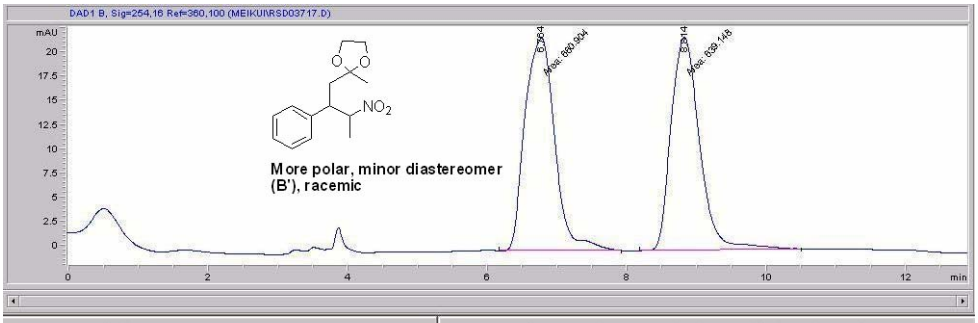


File Information	
LC-File	RSD03715.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	10-Apr-09, 13:53:11
Sample	mk-k-p101-rac
Sample Info	AS-H,0.5mL/min,;iPrOH:n-hexane=1:99,25deg
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	30.613 min

#	Time	Area	Height	Width	Area%	Symmetry
1	17.983	862.6	13.9	0.9739	48.716	0.815
2	20.437	908.1	14.5	0.983	51.284	0.867

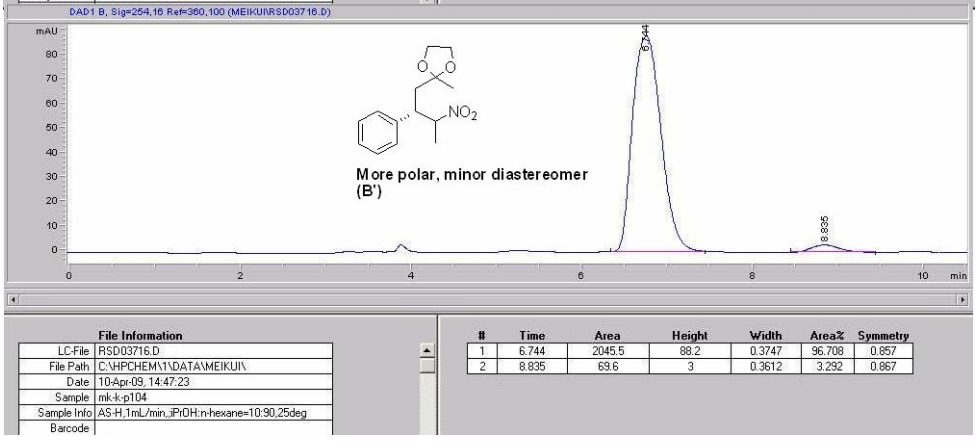
File Information	
LC-File	RSD03714.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	10-Apr-09, 13:19:30
Sample	mk-k-p103
Sample Info	AS-H,0.5mL/min,;iPrOH:n-hexane=1:99,25deg
Barcode	

#	Time	Area	Height	Width	Area%	Symmetry
1	18.397	7010.2	171.3	0.6274	96.808	0.389
2	21.29	231.1	6.1	0.5716	3.192	0.721



File Information	
LC-File	RSD03717.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	10-Apr-09, 15:01:15
Sample	mk-k-p102-rac
Sample Info	AS-H,1mL/min,;iPrOH:n-hexane=10:90,25deg
Barcode	
Operator	mk
Method	DEF_LC.M
Analysis Time	12.92 min

#	Time	Area	Height	Width	Area%	Symmetry
1	6.764	660.9	22.1	0.4991	50.837	1.12
2	8.814	639.1	22.1	0.4814	49.163	0.808



File Information	
LC-File	RSD03716.D
File Path	C:\HPCHEM\1\DATA\MEIKUI\
Date	10-Apr-09, 14:47:23
Sample	mk-k-p104
Sample Info	AS-H,1mL/min,;iPrOH:n-hexane=10:90,25deg
Barcode	

#	Time	Area	Height	Width	Area%	Symmetry
1	6.744	2045.5	88.2	0.3747	96.708	0.857
2	8.835	69.6	3	0.3612	3.292	0.867