Supporting Information

Iron Catalyzed Enantioselective Sulfa-Michael Addition: A Four-step Synthesis of the Anti-asthma Agent Montelukast

James D. White and Subrata Shaw*

Department of Chemistry, Oregon State University, Corvallis, Oregon 97331-4003

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Experimental Section

General

Starting materials and reagents were obtained from commercial sources and were used without further purification. Solvents were dried by distillation from the appropriate drying reagents immediately prior to use. All solvents used for routine isolation of products and chromatography were reagent grade. Moisture- and air-sensitive reactions were carried out under an atmosphere of argon. Reaction flasks were flame dried under a stream of argon gas, and glass syringes were oven dried at 120 °C prior to use.

Unless otherwise stated, concentration under reduced pressure refers to a rotary evaporator at water aspirator pressure. Residual solvent was removed by vacuum pump at a pressure less than 0.25 mm of mercury.

Analytical thin-layer chromatography (TLC) was conducted using precoated TLC plates (0.2 mm layer thickness of silica gel 60 F-254). Compounds were visualized by ultraviolet light and/or by heating the plate after dipping in a 3-5% solution of phosphomolybdic acid in ethanol, 10% ammonium molybdate in water, a 1% solution of vanillin in 0.1 M sulfuric acid in methanol or 2.5% *p*-anisaldehyde in 88% ethanol, 5% water, 3.5% concentrated sulfuric acid and 1% acetic acid. Flash chromatography was performed with the indicated eluents on 230 - 400 mesh silica gel.

Optical rotations were measured with a polarimeter at ambient temperature using a 0.9998 dm cell with 1 mL capacity. Infrared (IR) spectra were recorded on a FT-IR spectrometer. Proton and carbon nuclear magnetic resonance (NMR) spectra were obtained using either a 400, 500 or 700 MHz spectrometer. All chemical shifts were reported in parts per million (ppm) downfield from tetramethylsilane using the δ scale. ^{1}H NMR spectral data are reported in the

order: chemical shift, multiplicity (s = singlet, d = doublet, m = multiplet, and b = broad), coupling constant (*J*, in Hertz), and number of protons.

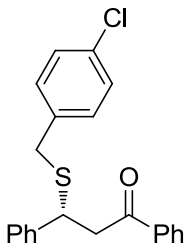
Low (MS) and high (HRMS) resolution mass spectra are reported with ion mass/charge (*m/z*) ratios as values in atomic mass units.

Representative Procedure for the Asymmetric Sulfa-Michael Addition of Thiols to Acyclic α,β-Unsaturated Ketones Catalyzed by Fe-salen Complex (+)-**2e:**

To an oven-dried vial were added Fe-salen complex (+)-**2e** (13.2 mg, 0.02 mmol, 20 mol%) and enone (0.1 mmol) followed by anhydrous DCE (1 mL) and the resulting brown suspension was stirred at room temperature for 10 min. To the suspension at -5 ^{o}C was added the thiol (0.12 mmol) and the mixture was stirred at that temperature for the length of time specified in Tables 4-5. The reaction mixture was concentrated under reduced pressure and the resulting crude residue was purified by flash chromatography on silica gel (15% hexane/ether) to give the product. The enantiomeric excess of the pure product was determined by HPLC on a Daicel Chiralcel OD, AD, OJ, OD-H or AS-H column.

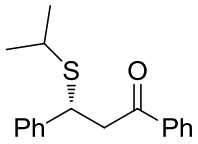
A procedure at 5 mmol scale was carried out with (*E*)-pent-3-en-2-one (421 mg, 5 mmol) and *p*-chlorobenzyl thiol (792 μL, 6 mmol) using (+)-**2e** (662.2 mg, 1.0 mmol, 1 mol%) in anhydrous DCE (50 mL). The SMA adduct was obtained in 96% yield and 94% ee.

(*R*)-3-(4-Chlorobenzylthio)-1,3-diphenylpropan-1-one (5)



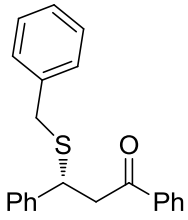
Colorless oil; $[\alpha]_D^{27}$ + 211.0 (*c* 0.1, $CHCl_3$), [lit.[1] for *(R)* enantiomer $[\alpha]_D^{25}$ + 209 (*c* 1.0, $CHCl_3$, 96% ee)]; 98% ee [Chiralcel OD-H, hexane:*i*-propanol 80:20, 0.8 mL/min, 215 nm, t_R (major) 19.5 min, t_R (minor) 24.0 min]; IR (neat) 2922, 1716, 1460, 1422, 1366, 1311, 1259, 1163, 1142, 1047, 748 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 3.47-3.61 (m, 4H), 4.42 (s, 1H), 7.15 (*J* = 7.3 Hz, 2H), 7.22-7.29 (m, 3H), 7.32-7.39 (m, 2H), 7.39-7.42 (m, 2H), 7.45-7.50 (m, 2H), 7.53-7.59 (m, 1H), 7.78-7.92 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 34.1, 44.1, 45.6, 127.2, 128.0, 128.9, 130.2, 133.2, 134.0, 136.4, 136.7, 141.8, 196.8.

(*R*)-3-(Isopropylthio)-1,3-diphenylpropan-1-one (8a)



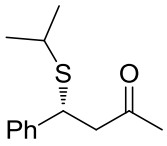
Colorless oil; $[\alpha]_D^{27}$ + 127.6 (*c* 0.1, $CHCl_3$), [lit.[1] for *(R)* enantiomer $[\alpha]_D^{25}$ + 107 (*c* 1.0, $CHCl_3$, 80% ee)]; 94% ee [Chiralcel OD, hexane:*i*-propanol 90:10, 0.8 mL/min, 215 nm, t_R (major) 21.6 min, t_R (minor) 25.5 min]; IR (neat) 3060, 2923, 1686, 1597, 1580, 1492, 1450, 1334, 1179, 979, 749, 697, 649 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 1.15 (d, *J* = 6.8 Hz, 3H), 1.30 (d, *J* = 6.8 Hz, 3H), 2.63-2.69 (m, 1H), 3.44-3.50 (m, 1H), 4.66-4.74 (m, 1H), 7.21-7.27 (m, 1H), 7.30-7.36 (m, 2H), 7.48-7.52 (m, 4H), 7.59-7.63 (m, 1H), 7.92-8.00 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.4, 22.7, 34.7, 43.5, 45.7, 127.1, 127.8, 128.1, 128.6, 133.2, 136.9, 142.7, 197.4.

(*R*)-3-(Benzylthio)-1,3-diphenylpropan-1-one (8b)



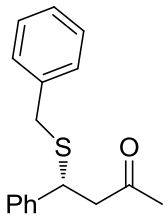
Colorless oil; $[\alpha]_D^{25}$ + 139.2 (*c* 0.14, $CHCl_3$), [lit.[1] for *(R)* enantiomer $[\alpha]_D^{25}$ + 139.7 (*c* 1.0, $CHCl_3$, 96% ee)]; 97% ee [Chiralcel OD, hexane:*i*-propanol 70:30, 0.8 mL/min, 215 nm, t_R (major) 40.7 min, t_R (minor) 45.9 min]; IR (neat) 3059, 1685, 1493, 1408, 1255, 1073, 1027, 980, 750, 696 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 3.53-3.57 (m, 1H), 3.59-3.62 (m, 1H), 3.63-3.70 (m, 2H), 4.54 (t, *J* = 7.2 Hz, 1H), 7.29-7.32 (m, 3H), 7.35-7.38 (m, 2H), 7.39-7.42 (m, 3H), 7.45-7.51 (m, 4H), 7.58-7.61 (m, 1H), 7.92 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 35.9, 44.2, 45.3, 127.0, 127.3, 128.1, 128.4, 128.5, 128.6, 133.2, 136.8, 137.9, 141.8, 196.8.

(*R*)-4-(Isopropylthio)-4-phenylbutan-2-one (8c)



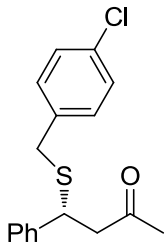
Colorless oil; $[\alpha]_D^{25}$ + 107.6 (*c* 0.1, $CHCl_3$); 97% ee [Chiralcel OD, hexane:*i*-propanol 70:30, 1.0 mL/min, 215 nm, t_R (major) 9.7 min, t_R (minor) 10.4 min]; IR (neat) 3028, 2924, 1717, 1492, 1361, 1152, 1021, 699, 534 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 1.11 (d, *J* = 6.5 Hz, 3H), 1.28 (d, *J* = 6.5 Hz, 3H), 2.08 (s, 3H), 2.59-2.64 (m, 1H), 2.91-2.98 (m, 2H), 4.50-4.54 (m, 1 H), 7.21-7.26 (m, 1H), 7.29-7.35 (m, 2H), 7.39-7.45 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.4, 22.7, 30.7, 34.2, 43.9, 50.8, 128.7, 129.1, 129.6, 143.1, 205.7; HRMS (EI) calcd for $C_{13}H_{18}OS$ *m/z* 222.1078, found 222.1074.

(*R*)-4-(Benzylthio)-4-phenylbutan-2-one (8d)



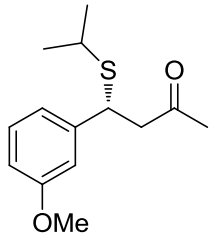
Colorless oil; $[\alpha]_D^{25}$ + 183.9 (*c* 0.1, $CHCl_3$), [lit.[2] for *(S)* enantiomer $[\alpha]_D^{25}$ - 162.5 (*c* 1.0, $CHCl_3$, 85% ee)]; 96% ee [Chiralcel OD, hexane:*i*-propanol 70:30, 1.0 mL/min, 215 nm, t_R (major) 13.0 min, t_R (minor) 16.2 min]; IR (neat) 3060, 2917, 1716, 1493, 1359, 1154, 1024, 762, 698, 531 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 2.06 (s, 3H), 2.95-3.03 (m, 2H), 3.50 (AB system, *J* = 13.3 Hz, 2H), 4.26 (t, *J* = 7.2 Hz, 1H), 7.23-7.29 (m, 3H), 7.32-7.41 (m, 7H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 30.3, 35.6, 44.2, 50.9, 127.4, 127.7, 127.9, 128.4, 128.5, 128.9, 138.6, 141.5, 207.4.

(*R*)-4-((4-Chlorobenzyl)thio)-4-phenylbutan-2-one (8e)



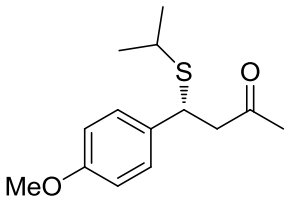
Colorless oil; $[\alpha]_D^{25}$ + 199.3 (*c* 0.1, $CHCl_3$); 97% ee [Chiralcel AD, hexane:*i*-propanol 85:15, 0.8 mL/min, 215 nm, t_R (major) 18.9 min, t_R (minor) 23.7 min]; IR (neat) 3028, 2919, 1716, 1598, 1490, 1452, 1092, 1015, 833, 699 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 2.06 (s, 3H), 2.90-3.00 (m, 2H), 3.50 (AB system, *J* = 13.2 Hz, 2H), 4.23 (t, *J* = 7.3 Hz, 1H), 7.16-7.20 (m, 2H), 7.27-7.33 (m, 3H), 7.37-7.42 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 30.2, 35.2, 43.4, 50.3, 128.9, 129.2, 129.4, 129.7, 130.4, 132.3, 138.8, 142.7, 207.3; HRMS (EI) calcd for $C_{17}H_{17}ClOS$ *m/z* 304.0689, found 304.0687.

(*R*)-4-(Isopropylthio)-4-(3-methoxyphenyl)butan-2-one (8f)



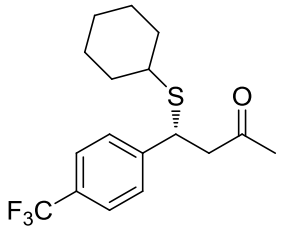
Colorless oil; $[\alpha]_D^{25}$ + 117.7 (*c* 0.12, $CHCl_3$); 95% ee [Chiralcel OD, hexane:*i*-propanol 85:15, 0.8 mL/min, 215 nm, t_R (major) 15.0 min, t_R (minor) 18.9 min]; IR (neat) 2959, 2921, 1716, 1599, 1261, 1153, 1046, 873, 697 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 1.13 (d, *J* = 6.6 Hz, 3H), 1.27 (d, *J* = 6.6 Hz, 3H), 2.11 (s, 3H), 2.59-2.65 (m, 1H), 2.90-2.99 (m, 2H), 3.84 (s, 3 H), 4.37 (t, J = 7.3 Hz, 1H), 6.75-6.83 (m, 1H), 6.90-7.0 (m, 2H), 7.21-7.29 (m, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.5, 22.7, 30.7, 34.9, 43.9, 50.9, 55.3, 113.2, 113.7, 120.6, 130.1, 143.1, 160.2, 207.4; HRMS (EI) calcd for $C_{14}H_{20}O_2S$ *m/z* 252.1184, found 252.1186.

(*R*)-4-(Isopropylthio)-4-(4-methoxyphenyl)butan-2-one (8g)



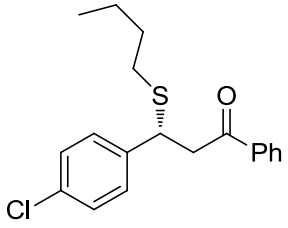
Colorless oil; $[\alpha]_D^{25}$ + 119.0 (*c* 0.14, $CHCl_3$); 92% ee [Chiralcel AD, hexane:*i*-propanol 80:20, 0.8 mL/min, 215 nm, t_R (major) 13.2 min, t_R (minor) 15.0 min]; IR (neat) 2958, 2926, 1716, 1610, 1461, 1175, 1035, 831, 805 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 1.10 (d, *J* = 6.5 Hz, 3H), 1.29 (d, *J* = 6.5 Hz, 3H), 2.06 (s, 3H), 2.50-2.61 (m, 1H), 2.89-2.98 (m, 2H), 3.82 (s, 3 H), 4.38 (t, *J* = 6.9 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.3, 22.5, 30.6, 34.5, 43.3, 50.2, 55.3, 114.1, 129.6, 134.8, 159.3, 207.9; HRMS (EI) calcd for $C_{14}H_{20}O_2S$ *m/z* 252.1184, found 252.1194.

(*R*)-4-(Cyclohexylthio)-4-(4-(trifluoromethyl)phenyl)butan-2-one (8h)



Colorless oil; $[\alpha]_D^{25}$ + 157.7 (*c* 0.27, $CHCl_3$); 98% ee [Chiralcel OD-H, hexane:*i*-propanol 70:30, 1.0 mL/min, 215 nm, t_R (major) 7.9 min, t_R (minor) 9.2 min]; IR (neat) 2930, 1718, 1418, 1163, 1016, 837, 604 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 1.08-1.79 (m, 10H), 1.88-2.00 (m, 1H), 2.08 (s, 3H), 2.33-2.41 (m, 1H), 2.89-3.02 (m, 2H), 4.47 (t, *J* = 7.2 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 25.4, 25.5, 30.8, 31.9, 32.0, 40.8, 41.3, 50.7, 123.1, 126.2, 129.1, 129.6 (q, *J* = 35.2 Hz), 139.3, 206.8; HRMS (EI) calcd for $C_{17}H_{21}OSF_3$ *m/z* 330.1265, found 330.1263.

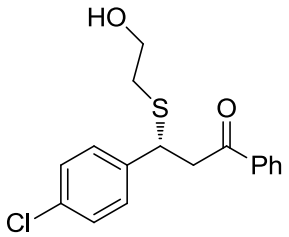
(*R*)-3-(Butylthio)-3-(4-chlorophenyl)-1-phenylpropan-1-one (8i)



Colorless oil; $[\alpha]_D^{25}$ + 204.7 (*c* 0.1, $CHCl_3$); 93% ee [Chiralcel OJ, hexane:*i*-propanol 70:30, 1.0 mL/min, 215 nm, t_R (major) 14.6 min, t_R (minor) 17.2 min]; IR (neat) 2957, 2871, 1686, 1448, 1351, 1226, 1091, 981, 821, 754, 689, 544 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 0.83 (t, *J* = 7.3 Hz, 3H), 1.20-1.40 (m, 2H), 1.40-1.55 (m, 2H), 2.31-2.41 (m, 2H), 3.52 (d, *J* = 7.2 Hz, 2H), 4.31 (t, *J* = 7.2 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 5H), 7.39 (d, *J* = 7.9 Hz, 2H), 7.41-7.49 (m, 2H), 7.51-

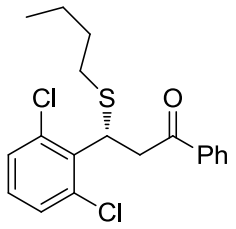
7.62 (m, 1H), 7.92 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 13.3, 21.9, 30.8, 43.2, 45.8, 128.3, 128.9, 129.2, 134.6, 135.1, 137.3, 140.9, 198.2; HRMS (EI) calcd for $C_{19}H_{21}OSCl$ *m/z* 332.1002, found 332.1010.

(*R*)-3-(4-Chlorophenyl)-3-((2-hydroxyethyl)thio)-1-phenylpropan-1-one (8j)



Colorless oil; $[\alpha]_D^{25}$ + 173.8 (*c* 0.1, $CHCl_3$); 96% ee [Chiralcel OD, hexane:*i*-propanol 80:20, 1.0 mL/min, 215 nm, t_R (major) 25.2 min, t_R (minor) 31.3 min]; IR (neat) 3370 (broad), 2970, 1700, 1456, 1242, 1079, 906, 755 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.59 (s, 2H), 3.48-3.51 (m, 1H), 3.58-3.61 (m, 1H), 3.66-3.71 (m, 1H), 3.88-3.93 (m, 2H), 4.51 (t, *J* = 7.2 Hz, 1H), 7.30-7.36 (m, 2H), 7.39-7.42 (m, 2H), 7.46-7.50 (m, 2H), 7.58-7.61 (m, 1H), 7.92-7.96 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 34.5, 43.6, 45.3, 60.3, 128.7, 129.1, 129.6, 129.9, 133.2, 133.6, 137.1, 140.9, 198.1; HRMS (EI) calcd for $C_{17}H_{18}O_2SCl$ *m/z* 321.0716, found 321.0729.

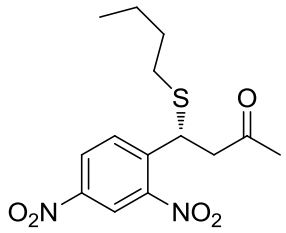
(*R*)-3-(Butylthio)-3-(2,6-dichlorophenyl)-1-phenylpropan-1-one (8k)



Colorless oil; $[\alpha]_D^{25}$ + 197.1 (*c* 0.1, $CHCl_3$); 96% ee [Chiralcel OJ, hexane:*i*-propanol 90:10, 1.0 mL/min, 215 nm, t_R (major) 34.3 min, t_R (minor) 41.5 min]; IR (neat) 2956, 2870, 1687, 1433,

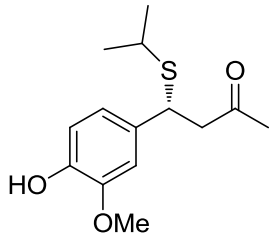
1358, 1218, 1085, 983, 772, 689 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.2 Hz, 3H), 1.29-1.43 (m, 2H), 1.55-1.68 (m, 2H), 2.60-2.79 (m, 2H), 3.80-3.88 (m, 1H), 3.97-4.09 (m, 1H), 5.52 (t, *J* = 7.2 Hz, 1H), 7.09-7.13 (m, 1H), 7.26-7.32 (m, 1H), 7.33-7.37 (m, 1H), 7.47-7.52 (m, 2H), 7.56-7.62 (m, 1H), 7.96 (d, *J* = 8.1 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 13.0, 21.9, 31.2, 32.0, 40.8, 42.3, 128.3, 128.9, 129.8, 133.8, 135.6, 135.8, 137.3, 138.9, 198.3; HRMS (EI) calcd for $C_{19}H_{20}OSClNa$ (M+H) *m/z* 389.0510, found 389.0505.

(*R*)-4-(Butylthio)-4-(2,4-dinitrophenyl)butan-2-one (8l)



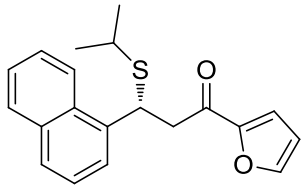
Colorless oil; $[\alpha]_D^{25}$ + 153.9 (*c* 0.1, $CHCl_3$); 95% ee [Chiralcel OD-H, hexane:*i*-propanol 80:10, 1.0 mL/min, 215 nm, t_R (major) 21.8 min, t_R (minor) 28.4 min]; IR (neat) 2958, 2930, 1708, 1348, 1276, 1158, 1065, 910, 835, 740 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.3 Hz, 3H), 1.34-1.42 (m, 2H), 1.49-1.56 (m, 2H), 2.36 (s, 3H), 2.38-2.44 (m, 1H), 2.50-2.58 (m, 1H), 3.37-3.44 (m, 1H), 3.59-3.65 (m, 1H), 3.69-3.74 (m, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 8.40 (d, *J* = 8.2 Hz, 1H), 8.83 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 13.7, 21.9, 28.0, 29.9, 30.8, 32.4, 52.1, 120.6, 128.1, 136.5, 141.2, 147.0, 149.8, 204.1; HRMS (EI) calcd for $C_{14}H_{18}N_2O_5S$ *m/z* 326.0936, found 326.0937.

(*R*)-4-(4-Hydroxy-3-methoxyphenyl)-4-(isopropylthio)butan-2-one (8m)



Colorless oil; $[\alpha]_D^{25}$ + 162.0 (*c* 0.1, $CHCl_3$); 96% ee [Chiralcel AD, hexane:*i*-propanol 85:15, 0.8 mL/min, 215 nm, t_R (major) 23.8 min, t_R (minor) 30.2 min]; IR (neat) 3432 (broad), 2960, 2926, 1711, 1600, 1462, 1363, 1269, 1153, 1122, 1033, 818, 792 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.12 (d, *J* = 6.8 Hz, 3H), 1.27 (d, *J* = 6.8 Hz, 3H), 2.09 (s, 3H), 2.58-2.69 (m, 1H), 2.87-2.98 (m, 2H), 3.89 (s, 3 H), 4.36 (t, *J* = 6.9 Hz, 1H), 6.80-6.89 (m, 2H), 6.92 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.7, 22.9, 30.5, 34.5, 43.3, 50.3, 56.8, 110.4, 114.9, 120.6, 135.3, 146.1, 148.0, 208.1; HRMS (EI) calcd for $C_{14}H_{20}O_3S$ *m/z* 268.1133, found 268.1134.

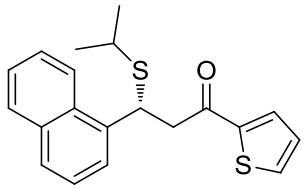
(*R*)-1-(Furan-2-yl)-3-(isopropylthio)-3-(naphthalen-1-yl)propan-1-one (8n)



Colorless oil; $[\alpha]_D^{25}$ + 206.3 (*c* 0.1, $CHCl_3$); 97% ee [Chiralcel AD, hexane:*i*-propanol 70:30, 1.0 mL/min, 215 nm, t_R (major) 8.6 min, t_R (minor) 9.9 min]; IR (neat) 3442, 2958, 2923, 1672, 1467, 1394, 1159, 1050, 981, 883, 776 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.17 (d, *J* = 6.9 Hz, 3H), 1.22 (d, *J* = 6.9 Hz, 3H), 2.78-2.88 (m, 1H), 3.03-3.16 (m, 2H), 3.49-3.68 (m, 1H), 6.48-6.55 (m, 1H), 7.13-7.19 (m, 1H), 7.46-7.57 (m, 2H), 7.59-7.63 (m, 2H), 7.76-7.84 (m, 1H), 7.86-7.99 (m, 2H), 8.37 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 21.9, 22.0, 32.5, 41.9, 44.2, 111.9,

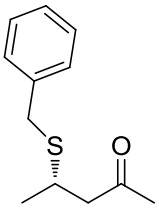
117.3, 120.8, 123.9, 125.8, 125.9, 126.3, 127.2, 128.7, 130.8, 134.1, 138.3, 147.1, 152.2, 201.3; HRMS (EI) calcd for $C_{20}H_{20}O_2S$ *m/z* 324.1184, found 324.1193.

(*R*)-3-(Isopropylthio)-3-(naphthalen-1-yl)-1-(thiophen-2-yl)propan-1-one (8o)



Colorless oil; $[\alpha]_D^{25}$ + 218.7 (*c* 0.1, $CHCl_3$); 94% ee [Chiralcel AD, hexane:*i*-propanol 80:20, 0.8 mL/min, 215 nm, t_R (major) 13.0 min, t_R (minor) 15.1 min]; IR (neat) 2959, 2922, 1660, 1453, 1414, 1355, 1237, 1060, 931, 858, 795, 776, 725 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.18 (d, *J* = 6.9 Hz, 3H), 1.22 (d, *J* = 6.9 Hz, 3H), 2.81-2.91 (m, 1H), 3.09-3.18 (m, 2H), 3.54-3.70 (m, 1H), 7.09-7.14 (m, 1H), 7.45-7.59 (2H), 7.60-7.67 (m, 2H), 7.69-7.74 (m, 1H), 7.77-7.83 (m, 1H), 7.88-7.95 (m, 2H), 8.49 (s, 1H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 21.7, 21.9, 32.7, 40.7, 42.9, 120.4, 126.7, 126.8, 127.2, 128.1, 128.2, 129.6, 130.9, 132.3, 134.7, 135.9, 139.0, 142.2, 145.9, 200.9; HRMS (EI) calcd for $C_{20}H_{20}OS_2$ *m/z* 340.0956, found 340.0949.

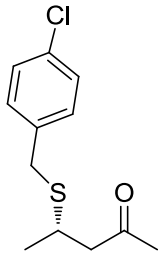
(*S*)-4-(Benzylthio)pentan-2-one (8p)



Colorless oil; $[\alpha]_D^{25}$ + 7.9 (*c* 0.1, $CHCl_3$); 96% ee [Chiralcel OD, hexane:*i*-propanol 92:8, 0.8 mL/min, 215 nm, t_R (major) 14.4 min, t_R (minor) 16.9 min]; IR (neat) 2962, 2922, 1714, 1494, 1359, 1158, 1070, 1028, 769 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 1.29 (d, *J* = 6.8 Hz, 3H), 2.10

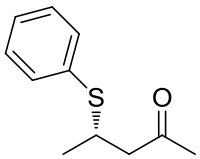
(s, 3H), 2.52-2.58 (m, 1H), 2.67-2.75 (m, 1H), 3.13-3.22 (m, 1H), 3.74-3.80 (m, 2H), 7.20-7.26 (m, 1H), 7.32-7.39 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 21.3, 30.9, 35.3, 35.8, 51.0, 127.7, 129.3, 129.4, 139.2, 208.8; HRMS (EI) calcd for $C_{12}H_{16}OS$ *m/z* 208.0922, found 208.0919.

(*S*)-4-((4-Chlorobenzyl)thio)pentan-2-one (8q)



Colorless oil; $[\alpha]_D^{25}$ + 10.5 (*c* 0.1, $CHCl_3$); 93% ee [Chiralcel OD, hexane:*i*-propanol 92:8, 0.8 mL/min, 215 nm, t_R (major) 19.3 min, t_R (minor) 22.5 min]; IR (neat) 2963, 2924, 1714, 1490, 1359, 1280, 1159, 1092, 1014, 962, 832, 747 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 1.28 (d, *J* = 6.8 Hz, 3H), 2.12 (s, 3H), 2.52-2.59 (m, 1H), 2.67-2.73 (m, 1H), 3.11-3.20 (m, 1H), 3.71-3.79 (m, 2H), 7.28-7.33 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.0, 30.6, 35.3, 35.9, 51.1, 128.9, 130.0, 134.1, 139.0, 208.7; HRMS (EI) calcd for $C_{12}H_{15}OClS$ *m/z* 242.0532, found 242.0530.

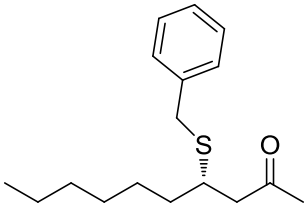
(S)-4-(Phenylthio)pentan-2-one (8r)



Colorless oil; $[\alpha]_D^{25}$ + 14.6 (*c* 0.1, $CHCl_3$); 98% ee [Chiralcel OD, hexane:*i*-propanol 98:2, 0.8 mL/min, 215 nm, t_R (major) 14.5 min, t_R (minor) 17.1 min]; IR (neat) 2968, 2925, 1715, 1583, 1476, 1360, 1157, 1091, 1024, 748, 693 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.30 (d, *J* = 6.7 Hz, 3H), 2.14 (s, 3H), 2.52-2.62 (m, 1H), 2.72-281 (m, 1H), 3.67-3.80 (m, 1H), 7.21-7.32 (m, 3H),

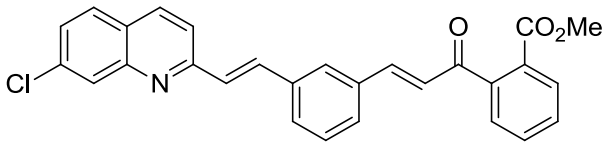
7.42-7.49 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 20.9, 30.8, 38.9, 50.6, 128.5, 129.6, 143.0, 144.8, 208.9.

(*S*)-4-(Benzylthio)decan-2-one (8s)



Colorless oil; $[\alpha]_D^{25}$ + 19.3 (*c* 0.1, $CHCl_3$); 98% ee [Chiralcel OD, hexane:*i*-propanol 90:10, 1.0 mL/min, 215 nm, t_R (major) 6.1 min, t_R (minor) 9.1 min]; IR (neat) 3028, 2927, 2856, 1716, 1494, 1454, 1359, 1154, 1070, 960, 766, 701 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.3 Hz, 3H), 1.22-1.48 (m, 10H), 2.09 (s, 3H), 2.59-2.63 (m, 1H), 2.65-2.72 (m, 1H), 3.04-3.09 (m, 1H), 3.70-3.79 (m, 2H), 7.21-7.26 (m, 1H), 7.30-7.39 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 14.1, 22.7, 26.4, 27.8, 30.0, 31.6, 34.9, 35.2, 40.8, 50.5, 128.4, 129.5, 129.8, 139.2, 208.7; HRMS (EI) calcd for $C_{17}H_{26}OS$ *m/z* 278.1704, found 278.1695.

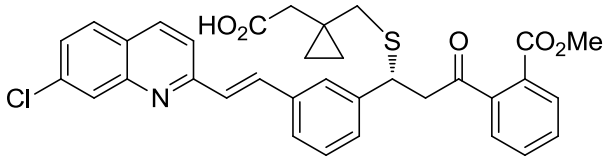
Methyl 2-((*E*)-3-(3-((*E*)-2-(7-chloroquinolin-2-yl)vinyl)phenyl)acryloyl)benzoate (10)



To a mixture of 7-chloroquinaldine (17.7 mg, 0.1 mmol) and 1,3-benzene dicarboxaldehyde (13.4 mg, 0.1 mmol) in dry toluene (2 mL) was added *p*-toluenesulfonamide (17.1 mg, 0.1 mmol) and the mixture was heated to reflux for 24 h. To the mixture was added a solution of methyl 2-acetylbenzoate (19.6 mg, 1.1 mmol) in toluene (0.5 mL) and reflux was continued for

an additional 16 h. The reaction mixture was concentrated under reduced pressure and the resulting crude residue was purified by flash chromatography on silica gel (5% ethyl acetate/hexane) to give the product (39 mg, 86% yield) as yellow solid; mp 119-120 ^{o}C; IR (neat) 3049, 2958, 2923, 2853, 1716, 1597, 1461, 1361, 1261, 797, 777, 736 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 3.91 (s, 3H), 7.42-7.51 (m, 4H), 7.59-7.64 (m, 2H), 7.67-7.74 (m, 2H), 7.76-7.81 (m, 2H), 7.83-7.86 (m, 2H), 7.88-7.91 (m, 1H), 7.93-7.98 (m, 1H), 8.11-8.15 (m, 1H), 8.16-8.21 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 50.9, 123.4, 125.3, 125.4, 127.6, 128.2, 128.4, 128.5, 128.6, 128.8, 129.0(x2), 129.2, 129.3, 129.6(x2), 133.1, 133.5, 134.5, 137.1, 138.6, 140.9, 142.8, 142.9, 144.9, 158.0, 161.6, 189.8; HRMS (EI) calcd for $C_{28}H_{21}O_3NCl$ *m/z* 454.1210, found 454.1202.

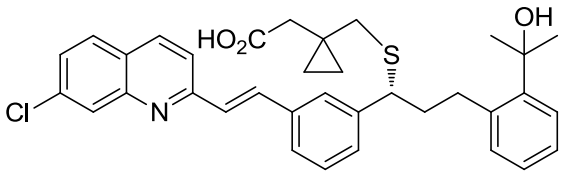
(*R*,*E*)-2-(1-(((1-(3-(2-(7-Chloroquinolin-2-yl)vinyl)phenyl)-3-(2-(methoxycarbonyl)phenyl)-3-oxopropyl)thio)methyl)cyclopropyl)acetic acid (21)



Pale yellow solid; mp 129-130 ^{o}C; $[\alpha]_D^{25}$ +93.3 (*c* 0.1, MeOH); 98% ee [Chiralcel AS-H, hexane:*i*-propanol 82:18, 0.8 mL/min, 215 nm, t_R (major) 20.7 min, t_R (minor) 27.3 min]; IR (neat) 3000 (broad), 1770, 1722, 1701, 1434, 1390, 1283, 1198, 1133, 1066, 982, 829, 764, 709 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 0.99-1.12 (m, 4H), 2.33-2.42 (m, 2H), 2.51-2.60 (m, 2H), 3.35-3.42 (m, 2H), 3.88-3.92 (m, 1H), 4.03 (s, 3H), 7.39-7.48 (m, 3H), 7.58-7.61 (m, 1H), 7.62-7.65 (m, 1H), 7.68-7.73 (m, 1H), 7.75-7.80 (m, 1H), 7.80-7.84 (m, 1H), 7.85-7.90 (m, 1H), 8.01-8.06 (m, 2H), 8.06-8.12 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 12.3, 17.6, 38.7, 40.9, 46.6, 49.7, 119.9, 126.1, 126.4, 127.7, 128.2, 129.0, 129.1, 129.3, 129.8, 130.4, 130.5, 131.0, 133.2,

134.8, 134.9, 135.2, 135.3, 137.8, 138.2, 138.4, 138.7, 139.1, 139.3, 149.3, 157.7, 169.1, 179.3, 199.9; HRMS (EI) calcd for $C_{34}H_{31}O_5NSCl$ *m/z* 600.1611, found 600.1614.

