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Supporting Information for

Enantioselective Desymmetrization of Prochiral Cyclohexanone Derivatives via the Organocatalytic Direct Aldol Reaction

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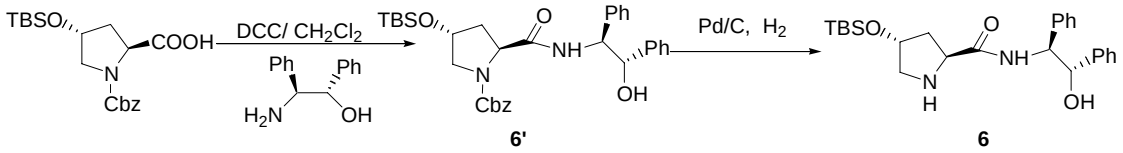
General Information: Chemicals and solvents were all purchased from commercial supplies and purified by standard techniques. NMR spectra were recorded on a Bruker-300 MHz spectrometer. High-resolution mass spectra were recorded on a Bruker BIO TOF Q mass spectrometer. Infrared spectra were recorded on a Nicolet MX-1E FT-IR spectrometer. HPLC analysis was performed on Waters-Breeze (2487 Dual λ Absorbance Detector and 1525 Binary HPLC Pump). Chiralpak AS, AD, OJ , and OD columns were purchased from Daicel Chemical Industries, LTD.

Typical procedure for the synthesis of 6: *N*-CBZ-O-TBS-L-proline (379 mg, 1.0 mmol) and amine (213 mg, 1mmol) were dissolved in Dicloromethane (15 ml), The solution was cooled down to 0 °C. To the solution, DCC (250 mg, 1.2 mmol) was added. After the resulting solution was stirred at 0 °C for 1 h and at room temperature for another 16 h, the mixture was filtered. The solvent was removed under the reduced pressure and Dicloromethane (10ml) was added to the residue. The solution was stirred at 0 °C for 12h and then was filtered to remove DCC. The solvent was removed under the reduced pressure and the residue was purified through column chromatography on silica gel(eluent: Dichloromethane: Ethyl acetate= 20:1) to give Compounds **6'**. A solution of **6'** (1.0 g), Pd/C (5%, 0.1 g) in methanol (30ml) was stirred under hydrogen (1 atm) in a two-neck flask (100 ml) for 1 h. The solution was filtered. After removal of solvent, the resulting residue was purified through a column chromatography on silica gel (eluent: Dichloromethane: methanol = 100:1) to give **6**.



(2S,1'S,2'S)-4-(*tert*-butyldimethylsiloxy)-*N*-(2-droxyl-1,2-diphenylethyl)pyrrolidine-2-caboxa mide (6): Yield: 70% mp 57-59 ^{o}C; $[\alpha]^{20}_{D}$ =-17.2 (c=0.5, CH_2Cl_2); ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.03 (s, 6H), 0.85 (s, 9H), 1.71-1.78 (m, 1 H), 2.08 (m, 1H), 2.66 (m, 1H), 2.87 (m, 1H), 3.87 (t, *J*= 8.1 Hz, 1H), 4.27 (brs, 1H), 4.99 (d, *J*= 4.4 Hz, 1H), 5.01 (m, 1H), 7.18-7.31 (m, 12H), 8.57 (d, *J*= 7.6 Hz, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) -5.03, 17.81, 25.61, 39.58, 55.62, 58.87, 59.38, 73.23, 126.08, 126.81, 127.03, 127.17, 127.74, 128.09, 174.81; HR-MS for $C_{25}H_{37}N_2O_3Si$, calc: 441.2568, found: 441.2553.

General procedure for the aldol reaction: To a solution of an aldehyde (0.5 mmol) and 4-substituted cyclohexanone (5 mmol) in anhydrous Dicloromethane (2 ml) was added L-prolinamide (11 mg, 0.025 mmol). The resulting mixture was stirred at –40 ^{o}C for 72 or 96 h (monitored by TLC). The reaction was quenched with saturated aqueous ammonium chloride (10 ml). The reaction mixture was extracted with ethyl acetate and the combined organic layers were dried over anhydrous $MgSO_4$. After removal of solvent, the residue was purified through a flash column chromatography on silica gel to give the corresponding aldol products.

2-[Hydroxy(4-nitrophenyl)methyl]-4-methylcyclohexanone (3aa): yield 90%; $[\alpha]^{30}_{D}$ = -44.4 (c= 0.5, Ethyl acetate); mp: 109-111°C; ^{1}H-NMR (300MHz, $CDCl_3$): δ (ppm) 1.05 (d, *J*= 6.9 Hz, 3H), 1.33 (m, 1H), 1.54-1.60 (m, 1H), 1.78-1.81 (m, 1H), 1.89-1.93 (m,1H), 2.07-2.09 (m, 1H), 2.36-2.43 (m, 1H), 2.48-2.50 (m, 1H), 2.72-2.78 (m, 1H), 3.82-3.89 (b, 1H), 4.92 (d, *J*= 8.6 Hz, 1H), 7.47-7.52 (m, 2H), 8.18-8.23 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.144, 26.599, 32.874, 36.031, 38.115, 52.827, 74.106, 123.627, 127.783, 147.600, 148.376, 214.887; IR(KBr) 3499, 3109, 2957, 1702, 1606, 1522, 1345, 699 cm^{-1}; Enantiomeric excess: >99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 20/ 80), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 11.749 min; t_{Rminor}= 18.949 min; HR-MS for $C_{14}H_{17}N_1O_4$ +Na^+, calc: 286.1050, found: 286.1043.

2-[(2-Fluorophenyl)hydroxymethyl]-4-methylcyclohexanone (3ab): yield 93%, $[\alpha]^{30}_{D}$ = -32.6 (c=0.5, Ethyl acetate); mp: 81.7-82.5 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.05 (d, *J*= 6.9 Hz, 3H), 1.39-1.40 (m, 1H), 1.62-1.63 (m, 1H), 1.72-1.76 (m, 1H), 1.93-1.94 (m, 1H), 2.08 (m, 1H), 2.43-2.52 (m, 2H), 2.80-2.82 (m, 1H), 3.61 (bs, 1H), 5.21 (d, *J*= 9.0 Hz, 1H), 7.00-7.06 (m, 1H), 7.16-7.19 (m, 1H), 7.26-7.29 (m, 1H), 7.42-7.45 (m, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm)

18.540, 26.683, 33.370, 35.883, 53.273, 68.232, 115.084 (d, *J*= 22.2 Hz), 124.566, 128.155, 129.273, 129.383, 158.533 (d, *J*= 244.3 Hz), 215.304; IR(KBr) 3397, 3109, 2928, 2868, 1689, 1615, 1585, 1044, 760 cm^{-1}; Enantiomeric excess: >99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 5/95), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 6.283 min; t_{Rminor}= 9.912 min; HR-MS for $C_{14}H_{17}F_1O_2$ +Na^+, calc: 259.1105, found: 259.1093.

2-[(4-Fluorophenyl)hydroxymethyl]-4-methylcyclohexanone (3ac): yield 76%; $[\alpha]^{30}_D$ = -36.8 (c= 0.5, Ethyl acetate); mp: 91.8-93.6°C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.03 (d, *J*= 6.9 Hz, 3H), 1.32 (m, 1H), 1.46-1.50 (m, 1H), 1.74 (m, 1H), 1.91-1.93 (m,1H), 2.04 (m, 1H), 2.41-2.52 (m, 2H), 2.70-2.72 (m, 1H), 4.81 (d, *J*= 9 Hz, 1H), 7.00-7.07 (m, 2H), 7.25-7.31 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.491, 26.671, 33.226, 36.158, 38.190, 53.495, 74.245, 115.129 (d, *J*= 21.3 Hz), 128.491, 128.598, 136.901, 160.796 (d, *J*= 244.5 Hz), 215.412; IR(KBr) 3390, 3966, 2931, 1690, 1602, 1507, 1052, 840 cm^{-1}; Enantiomeric excess: >99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 5.59 min; t_{Rminor}= 8.55 min; HR-MS for $C_{14}H_{17}F_1O_2$ +Na^+, calc: 259.1105, found: 259.1098.

2-[Hydroxy(2-nitrophenyl)methyl]-4-methylcyclohexanone (3ad): yield 84%; $[\alpha]^{30}_D$ = +16 (c= 0.5, Ethyl acetate); mp. 103.5-105.7 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.07 (d, *J*= 6.9 Hz, 3H), 1.52 (m, 1H), 1.74-1.93 (m, 3H), 2.09-2.11 (m, 1H), 2.33-2.39 (m, 2H), 2.44-2.46 (m, 1H), 2.89-2.92 (m, 1H), 3.95-3.98 (b, 1H), 5.42 (d, *J*= 7.2 Hz, 1H), 7.40-7.45 (m, 1H), 7.62 (m, 1H); 7.72-7.74 (m, 1H); 7.81-7.84 (m, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.172, 26.814, 33.135, 35.719, 36.601, 38.460, 52.848, 69.804, 124.038, 128.442, 128.838, 133.092, 136.686, 148.759, 214.974; IR(KBr) 3333, 3109, 2961, 2928, 2853, 1704, 1604, 1579, 1535, 1371, 848, 779 cm^{-1}; Enantiomeric excess: >99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 8.229 min; t_{Rminor}= 10.209 min; HR-MS for $C_{14}H_{17}N_1O_4$ +Na^+, calc: 286.1050, found: 286.1059.

2-[Hydroxy(4-trifluoromethylphenyl)methyl]-4-methylcyclohexanone (3ae): yield: 70%; $[\alpha]^{30}_D$ = -35.2 (c= 0.5, Ethyl acetate); mp: 110.6-111.4 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.05 (d, *J*= 6.9 Hz, 3H), 1.33 (m, 1H), 1.50-1.60 (m, 1H), 1.77 (m, 1H), 1.90-1.93 (m,1H), 2.06-2.08 (m, 1H), 2.38-2.44 (m, 1H), 2.48-2.52 (m, 1H), 2.74-2.79 (m, 1H), 3.80 (b, 1H), 4.87 (d, *J*= 8.7 Hz, 1H), 7.44 (d, *J*= 8.1 Hz, 2H), 7.61 (d, *J*= 8.1 Hz, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.236, 26.617, 33.072, 36.072, 38.140, 53.024, 74.389, 118.625 (q, *J*= 270.3 Hz), 125.393 (q, *J*= 3.5 Hz), 127.278, 129.491 (q, *J*= 32.1 Hz), 144.972, 215.261; IR(KBr) 3363, 3045, 2959, 2913, 2875, 1694,

1455, 1322, 1182, 1168.2, 1069, 608 cm^{-1}; Enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 5.966 min; t_{Rminor}= 8.184 min; HR-MS for $C_{15}H_{17}F_3O_2+Na^+$, calc: 309.1073, found: 309.1083.