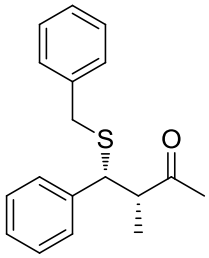
(*R*,*E*)-2-(1-(((1-(3-(2-(7-Chloroquinolin-2-yl)vinyl)phenyl)-3-(2-(2-hydroxypropan-2-yl)phenyl)propyl)thio)methyl)cyclopropyl)acetic acid (9)



To a solution of **21** (38 mg, 0.06 mmol) in MeOH (1.5 mL) at 25 ^{o}C was added tosylhydrazine (14.2 mg, 0.08 mmol) and the mixture was stirred for 6 h. To the reaction mixture at room temperature was added sodium borohydride (5 mg, 0.13 mmol) and the mixture was stirred for an additional 3 h. Saturated NH_4Cl was added to the reaction mixture and subsequently extracted in ethyl acetate (2x50 mL). The organic layer was dried (anhyd. Na_2SO_4) and evaporated to achieve crude **23** (45 mg). To a solution of crude **23** (45 mg) in anhydrous THF (3 mL) at 0 ^{o}C was added methylmagnesium bromide (126 μL, 0.38 mmol, 3M in Et_2O) dropwise. After the addition was over the mixture was allowed to warm to room temperature and was stirred for an additional 2 h. Saturated NH_4Cl was added to the reaction mixture and subsequently extracted in ethyl acetate (3x50 mL). The crude residue was purified by flash chromatography on silica gel (15% ether/hexane) to give the product (32 mg, 87% yield) as yellow solid; mp 147-148 ^{o}C, [lit.[3] 145-148 ^{o}C]; $[\alpha]_D^{26}$ + 101.4 (*c* 0.5, MeOH), [lit.[3] for *(S)* enantiomer $[\alpha]_D^{25}$ + 102 (*c* 1.0, $CHCl_3$)]; IR (neat) 3440 (broad), 1762, 1708, 1436, 1309, 1259, 1190, 1118, 1070, 1026, 997, 750, 721, 695 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 0.41-0.52 (m, 4H), 1.37 (s, 6H), 2.02-2.16 (m, 2H), 2.29-2.42 (m, 2H), 2.62-2.71 (m, 2H), 3.01-3.10 (m, 1H), 3.24-3.32 (m, 1H), 3.79-3.88 (m, 1H), 7.20-7.29 (m, 2H), 7.32-7.38 (m, 1H), 7.40-7.45 (m, 1H), 7.51-7.55 (m, 1H), 7.57-7.63 (m, 5H),

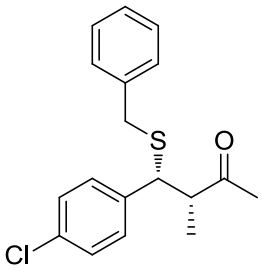
7.67-7.73 (m, 1H), 7.73-7.77 (m, 1H), 7.79-7.85 (m, 1H), 7.90-7.96 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 12.3, 17.3, 31.6, 31.7, 39.7, 40.9, 44.4, 45.2, 74.3, 119.9, 126.8, 127.7, 128.4, 128.6, 129.0, 129.4, 129.7, 129.8, 132.0, 132.9, 134.5, 135.6, 138.1, 138.4, 139.1, 140.3, 141.0, 141.7, 142.3, 144.2, 146.9, 159.1, 157.3, 179.8.

(3*S*,4*R*)-4-(Benzylthio)-3-methyl-4-phenylbutan-2-one (25a)



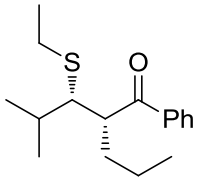
Colorless oil; *syn*:*anti* > 23:1; 98% ee [Chiralcel OD-H, hexane:*i*-propanol 95:5, 0.8 mL/min, 215 nm, t_R (*syn*, major) 15.4 min, t_R (*syn*, minor) 18.3 min]; $[\alpha]_D^{25}$ + 160.2 (*c* 0.1, $CHCl_3$) [lit.[4] for *(3R,4S)* enantiomer $[\alpha]_D^{25}$ - 140.7 (*c* 0.55, $CHCl_3$, 85% ee)]; IR (neat) 3060, 3027, 2970, 2928, 1714, 1665, 1492, 1452, 1357, 1244, 1215, 1157, 1073, 698 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 0.82 (d, *J* = 5.6 Hz, 3H, minor), 1.24 (d, *J* = 6.0 Hz, 3H, major), 1.82 (s, 3H, major), 2.08 (s, 3H, minor), 2.98-3.07 (m, 1H), 3.34 (d, *J* = 13.1 Hz, 1H), 3.48 (d, *J* = 13.1 Hz, 1H), 3.97 (d, *J* = 10.2 Hz, 1H), 7.16-7.28 (m, 8H), 7.42-7.50 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 16.3, 29.6, 35.9, 52.4, 52.8, 127.1, 127.5, 128.5, 128.7, 129.0, 129.1, 137.7, 140.9, 210.1; HRMS (EI) calcd for $C_{18}H_{20}OS$ *m/z* 284.1235, found 284.1232.

(3*S*,4*R*)-4-(Benzylthio)-4-(4-chlorophenyl)-3-methylbutan-2-one (25b)



Colorless oil; *syn*:*anti* > 31:1; 96% ee [Chiralcel AS-H, hexane:*i*-propanol 95:5, 0.8 mL/min, 215 nm, t_R (*syn*, major) 19.5 min, t_R (*syn*, minor) 22.6 min]; $[\alpha]_D^{25}$ + 148.2 (*c* 0.1, $CHCl_3$); IR (neat) 3061, 3028, 2969, 2928, 1714, 1600, 1491, 1453, 1409, 1355, 1233, 1157, 1090, 1070, 1013, 822, 764, 699 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 0.84 (d, *J* = 6.4 Hz, 3H, minor), 1.23 (d, *J* = 7.4 Hz, 3H, major), 1.86 (s, 3H, major), 2.17 (s, 3H, minor), 2.91-3.00 (m, 1H), 3.36 (d, *J* = 12.9 Hz, 1H), 3.45 (d, *J* = 12.9 Hz, 1H), 3.93 (d, *J* = 10.1 Hz, 1H), 7.18-7.22 (m, 2H), 7.25-7.40 (m, 7H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 14.3, 29.8, 35.1, 50.7, 52.3, 127.9, 128.3, 128.9, 129.2, 130.0, 130.4, 138.8, 140.9, 200.1; HRMS (EI) calcd for $C_{18}H_{19}OSCl$ *m/z* 318.0845, found 318.0850.

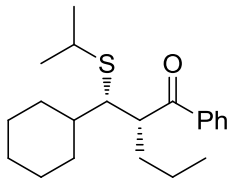
(2*S*,3*S*)-3-(Ethylthio)-4-methyl-1-phenyl-2-propylpentan-1-one (25c)



Colorless oil; *syn*:*anti* > 50:1; 97% ee [Chiralcel OD-H, hexane:*i*-propanol 97:3, 0.8 mL/min, 215 nm, t_R (*anti*, minor) 22.3 min, t_R (*syn*, minor) 26.4 min, t_R (*anti*, major) 34.6 min, t_R (*syn*, major) 39.8 min]; $[\alpha]_D^{25}$ + 37.5 (*c* 0.1, $CHCl_3$); IR (neat) 2926, 2851, 1699, 1648, 14.86, 1437, 1388, 1247, 1021, 757 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 0.61 (d, *J* = 6.3 Hz, 3H), 0.72 (d, *J* = 6.3 Hz, 3H), 0.83-1.07 (m, 4H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.41-1.49 (m, 2H), 1.72-1.82 (m, 2H),

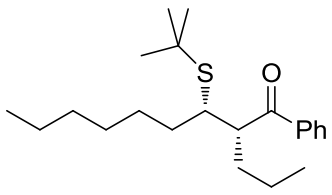
2.96-3.05 (m, 2H), 3.50 (d, *J* = 12.2 Hz, 1H), 3.83 (d, *J* = 12.2 Hz, 1H), 7.42-7.51 (m, 2H), 7.57-7.61 (m, 1H), 7.98-8.04 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 12.9, 13.2 (x2), 19.8, 20.2, 27.3, 31.6, 38.6, 49.6, 119.2, 119.8, 124.7, 138.3, 201.5; HRMS (EI) calcd for $C_{17}H_{27}OS$ *m/z* 279.1783, found 279.1789.

(*S*)-2-((*S*)-Cyclohexyl(isopropylthio)methyl)-1-phenylpentan-1-one (25d)



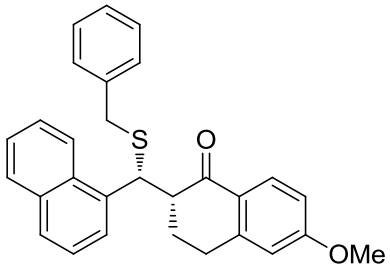
Colorless oil; *syn*:*anti* > 50:1; 96% ee [Chiralcel OD-H, hexane:*i*-propanol 92:8, 0.8 mL/min, 215 nm, t_R (*syn*, major) 16.1 min, t_R (*syn*, minor) 19.2 min]; $[\alpha]_D^{25}$ + 29.3 (*c* 0.1, $CHCl_3$); IR (neat) 3056, 2957, 2919, 1685, 1597, 1448, 1346, 1217, 1179, 1007, 977, 778, 689 cm^{-1}; ^{1}H NMR (700 MHz, $CDCl_3$) δ 0.81-1.12 (m, 19H), 1.39-1.47 (m, 2H), 1.72-1.80 (m, 2H), 2.13-2.22 (m, 2H), 3.18 (d, *J* = 12.5 Hz, 1H), 3.96 (d, *J* = 12.5 Hz, 1H), 7.43-7.49 (m, 2H), 7.54-7.58 (m, 1H), 7.94-7.98 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 13.9, 22.7, 26.2 (x2), 26.6, 27.3, 30.9, 46.9, 47.3, 39.0, 50.2, 128.8, 129.0, 134.0, 138.1, 200.8; HRMS (EI) calcd for $C_{21}H_{33}OS$ *m/z* 333.2252, found 333.2245.

(2*S*,3*S*)-3-(Tert-butylthio)-1-phenyl-2-propylnonan-1-oneone (25e)



Colorless oil; *syn*:*anti* > 50:1; 95% ee [Chiralcel OD, hexane:*i*-propanol 97:3, 0.8 mL/min, 215 nm, t_R (*syn*, major) 21.3 min, t_R (*syn*, minor) 25.0 min]; $[\alpha]_D^{25}$ + 17.0 (*c* 0.1, $CHCl_3$); IR (neat) 3058, 2923, 1685, 1597, 1448, 1346, 1019, 978, 778, 760, 690 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 0.52-0.68 (m, 9H), 0.87-1.02 (m, 6H), 1.09-1.31 (m, 6H), 1.42-1.49 (m, 4H), 1.74-1.83 (m, 4H), 2.98 (d, *J* = 11.8 Hz, 1H), 3.40 (d, *J* = 11.8 Hz, 1H), 7.46-7.52 (m, 2H), 7.56-7.61 (m, 1H), 7.98-8.03 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 14.2, 22.3, 24.1, 25.4, 25.9, 27.7, 28.9, 29.6 (x2), 30.4, 32.4, 46.0, 53.4, 119.7, 120.4, 134.8, 139.5, 200.9; HRMS (EI) calcd for $C_{22}H_{36}OS$ *m/z* 348.5932, found 348.5943.

(*S*)-2-((*R*)-(Benzylthio)(naphthalen-1-yl)methyl)-6-methoxy-3,4-dihydronaphthalen-1(2H)-one (25f)

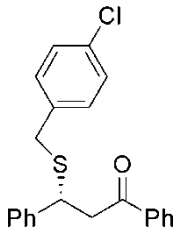


White solid; mp 105-106 ^oC; *syn*:*anti* > 50:1; 98% ee [Chiralcel OD, hexane:*i*-propanol 99:1, 0.8 mL/min, 215 nm, t_R (*syn*, minor) 47.4 min, t_R (*syn*, major) 53.5 min]; $[\alpha]_D^{25}$ + 103.1 (*c* 0.1, $CHCl_3$); IR (neat) 3440, 2922, 1669, 1599, 1493, 1250, 1123, 1023, 920, 778, 699 cm^{-1}; ^1H NMR (700 MHz, $CDCl_3$) δ 2.02-2.09 (m, 1H), 2.17-2.25 (m, 1H), 2.67-2.73 (m, 1H), 2.84-2.93 (m, 2H), 3.60-3.71 (m, 2H), 3.89 (s, 3H), 4.78 (d, *J* = 12.0 Hz, 1H), 6.57 (s, 1H), 6.86-6.92 (m, 1H), 7.13-7.22 (m, 5H), 7.51-7.59 (m, 3H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 8.09-8.20 (m, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 22.5, 28.9, 37.3, 39.6, 53.0, 55.1, 113.2, 113.7, 124.5, 126.1, 127.0, 127.2, 127.9 (x2), 128.1 (x2), 129.1, 129.3, 130.6, 130.9, 131.3, 135.5,

138.1, 138.9, 148.1, 165.3, 197.1; HRMS (EI) calcd for $C_{29}H_{26}O_2S$ *m/z* 438.1653, found 438.1643.

References:

1. Dai, L.; Wang, S. -X.; Chen,F. -E. *Adv. Syth. Catal.* **2010**, *352*, 2137.
2. Ricci, P.; Carone, A.; Bartoli, G.; Bosco, M.; Sambri, L.; Melchiorre, P. *Adv. Synth. Catal.* **2008**, *350*, 49.
3. B. Satyanarayana, P. P. Reddy, *Synth. Comm.* **2007**, *37*, 545.
4. X. Tian, C. Cassani, Y. Liu, A. Moran, A. Urakawa, P. Galzerano, E. Arceo, P. Melchiorre, *J. Am. Chem. Soc.* **2011**, *133*, 17934.



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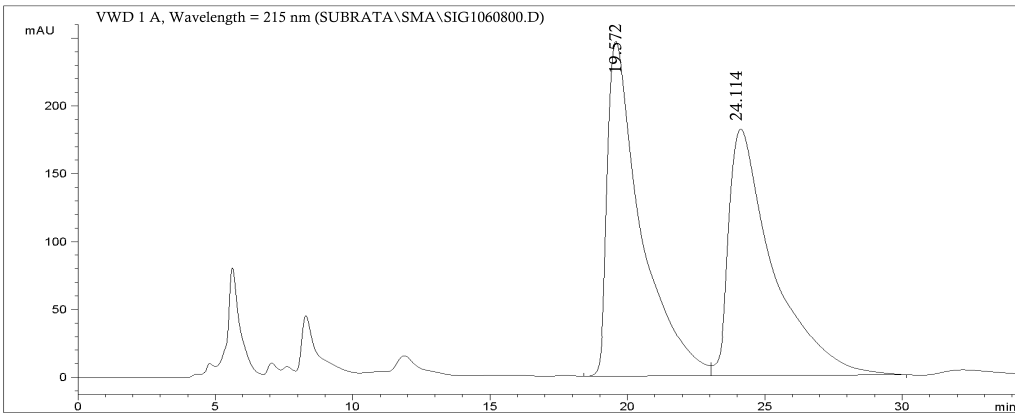
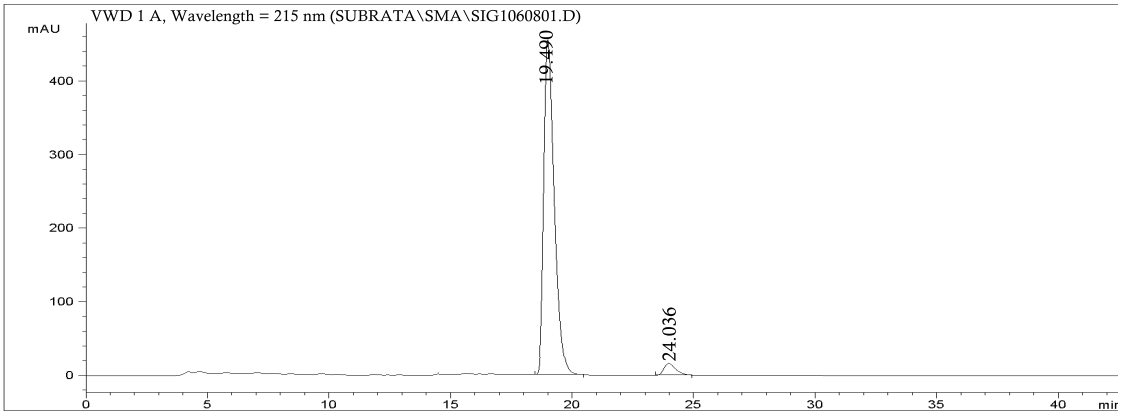
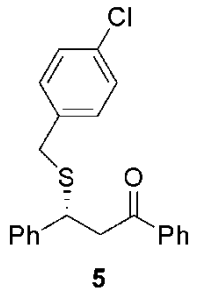


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.572	VB	1.2159	2.10023e4	246.76242	57.5868
2	24.114	BB	1.6117	2.04180e4	181.34812	42.4132



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.490	VB	0.4698	1.39329e4	224.38745	99.1107
2	24.036	VB	0.5372	125.01738	180.58675	0.8893



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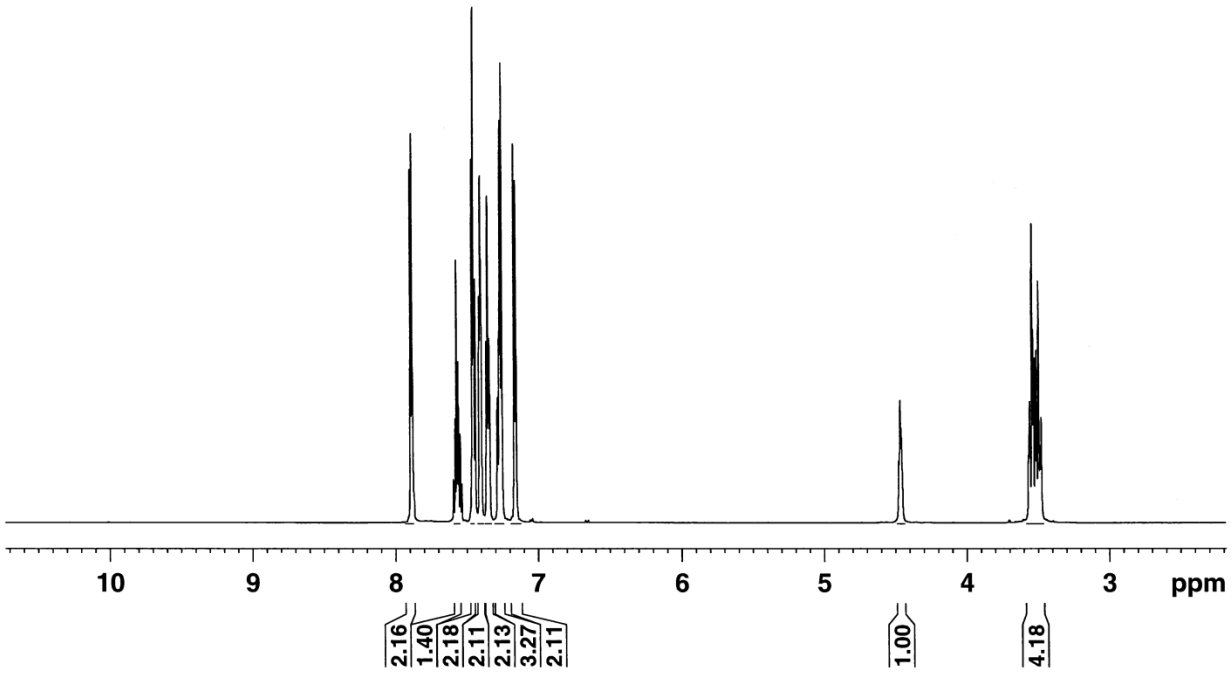
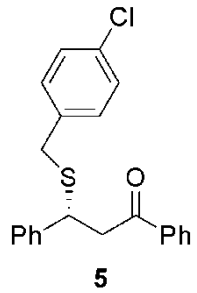


NAME	SS-06-26
EXPNO	1
PROCNO	1
Date_	20121213
Time	15.08
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	28
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	20.2
DW	42.000 usec
DE	6.50 usec
TE	303.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 usec
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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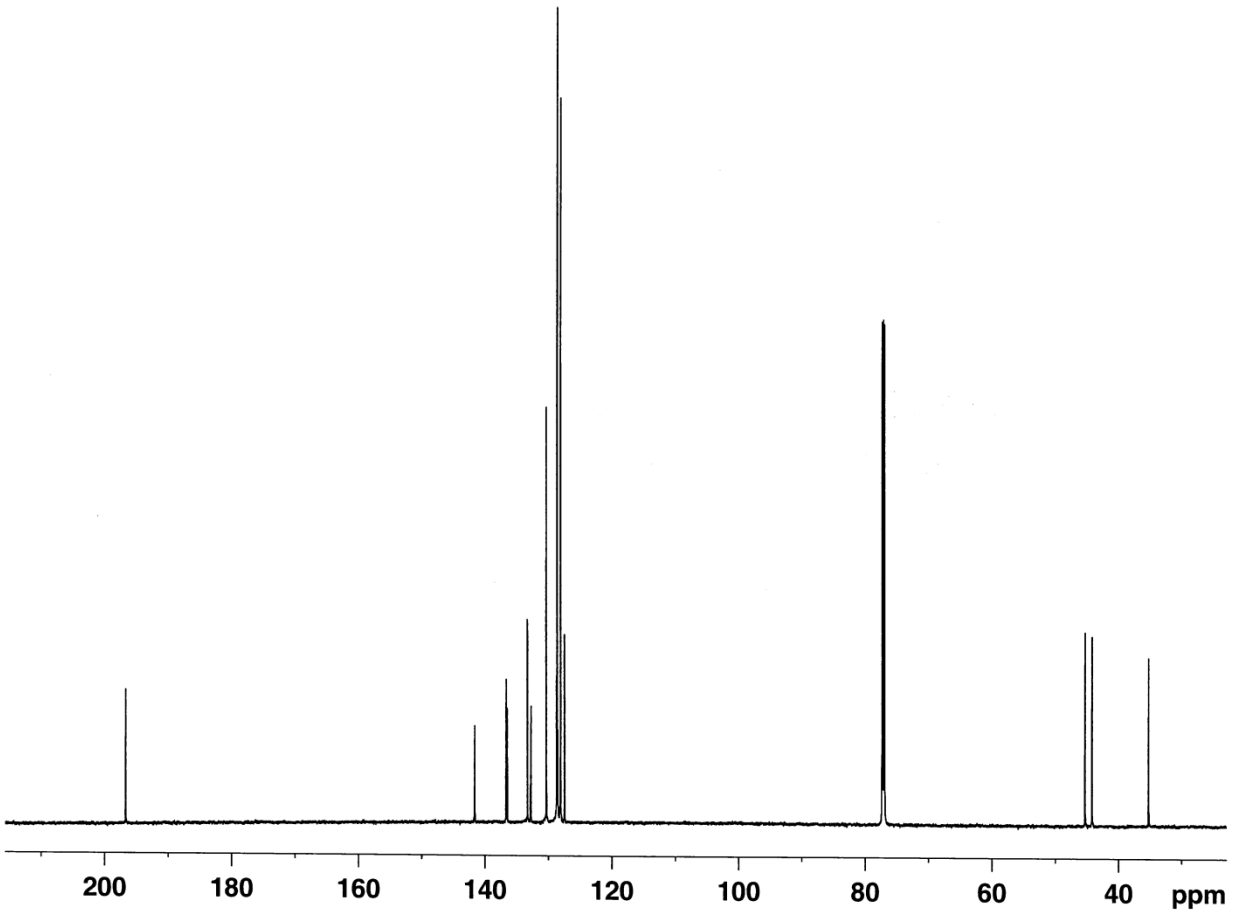
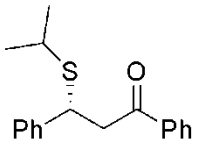


NAME	SS-06-26
EXPNO	2
PROCNO	1
Date_	20121213
Time	15.14
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	38
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	303.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



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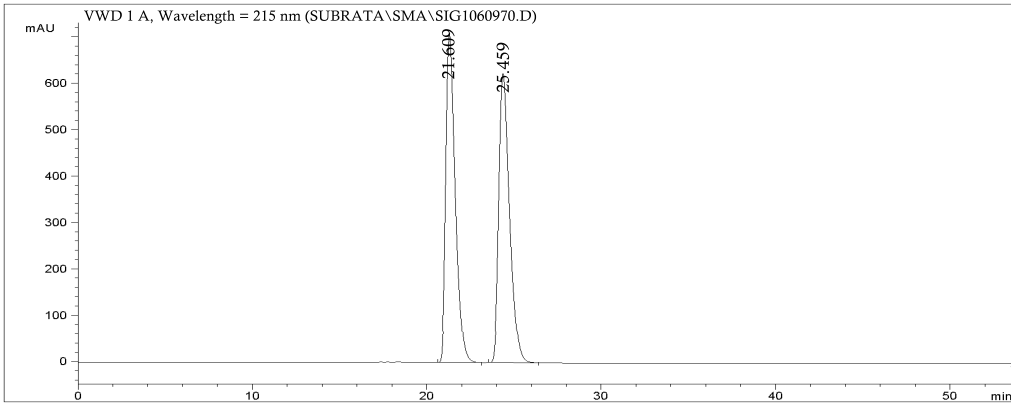
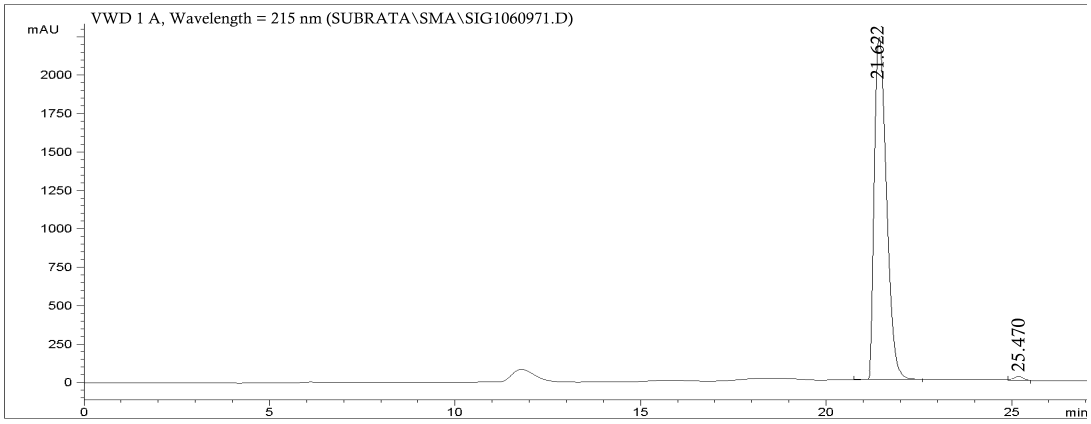
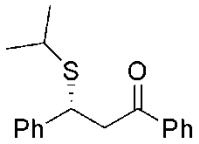


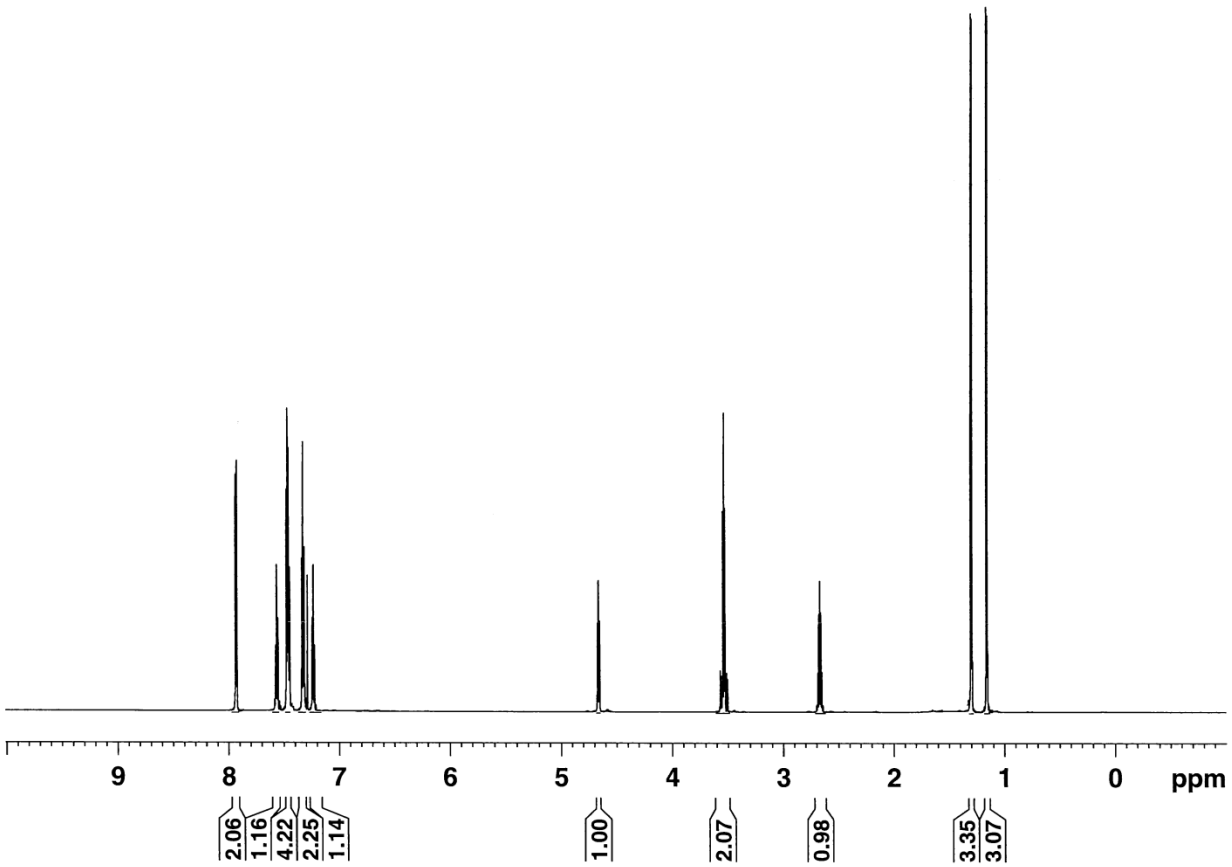
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.609	BV	0.3278	8629.01477	705.06243	53.4969
2	25.459	BB	0.3026	7500.94152	621.63450	46.5031



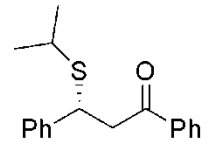
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.622	VB	0.3431	3.28911e4	2201.34421	97.0996
2	25.470	BB	0.0373	982.46896	21.91663	2.9004



8a



NAME	SS-06-97	
EXPNO	1	
PROCNO	1	
Date_	20130323	
Time	15.59	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zg30	
TD	95236	
SOLVENT	CDCl3	
NS	7	
DS	2	
SWH	11904.762	Hz
FIDRES	0.125003	Hz
AQ	3.9999621	sec
RG	18	
DW	42.000	use
DE	6.50	use
TE	298.2	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 =======		
NUC1	1H	
P1	9.40	use
PL1	-3.20	dB
PL1W	33.59817505	W
SFO1	700.1516910	MHz
SI	131072	
SF	700.1471400	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



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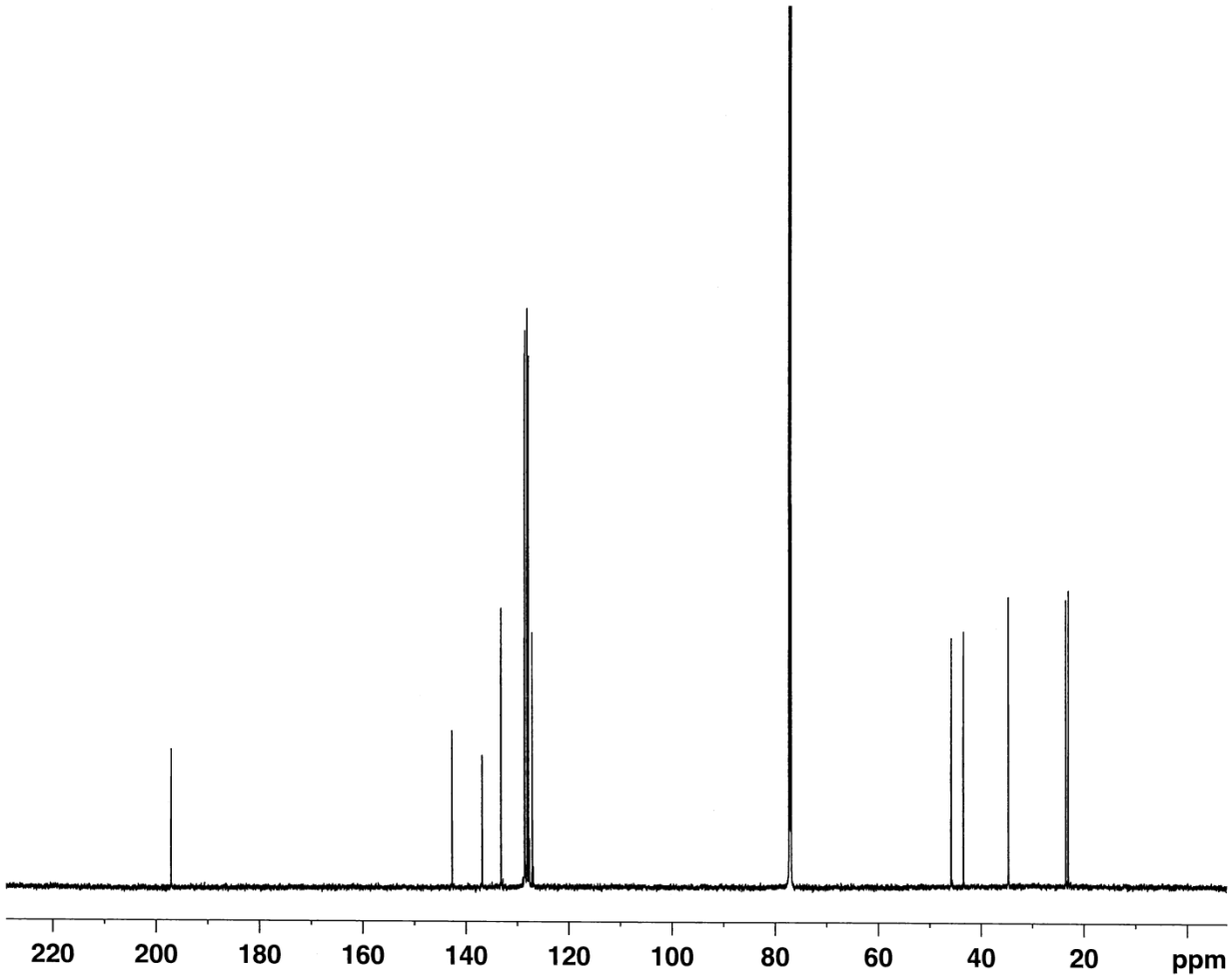
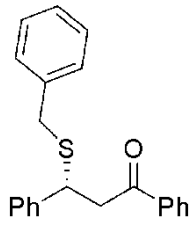
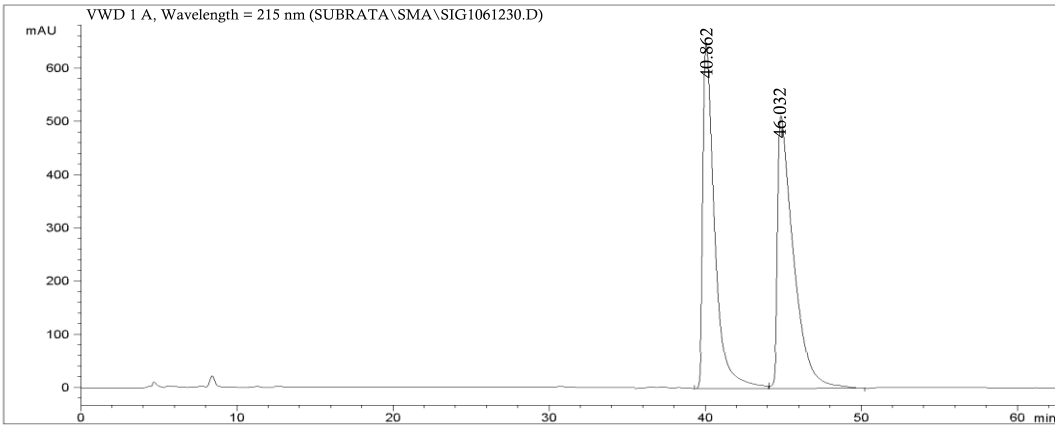


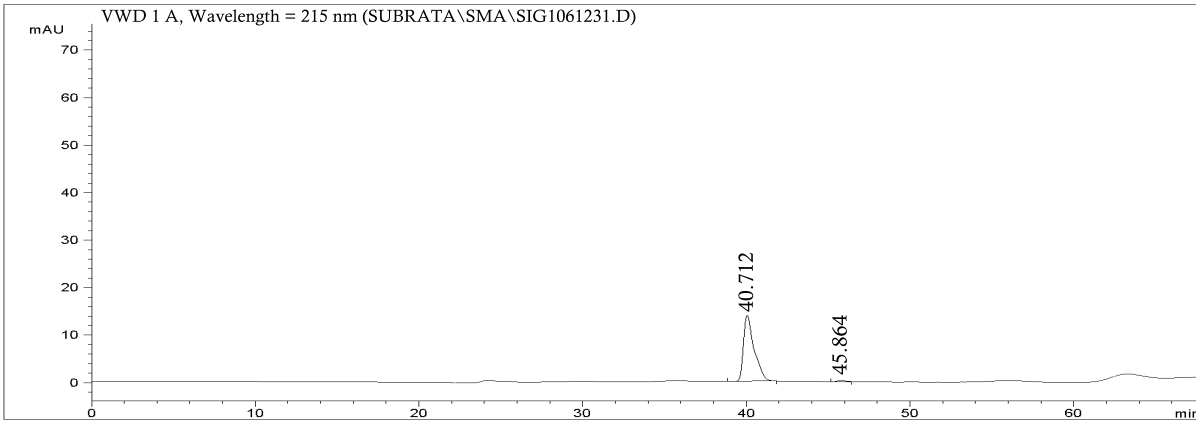
NAME	SS-06-97
EXPNO	2
PROCNO	1
Date_	20130323
Time	16.05
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



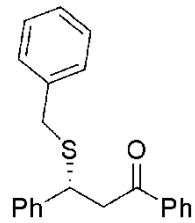
8b



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	40.862	BB	0.7856	3.34754e4	649.52328	44.0168
2	46.032	BB	1.2356	3.65632e4	511.06427	55.9832



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	40.712	BB	0.4645	7635.65343	14.45315	98.6092
2	45.864	BV	0.0365	107.69448	0.53745	1.3908



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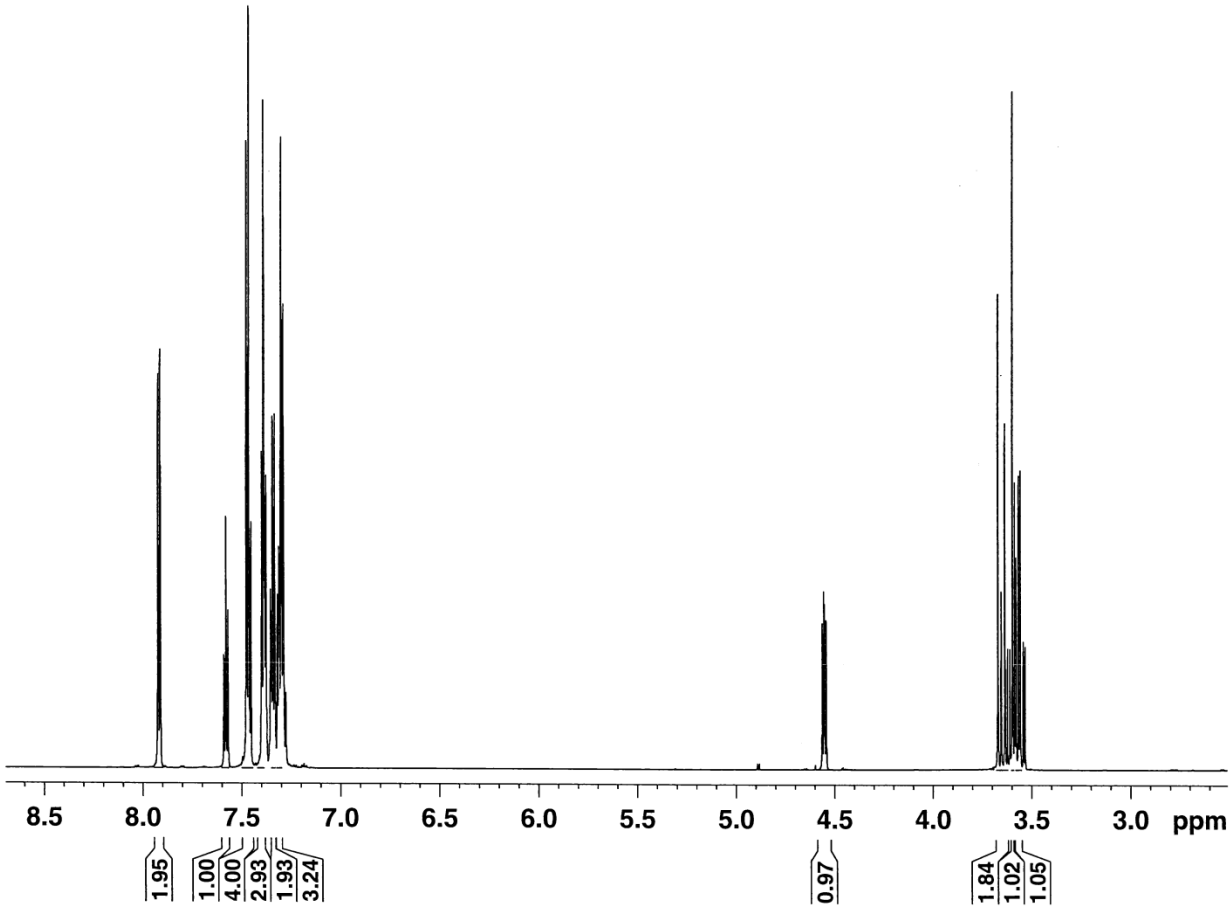
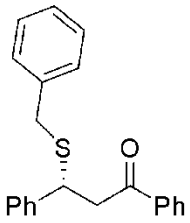
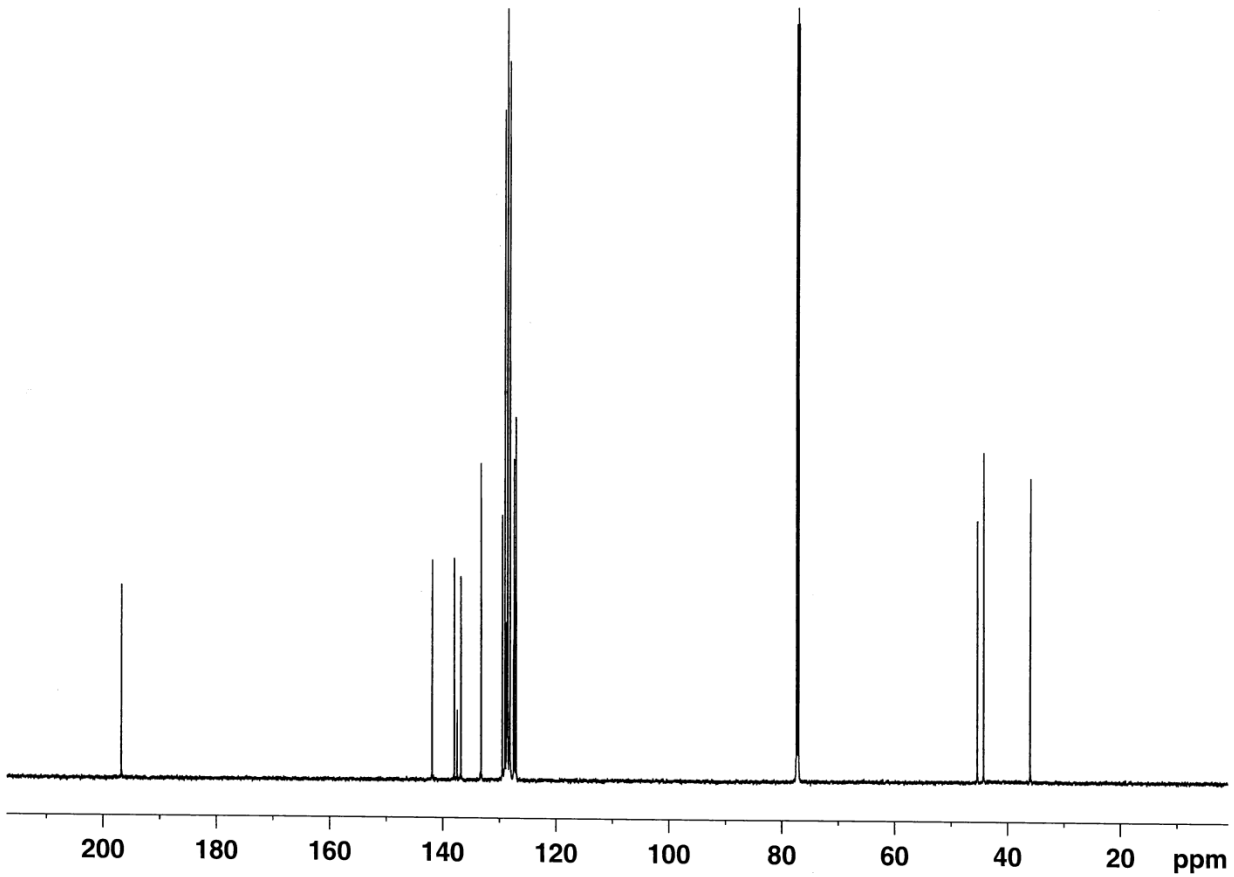


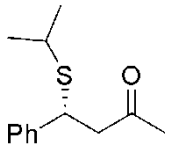
NAME	SS-06-123
EXPNO	1
PROCNO	1
Date_	20130323
Time	16.11
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	32
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	14.2
DW	42.000 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 usec
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



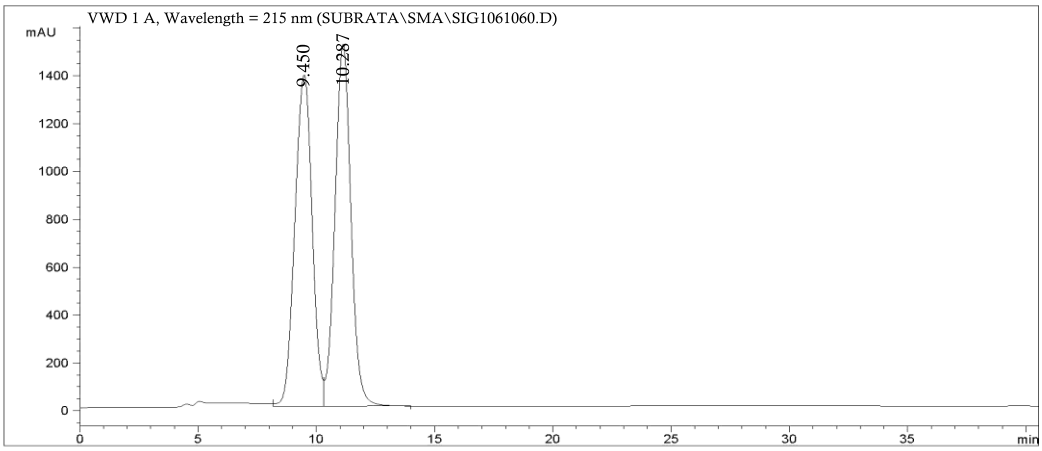
8b



NAME	SS-06-123	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	16.21	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	13	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	use
DE	16.50	use
TE	298.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 =======		
NUC1	13C	
P1	9.00	use
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 =======		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	use
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



8c



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
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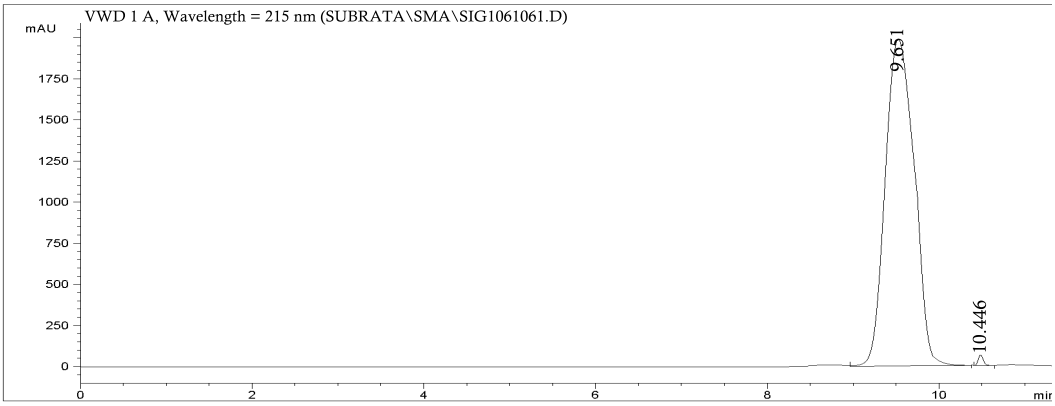

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
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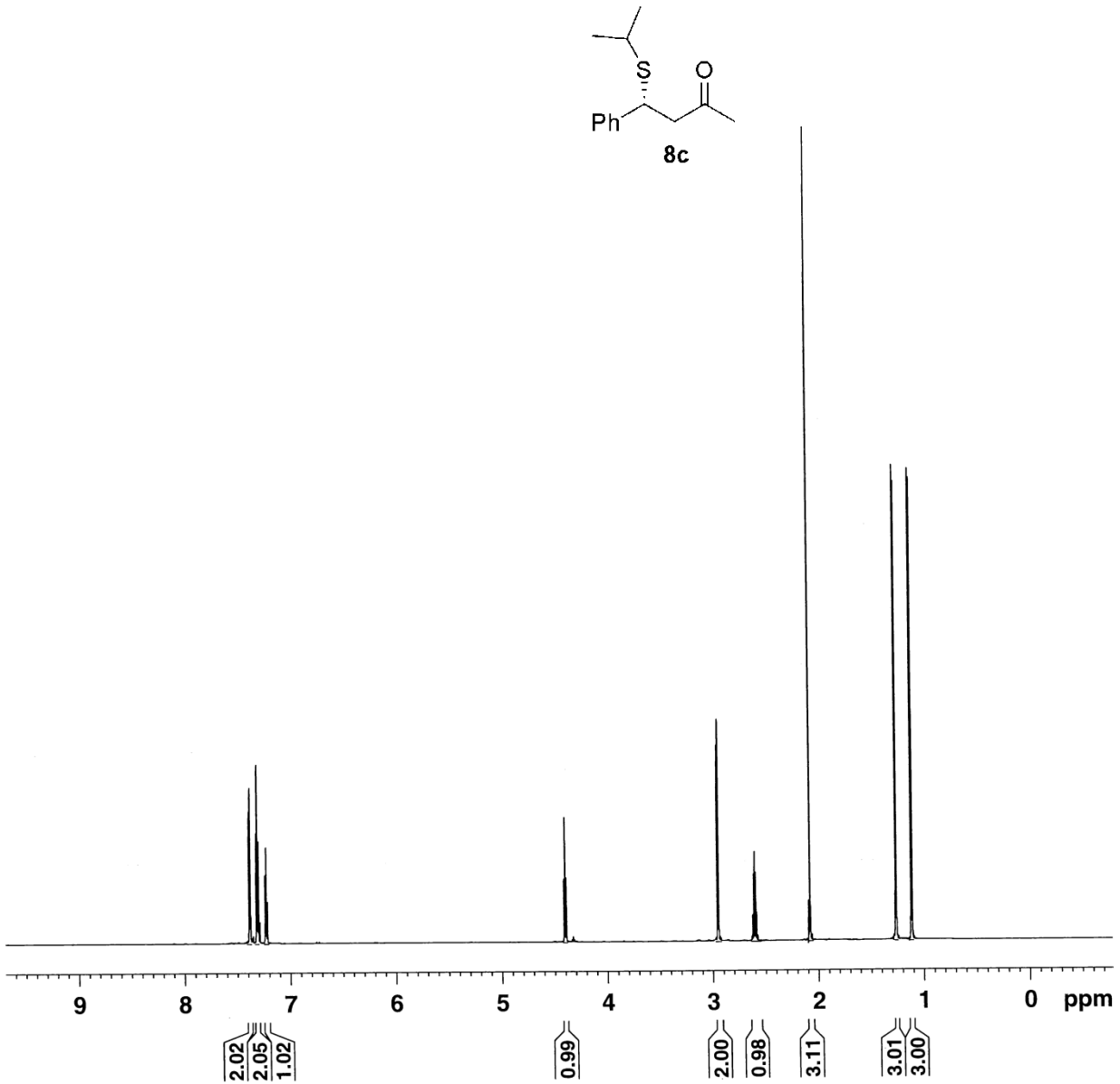
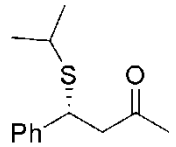
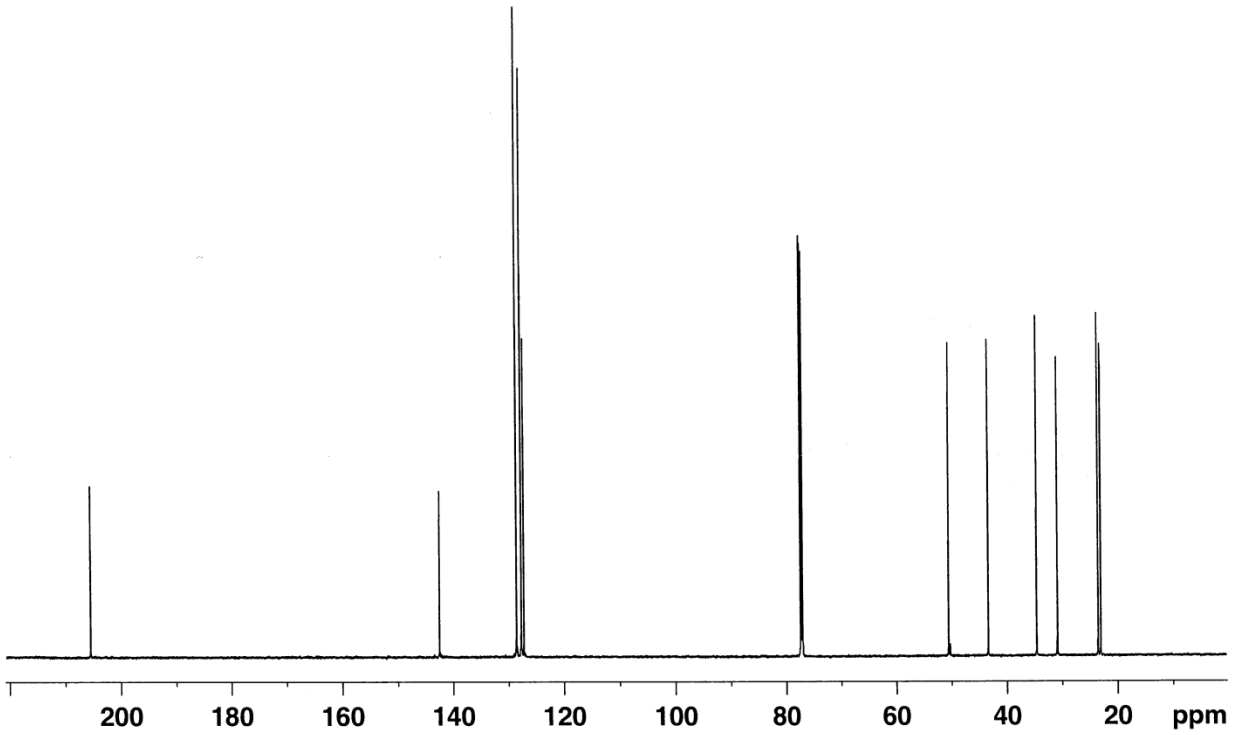
2	10.446	VB	0.0605	18.22251	49.08568	1.8959



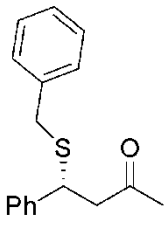
NAME	SS-06-106
EXPNO	1
PROCNO	1
Date_	20130323
Time	16.27
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	11
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	12.7
DW	42.000 use
DE	6.50 use
TE	298.3 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



8c



NAME	SS-06-106	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	16.30	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	17	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	usec
DE	16.50	usec
TE	298.2	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	usec
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	usec
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



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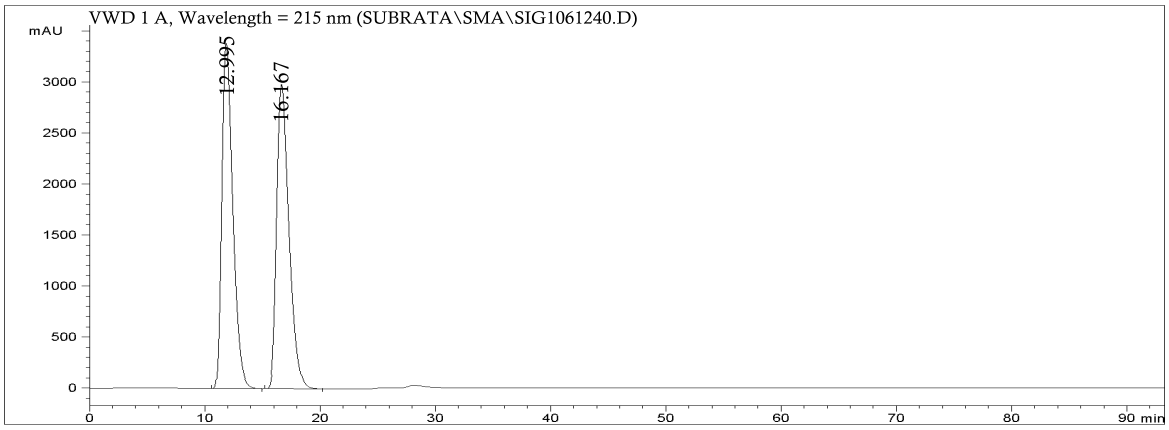
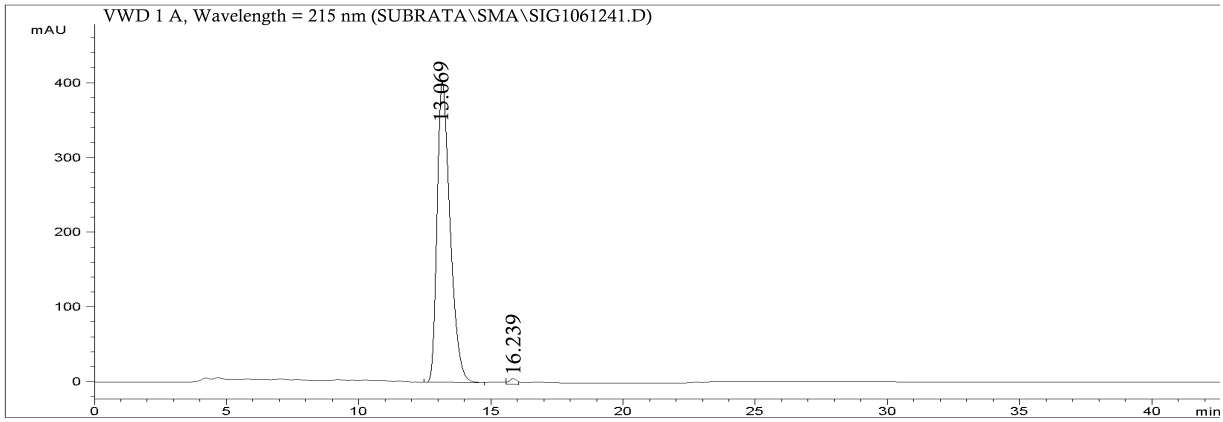
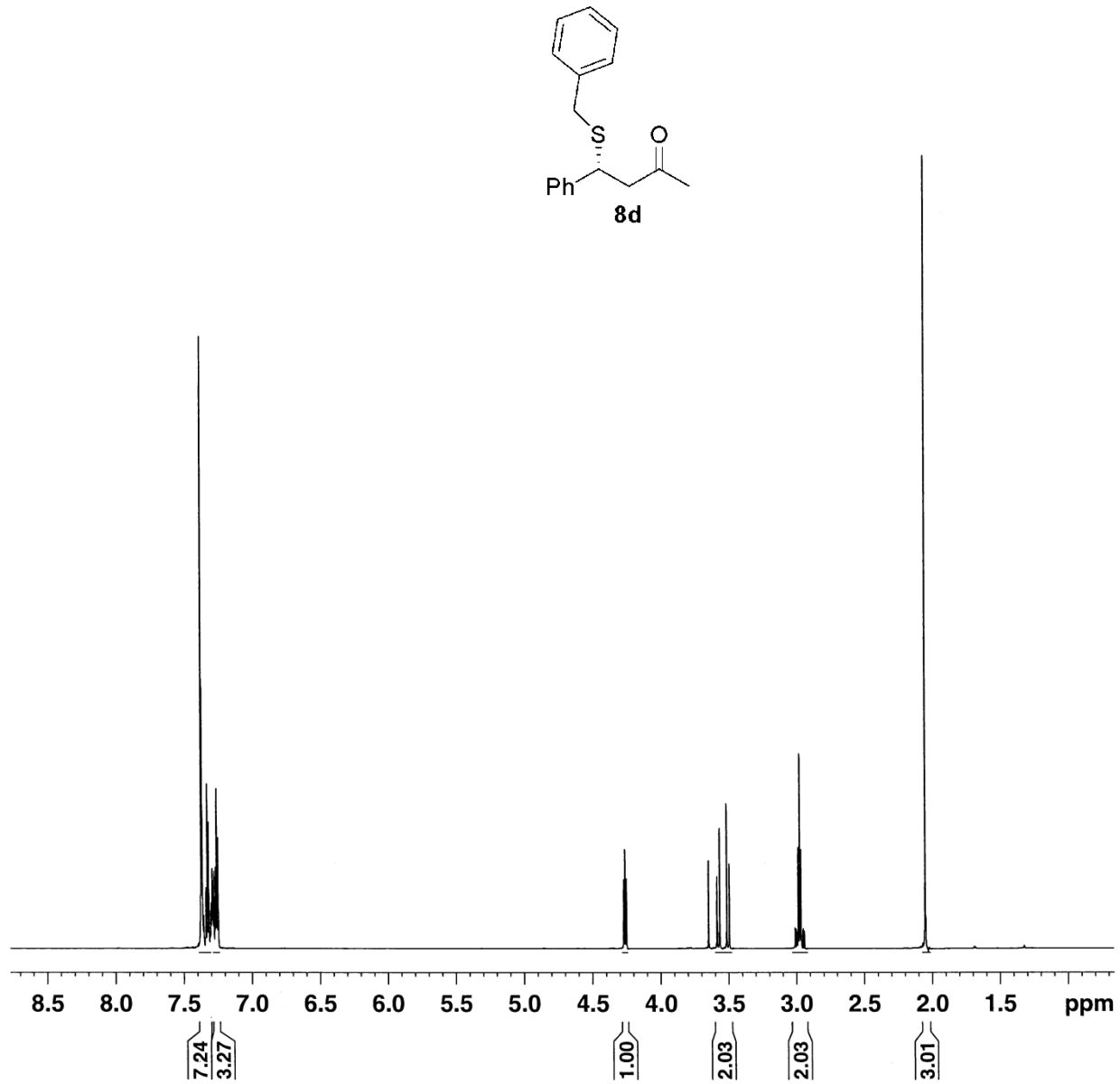


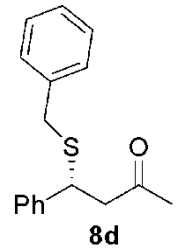
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.995	BB	0.4205	2.27691e4	3398.70152	50.1233
2	16.167	BB	0.4597	2.26572e4	2994.45061	49.8767



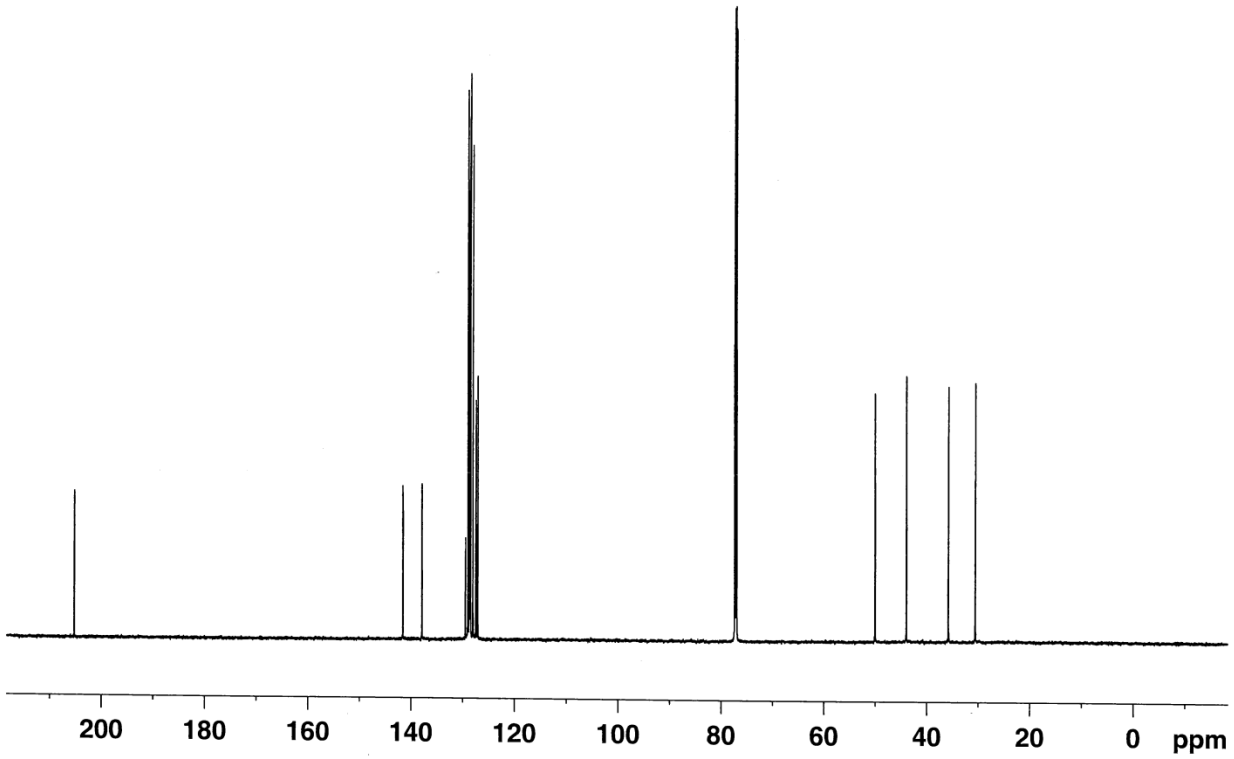
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.069	VB	0.3106	7635.65343	409.65349	98.2336
2	16.239	BV	0.0565	137.30141	3.9645	1.7664