4-[(Hydroxy(5-methyl-2-oxocyclohexyl)methyl)benzonitrile(3af): yield 80%; $[\alpha]^{30}_D$ = -51.4 (c= 0.5, Ethyl acetate); mp: 93.4-95.1 °C; ^{1}H-NMR (300MHz, $CDCl_3$): δ (ppm) 1.05 (d, *J*= 6.9 Hz, 3H), 1.28-1.32 (m, 1H), 1.52-1.62 (m, 1H), 1.77-1.81 (m, 1H), 1.89-1.93 (m,1H), 2.04-2.09 (m, 1H), 2.36-2.43 (m, 1H), 2.48-2.50 (m, 1H), 2.72 (m, 1H), 4.85 (d, *J*= 8.7 Hz, 1H), 7.42-7.45 (m, 2H), 7.63-7.66 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.142, 26.610, 32.888, 36.035, 38.126, 52.755, 74.391, 111.833, 118.669, 127.696, 132.287, 146.353, 215.029; IR(KBr) 3422, 3050, 2938, 2927, 2854, 2871, 2227, 1698, 1606, 1503, 842 cm^{-1}; Enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 12.009 min; t_{Rminor}= 19.724 min; HR-MS for $C_{15}H_{17}N_1O_2+Na^+$ calc: 266.1151; found: 266.1140.

2-[(4-Bromo-phenyl)hydroxymethyl]-4-methylcyclohexanone (3ag): yield 61%; $[\alpha]^{30}_D$ = -27.4 (c= 0.5, Ethyl acetate); mp: 103.1-104.5 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.02 (d, *J*= 6.9 Hz, 3H), 1.29-1.31 (m, 1H), 1.45-1.50 (m, 1H), 1.73-1.75 (m, 1H), 1.92 (m,1H), 2.03 (m, 1H), 2.36-2.50 (m, 2H), 2.67-2.69 (m,1H), 3.71 (b, 1H), 4.81 (d, *J*= 9.0 Hz, 1H), 7.15-7.20 (m, 2H), 7.44-7.49 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.416, 26.620, 33.190, 36.093, 38.145, 53.283, 74.263, 121.806, 128.614, 131.565, 140.067, 215.304; IR(KBr) 3371, 3023, 2963.6, 2933, 2911, 2872, 1700, 1590, 1455, 1059, 1006, 823 cm^{-1}; Enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 7.262 min; t_{Rminor}= 10.747 min; HR-MS for $C_{14}H_{17}Br_1O_2+Na^+$, calc: 319.0304, found : 319.0310.

2-[(4-Chlorophenyl)hydroxymethyl]-4-methylcyclohexanone (3ah): yield 70%; $[\alpha]^{30}_D$ = -30.8 (c= 0.5, Ethyl acetate); mp: 102.7-104.5 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.02 (d, *J*= 6.9 Hz, 3H), 1.29-1.32 (m, 1H), 1.46-1.50 (m, 1H), 1.74-1.76 (m, 1H), 1.92 (m,1H), 2.03 (m, 1H), 2.37-2.51 (m, 2H), 2.68-2.70 (m,1H), 3.71 (b, 1H), 4.79 (d, *J*= 9 Hz, 1H), 7.22-7.25 (m, 2H), 7.30-7.33 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.414, 26.630, 33.184, 36.103, 38.155, 53.319, 74.228, 128.273, 128.630, 133.661, 139.552, 215.339; IR(KBr) 3451, 3051, 2953, 2925, 2850, 1697, 1489, 1455, 832, 735 cm^{-1}; Enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 7.009 min; t_{Rminor}= 10.091 min; HR-MS for $C_{14}H_{17}Cl_1O_2+Na^+$, calc: 275.0809, found: 275.0822.

2-[(3,5-Dibromophenyl)hydroxymethyl]-4-methylcyclohexanone (3ai): yield 82%; $[\alpha]^{30}_D$ =

-24.4 (c= 0.5, Ethyl acetate); ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.08 (d, *J*= 6.9 Hz, 3H), 1.38 (m, 1H), 1.53-1.61 (m, 1H), 1.79-1.81 (m, 1H), 1.88-1.94 (m,1H), 2.07-2.09 (m, 1H), 2.35-2.41 (m, 1H), 2.47-2.53 (m, 1H), 2.68 (m,1H), 3.85 (b, 1H), 4.71 (d, *J*= 8.7 Hz, 1H), 7.39-7.40 (m, 2H), 7.58-7.60 (m, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.256, 26.642, 32.953, 36.064, 38.130, 52.801, 73.922, 122.972, 128.837, 133.569, 145.065, 215.029; IR(Neat) 3428, 3071, 2953, 2927, 1868, 1703, 1584, 1556, 857, 740, 686 cm^{-1}; Enantiomeric excess: 96%, determined by HPLC (Daicel Chiralpak OJ-H, i-PrOH/ Hexane= 5/ 95), UV 254 nm, flow rate 1.0 mL/min; t_{Rmajor}= 8.731 min; t_{Rminor}= 10.084 min; HR-MS for $C_{14}H_{16}Br_2O_2$ +Na^+, calc: 396.9409, found: 396.9400.

2-[(3,5-Bistrifluoromethylphenyl)hydroxymethyl]-4-methylcyclohexanone (3aj): yield 55%; $[\alpha]^{30}_D$ = -25.4 (c= 0.5, Ethyl acetate); mp: 90.5-90.9 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.07 (d, *J*= 6.9 Hz, 3H), 1.33 (m, 1H), 1.58-1.62 (m, 1H), 1.81-1.83 (m, 1H), 1.90-1.94 (m,1H), 2.09-2.11 (m, 1H), 2.36-2.43 (m, 1H), 2.50-2.54 (m,1H), 2.75-2.79 (m, 1H), 4.00 (b, 1H), 4.93 (d, *J*= 8.5 Hz, 1H), 7.78-7.82 (m, 3H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.027, 26.598, 32.764, 35.954, 38.085, 52.615, 74.050, 117.821 (q, *J*= 271.1 Hz); 121.931, 127.203, 131.040 (q, *J*= 33 Hz), 143.717, 214.860; IR(KBr) 3425, 2957, 2930, 2874, 1694, 1619, 1458, 1380, 1275, 1174, 1138, 898, 845, 680 cm^{-1}; Enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak AD, i-PrOH/ Hexane= 5/95), UV 254 nm, flow rate 1.0 mL/min, t_{Rminor}= 5.238 min; t_{Rmajor}= 11.863 min; HR-MS for $C_{16}H_{16}F_6O_2$ +Na^+, calc: 377.0947, found: 377.0951.

2-[(2,6-Dichlorophenyl)hydroxymethyl]-4-methylcyclohexanone(3ak): yield 95%; $[\alpha]^{30}_D$ = -92.6 (c= 0.5, Ethyl acetate); mp: 95.8-97.3 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.06 (d, *J*= 6.9 Hz, 3H), 1.27-1.32 (m, 1H), 1.52-1.54 (m, 1H), 1.66-1.71 (m, 1H), 1.96-1.98 (m,1H), 2.16-2.18 (m, 1H), 2.48-2.53 (m, 2H), 3.47 (d, *J*= 12 Hz, 1H), 3.54-3.57 (m, 1H), 5.83 (m, 1H), 7.13-7.19 (m, 1H), 7.25-7.33 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.882, 26.858, 33.523, 35.666, 38.470, 50.700, 70.760, 129.430, 134.942, 214.024; IR(KBr) 3405, 3082, 2959, 2933, 2905, 1703, 1580, 1559, 779, 763, 732, cm^{-1}; Enantiomeric excess: >99%, determined by HPLC (Daicel Chiralpak OJ, *i*-PrOH/ Hexane= 5/95), UV 254 nm, flow rate: 1.0 mL/min; t_{Rminor}= 9.041 min; t_{Rmajo}= 9.782 min; HR-MS for $C_{14}H_{16}Cl_2O_2$ +Na^+, calc: 309.0420, found: 309.0419.

2-(Hydroxyphenylmethyl)-4-methylcyclohexanone (3al): yield 46%; $[\alpha]^{30}_D$ = -43.8 (c= 0.5, Ethyl acetate); mp: 52.2-54 °C; ^{1}H-NMR (300MHz, $CDCl_3$): δ (ppm) 1.02 (d, *J*= 6.9 Hz, 3H), 1.30-1.34 (m, 1H), 1.52 (m, 1H), 1.70-1.74 (m, 1H), 1.94 (m,1H), 2.04-2.06 (m, 1H), 2.43-2.52 (m, 2H), 2.75-2.78 (m, 1H), 4.84 (d, *J*= 9.3 Hz, 1H), 7.25-7.38 (m, 5H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ

(ppm) 18.672, 26.729, 33.454, 36.291, 38.263, 53.705, 74.920, 126.927, 128.050, 128.512, 141.084, 215.446; IR(KBr) 3409, 3018, 3061, 2868, 2852, 1696, 1415, 1038, 742, 697cm^{-1}; Enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 6.515 min; t_{Rminor}= 9.992 min; HR-MS for $C_{16}H_{18}F_6O_2$ +Na$^+$, calc: 241.1199, found: 241.1217.

4-Ethyl-2-[hydroxy(4-nitrophenyl)methyl]cyclohexanone (3ba): yield 90%; $[\alpha]^{30}_D$ = -51.8 (c= 0.5, Ethyl acetate); mp: 120-122 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.807 (d, *J*= 7.5 Hz, 3H), 1.35-1.54 (m, 4H), 1.70-1.74 (m, 1H), 1.85-1.90 (m, 1H), 2.39-2.42 (m, 1H), 2.68 (m, 1H), 4.91 (d, *J*= 9 Hz, 1H), 7.48-7.52 (m, 2H), 8.19-8.24 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 11.985, 24.725, 30.461, 33.517, 33.680, 38.380, 52.946, 74.164, 123.641, 127.815, 147.642, 148.356, 215.027; IR(KBr) 3497, 3109, 3074, 2968, 2924, 2848, 1700, 1605, 1595, 1516, 1342, 862 cm^{-1}; Enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 13.662 min; t_{Rminor}= 19.067 min; HR-MS for $C_{15}H_{19}N_1O_4$ +Na$^+$, calc: 300.1206, found: 300.1229.

2-[Hydroxy(4-nitrophenyl)methyl]-4-propylcyclohexanone (3ca): yield: 90%; $[\alpha]^{30}_D$ = -36.4 (c= 0.5, Ethyl acetate); mp: 109-111 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.86 (d, *J*= 6.9 Hz, 3H), 1.16-1.38 (m, 5H), 1.50-1.58 (m, 1H), 1.84-1.88 (m, 3H), 2.40-2.47 (m, 2H), 2.69 (m, 1H), 3.93 (b, 1H), 4.91 (d, *J*= 8.7 Hz, 1H), 7.47-7.51 (m, 2H), 8.19-8.22 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 14.047, 20.586, 30.733, 31.576, 33.991, 34.151, 38.371, 53.031, 74.117, 123.615, 127.794, 147.604, 148.378, 215.021; IR(KBr) 3487, 3108, 2949, 2926, 2867, 2853, 1702, 1605, 1521, 1344, 859, 838 cm^{-1}; Enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 10.529 min; t_{Rminor}= 13.668 min; HR-MS for $C_{16}H_{21}N_1O_4$ +Na$^+$, calc: 314.1363; found: 314.1360.

4-*tert*-Butyl-2-[hydroxy(4-nitrophenyl)methyl]cyclohexanone (3da): yield 52%; $[\alpha]^{30}_D$ = -86.6 (c= 0.5, Ethyl acetate); mp: 178.1-179.9 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.78 (s, 9H), 1.40-1.62 (m, 4H), 1.94-1.99 (m,1H), 2.41-2.51 (m, 2H), 2.64-2.67 (m, 1H), 3.63 (b, 1H), 4.96 (d, *J*= 9 Hz, 1H), 7.52-7.55 (m, 2H), 8.21-8.24 (m, 2H); ^{13}C-NMR (75MHz, $CDCl_3$): δ (ppm) 24.113, 26.881, 26.992, 32.892, 39.314, 42.381, 54.283, 74.002, 123.705, 127.765, 147.753, 148.524, 215.814; IR(KBr) 3462, 2952, 2924, 2865, 1702, 1604, 1520, 1390, 1344, 1258, 1222, 854 cm^{-1}; Enantiomeric excess: 93%, determined by HPLC (Daicel Chiralpak AD, i-PrOH/ Hexane= 15/ 85),

UV 254 nm, flow rate 1.0 mL/min, t_{Rminor} = 7.93 min; t_{Rmajor} = 17.47 min; HR-MS for $C_{17}H_{23}N_1O_4$ $+Na^+$, calc: 328.1519, found: 328.1507.

2-[Hydroxy(4-nitrophenyl)methyl]-4-phenylcyclohexanone (3ea): yield: 74%; $[\alpha]^{30}_D$ = -48.2 (c= 0.5, Ethyl acetate); mp: 140.5-141.7 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.79-1.84 (m, 1H), 1.94-1.96 (m, 1H), 2.19 (m, 1H), 2.35-2.40 (m, 1H), 2.53-2.58 (m, 2H), 2.76-2.79 (m, 1H), 3.16-3.17 (m, 1H), 3.70 (d, *J*= 3.0 Hz, 1H), 5.05 (dd, J_1= 3 Hz, J_2= 8.8 Hz, 1H), 7.12-7.15 (m, 2H), 7.22-7.26 (m, 1H), 7.28-7.33 (m, 2H), 7.51-7.54 (m, 2H), 8.21-8.24 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 31.041, 34.056, 36.725, 39.052, 53.983, 73.907, 123.745, 126.355, 126.660, 127.786, 128.791, 142.198, 147.671, 148.200, 213.944; IR(KBr) 3380, 3034, 2941, 2918, 2887, 1703, 1604, 1515, 1399, 1055, 847, 772 cm^{-1}; Enantiomeric excess: 94%, determined by HPLC (Daicel Chiralpak AD, i-PrOH/ Hexane= 20/ 80), UV 254 nm, flow rate 1.0 mL/min, t_{Rminor} = 15.697 min; t_{Rmajor} = 22.640 min; HR-MS for $C_{19}H_{19}N_1O_4$ $+Na^+$, calc: 348.1206, found: 348.1208.

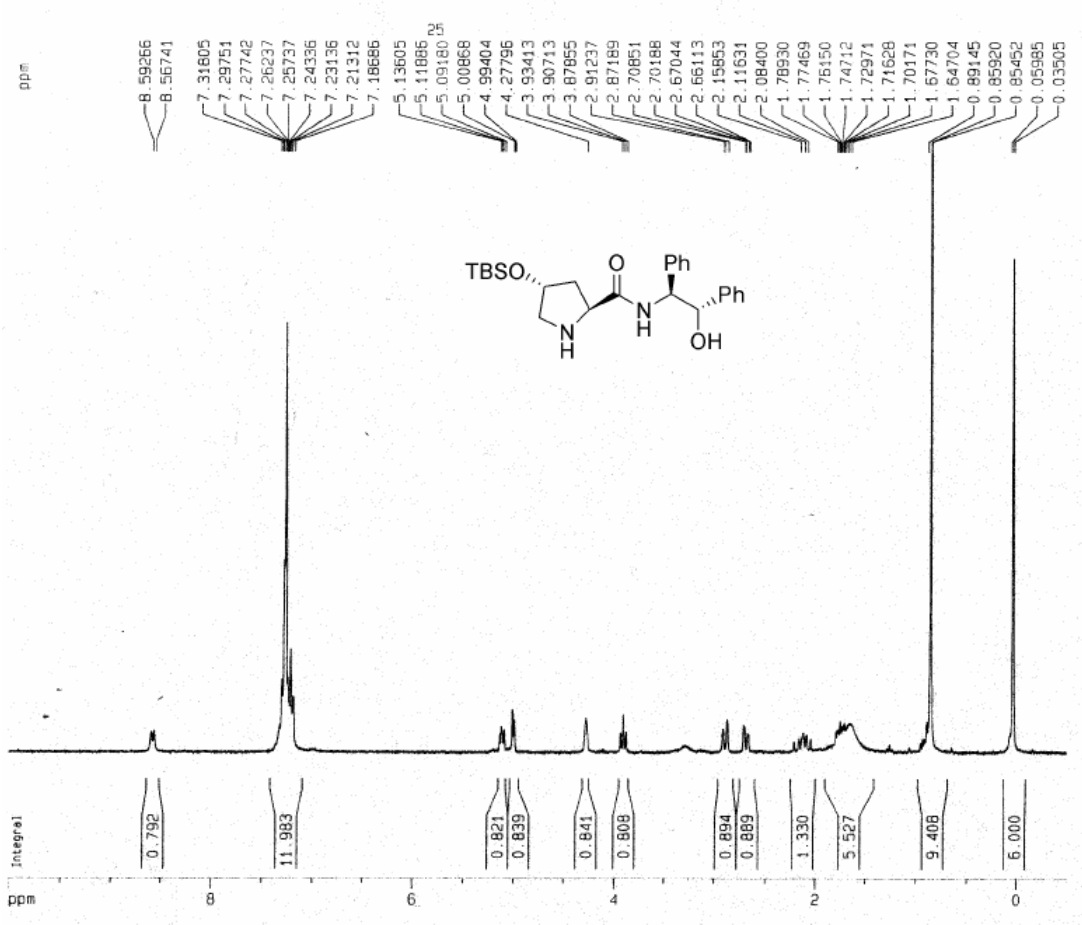
General procedure for the synthesis of 2-arylidene-4-methylcyclohexanones: The crude product of the enantioselective desymmetrization was dissolved in anhydrous Dicloromethane (5 ml), then TsCl (0.2 ml), triethylamine (1.0 ml), and DMAP (5 mg) were added at 0 °C. The mixture was stirred at 0°C for 30 minute and then refluxed for 2 days at 40 °C. The reaction was quenched with water (10 ml). The resultant mixture was extracted with ethyl acetate and the combined organic layers were dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was purified through flash column chromatography on a silica gel to give the corresponding dehydroxylation products.

2-(2-Fluoro-benzylidene)4-methylcyclohexanone (7): yield: 60%; $[\alpha]^{30}_D$ = +136.2 (c= 0.5, CH_3CO_2Et); mp: 81.7-82.5 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 1.03 (d, *J*= 6.3 Hz, 3H), 1.60-1.62 (m, 1H), 1.82-1.88 (m, 1H), 1.92-2.00 (m, 1H), 2.23-2.24 (m,1H), 2.44-2.50 (m, 1H), 2.61-2.64 (m, 1H), 2.83-2.88 (m, 1H), 7.05-7.16 (m, 2H), 7.26-7.34 (m, 2H), 7.45 (s, 1H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 21.564, 30.269, 31.498, 37.302, 39.366, 115.505 (d, *J*= 21.8 Hz), 123.620, 127.907, 130.144, 130.675, 138.295, 159.138(d, *J*= 248.8 Hz), 201.323; IR(KBr) 3076, 2952, 2927, 2881, 1686, 1613, 1600, 1572, 1451, 1140, 755 cm^{-1}; Enantiomeric excess: 99%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rminor} = 5.571 min; t_{Rmajor} = 6.135 min; HR-MS for $C_{14}H_{15}F_1O_1$ $+Na^+$, calc: 241.0999, found: 241.0983.

The synthesis of 7-[Hydroxy(4-nitrophenyl)methyl]-5-methyloxepan-2-one (8): To solution of **3aa** (131 mg, 0.5 mmol) in anhydrous Dicloromethane (5 ml) were added $NaHCO_3$ (87 mg) and m-CPBA (270 mg, 1.5mmol). The reaction mixture was stirred at 25 °C until the reaction was complete (monitored by TLC). The reaction was quenched with saturated aqueous $Na_2S_2O_3$ (10 ml). The mixture was extracted with ethyl acetate and the combined organic layers were dried over anhydrous $MgSO_4$. After removal of solvent, the residue was purified through flash column chromatography on a silica gel (eluent: Petroleum: Ethyl acetate= 2:1) to give the **8** as a white solid in 81% yield. $[\alpha]^{30}_D$= -9.2 (c= 0.5, Ethyl acetate); mp: 148.9-149.4 °C; ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.90 (d, *J*= 6.9 Hz, 3H), 1.30-1.34 (m, 1H), 1.574-1.59 (m, 1H), 1.75-1.83 (m, 2H), 2.01-2.03 (m,1H), 2.54-2.59 (m, 1H), 2.77-2.82 (m, 1H), 4.44-4.51 (m, 1H), 4.78 (d, *J*= 6.9 Hz, 1H), 7.57-7.60 (m, 2H), 8.21-8.24 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 18.894, 27.829, 27.937, 30.007, 36.129, 75.443, 78.731, 123.704, 128.234, 146.244, 147.943, 174.231; IR(KBr) 3383, 3105, 3075.0, 2942, 2889, 1707, 1604, 1596, 1517, 1465, 1344, 1161, 859 cm^{-1}; Enantiomeric excess: 98%, determined by HPLC (Daicel Chiralpak AS, i-PrOH/ Hexane= 30/ 70), UV 254 nm, flow rate 1.0 mL/min, t_{Rmajor}= 9.307 min; t_{Rminor}= 10.938 min; HR-MS for $C_{14}H_{17}N_1O_5$ +Na^+, calc: 302.0999, found: 302.1099.