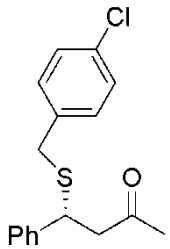

```
NAME            SS-06-124
EXPNO                   1
PROCNO                  1
Date_            20130323
Time                16.35
INSTRUM             spect
PROBHD    5 mm CPDCH 13C
PULPROG              zg30
TD                  95236
SOLVENT             CDCl3
NS                      8
DS                      2
SWH            11904.762 Hz
FIDRES           0.125003 Hz
AQ               3.9999621 sec
RG                     16
DW                  42.000 usec
DE                   6.50 usec
TE                  298.2 K
D1             2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.40 usec
PL1                 -3.20 dB
PL1W         33.59817505 W
SFO1        700.1516910 MHz
SI                  131072
SF          700.1471400 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



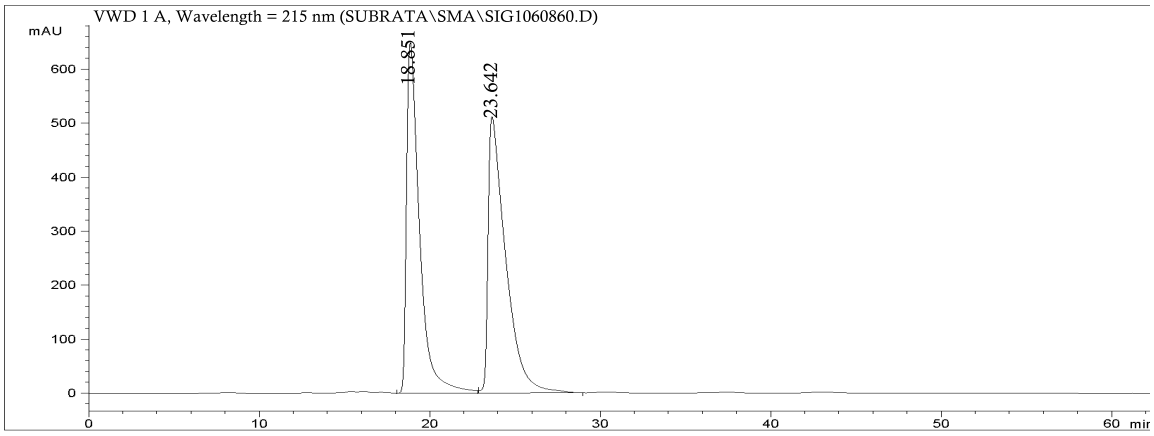
8d



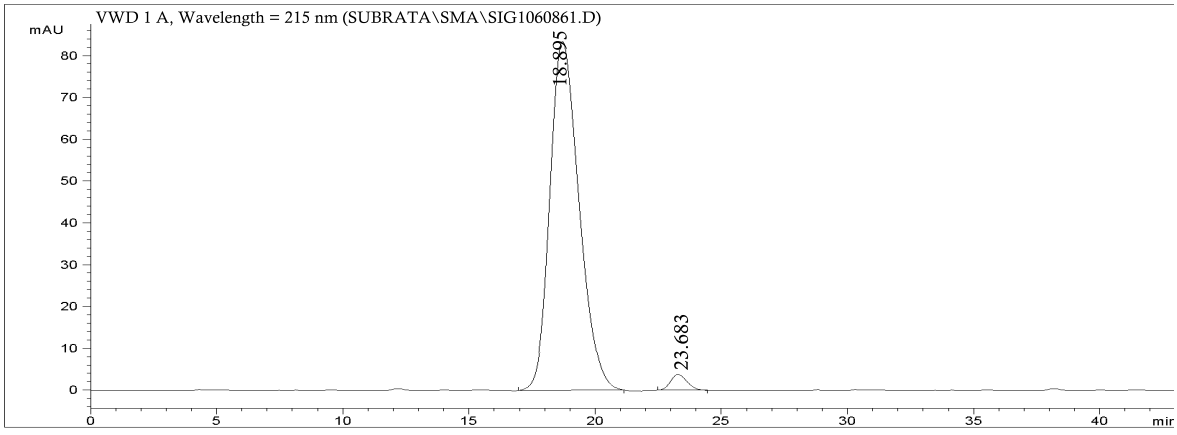
NAME	SS-06-124
EXPNO	2
PROCNO	1
Date_	20130323
Time	16.38
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	12
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



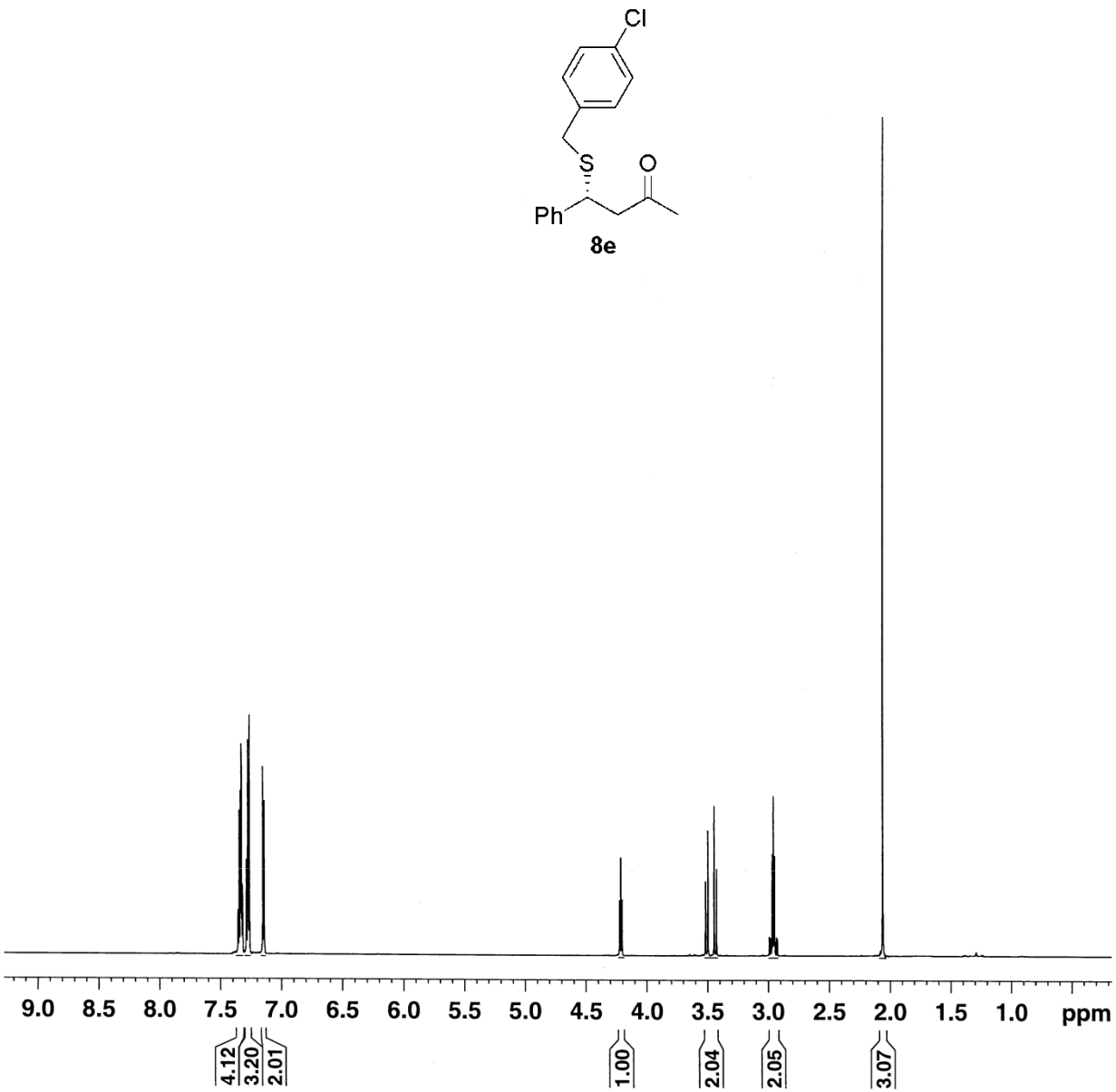
8e



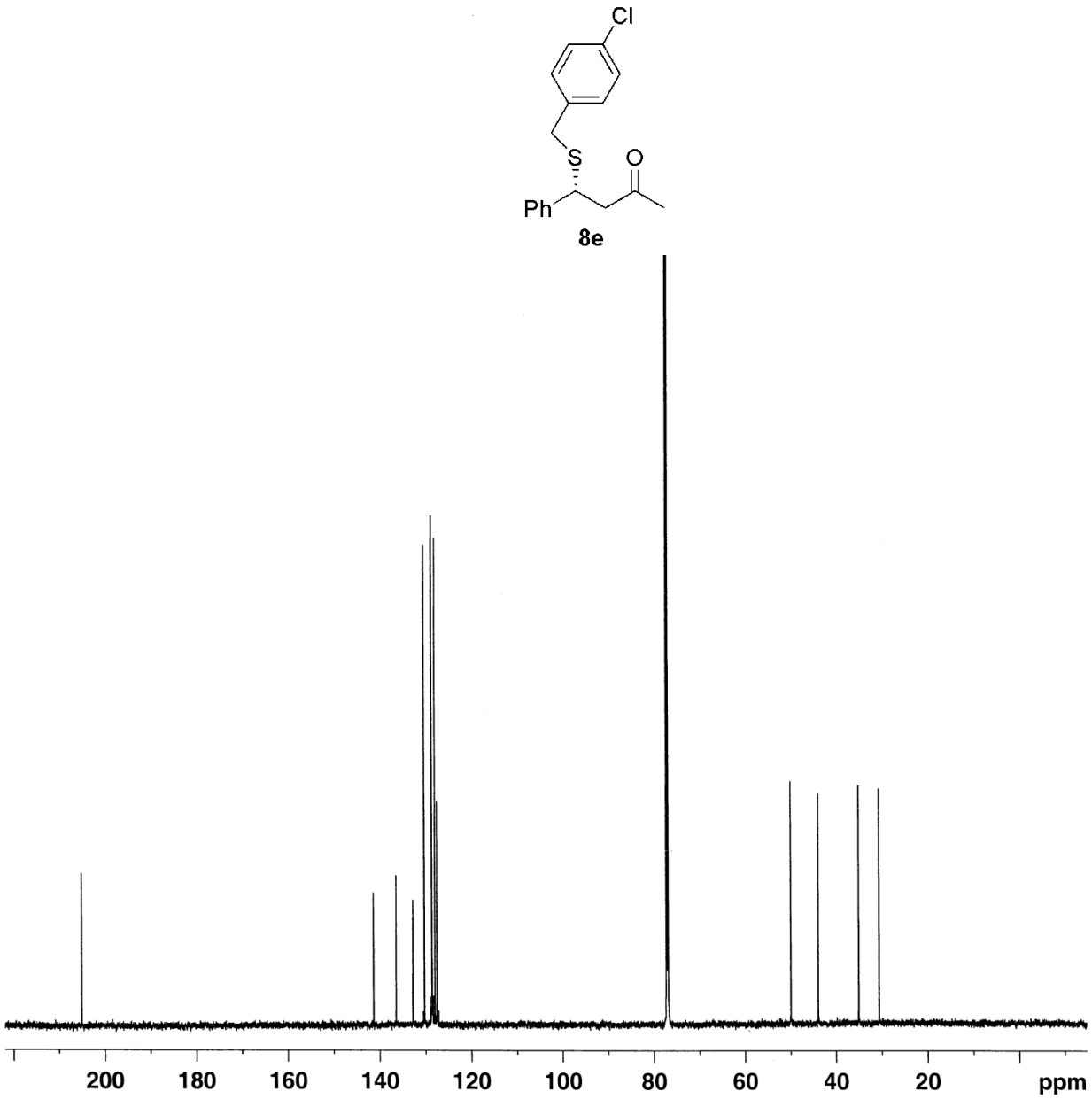
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.851	BB	0.7889	3.44955e4	649.09906	48.5628
2	23.642	BB	1.0161	3.65373e4	511.06638	51.4372



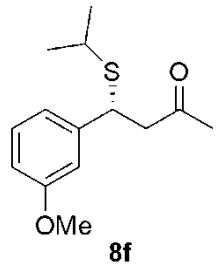
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	18.895	BV	1.2599	6856.05349	83.96743	98.4914
2	23.683	BB	0.6973	105.01582	3.96443	1.5086



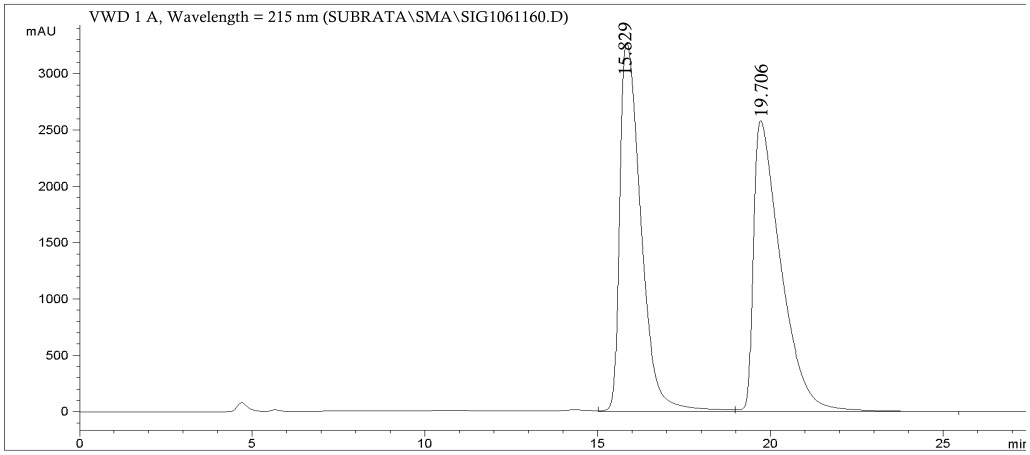
NAME	SS-06-86
EXPNO	3
PROCNO	1
Date_	20130323
Time	16.42
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	10
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	25.4
DW	42.000 use
DE	6.50 use
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



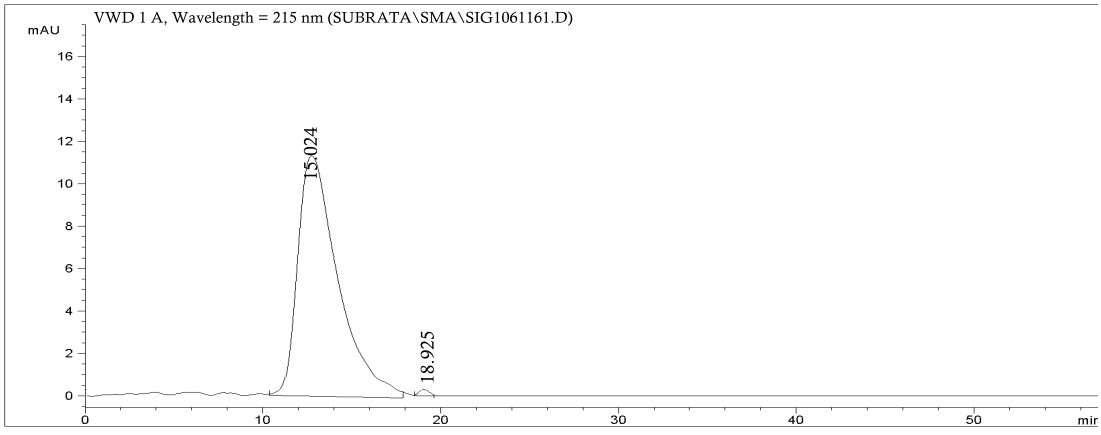
NAME	SS-06-86
EXPNO	4
PROCNO	1
Date_	20130323
Time	16.45
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	12
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



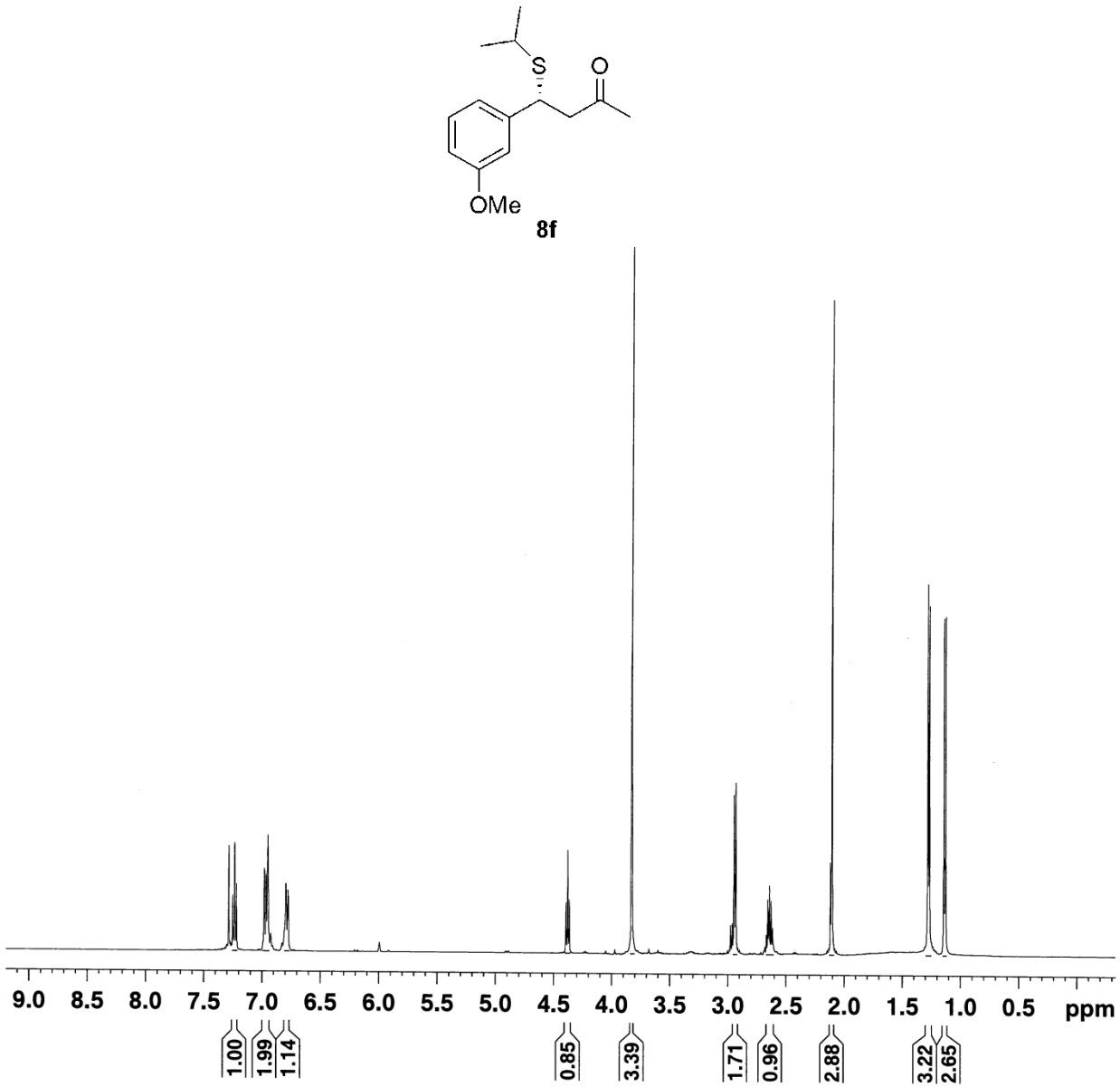
8f



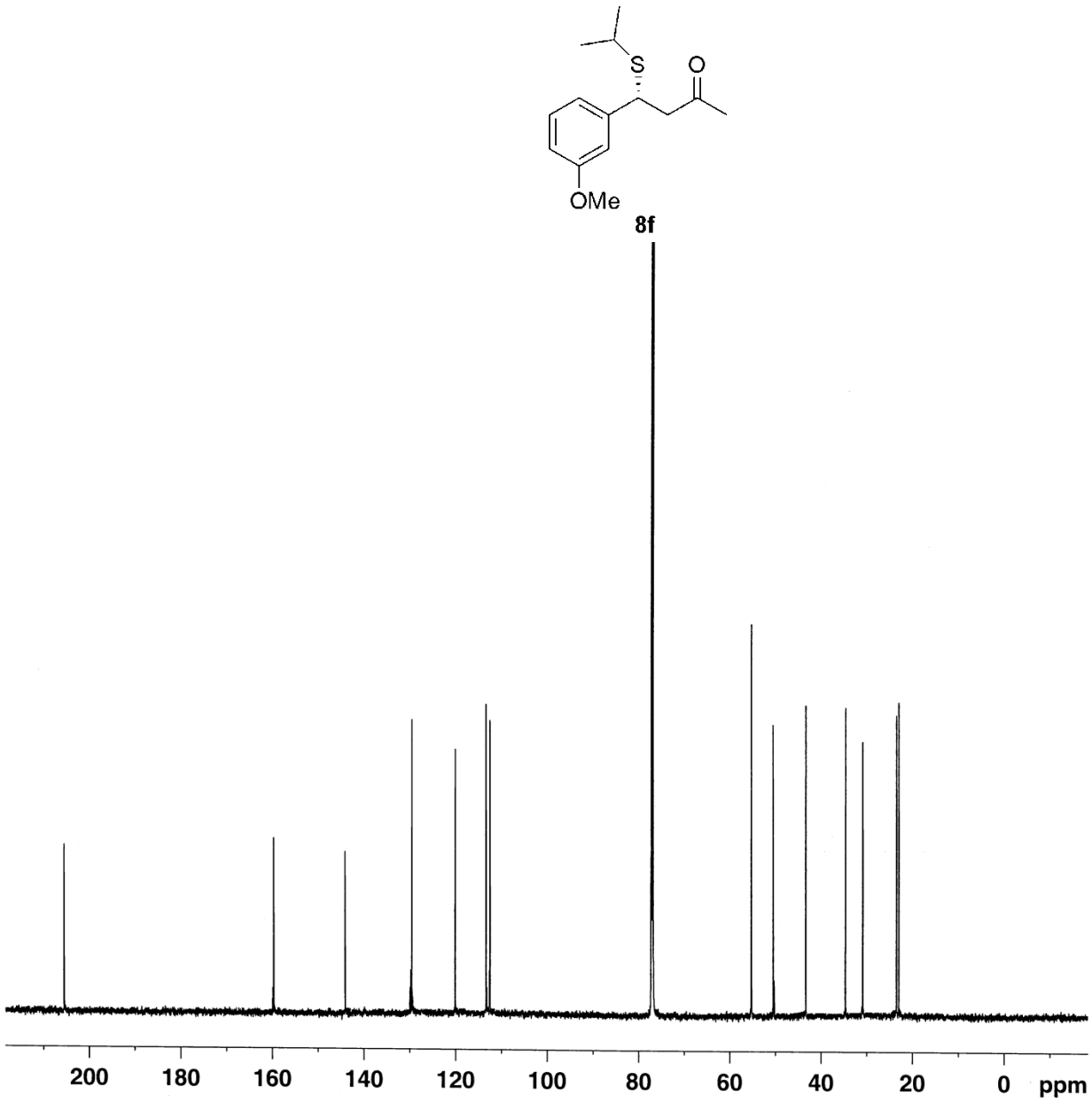
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.829	VV	0.6616	1.40223e5	3272.11230	49.5933
2	19.706	VB	0.8112	1.42523e5	2582.92505	50.4067



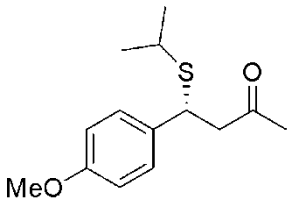
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.024	MM	2.6434	1807.75098	11.39789	97.6990
2	18.925	MM	0.0185	42.57597	0.10645	2.3010



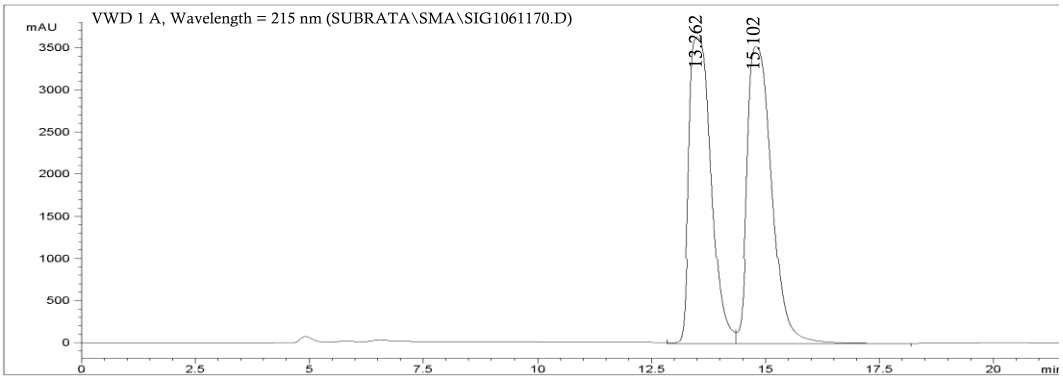

```
Current Data Parameters
NAME                  SS-6-116
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130302
Time                     21.39
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                       131.79
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               500.1330008 MHz
NUC1                        1H
P1                        7.80 usec
PLW1               12.00000000 W

F2 - Processing parameters
SI                      65536
SF                 500.1300000 MHz
WDW                        EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```



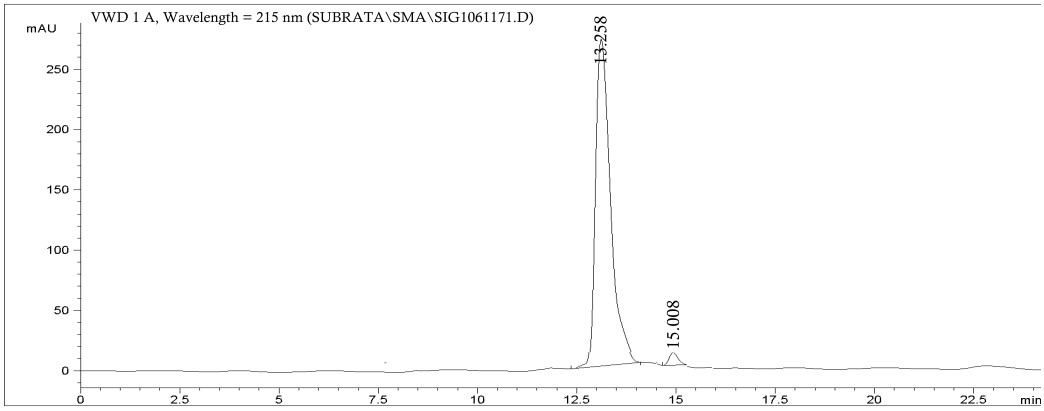
NAME	SS-06-116
EXPNO	2
PROCNO	1
Date_	20130323
Time	18.18
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	56
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



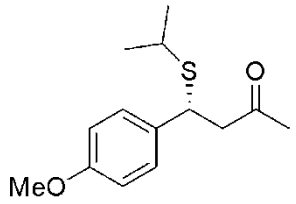
8g



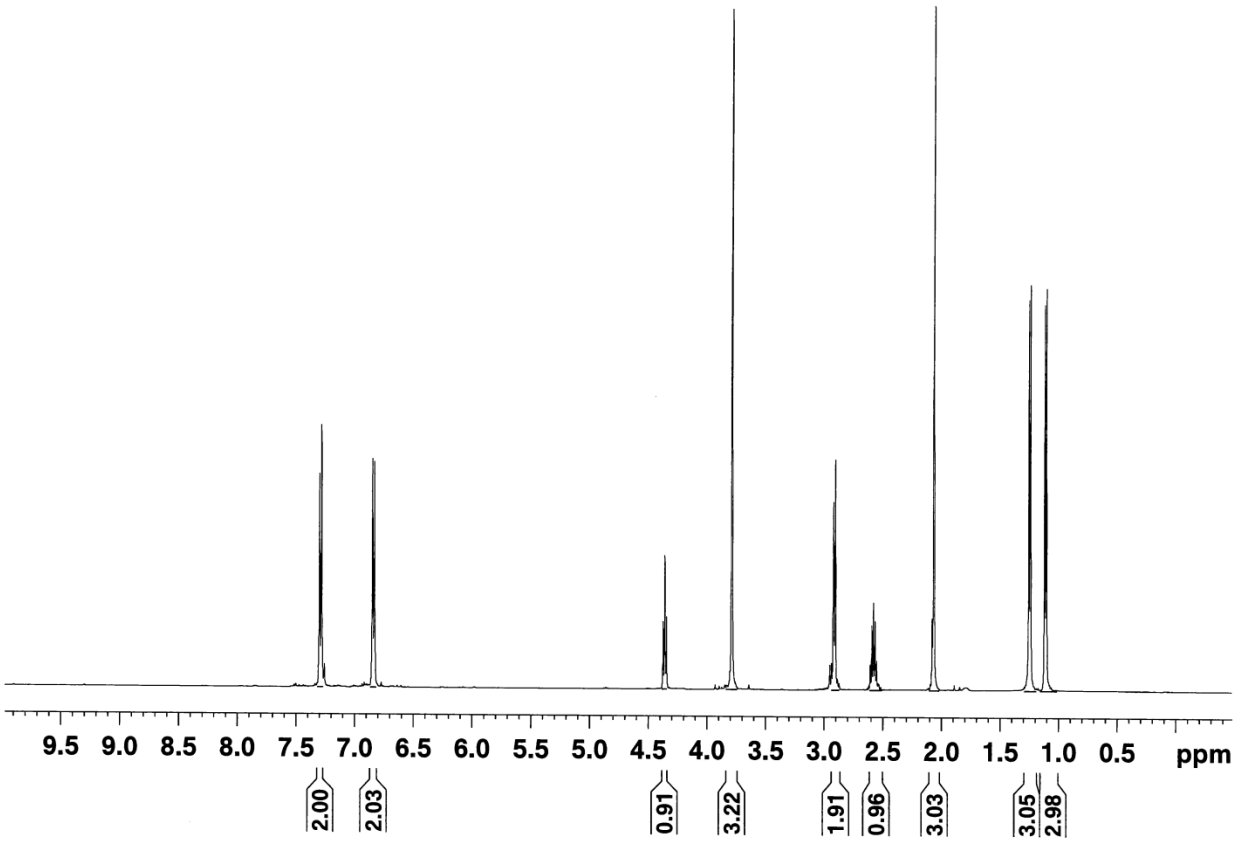
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.262	VV	0.4592	1.22381e5	3626.61401	48.1463
2	15.102	VB	0.5886	1.31805e5	3517.02368	51.8537



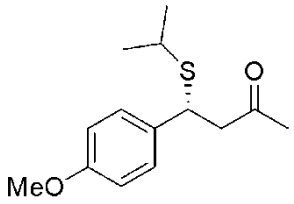
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.258	VB	0.4193	7350.96351	271.96431	96.2340
2	15.008	BB	0.0896	287.67097	7.45653	3.7660