The synthesis of 6,7-Dihydroxy-4-methyl-7-(4-nitrophenyl)heptanoic acid ethyl ester (9): After a solution of **8** (50 mg, 0.18mmol) and EtONa (2.5 mg) in ethanol (3 ml) was stirred at room temperature for 1 hour, water (5 ml) was added to quench the reaction. The reaction mixture was extracted with ethyl acetate and the combined organic layers were dried over anhydrous $MgSO_4$. After removal of solvent, the residue was purified through flash column chromatography on a silica gel (eluent: Petroleum: Ethyl acetate= 2:1) to give the **9** as s colorless oil in 90% yield. $[\alpha]^{30}_D$ = -2.2 (c= 0.5, Ethyl acetate); ^{1}H-NMR (300 MHz, $CDCl_3$): δ (ppm) 0.99 (d, *J*= 6.6 Hz, 3H), 1.07-1.16 (m, 2H), 1.24 (t, *J*= 7.2 Hz, 3H), 1.39-1.48 (m, 2H), 1.61-1.64 (m,1H), 1.69-1.80 (m, 1H), 2.26-2.32 (m, 2H), 3.82-3.87 (m,1H), 4.07-4.15 (q, 2H), 4.55 (d, *J*= 6 Hz, 1H), 7.53-7.56 (m, 2H), 8.19-8.22 (m, 2H); ^{13}C-NMR (75 MHz, $CDCl_3$): δ (ppm) 14.159, 20.333, 28.628, , 29.354, 31.396, 39.946, 60.688, 73.233, 76.934, 123.574, 127.792, 147.601, 148.620, 174.709; IR(Neat) 3440, 3127, 3076, 2955, 2871, 1715, 1604, 1519, 1462, 1347, 1191, 1105, 855 cm^{-1}; Enantiomeric excess: 97%, determined by HPLC (Daicel Chiralpak OD, i-PrOH/ Hexane= 15/ 85), UV 254 nm, flow rate: 1.0 mL/min, t_{Rmajor}= 9.408 min; t_{Rminor}= 15.382 min; HR-MS for $C_{16}H_{23}N_1O_6$ +Na^+, calc: 348.1418,