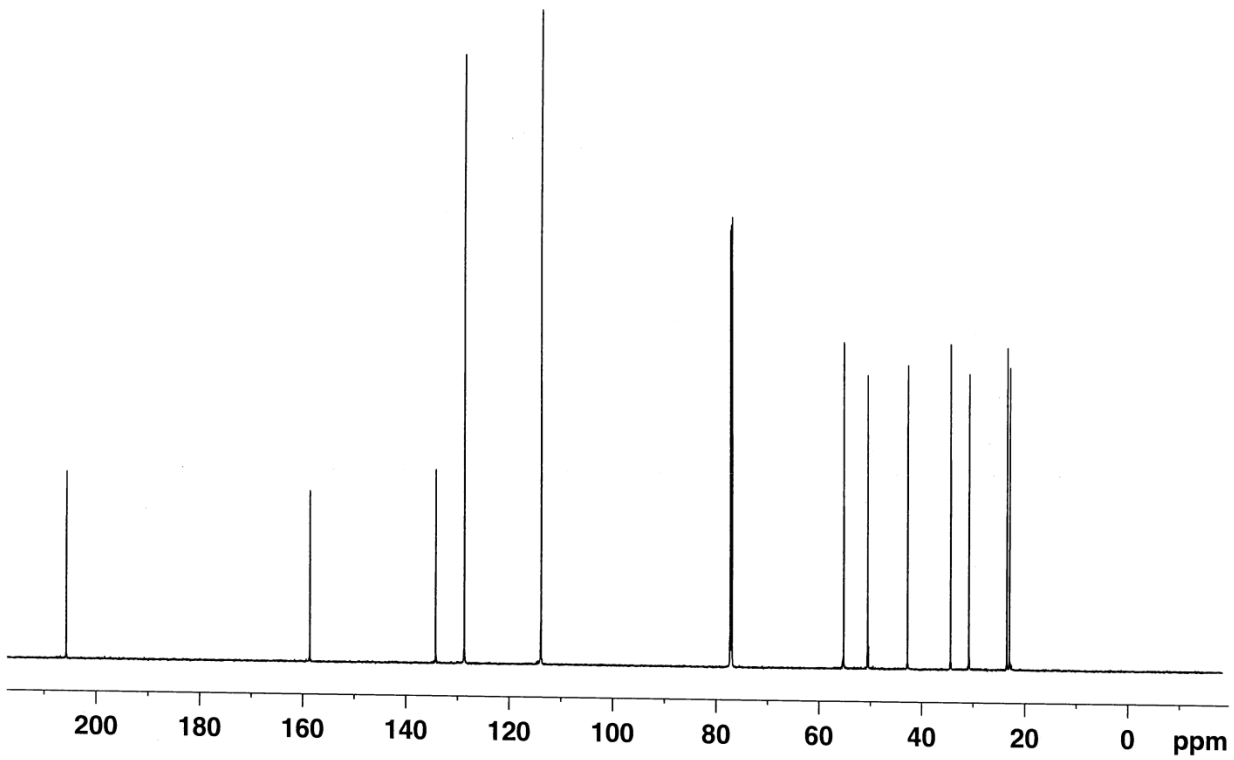
8g



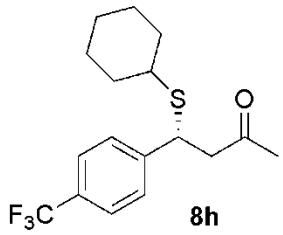

```
Current Data Parameters
NAME            SS-6-117
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130302
Time               23.06
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 25.78
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330008 MHz
NUC1                   1H
P1                 7.80 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



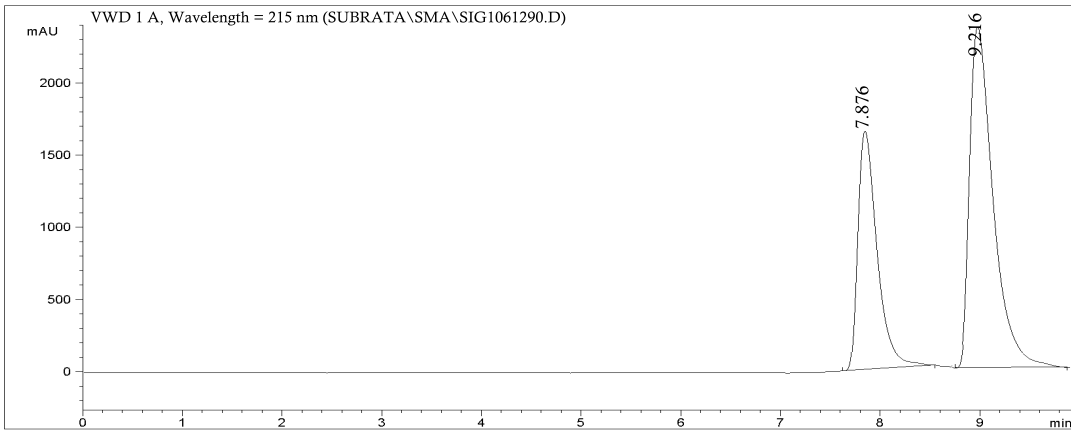
8g



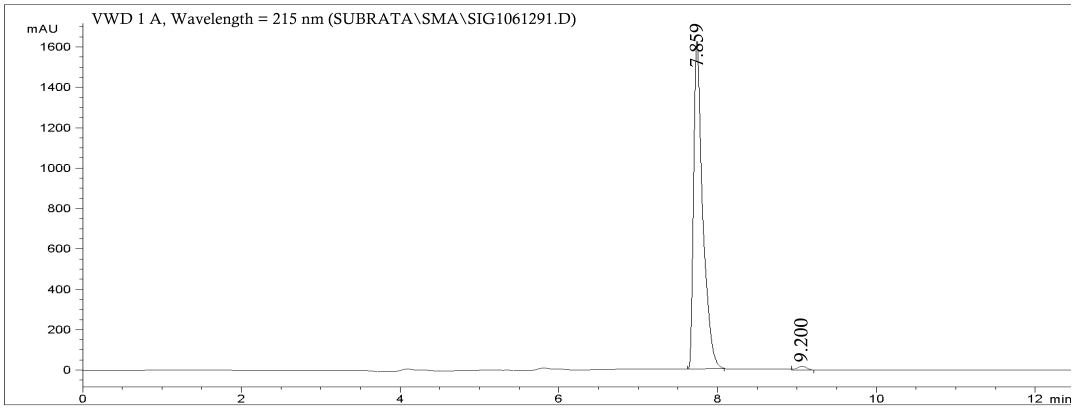
NAME	SS-06-117
EXPNO	2
PROCNO	1
Date_	20130323
Time	18.29
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	35
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



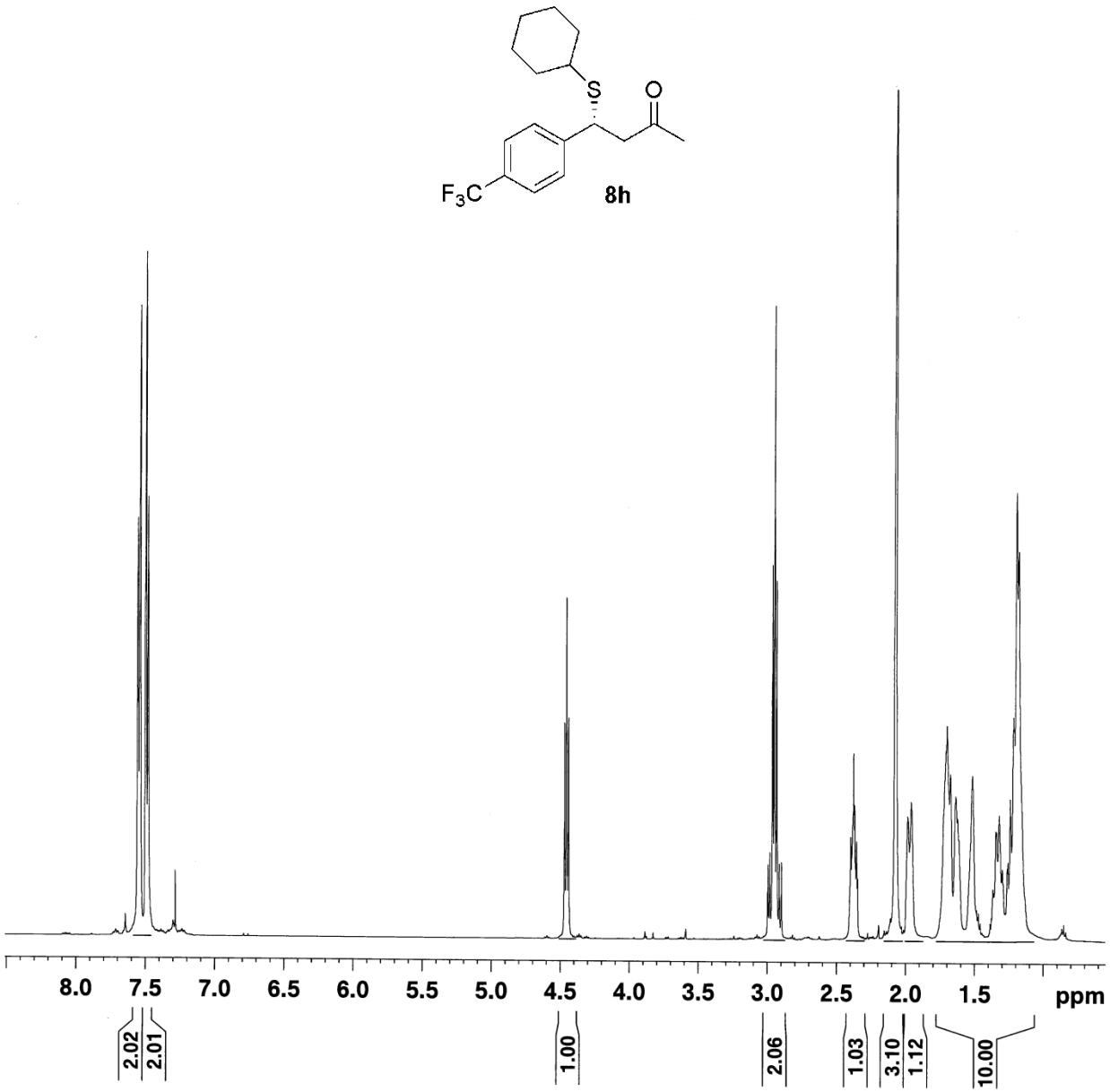
8h



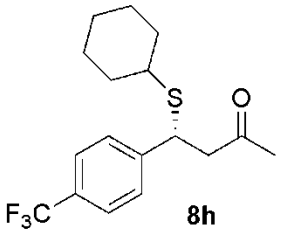
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.876	BV	0.2609	1.64212e4	1821.27061	37.0926
2	9.216	VB	0.3213	2.78496e4	2387.03215	62.9074



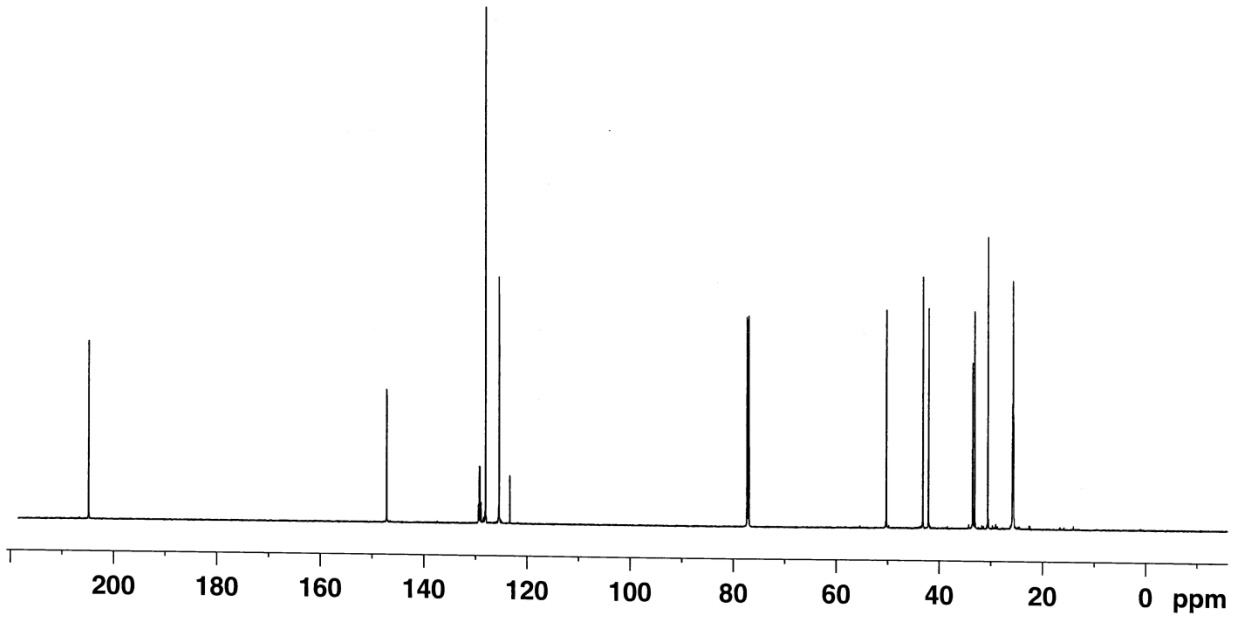
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.859	VV	0.1573	9956.07299	1559.67036	98.8983
2	9.200	VV	0.1422	110.90825	11.49801	1.1017



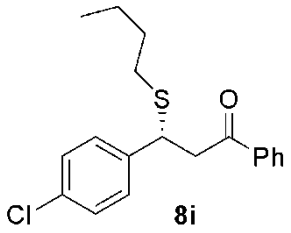

```
Current Data Parameters
NAME                  SS-6-129
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130309
Time                     17.37
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       10.37
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1           500.1330008 MHz
NUC1                       1H
P1                       7.80 usec
PLW1             12.00000000 W

F2 - Processing parameters
SI                      65536
SF             500.1300000 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



8h



NAME	SS-06-129	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	18.50	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	25	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	usec
DE	16.50	usec
TE	298.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	usec
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	usec
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



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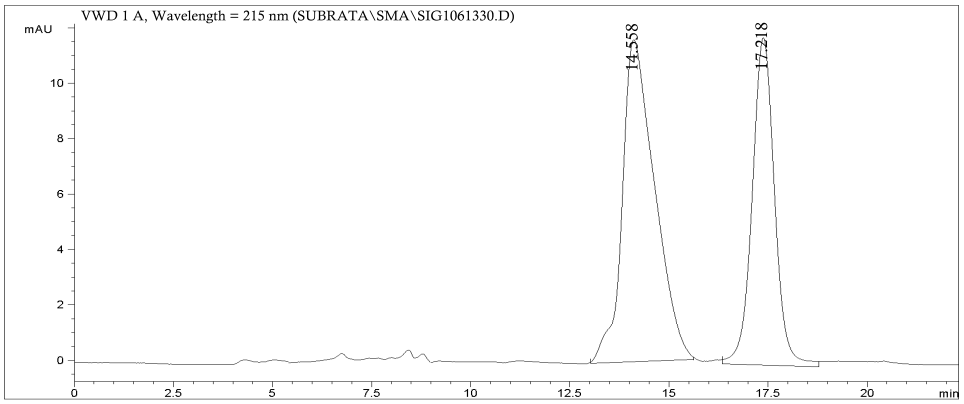
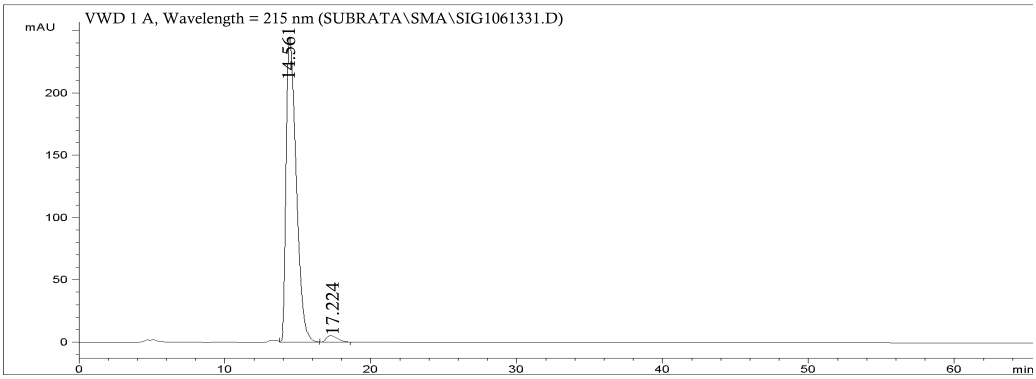
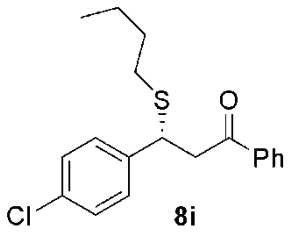


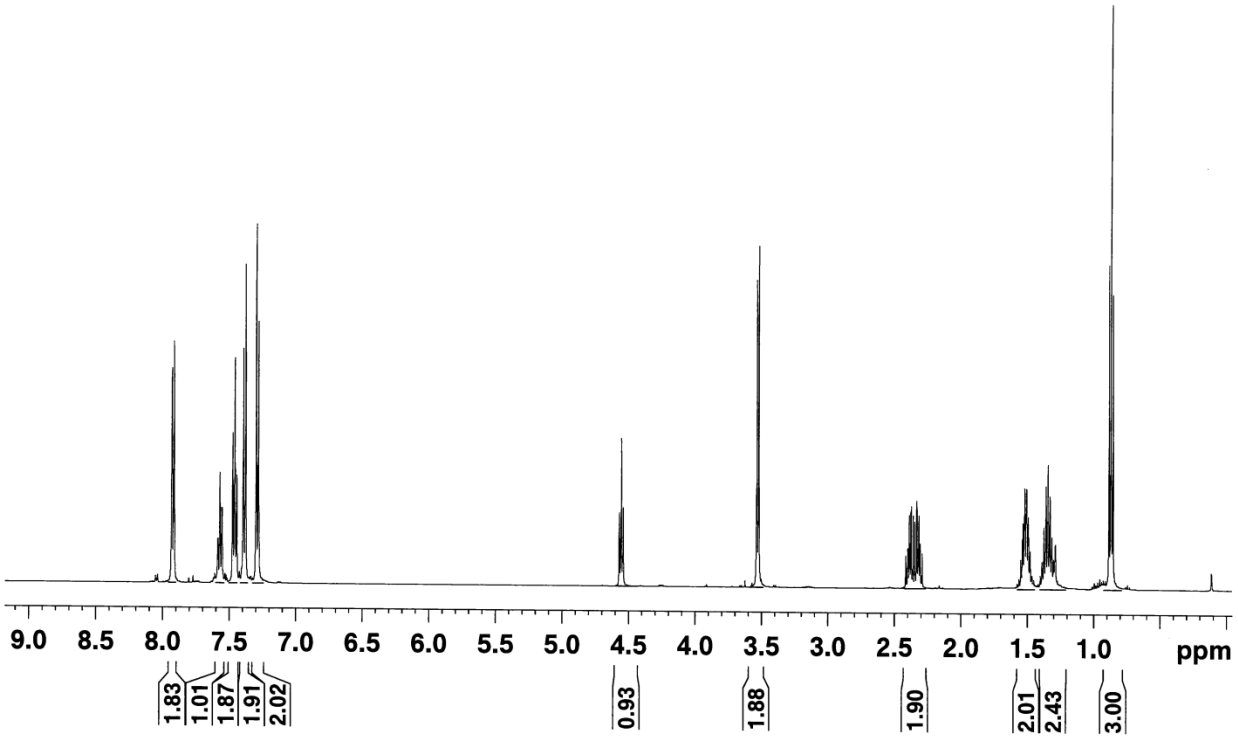
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.558	BB	0.7605	1953.03961	11.52154	54.2108
2	17.218	BV	0.4041	1649.63641	11.21972	45.7892



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.561	VB	0.6799	1.06673e4	238.99613	96.7308
2	17.224	VB	0.6486	360.53291	11.49801	3.2692



8i

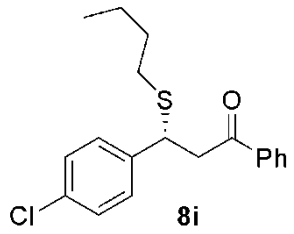



```
Current Data Parameters
NAME                  SS-6-133
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130309
Time                     20.42
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       25.78
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1          500.1330008 MHz
NUC1                    1H
P1                    7.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                      65536
SF            500.1300000 MHz
WDW                       EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



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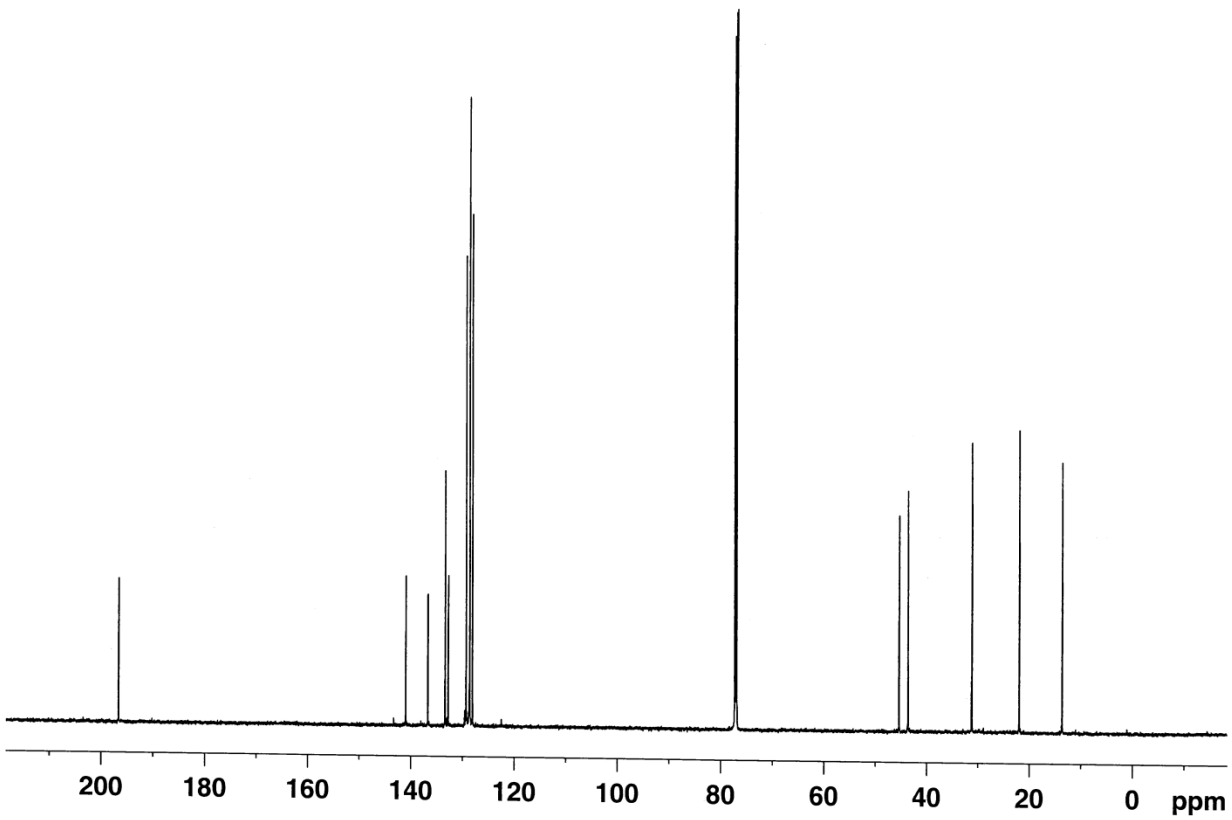
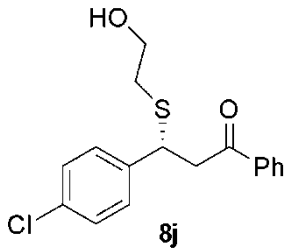
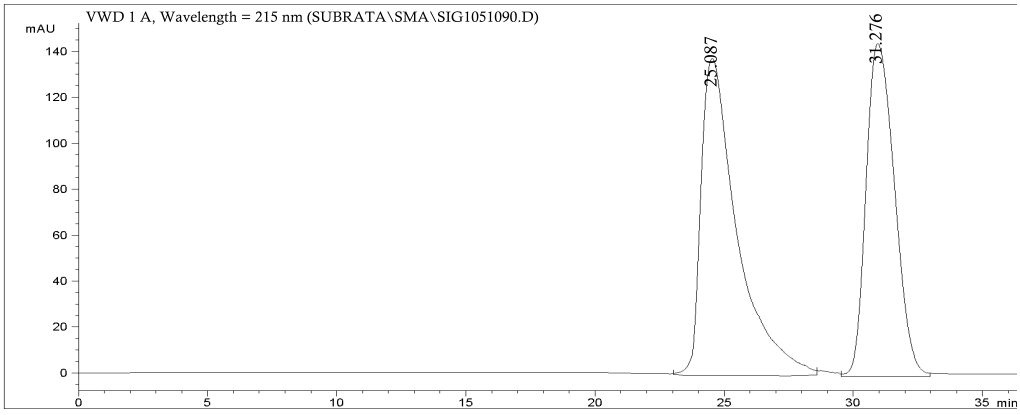


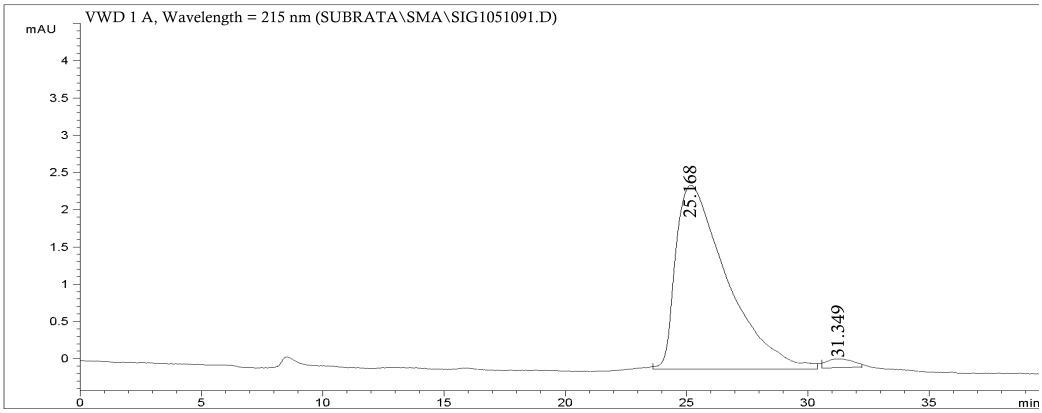
NAME	SS-06-133
EXPNO	2
PROCNO	1
Date_	20130323
Time	19.03
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	15
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



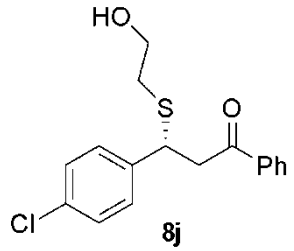
8j



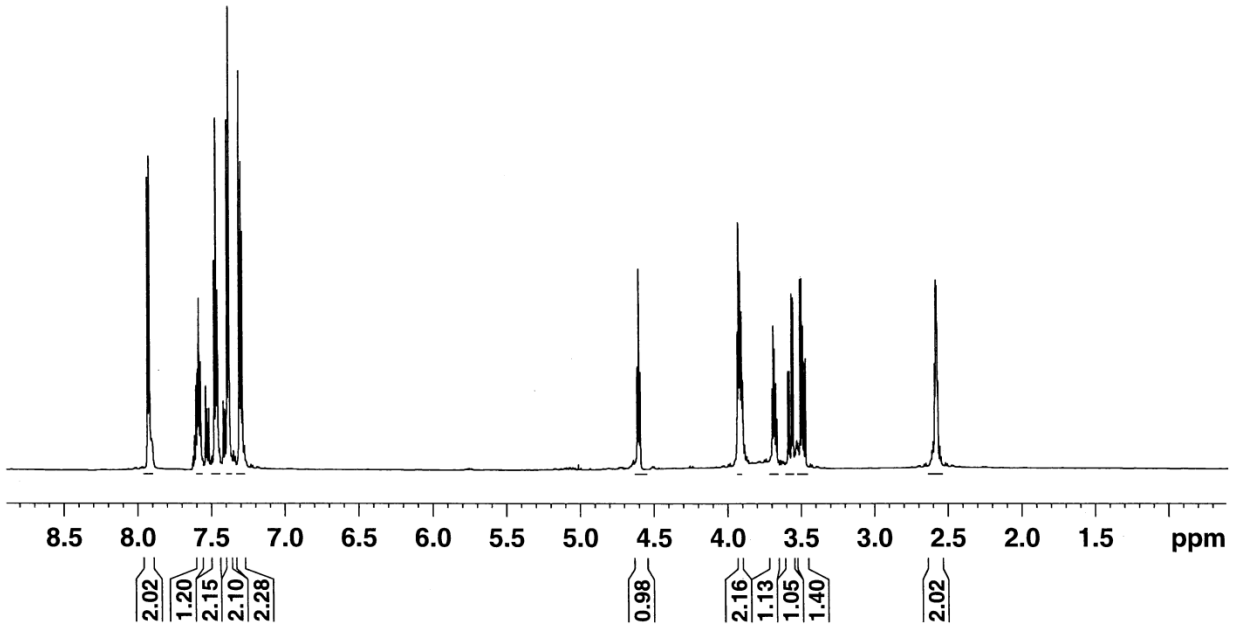
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	25.087	VV	0.9806	4689.27086	137.69165	50.8632
2	31.276	BV	0.3851	4530.10713	142.39542	49.1368



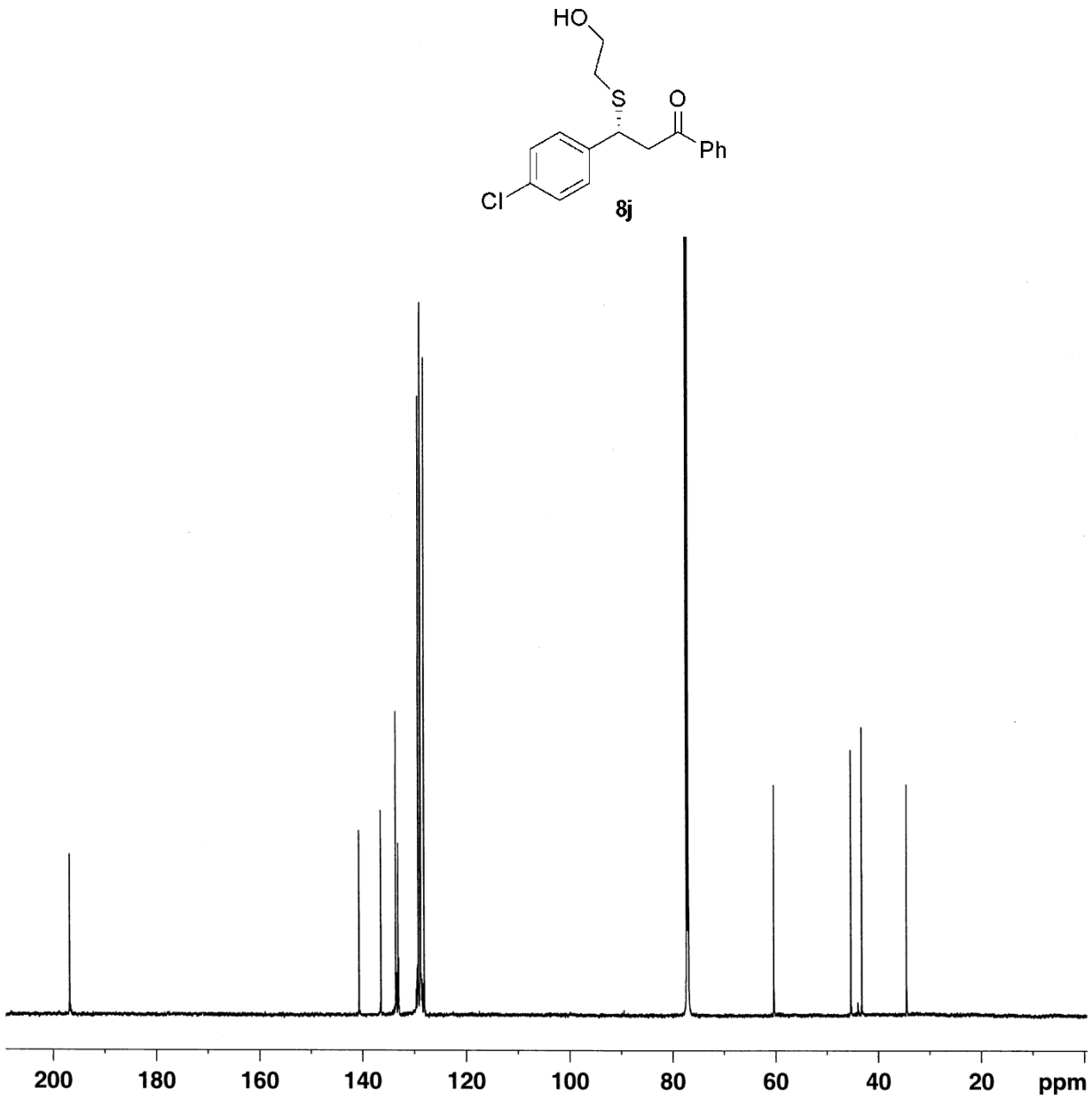
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	25.168	BB	1.1038	629.97602	2.69181	97.7972
2	31.349	VV	0.4194	14.18964	0.13498	2.2028



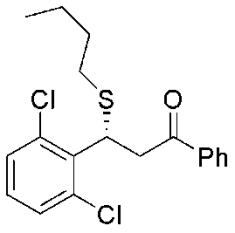
8j



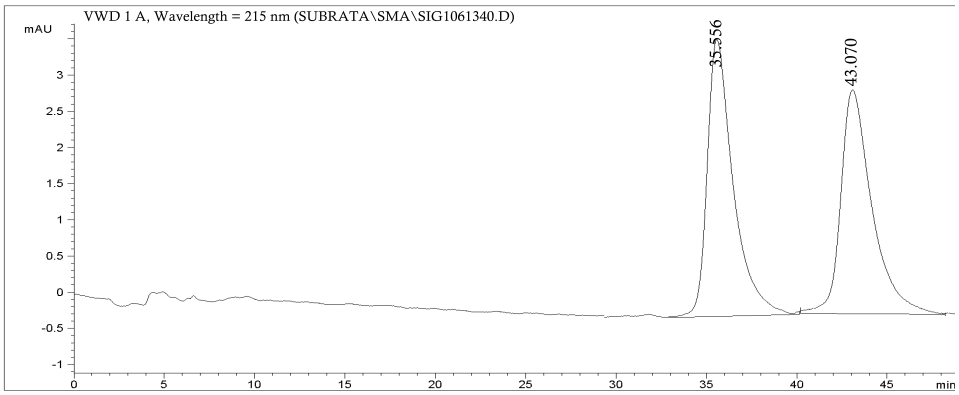
NAME	SS-06-145
EXPNO	4
PROCNO	1
Date_	20130916
Time	17.30
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	16
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	22.6
DW	42.000 use
DE	6.50 use
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



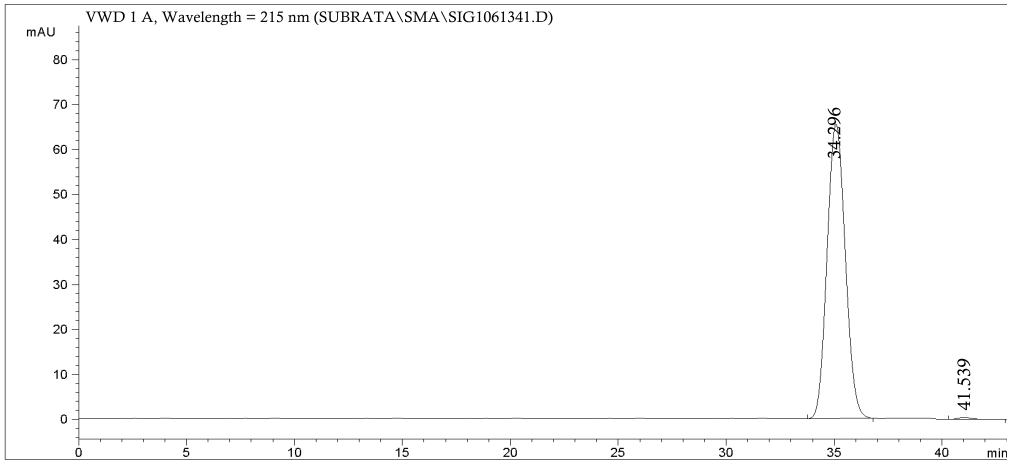
NAME	SS-06-145
EXPNO	5
PROCNO	1
Date_	20130916
Time	17.42
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	192
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



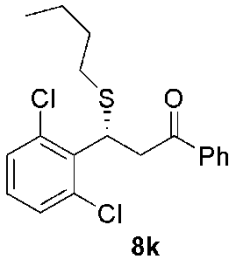
8k



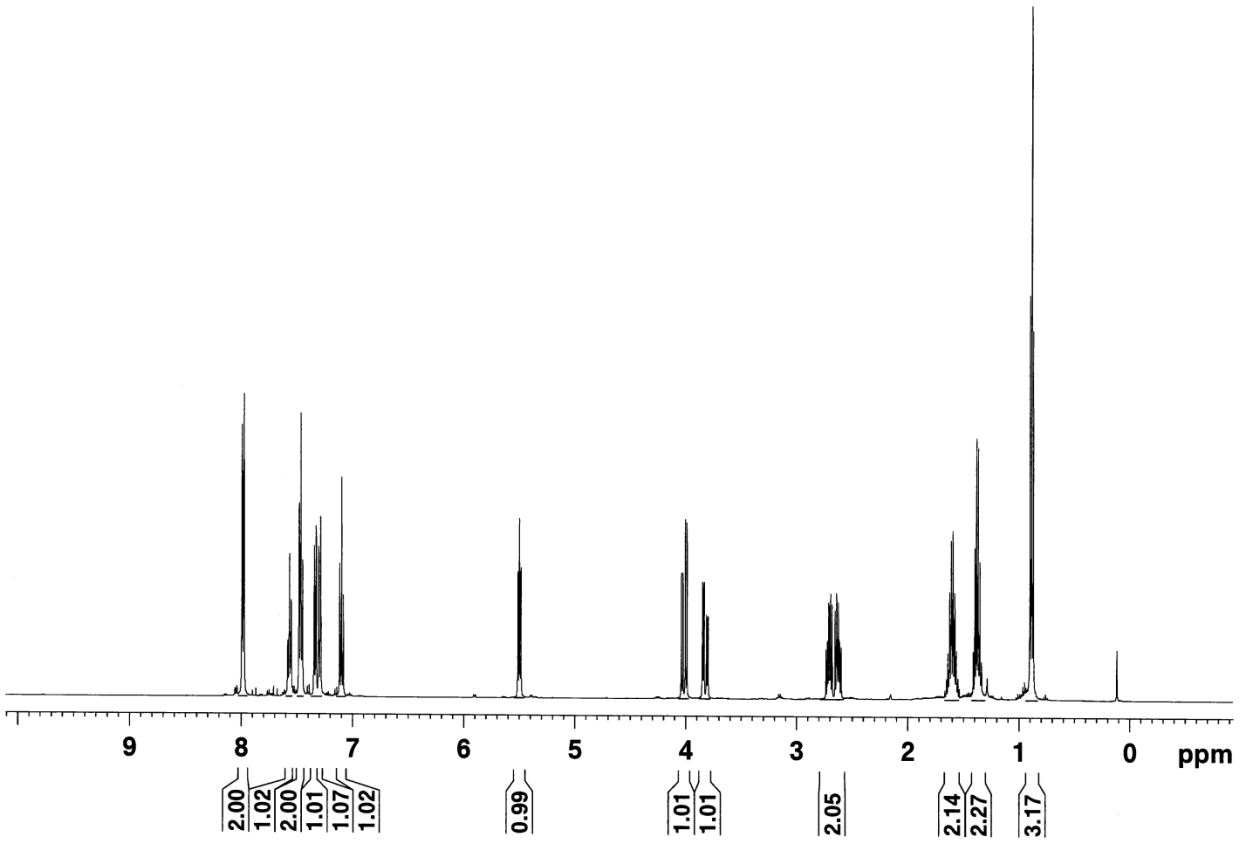
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	35.556	MM	1.5780	407.90018	3.62047	49.9642
2	43.070	MM	1.9890	408.48471	2.69828	50.0358



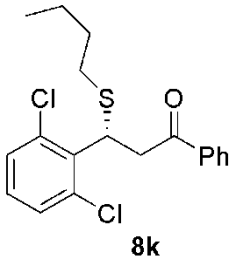
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	34.296	BV	0.3863	893.17631	72.45066	97.3961
2	41.539	VB	0.2316	23.88012	0.61832	2.6039



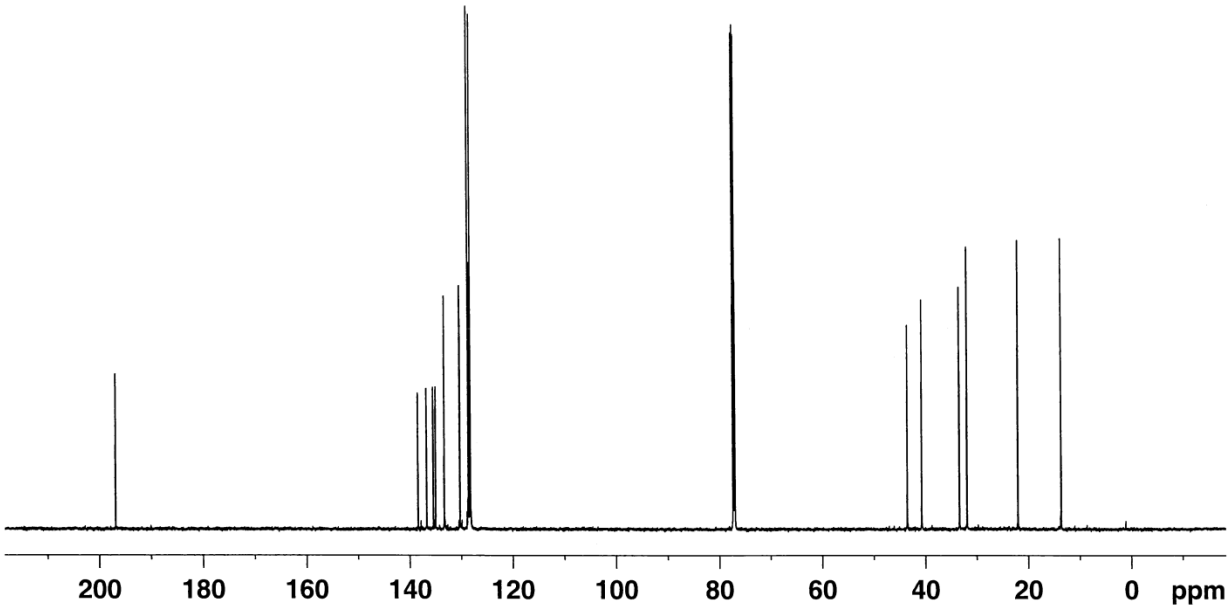
8k



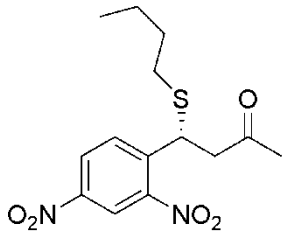