found: 348.1419.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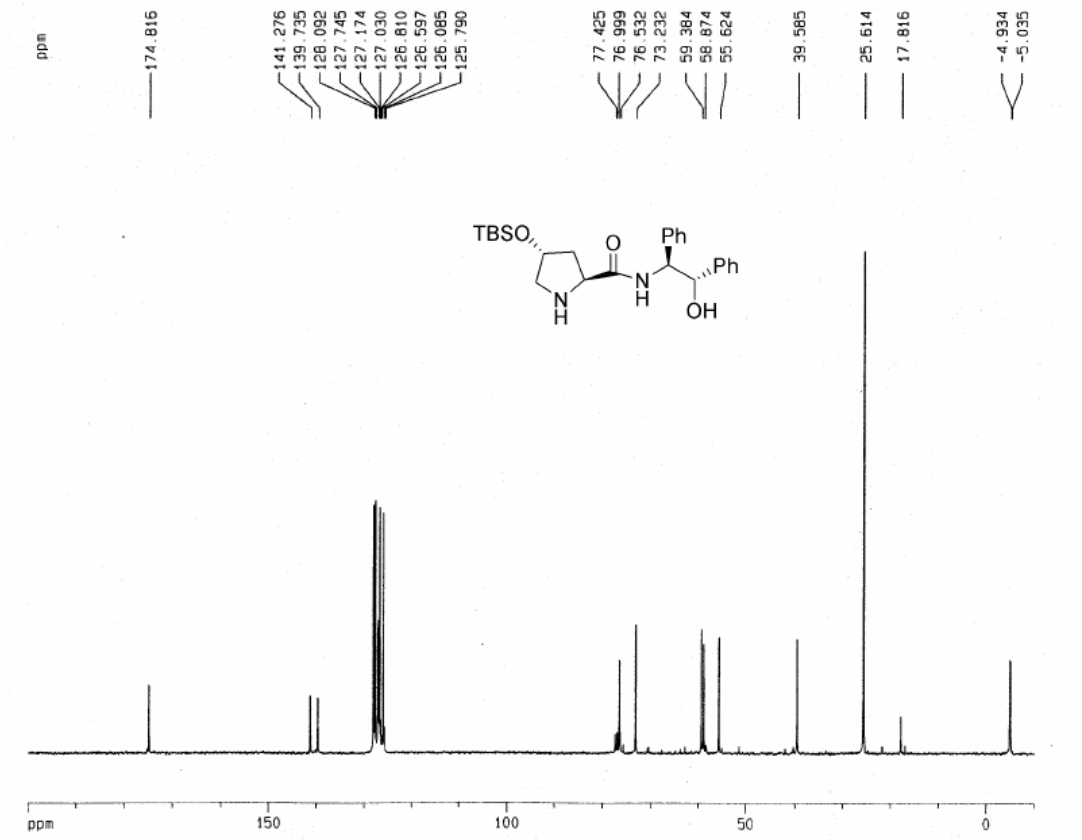
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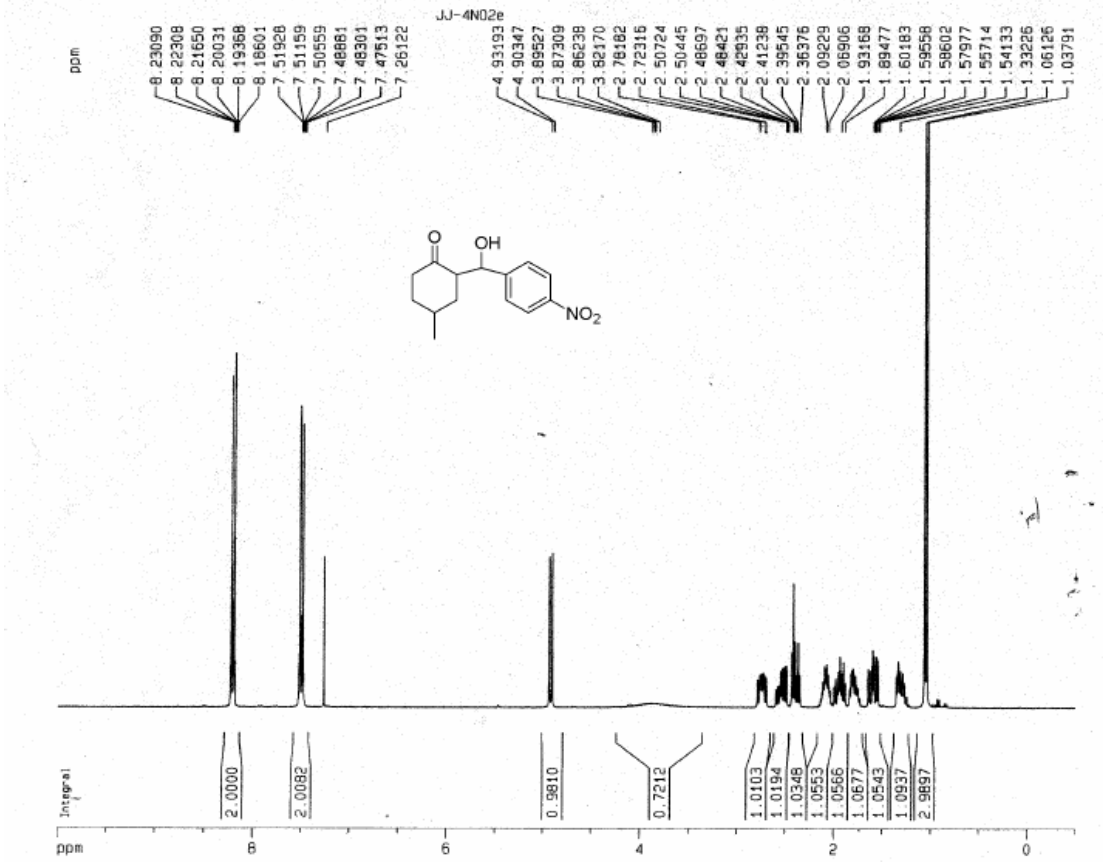
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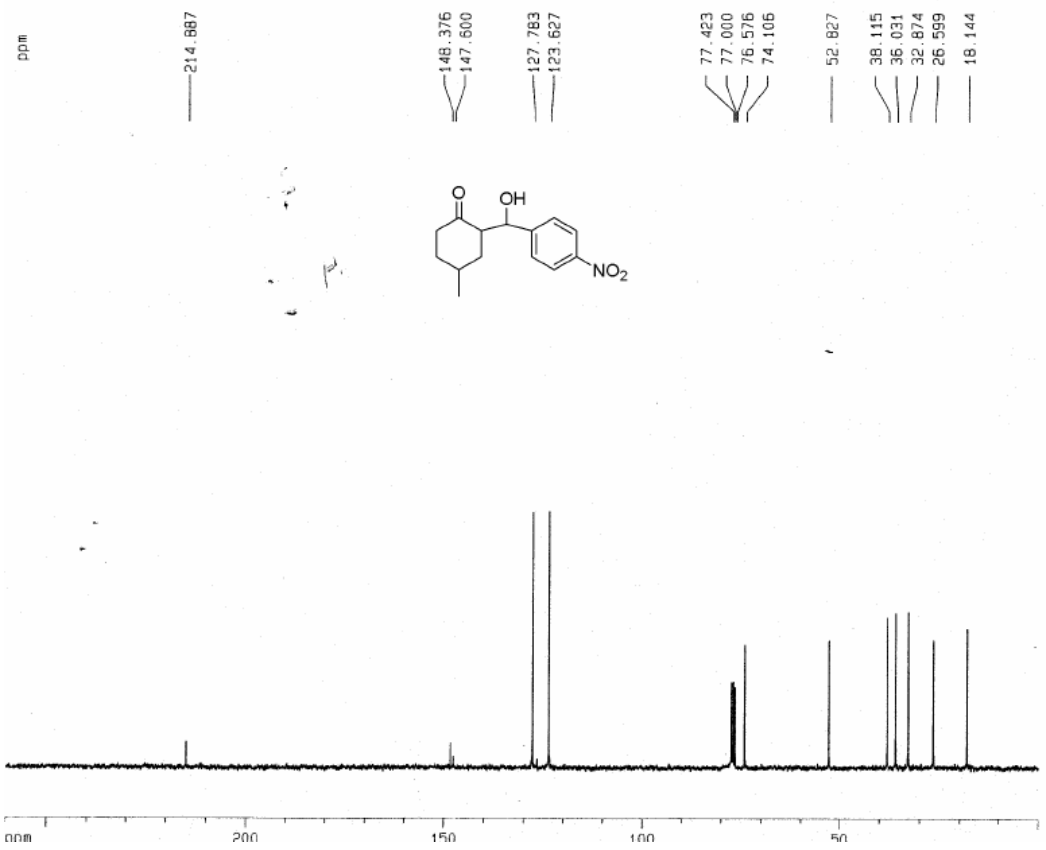
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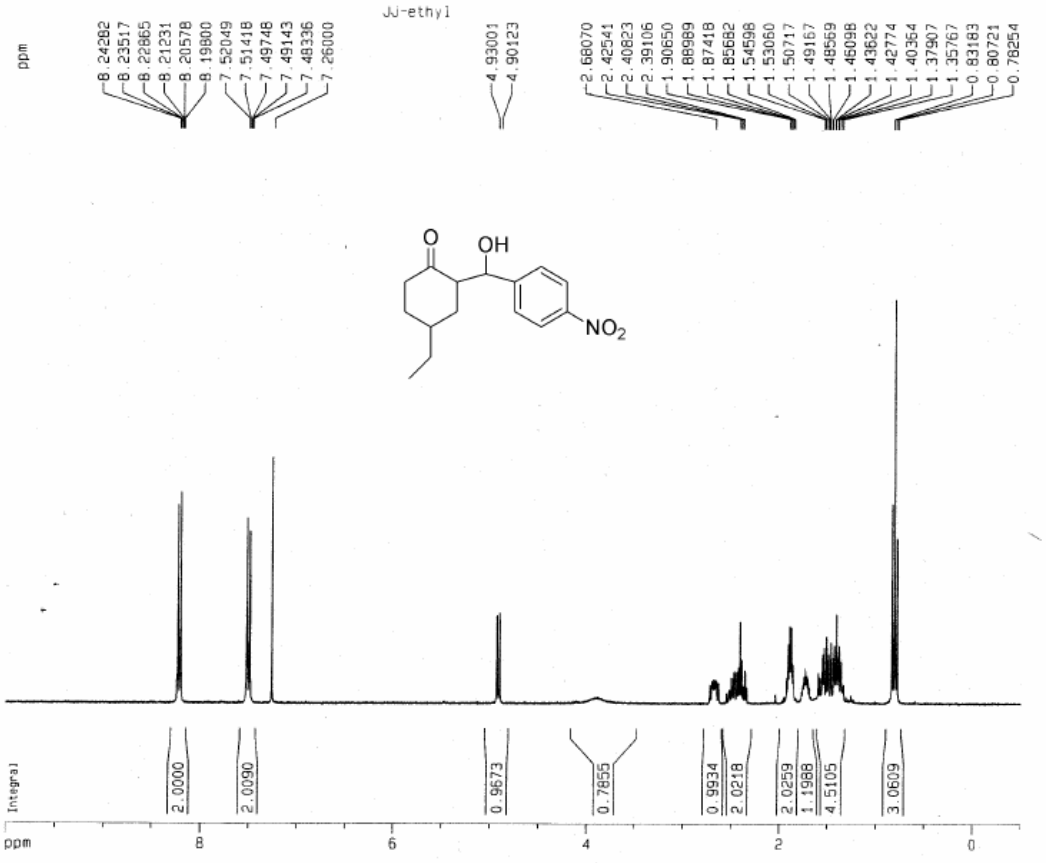
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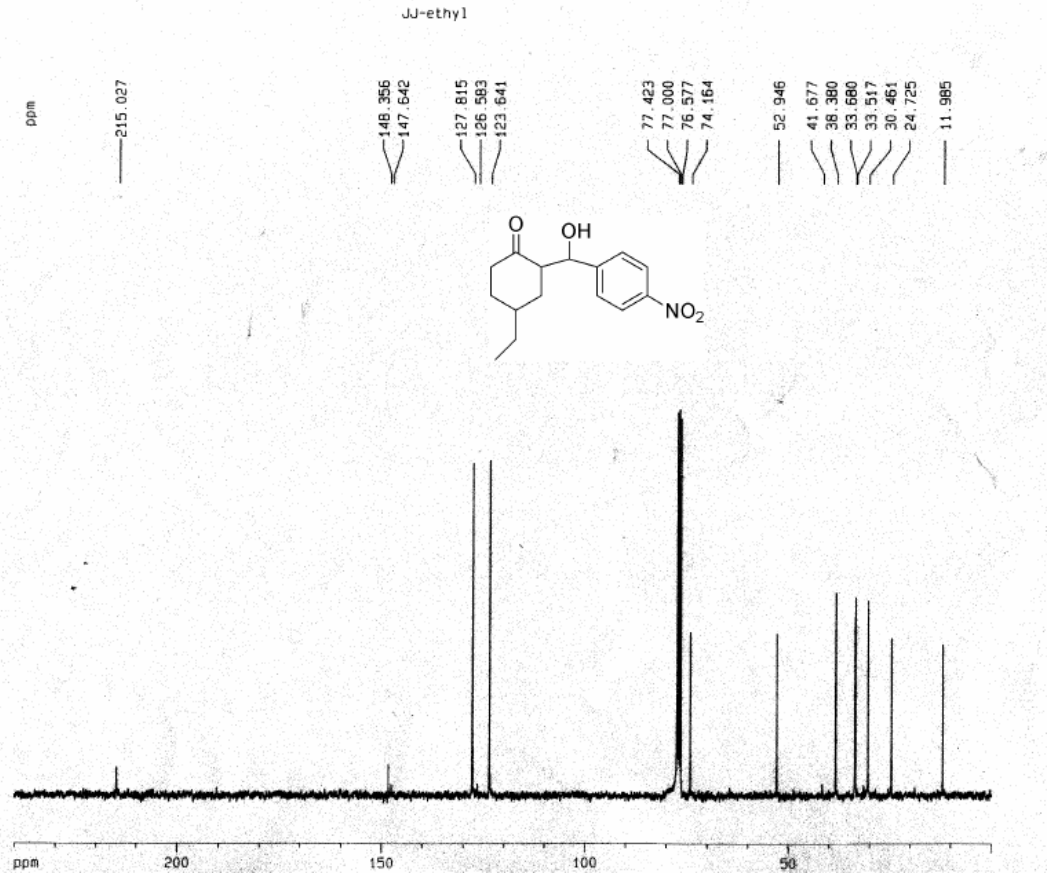
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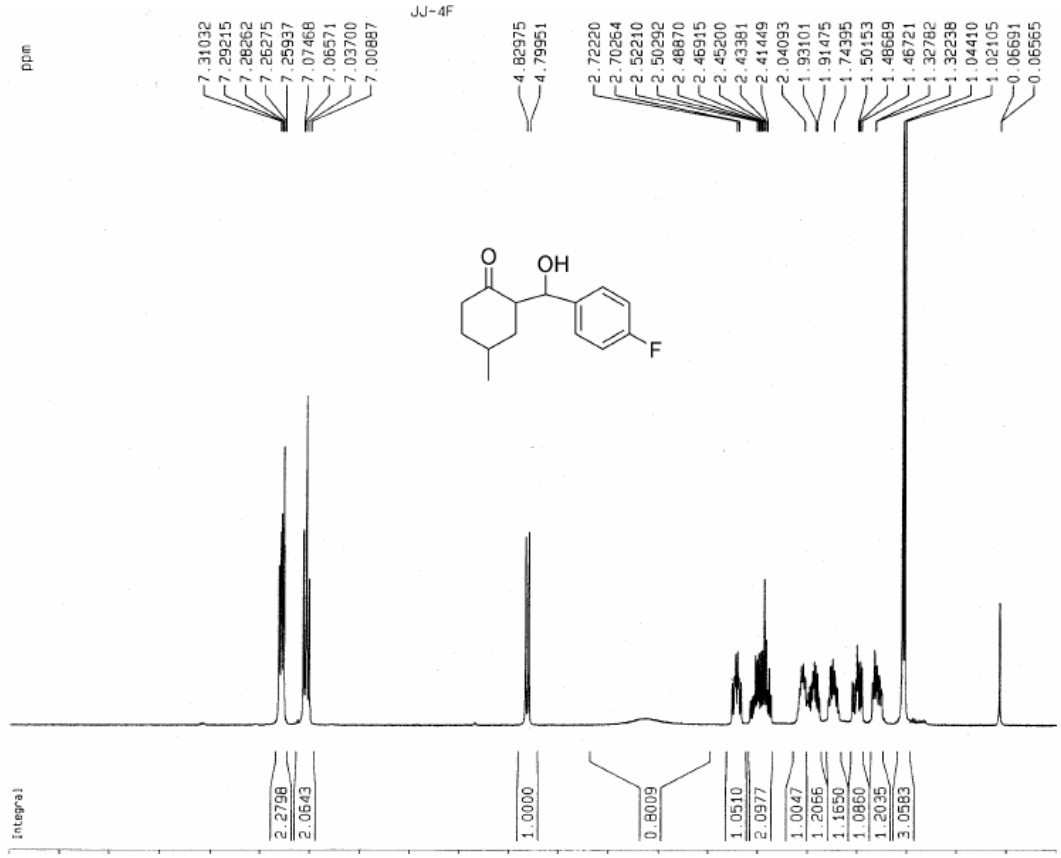
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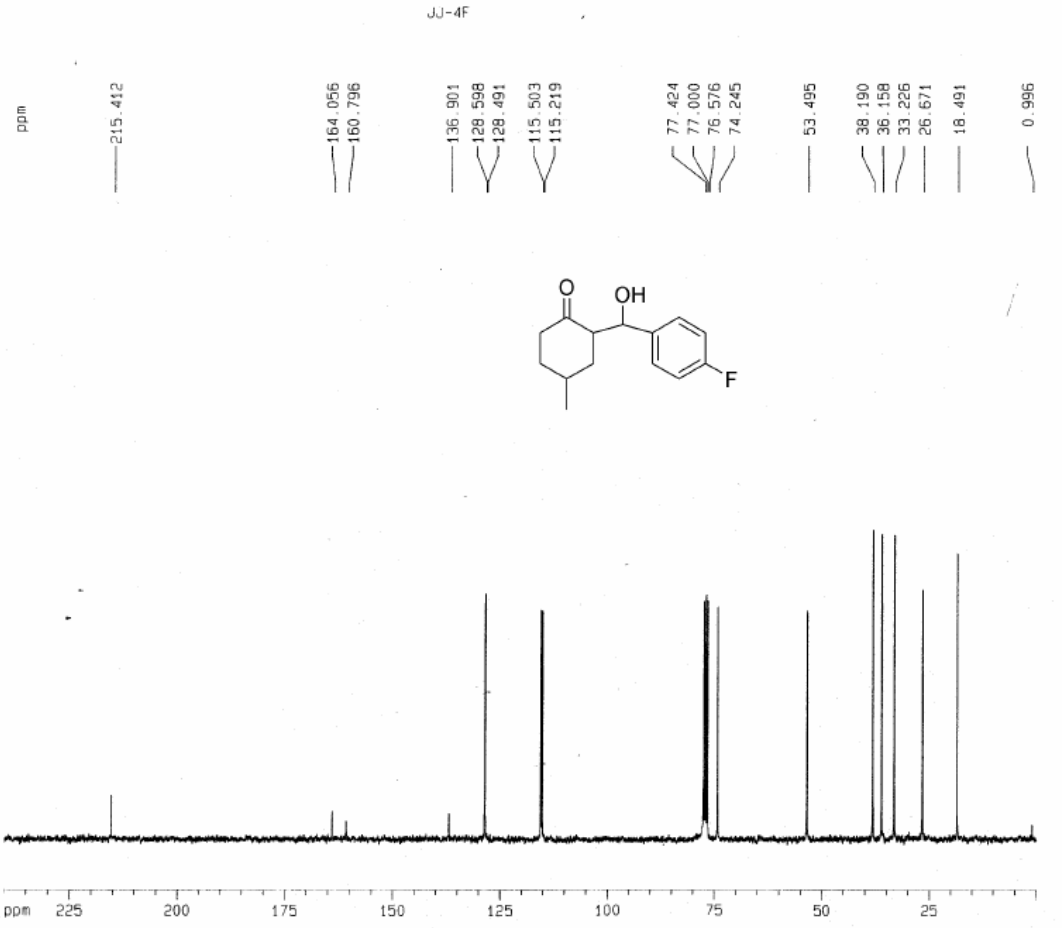
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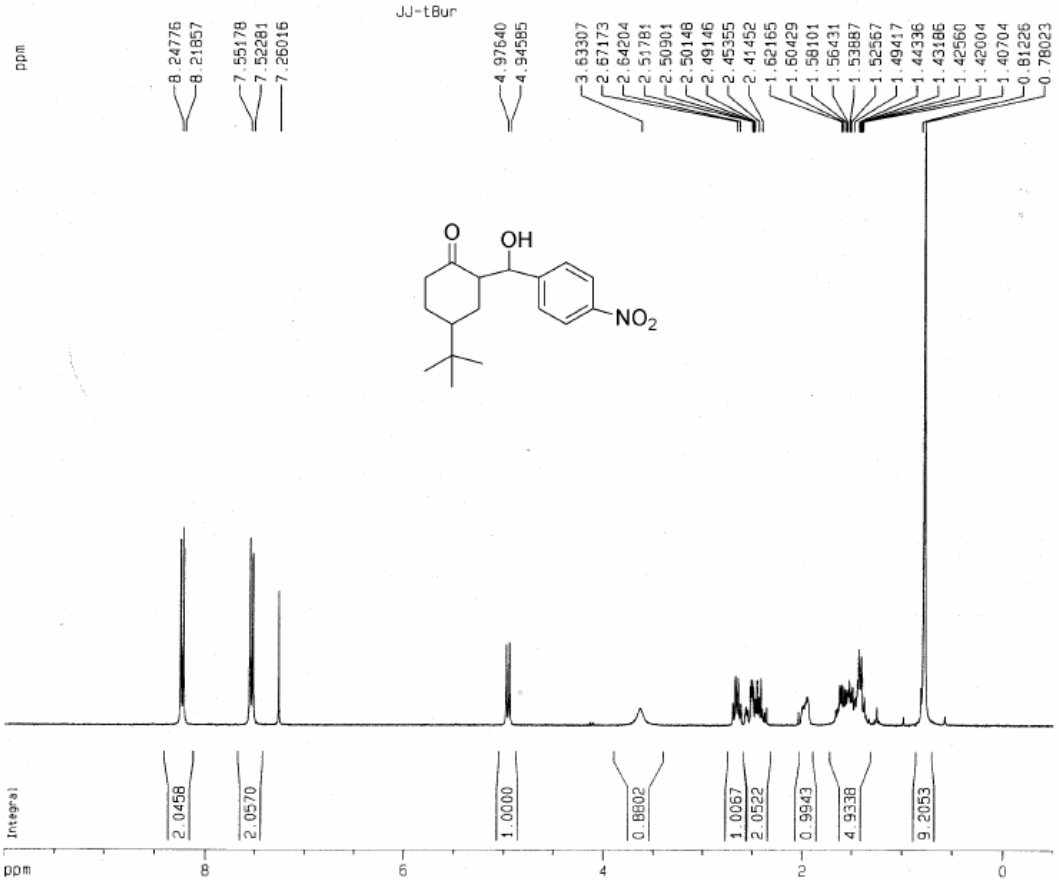
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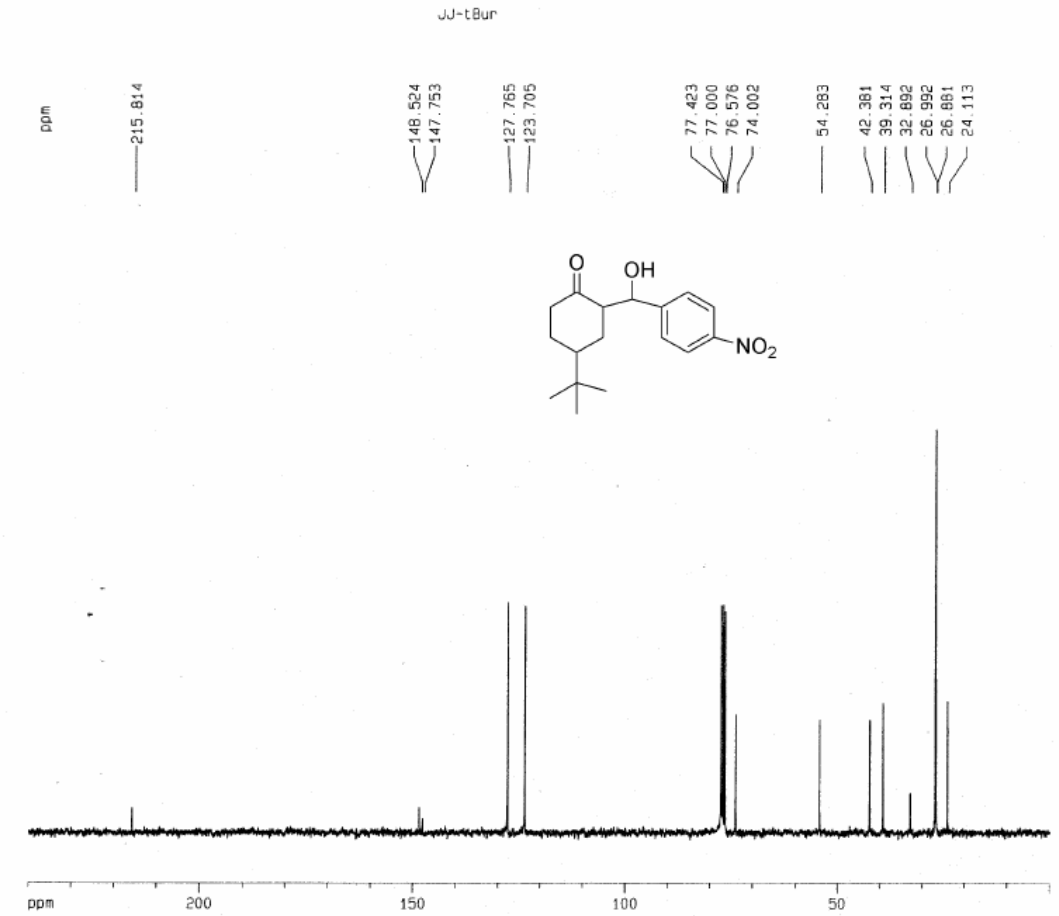
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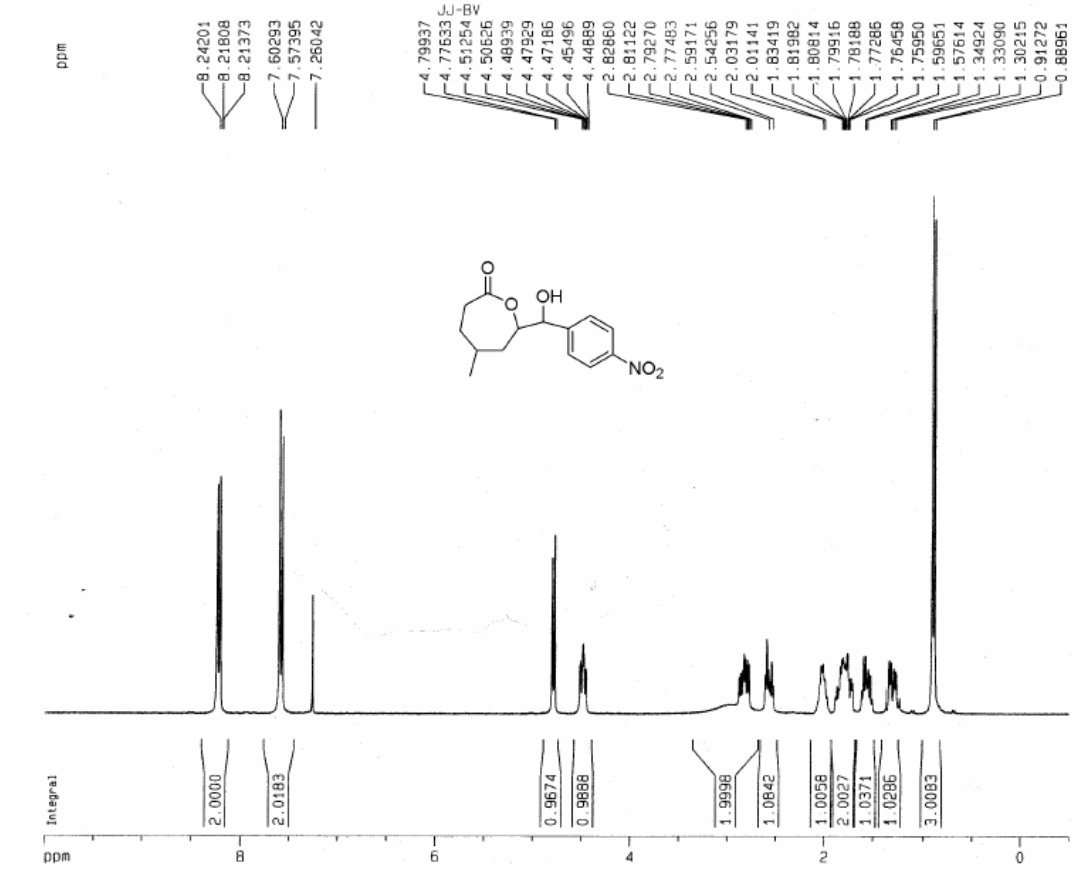
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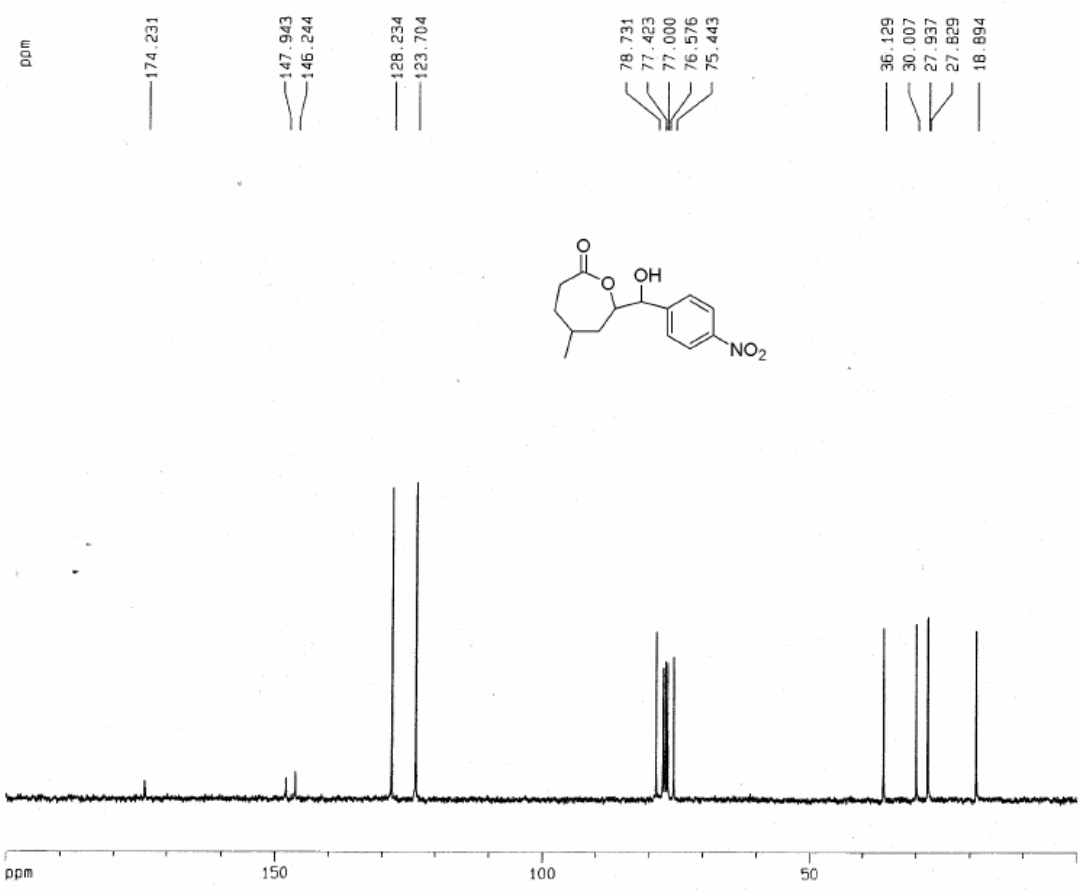
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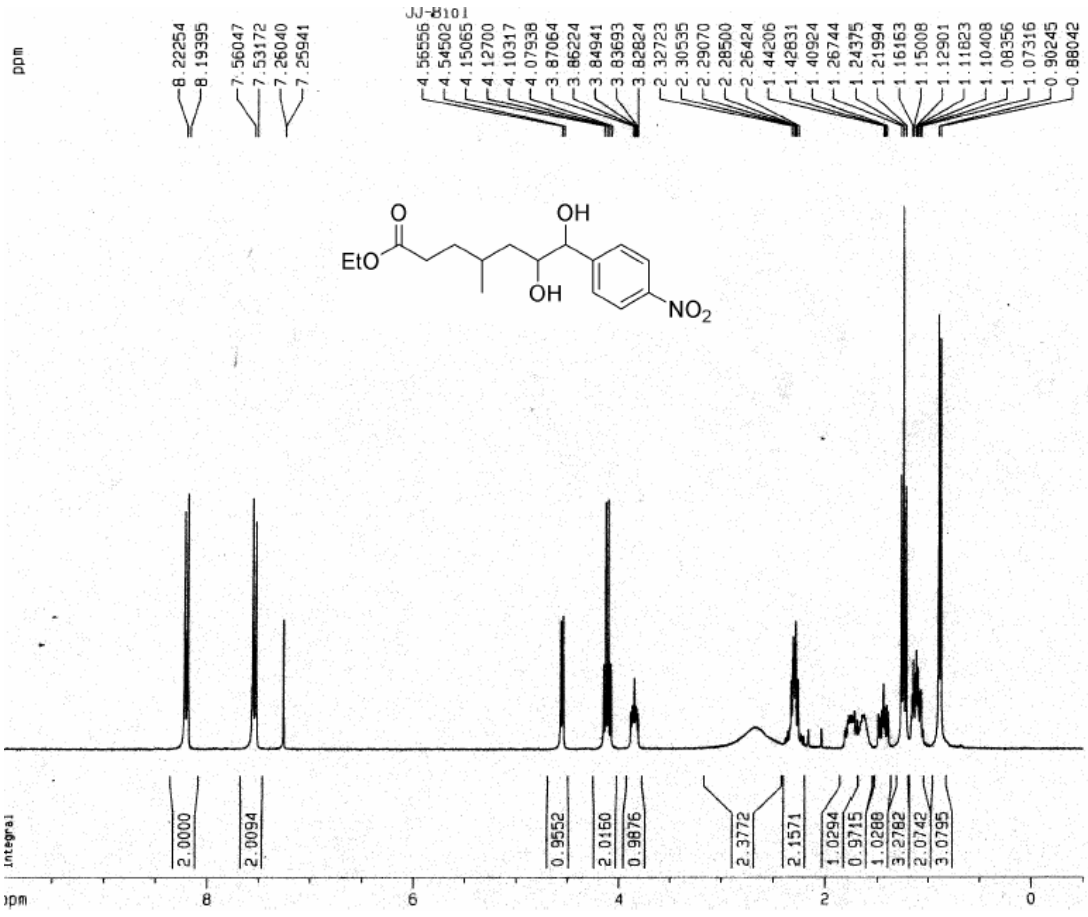
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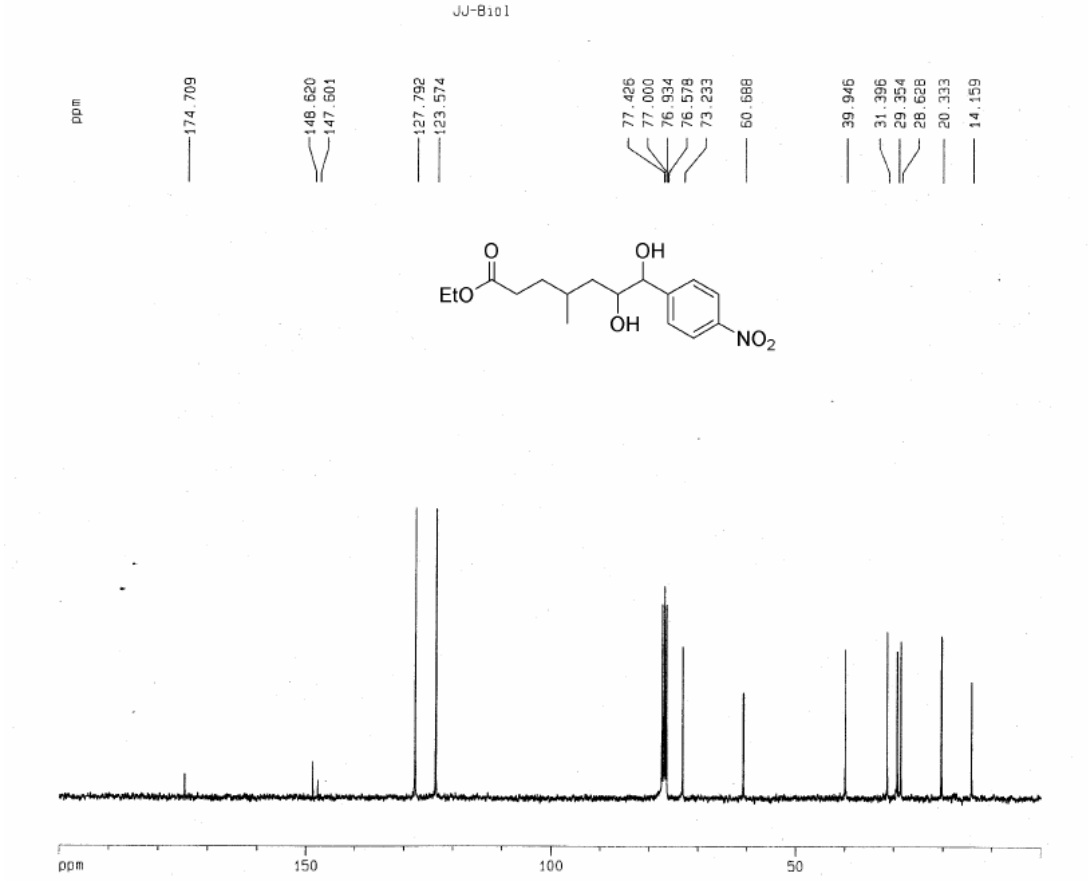
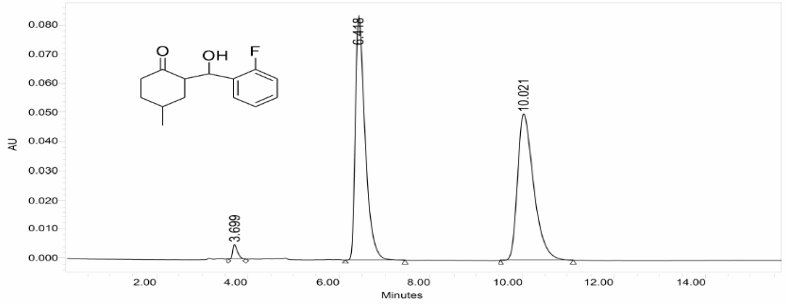