```
Current Data Parameters
NAME                  SS-6-134
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130309
Time                     20.55
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       20.49
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               500.1330008 MHz
NUC1                       1H
P1                       7.80 usec
PLW1              12.00000000 W

F2 - Processing parameters
SI                      65536
SF                 500.1300000 MHz
WDW                        EM
SSB       0
LB                       0.30 Hz
GB        0
PC                       1.00
```



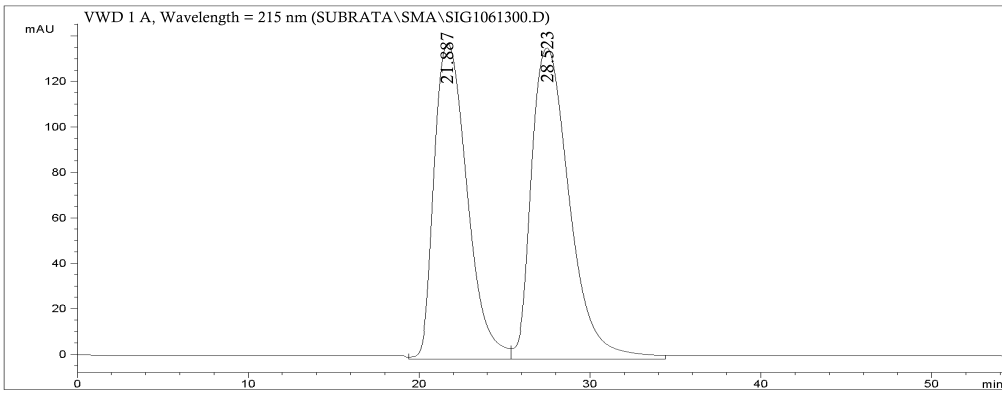
8k



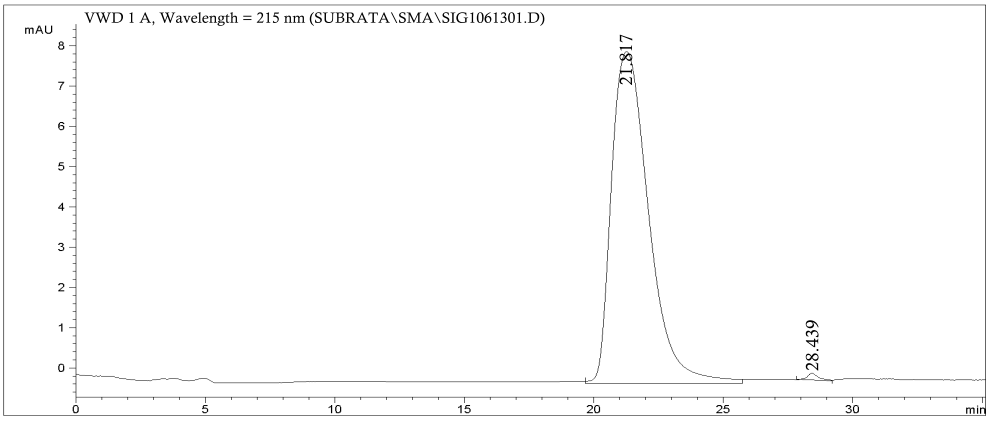
NAME	SS-06-134
EXPNO	2
PROCNO	1
Date_	20130323
Time	19.10
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



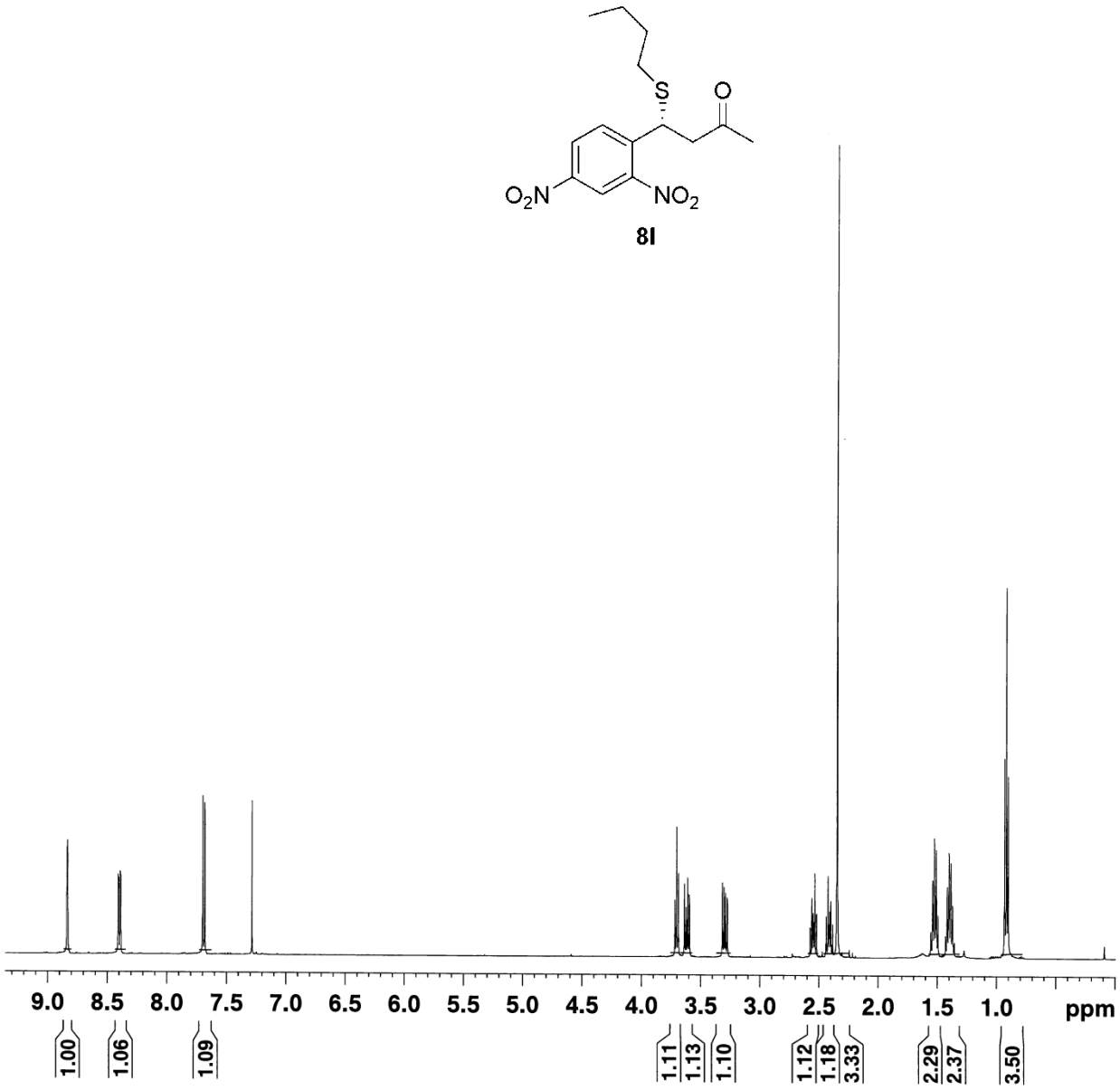
8l



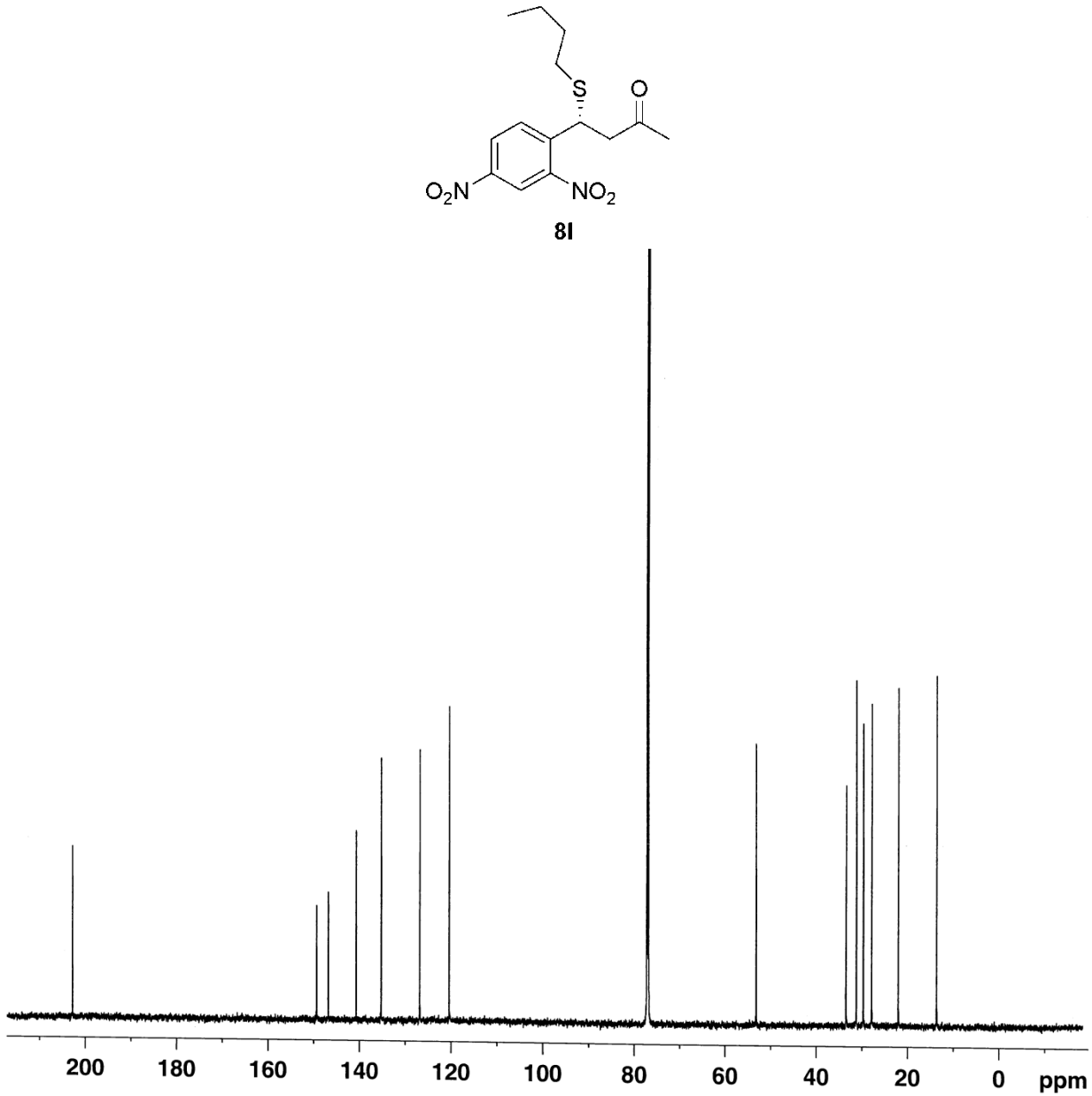
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.887	BB	1.0627	9818.74061	141.99027	48.4391
2	28.523	BB	1.1683	1.04515e4	136.75107	51.5609



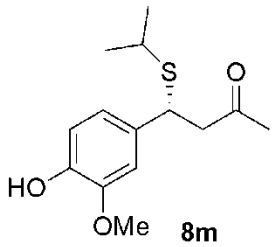
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.817	BB	1.0236	826.63911	7.78795	97.4453
2	28.439	VV	0.0139	21.67175	0.16871	2.5547




```
Current Data Parameters
NAME                  SS-6-130
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130309
Time                     17.43
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                         97.9
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                500.1330008 MHz
NUC1                        1H
P1                        7.80 usec
PLW1               12.00000000 W

F2 - Processing parameters
SI                          65536
SF                  500.1300000 MHz
WDW                            EM
SSB       0
LB                        0.30 Hz
GB        0
PC                        1.00
```



NAME	SS-06-130
EXPNO	2
PROCNO	1
Date_	20130323
Time	18.57
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	20
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



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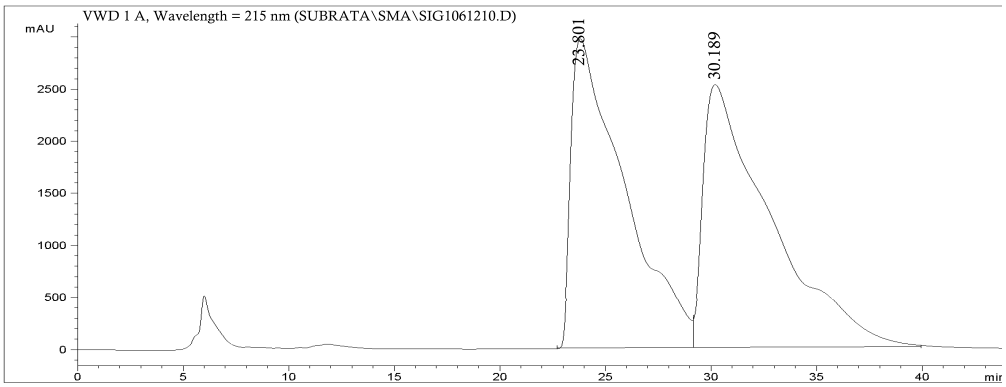
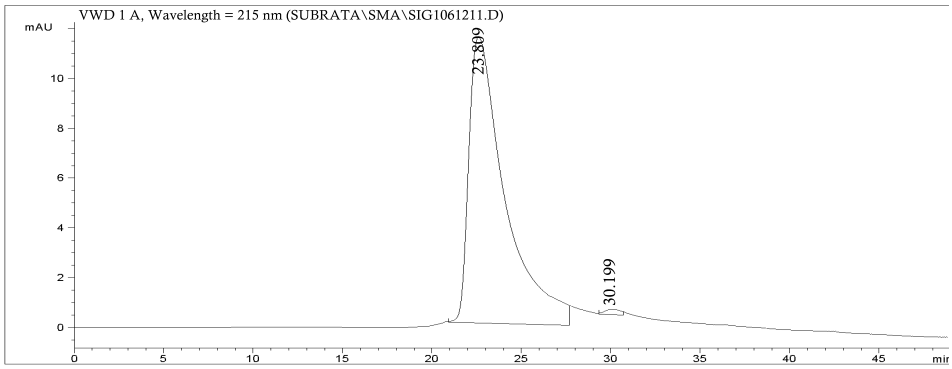
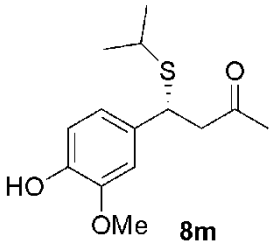


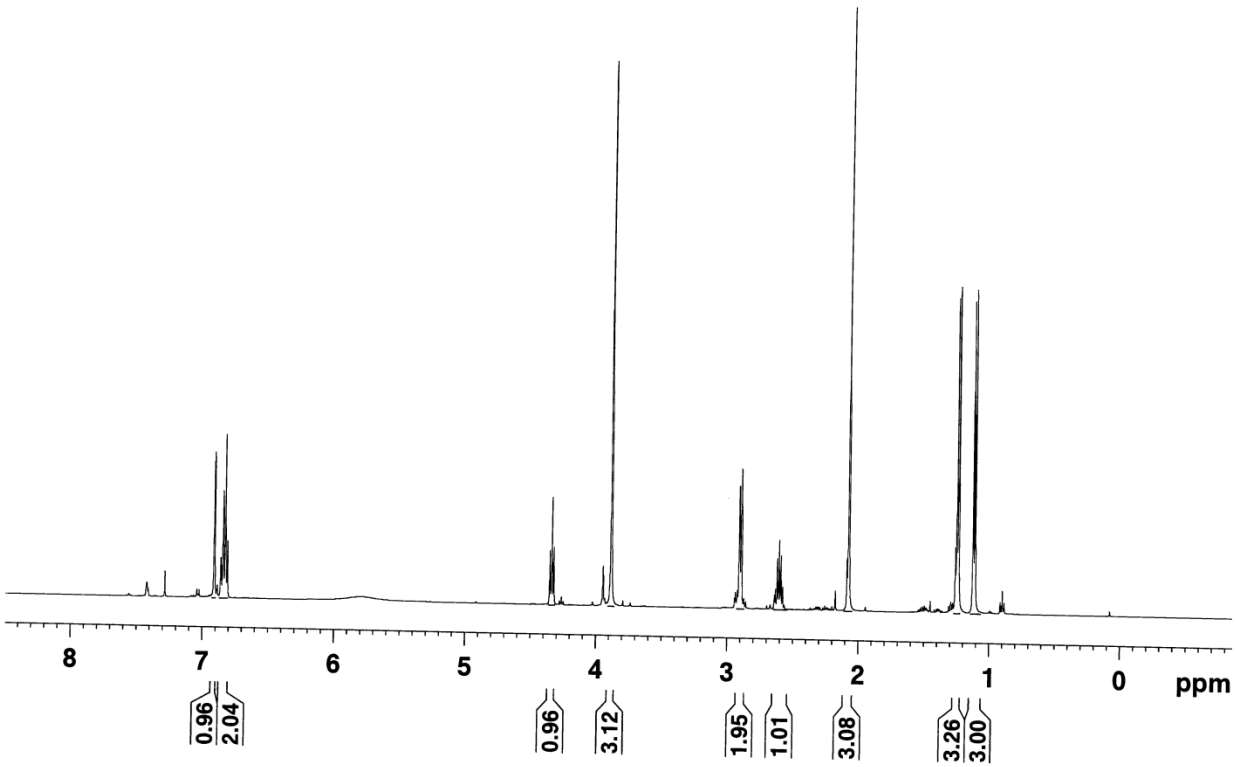
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	23.801	MM	2.9307	5.22157e5	2969.45239	48.3430
2	30.189	MM	3.6872	5.57951e5	2522.02271	51.6570



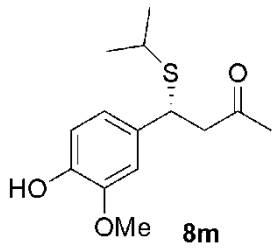
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	23.809	MM	2.3276	1589.06414	11.47271	98.2419
2	30.199	MM	3.5403	28.43728	0.22972	1.7581



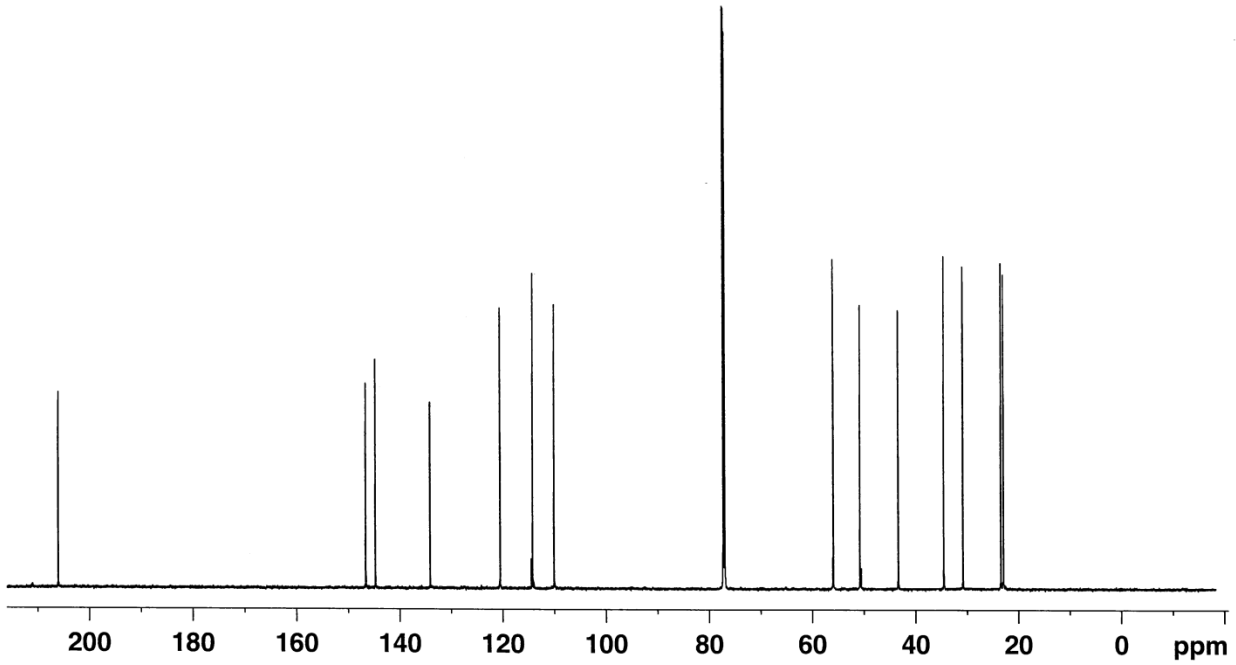
8m



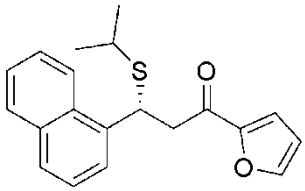

```
Current Data Parameters
NAME                  SS-6-121
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130303
Time                      0.41
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                        25.78
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                500.1330008 MHz
NUC1                        1H
P1                        7.80 usec
PLW1               12.00000000 W

F2 - Processing parameters
SI                       65536
SF                  500.1300000 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```



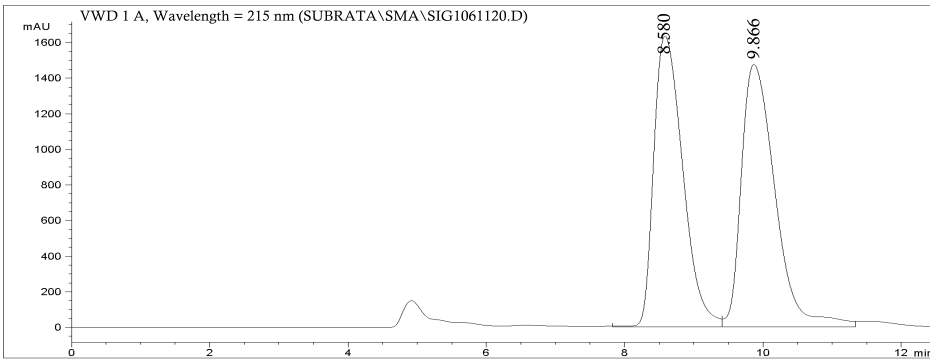
8m



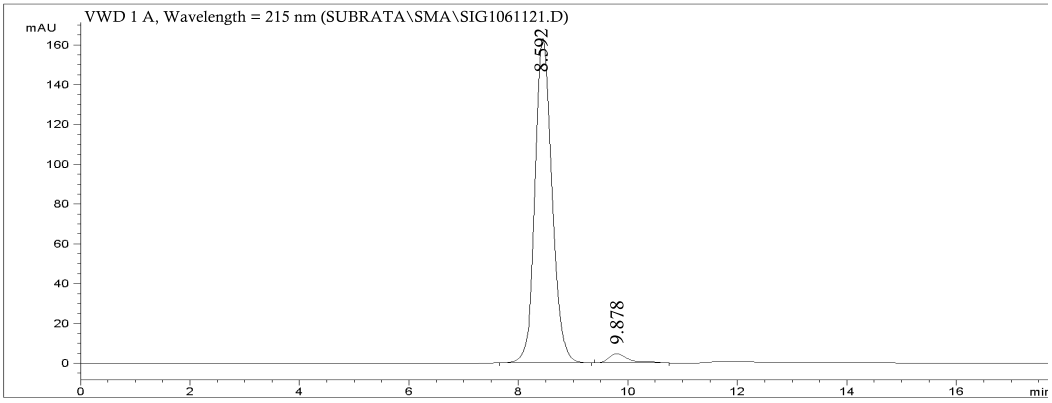
NAME	SS-06-121	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	18.36	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	22	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	usec
DE	16.50	usec
TE	298.2	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	usec
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	usec
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



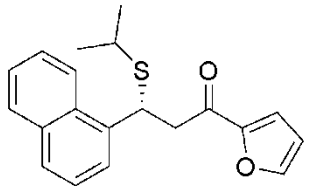
8n



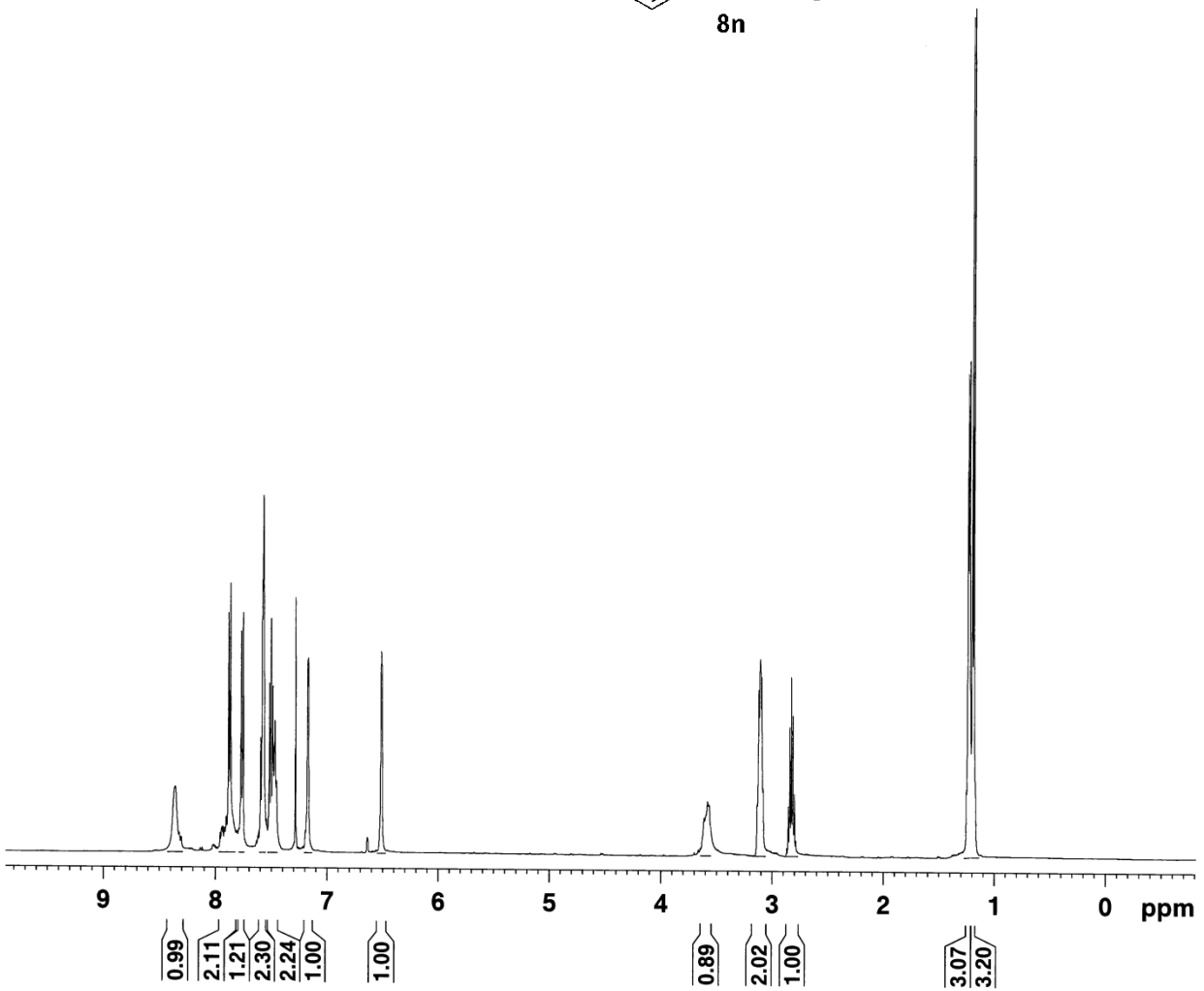
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.580	VV	0.4653	4.79540e4	1637.84460	48.7244
2	9.866	VV	0.5381	5.04649e4	1478.10620	51.2756



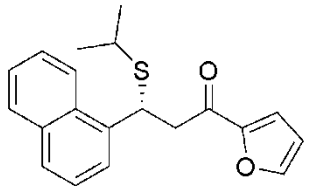
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.592	VB	0.3534	6390.63819	164.93804	98.2993
2	9.878	VB	0.3985	110.57623	4.61011	1.7007