JJ-B101
ppm
174.709
148.620
147.601
127.792
123.574
77.426
77.000
76.934
76.578
73.233
60.688
39.946
31.396
29.354
28.628
20.333
14.159
O
OH
EtO
OH
NO2
ppm
150
100
50

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	11/19/05 11:09:20 AM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	11/19/05 11:25:06 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.699	41540	1.64	5190	3.73
2	6.418	1243820	49.25	83576	60.08
3	10.021	1239975	49.10	50339	36.19

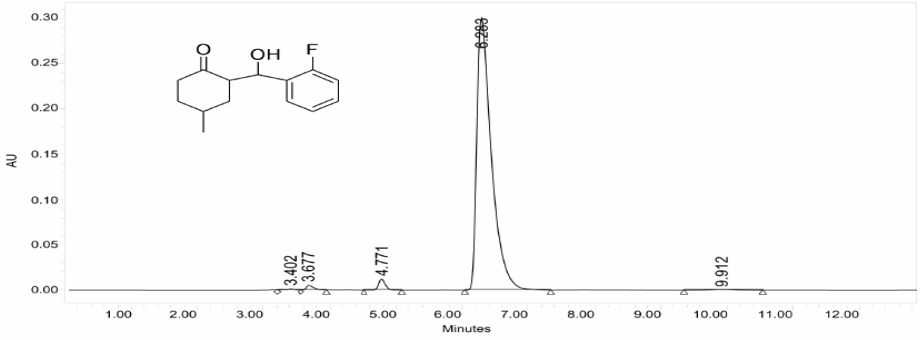
Report Method: Untitled Printed 4:33:18 PM 8/15/06 Page: 1 of 1

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	11/19/05 11:26:06 AM
Vial:	1	Acq. Method:	100A
Injection #:	2	Date Processed:	11/19/05 11:39:13 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.402	10601	0.22	1195	0.37
2	3.677	38157	0.80	5224	1.63
3	4.771	86245	1.80	12169	3.80
4	6.283	4626640	96.77	300741	93.94
5	9.912	19603	0.41	829	0.26

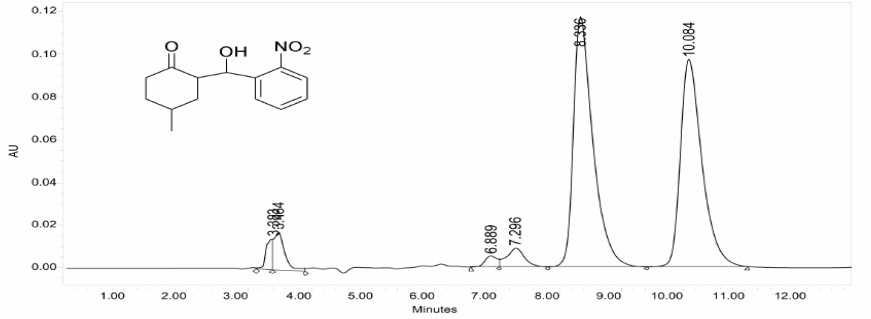
Report Method: Untitled Printed 4:33:42 PM 8/15/06 Page: 1 of 1

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1/6/06 9:37:32 AM
Vial:	1	Acq. Method:	100A
Injection #:	3	Date Processed:	1/6/06 9:50:41 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:	



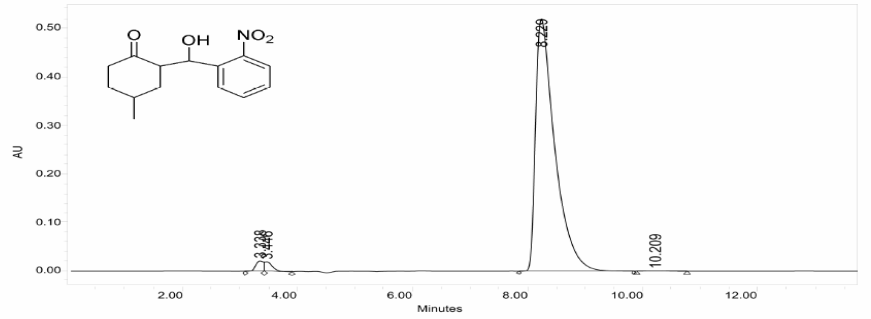
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.383	115943	2.12	14409	5.55
2	3.464	212277	3.88	17709	6.82
3	6.889	69690	1.27	5122	1.97
4	7.296	172189	3.14	8766	3.38
5	8.336	2564417	46.83	116825	44.98
6	10.084	2341691	42.76	96877	37.30

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	1/6/06 9:54:12 AM
Vial:	1	Acq. Method:	100A
Injection #:	4	Date Processed:	1/6/06 10:08:06 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	50.00 Minutes	Sample Set Name:	



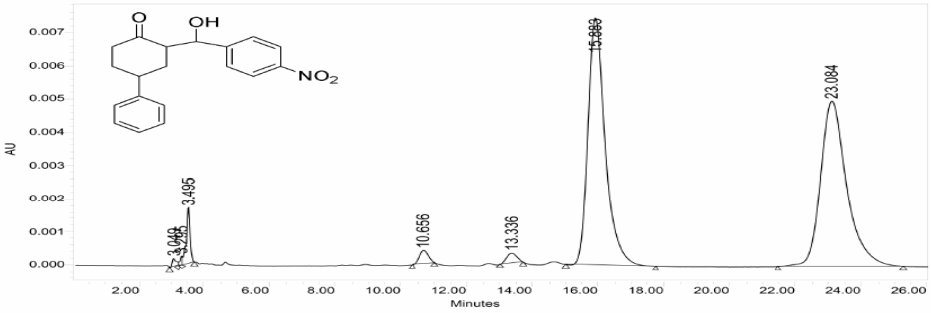
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.338	216873	1.73	21926	3.89
2	3.446	207064	1.65	20446	3.63
3	8.229	12125765	96.51	520418	92.36
4	10.209	14728	0.12	680	0.12

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	jj-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	12/2/05 6:35:21 PM
Vial:	1	Acq. Method:	100A
Injection #:	3	Date Processed:	12/2/05 7:03:40 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.049	2434	0.42	257	1.67
2	3.295	1682	0.29	283	1.84
3	3.495	13480	2.32	1691	10.98
4	10.656	7978	1.37	414	2.69
5	13.336	6745	1.16	307	1.99
6	15.883	272618	46.93	7456	48.42
7	23.084	275969	47.51	4992	32.42

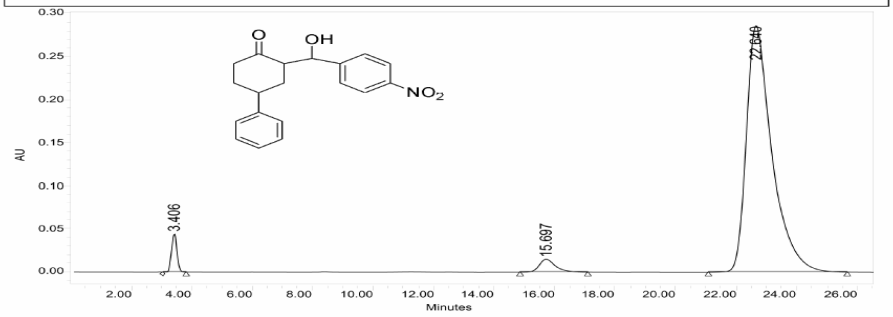
Report Method: Untitled Printed 4:29:34 PM 8/15/06 Page: 1 of 1

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	12/23/05 4:52:43 PM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	12/23/05 5:19:20 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	45.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	3.406	544129	3.03	44233	12.79
2	15.697	561781	3.13	15071	4.36
3	22.640	16851565	93.84	286669	82.86

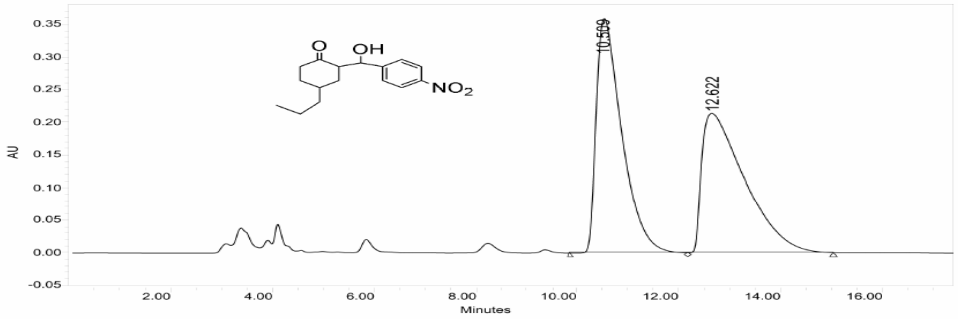
Report Method: Untitled Printed 4:30:55 PM 8/15/06 Page: 1 of 1

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/18/06 6:31:01 PM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	5/18/06 6:49:32 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



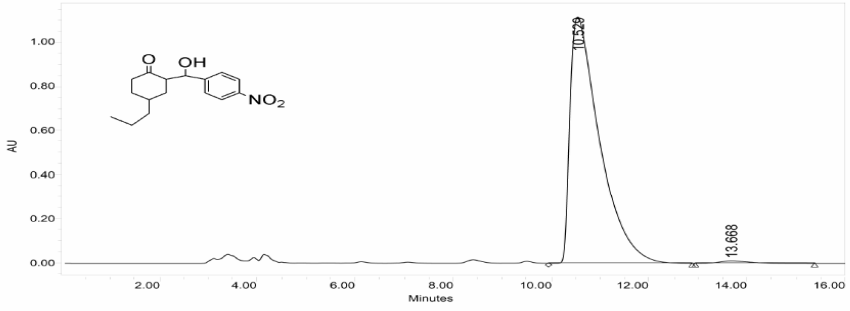
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.509	12627281	50.08	359991	62.71
2	12.622	12588560	49.92	214079	37.29

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	5/19/06 2:44:10 PM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	5/19/06 3:00:25 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



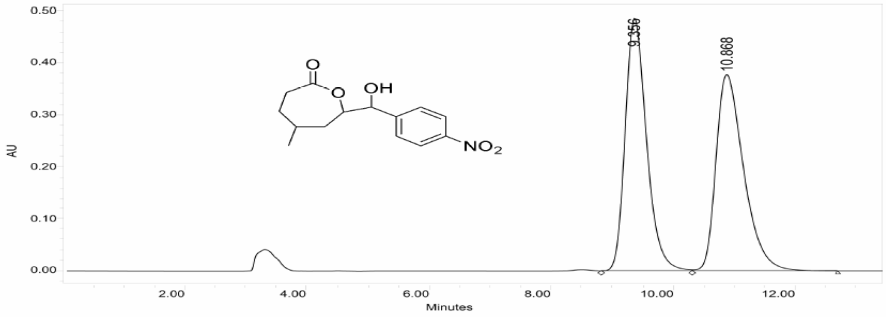
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	10.529	46878394	99.03	1114915	99.04
2	13.668	461088	0.97	10779	0.96

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/4/06 11:23:08 AM
Vial:	1	Acq. Method:	100A
Injection #:	2	Date Processed:	7/4/06 11:36:47 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



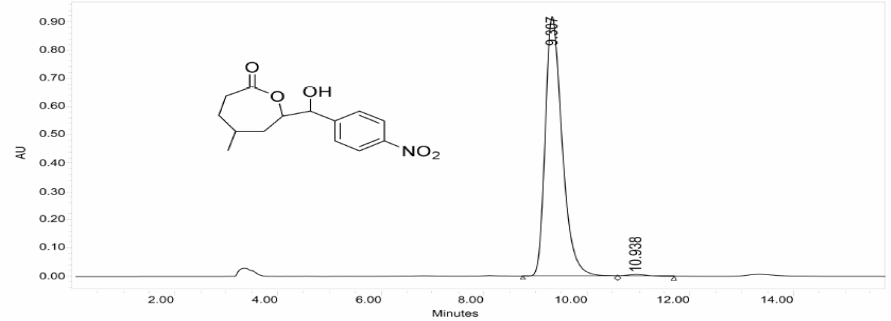
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.356	11881637	49.84	486823	56.25
2	10.868	11959451	50.16	378623	43.75

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/4/06 11:37:28 AM
Vial:	1	Acq. Method:	100A
Injection #:	3	Date Processed:	7/4/06 11:53:44 AM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



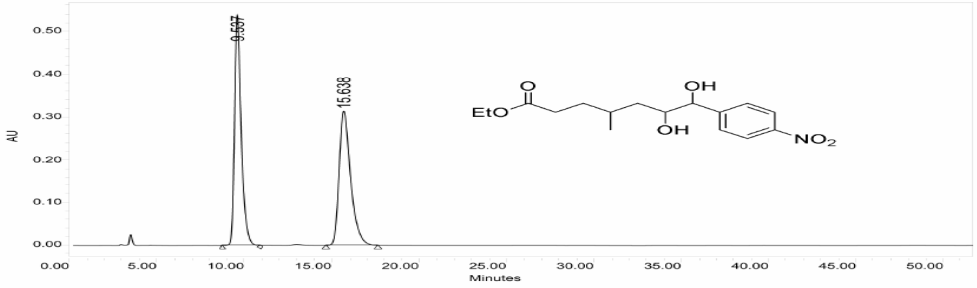
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.307	20991489	99.19	918920	99.31
2	10.938	171128	0.81	6340	0.69

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ-0	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/06 1:25:54 PM
Vial:	1	Acq. Method:	100A
Injection #:	1	Date Processed:	7/6/06 2:17:55 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	60.00 Minutes	Sample Set Name:	



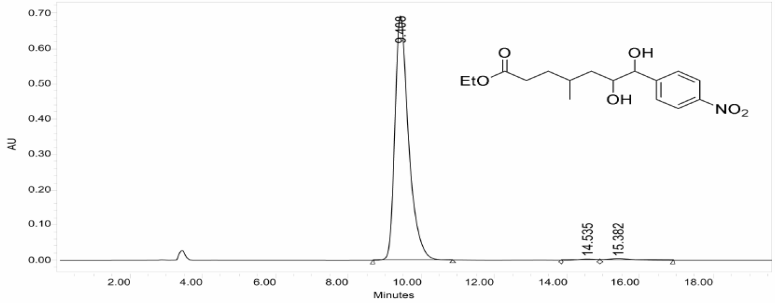
	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.537	14386608	50.04	537631	63.11
2	15.638	14362599	49.96	314197	36.89

ulas
Project Name: Defaults
Reported by User: System

Breeze

SAMPLE INFORMATION

Sample Name:	JJ	Acquired By:	System
Sample Type:	Unknown	Date Acquired:	7/6/06 2:21:15 PM
Vial:	1	Acq. Method:	100A
Injection #:	2	Date Processed:	7/6/06 2:41:17 PM
Injection Volume:	20.00 ul	Channel Name:	2487Channel 1
Run Time:	40.00 Minutes	Sample Set Name:	



	RT (min)	Area (V*sec)	% Area	Height (V)	% Height
1	9.408	18156562	98.05	693844	98.85
2	14.535	121050	0.65	3338	0.48
3	15.382	240801	1.30	4737	0.67