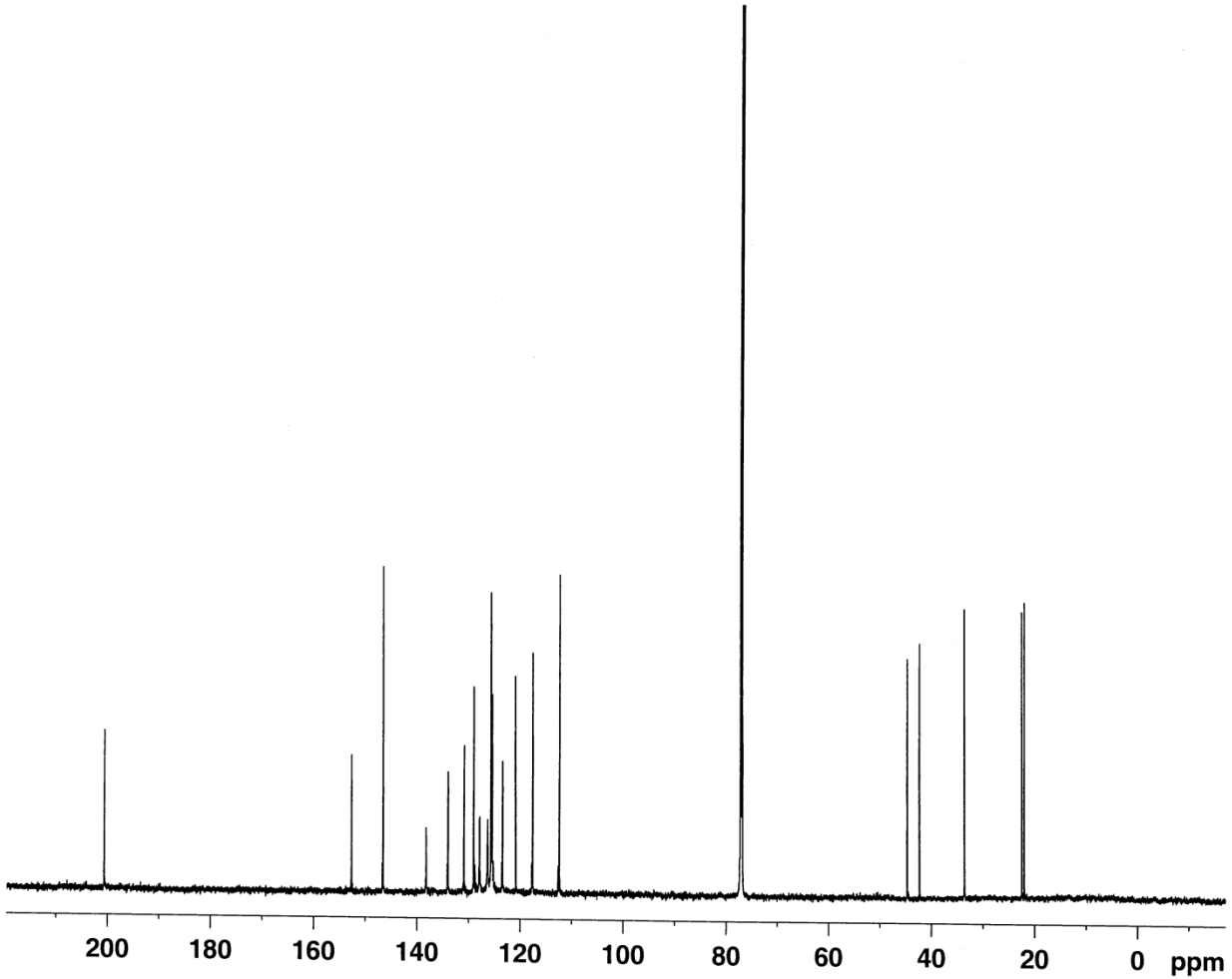
8n



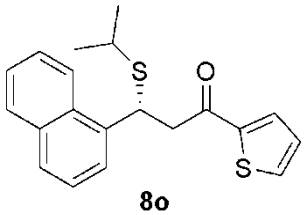

```
Current Data Parameters
NAME            SS-6-112
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130302
Time               20.00
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                  97.9
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1330008 MHz
NUC1                  1H
P1                 7.80 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



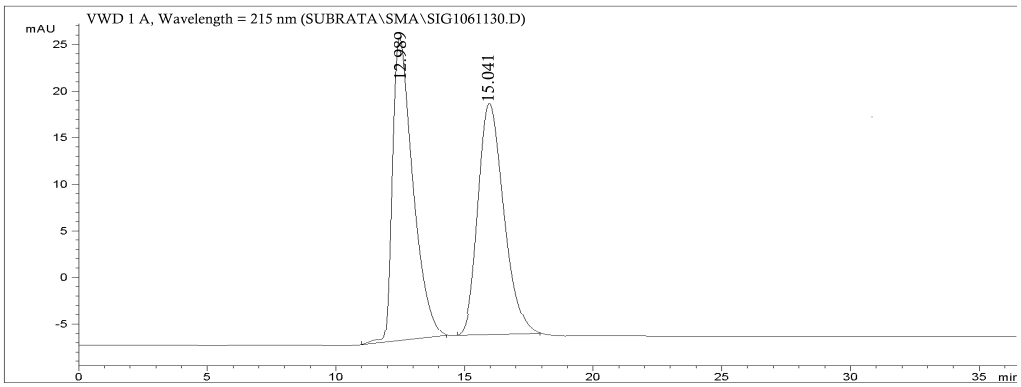
8n



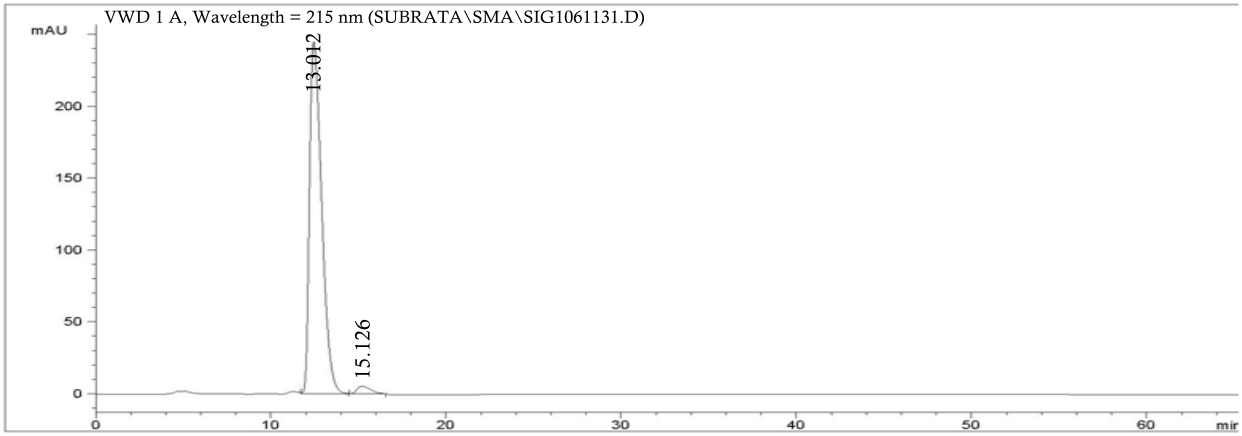
NAME	SS-06-112
EXPNO	2
PROCNO	1
Date_	20130323
Time	17.43
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	52
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 se
RG	203
DW	12.000 us
DE	16.50 us
TE	298.2 K
D1	2.00000000 se
D11	0.03000000 se
TD0	1
======== CHANNEL f1 =======	
NUC1	13C
P1	9.00 us
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MH
======== CHANNEL f2 =======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 us
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MH
SI	32768
SF	176.0521380 MH
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



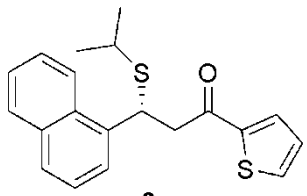
8o



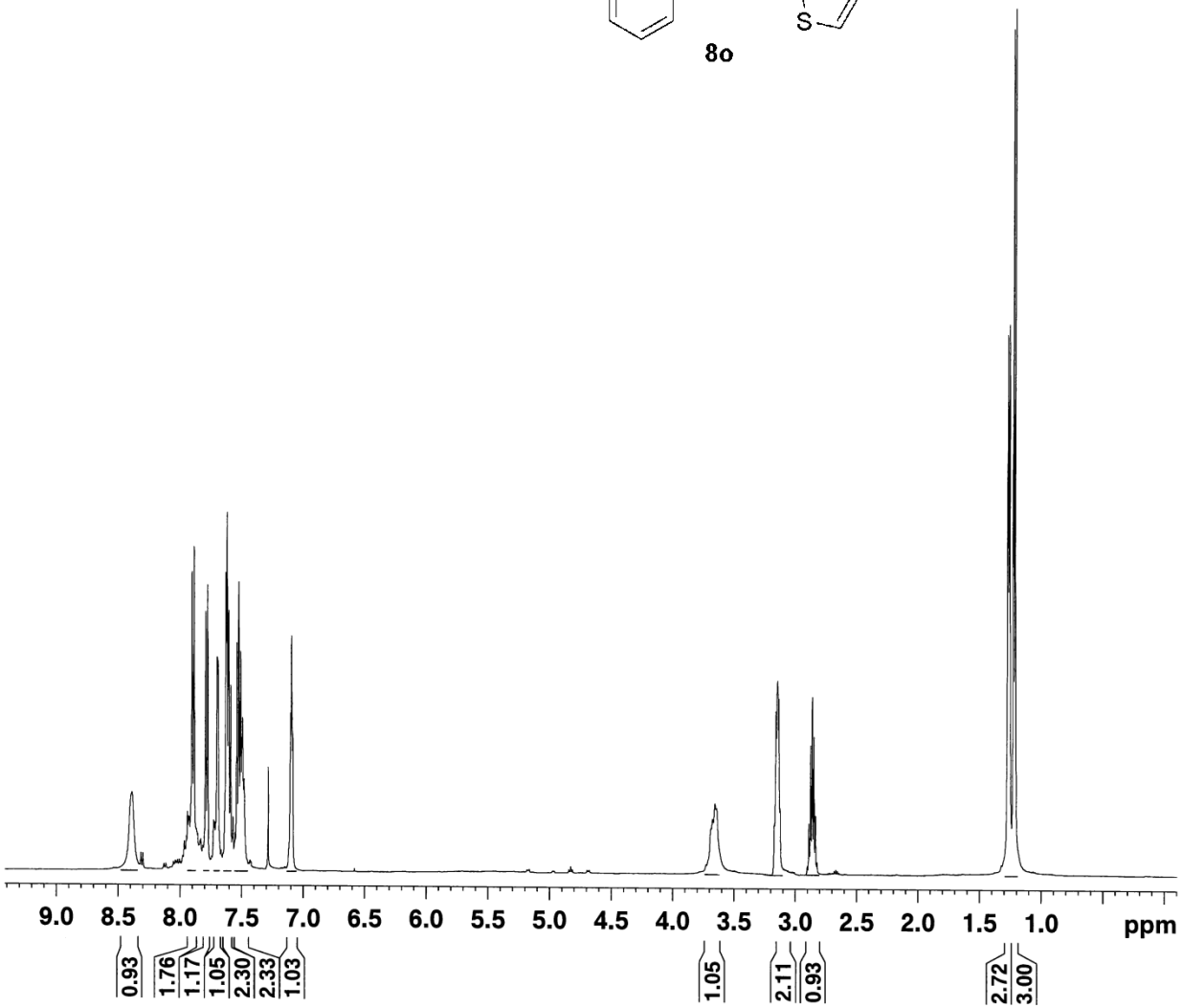
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.989	BB	0.8174	1824.29565	26.74717	51.0718
2	15.041	BB	1.0487	1747.72729	19.86244	48.9282



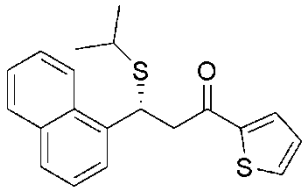
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	13.012	VB	0.7634	2.29458e4	243.87971	96.8523
2	15.126	VB	0.7596	745.73853	5.39673	3.1477



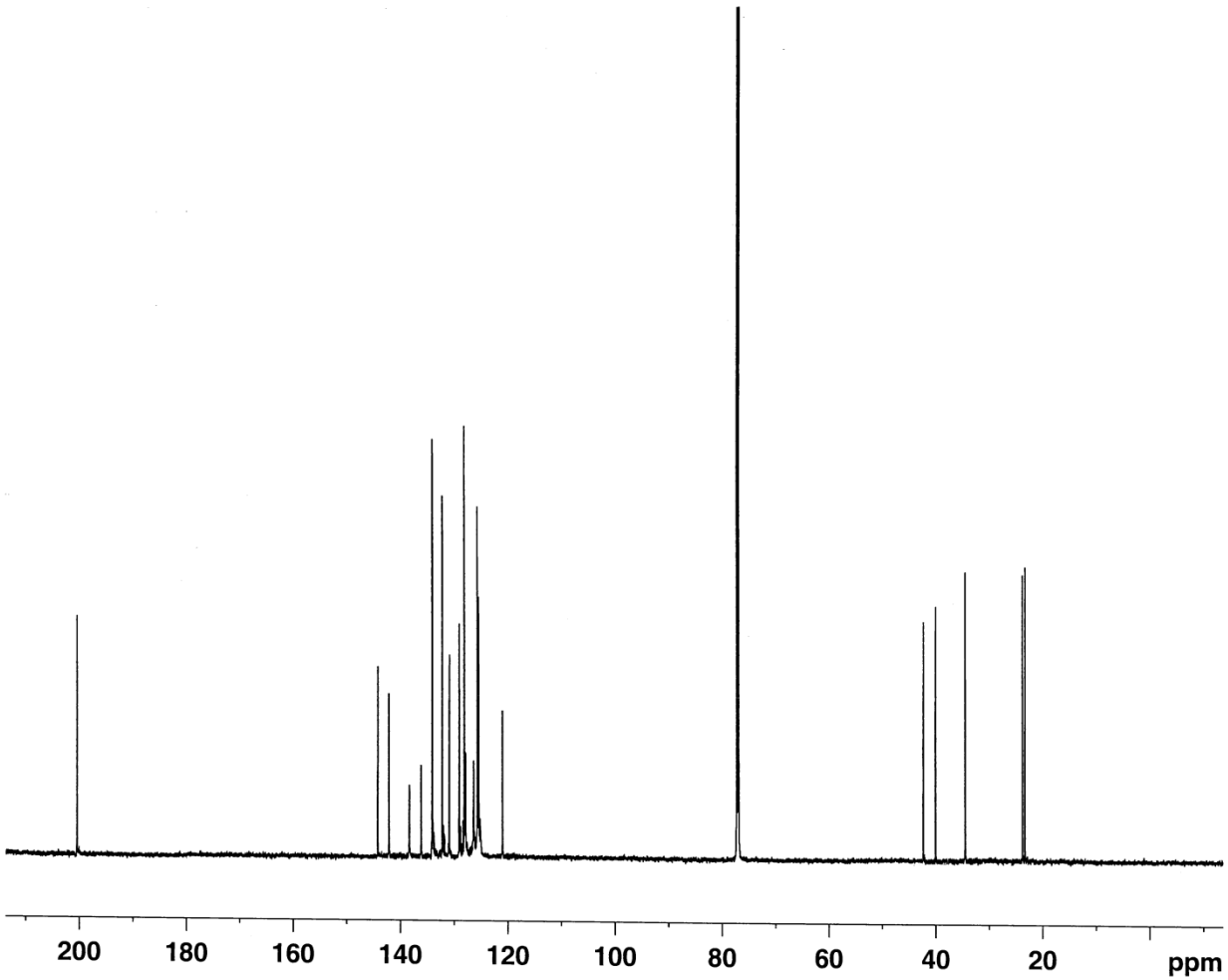
8o



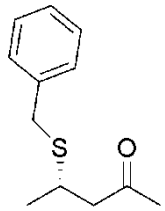

```
Current Data Parameters
NAME            SS-6-113
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130302
Time               20.20
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 33.71
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          500.1330008 MHz
NUC1                  1H
P1                 7.80 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



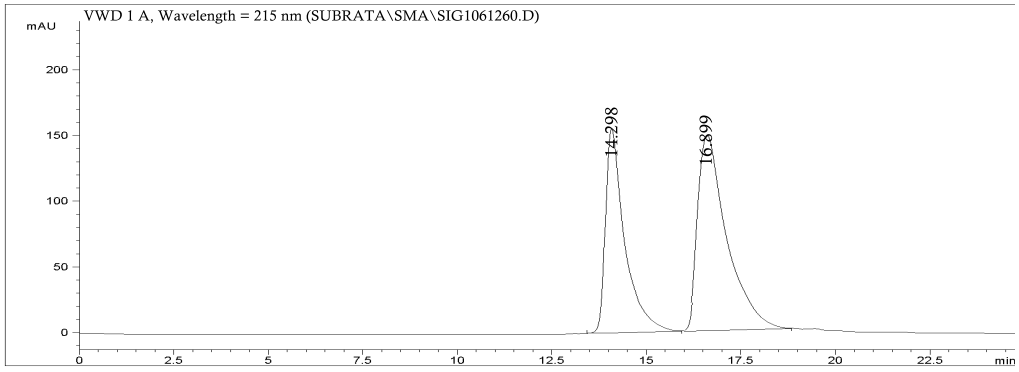
8o



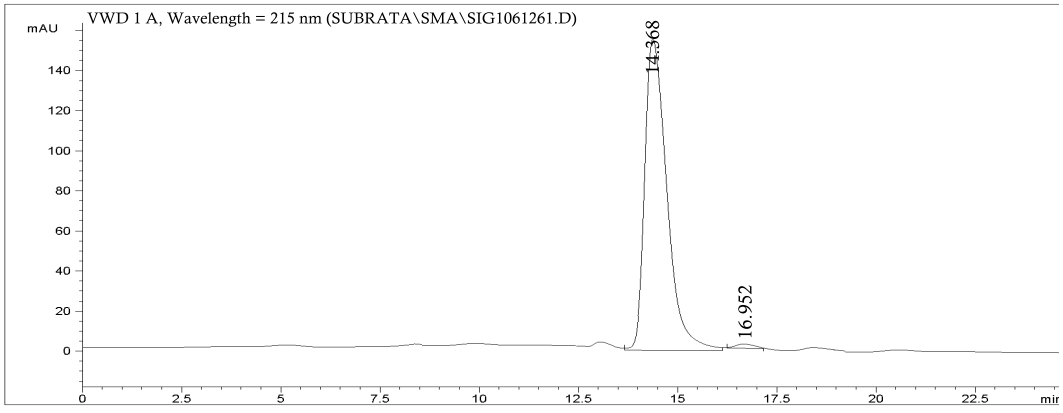
NAME	SS-06-113	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	17.51	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	36	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	use
DE	16.50	use
TE	298.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	use
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	use
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



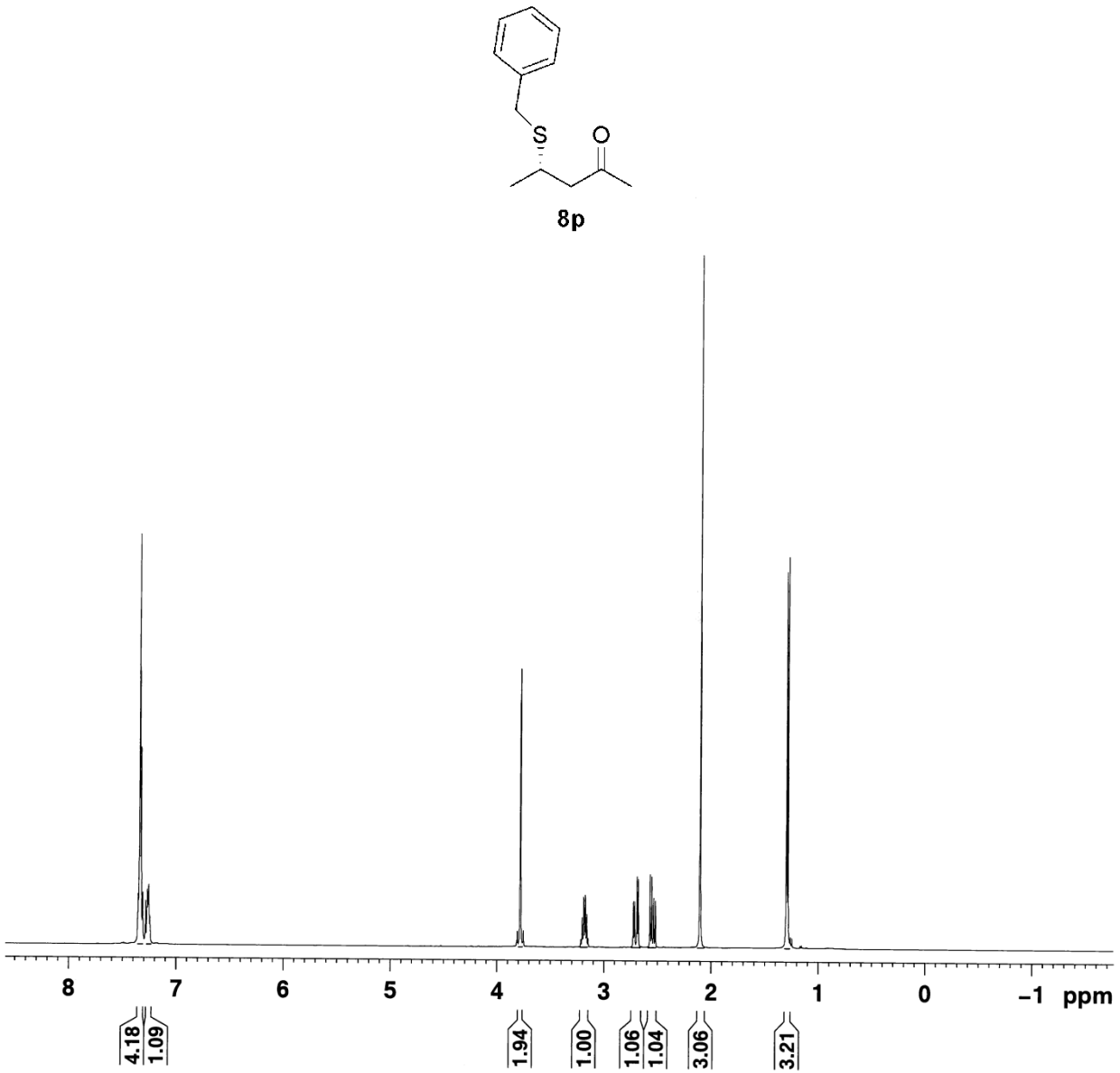
8p



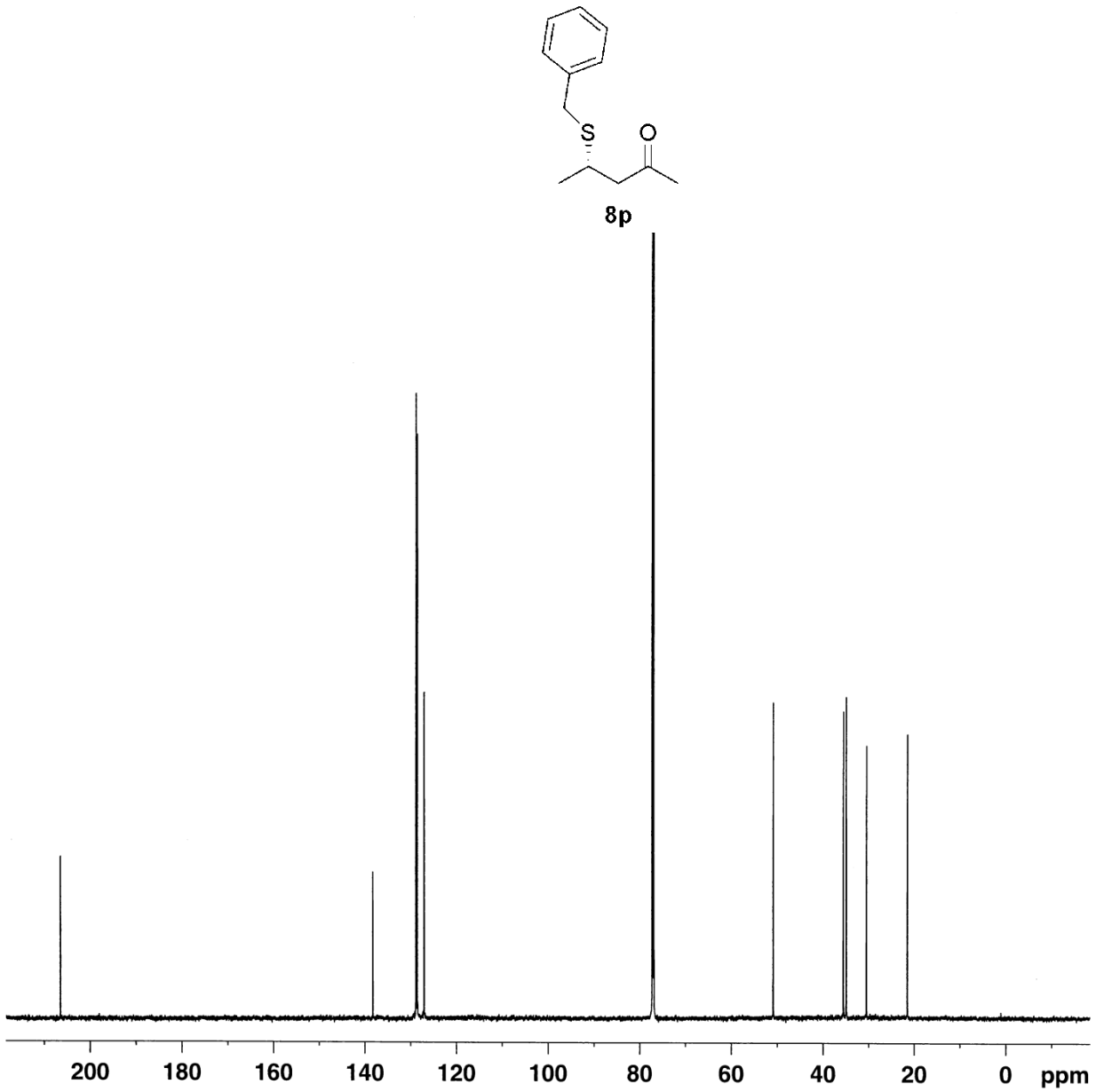
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.298	VV	0.5344	5876.37256	155.39836	42.1923
2	16.899	VV	0.7982	8051.19287	148.90695	57.8077



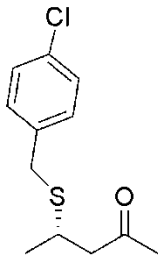
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.368	BB	0.6231	8759.02667	157.97361	97.6641
2	16.952	VB	0.5986	209.49926	2.48927	2.3359



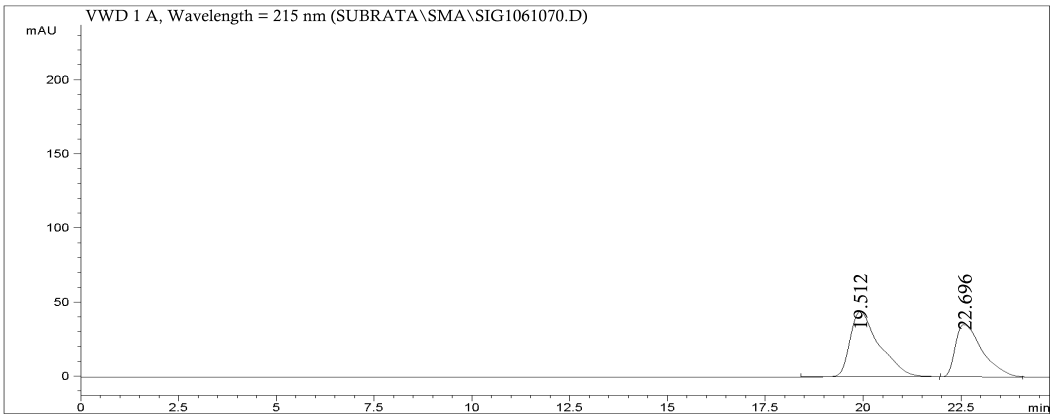

```
Current Data Parameters
NAME                  SS-6-126
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130303
Time                      2.08
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                        67.68
DW                       62.400 usec
DE                        6.50 usec
TE                       298.0 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               500.1330008 MHz
NUC1                        1H
P1                        7.80 usec
PLW1              12.00000000 W

F2 - Processing parameters
SI                       65536
SF                 500.1300000 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```



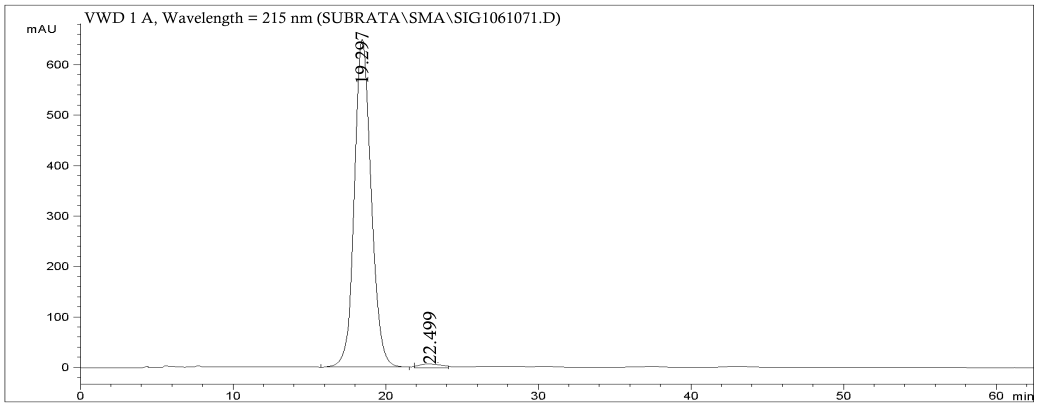
NAME	SS-06-126
EXPNO	2
PROCNO	1
Date_	20130323
Time	16.54
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	15
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 =======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



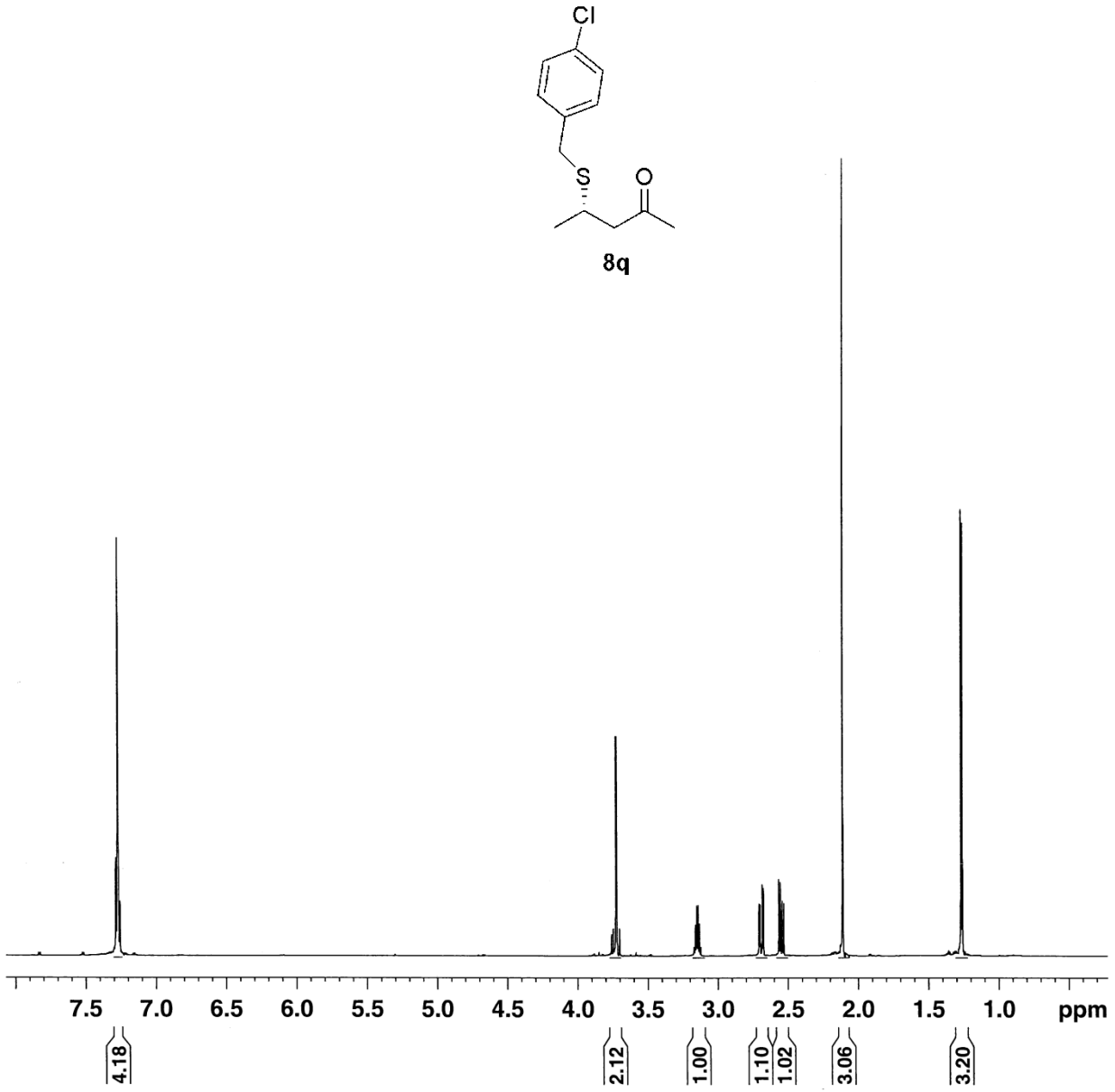
8q



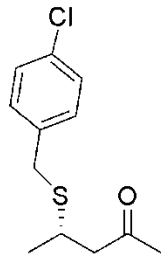
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.512	VB	0.7961	1067.36856	48.06591	55.5083
2	22.696	VB	0.7636	855.53142	42.72204	44.4917



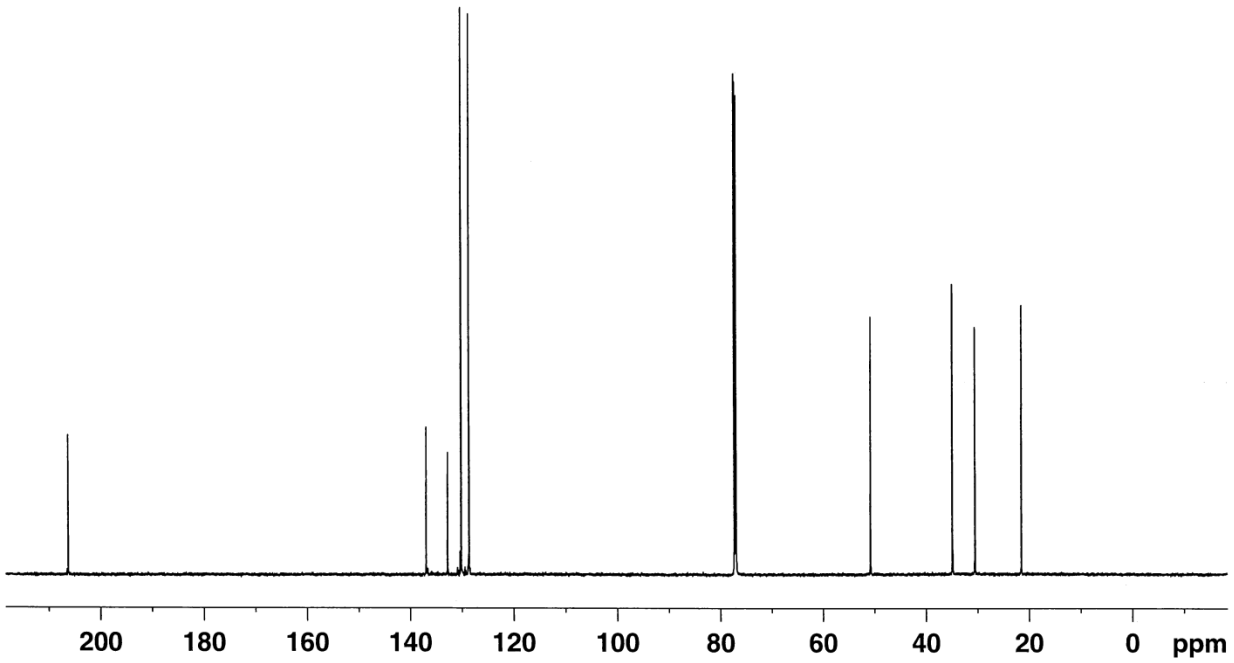
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.297	BB	1.2991	1.74924e4	649.93282	96.5435
2	22.499	VB	0.9083	626.27187	8.99530	3.4565



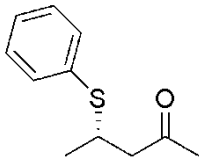
NAME	SS-06-107
EXPNO	1
PROCNO	1
Date_	20130323
Time	16.59
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	8
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	18
DW	42.000 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 usec
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



8q



NAME	SS-06-107
EXPNO	2
PROCNO	1
Date_	20130323
Time	17.02
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	13
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



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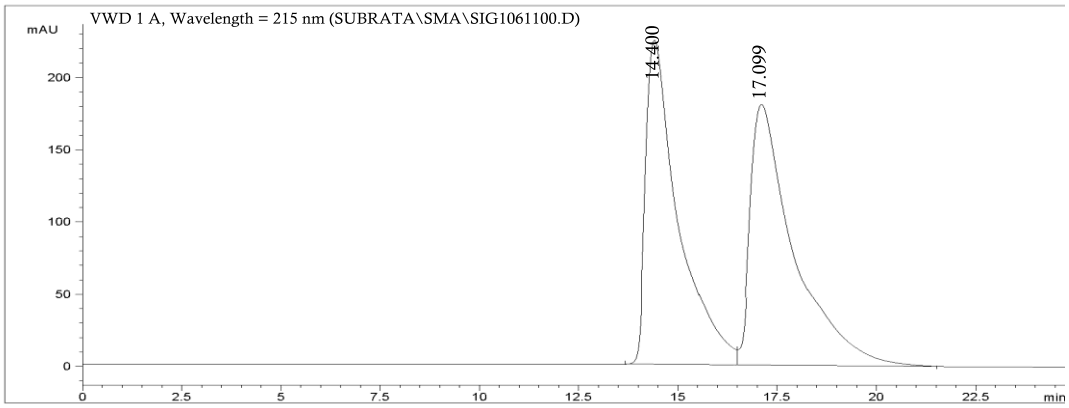
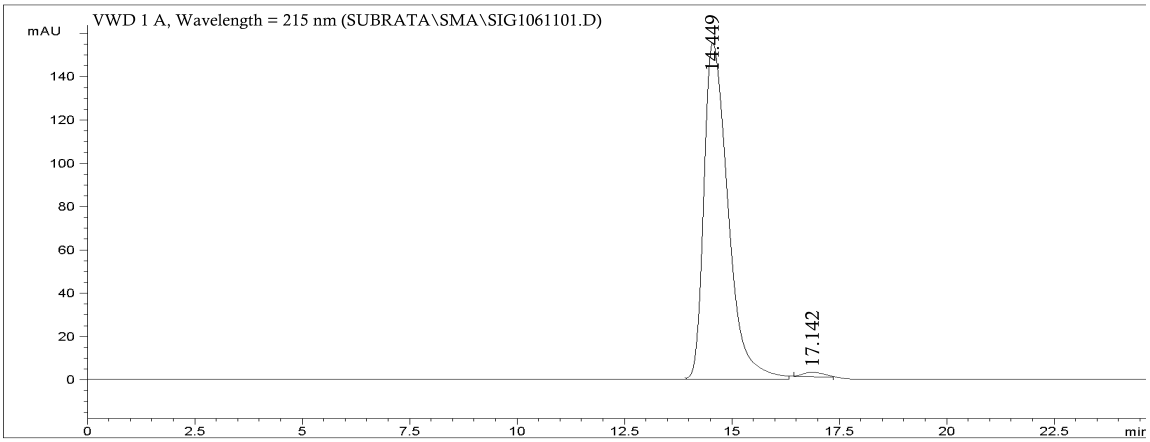
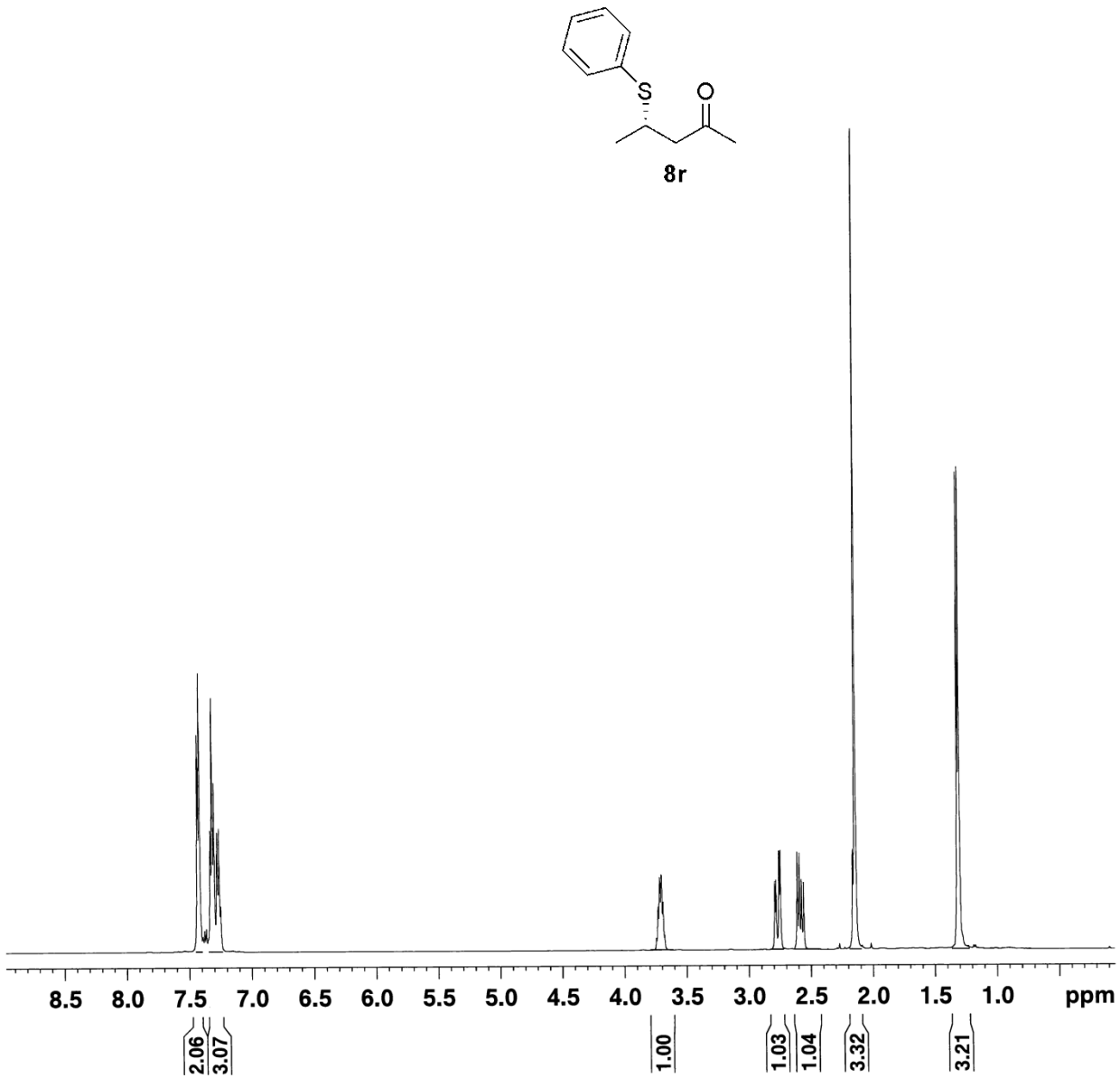


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.400	BV	0.8241	1.28537e4	224.38745	44.4555
2	17.099	VB	1.0900	1.37837e4	180.58675	55.5445



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.449	VB	0.6293	4856.98037	158.97015	98.8246
2	17.142	VB	0.5803	57.76795	2.26903	1.1754

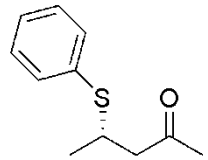



```
Current Data Parameters
NAME            SS-6-110
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130220
Time               12.28
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 29.88
DW                62.400 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         500.1330008 MHz
NUC1                   1H
P1                  7.80 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



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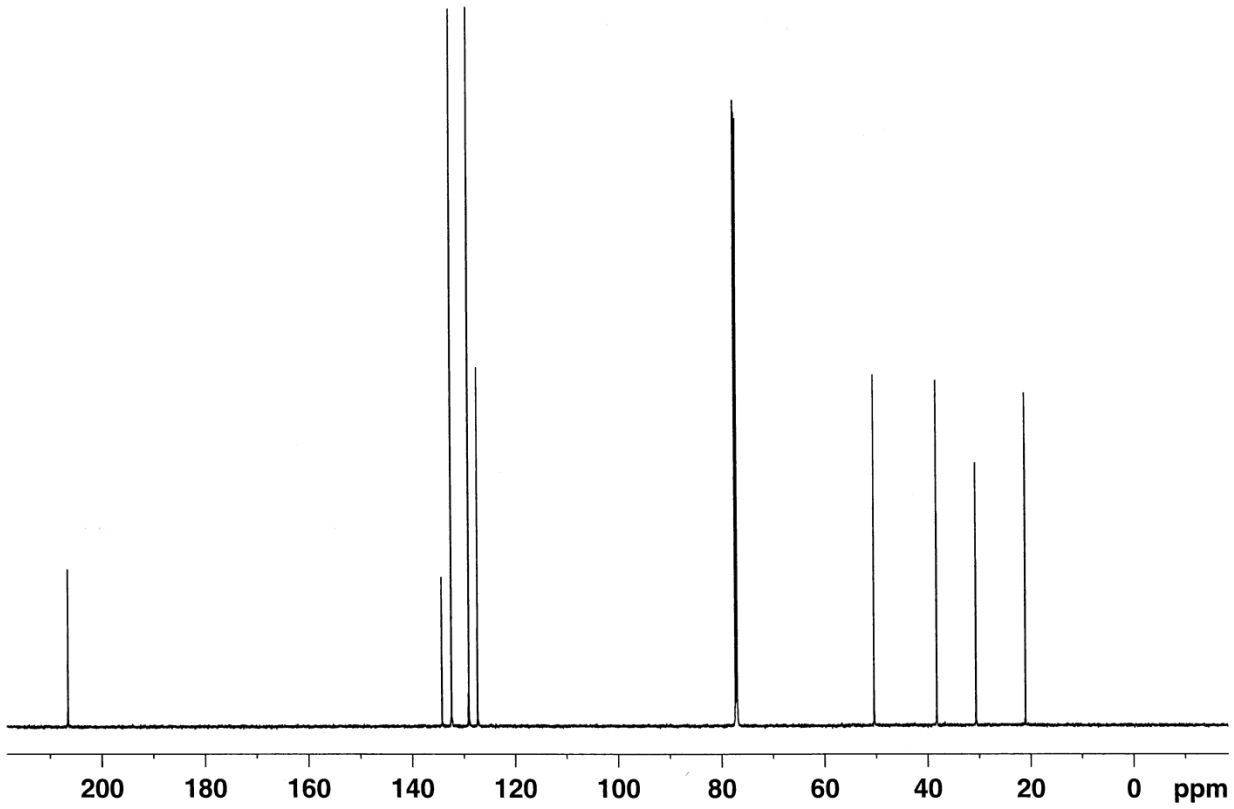
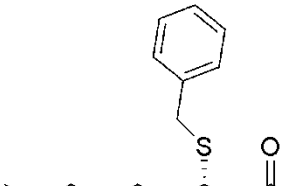


NAME	SS-06-110	
EXPNO	2	
PROCNO	1	
Date_	20130323	
Time	17.08	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	14	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	usec
DE	16.50	usec
TE	298.2	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	usec
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	usec
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	



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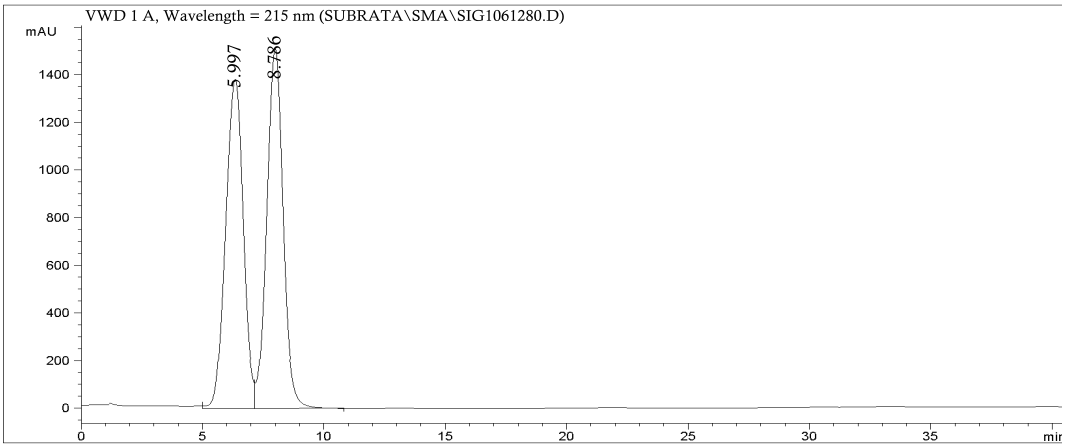
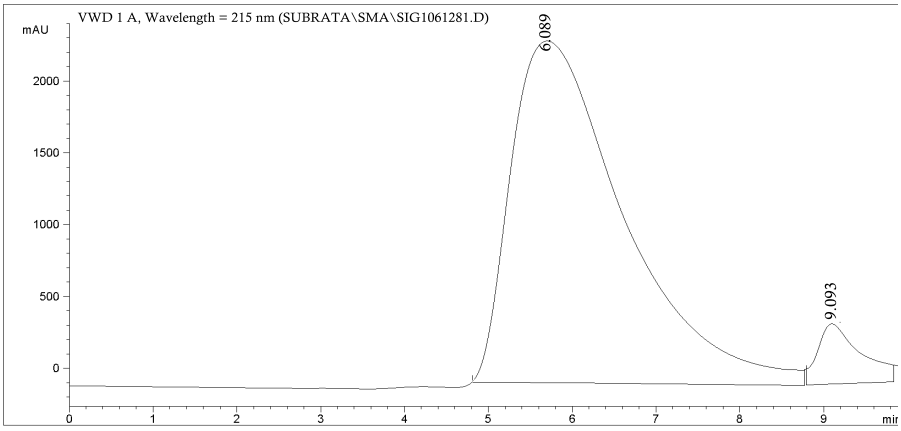
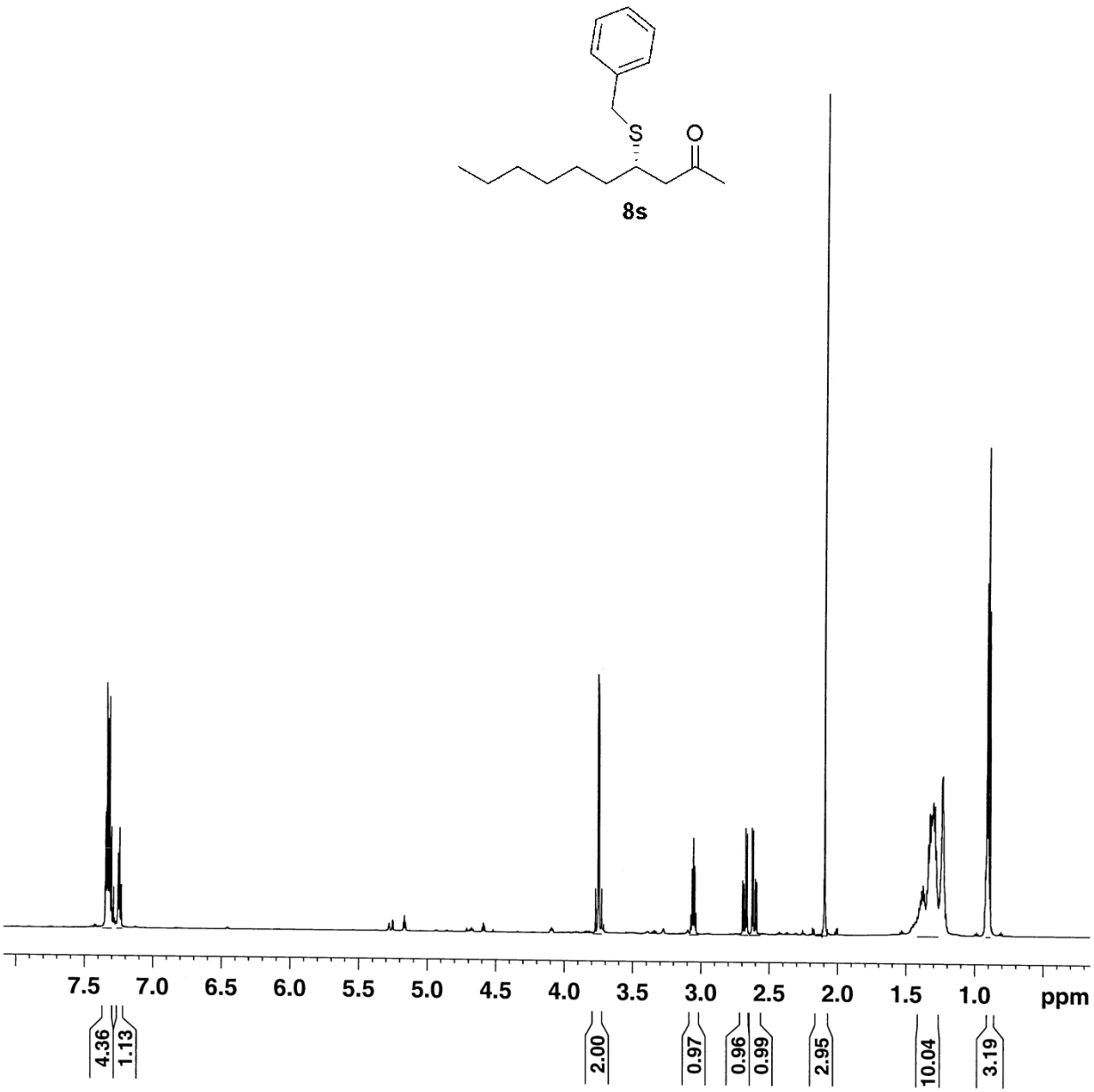


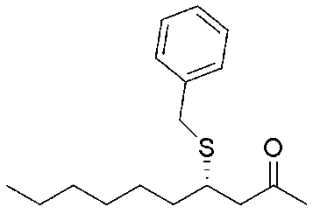
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.997	VV	0.8042	7.03961e4	1384.70068	47.7812
2	8.786	VB	0.7302	7.12962e4	1513.39014	52.2188



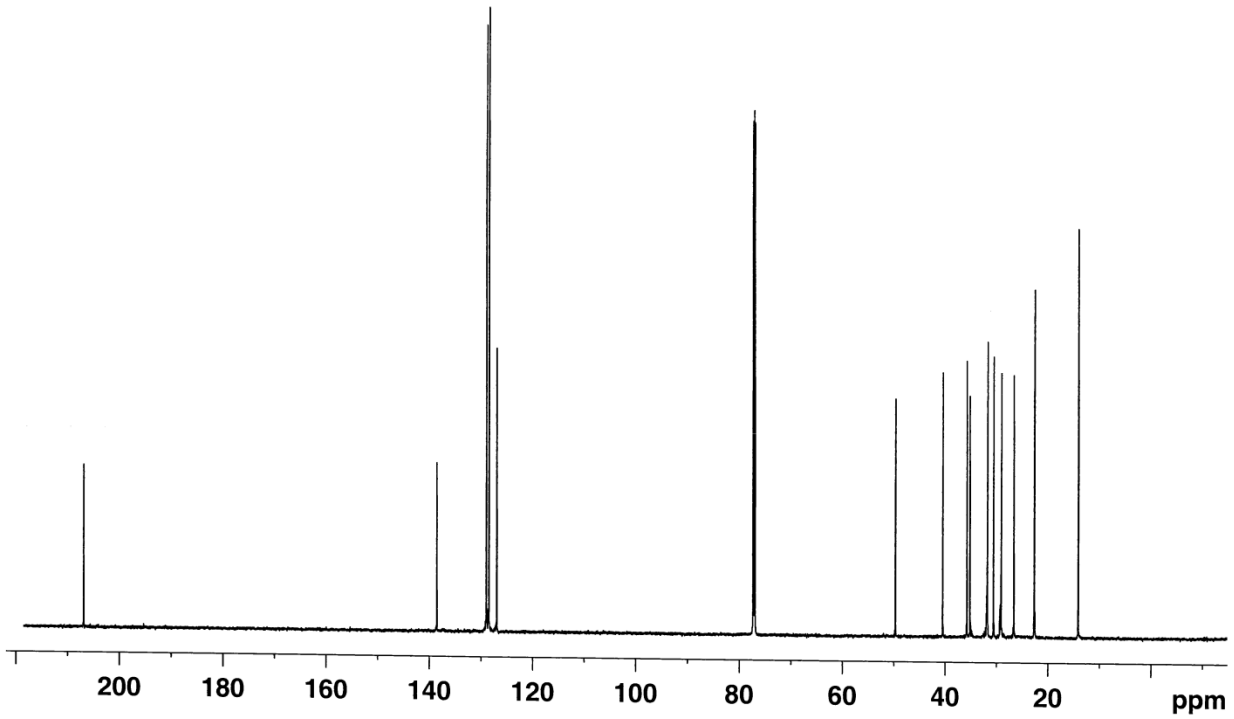
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.089	MM	1.6571	2.41504e4	2429.00000	98.8421
2	9.093	MM	0.5983	282.90759	419.35223	1.1579



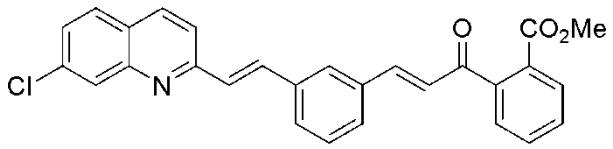

```
NAME            SS-06-128
EXPNO                   1
PROCNO                  1
Date_            20130323
Time                18.40
INSTRUM             spect
PROBHD    5 mm CPDCH 13C
PULPROG              zg30
TD                  95236
SOLVENT             CDCl3
NS                      9
DS                      2
SWH           11904.762 Hz
FIDRES         0.125003 Hz
AQ            3.9999621 sec
RG                      9
DW               42.000 use
DE                6.50 use
TE                298.2 K
D1           2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  9.40 use
PL1                -3.20 dB
PL1W        33.59817505 W
SFO1       700.1516910 MHz
SI              131072
SF         700.1471400 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



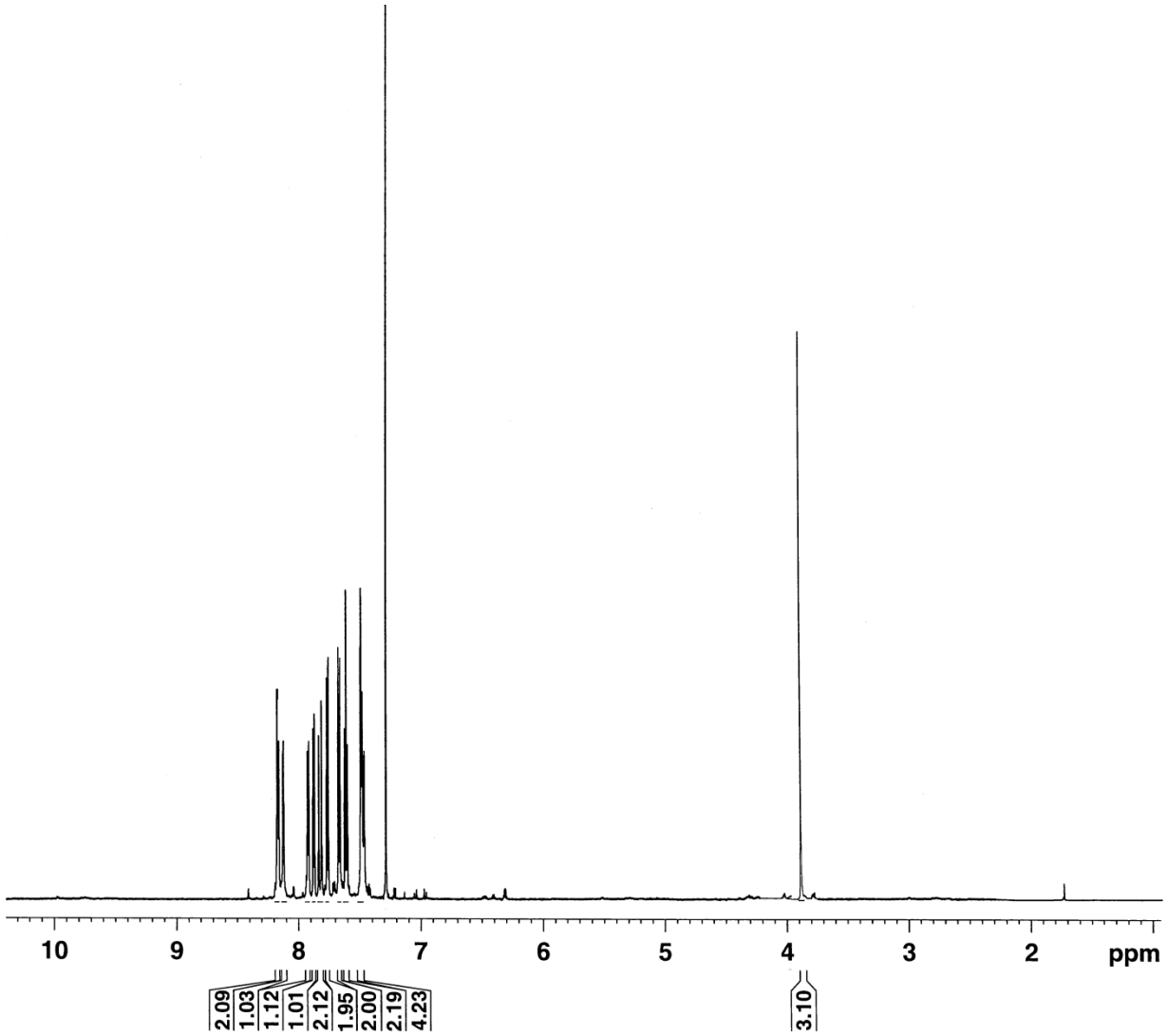
8s



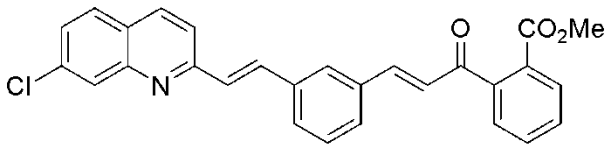
NAME	SS-06-128
EXPNO	2
PROCNO	1
Date_	20130323
Time	18.43
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	12
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



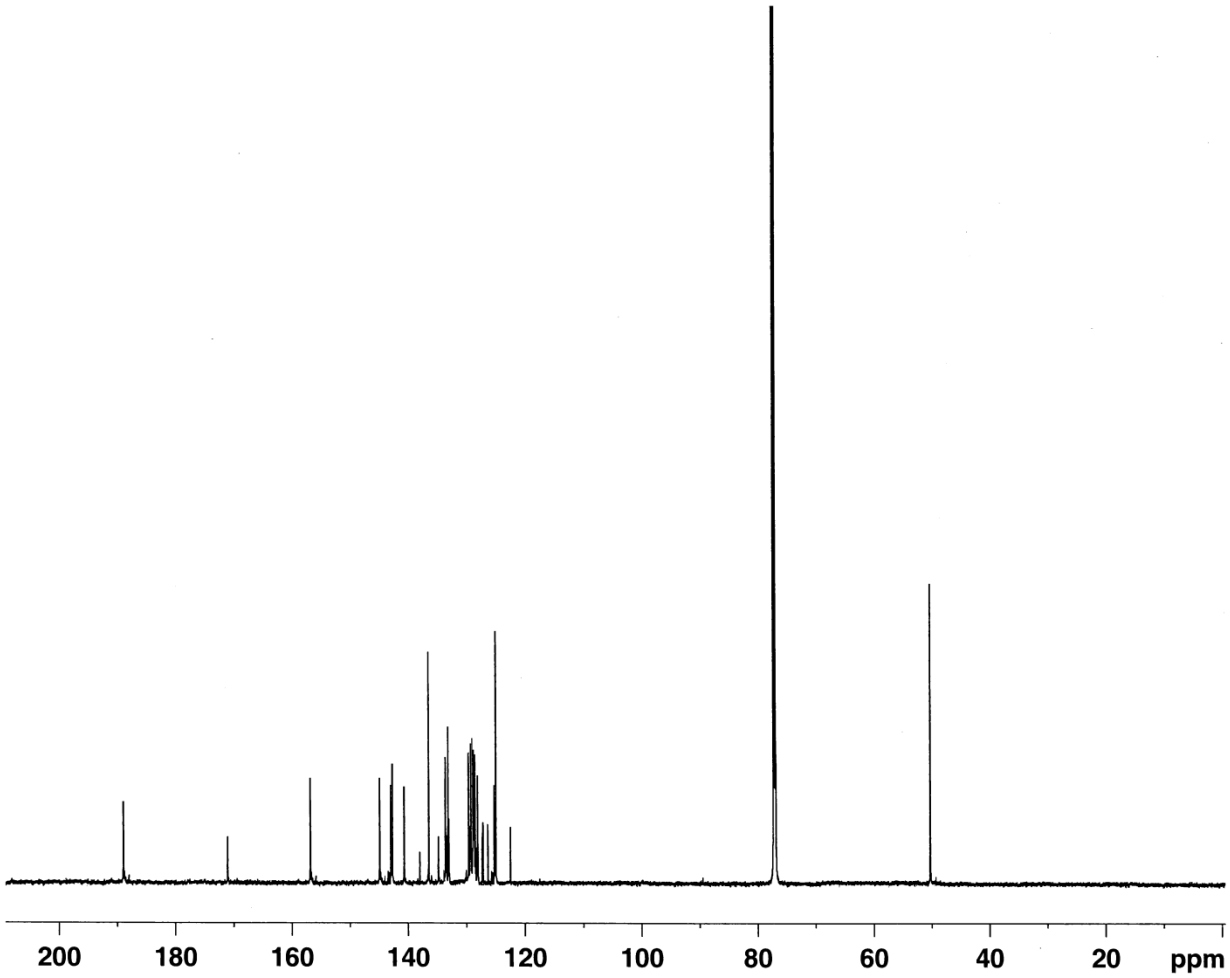
10



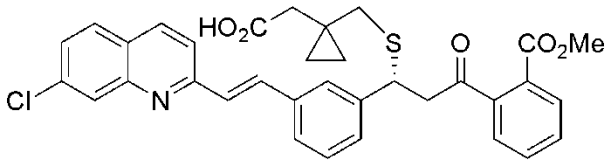
NAME	SS-05-90
EXPNO	1
PROCNO	1
Date_	20130903
Time	18.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	23
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	90.5
DW	42.000 use
DE	6.50 use
TE	297.8 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.75 use
PL1	-3.00 dB
PL1W	32.08600616 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



10



NAME	SS-06-145	
EXPNO	5	
PROCNO	1	
Date_	20130916	
Time	17.42	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	192	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	usec
DE	16.50	usec
TE	298.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	usec
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	usec
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.40	



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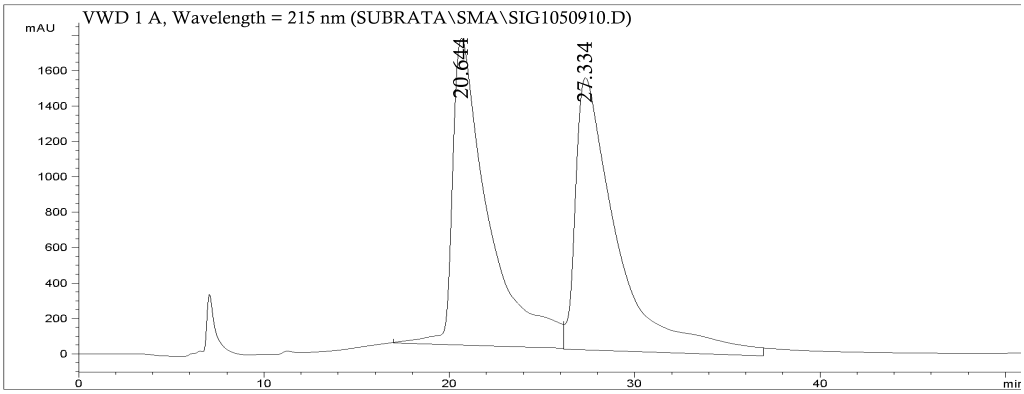
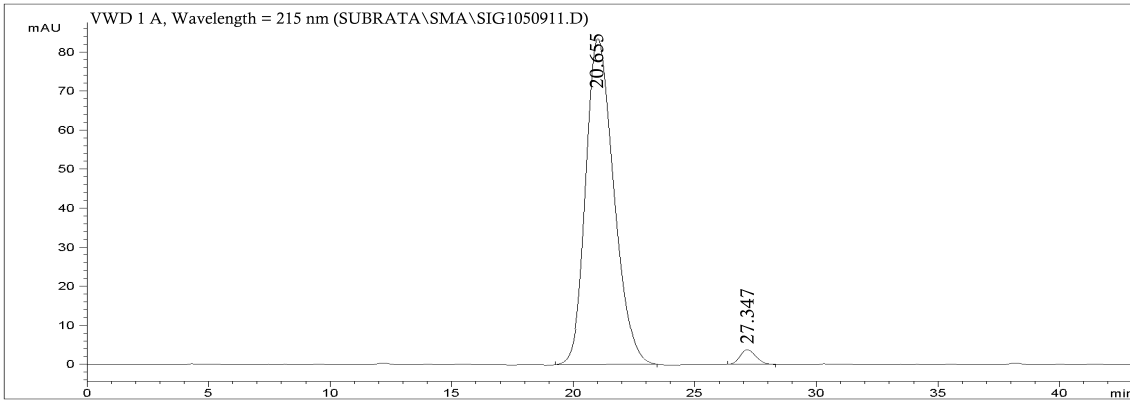
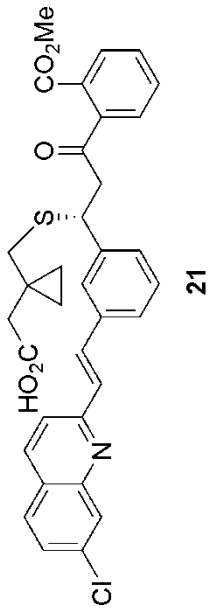


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	20.644	MM	2.2462	2.33987e5	1736.15942	49.2668
2	27.334	MM	2.6082	2.40952e5	1539.72363	50.7332



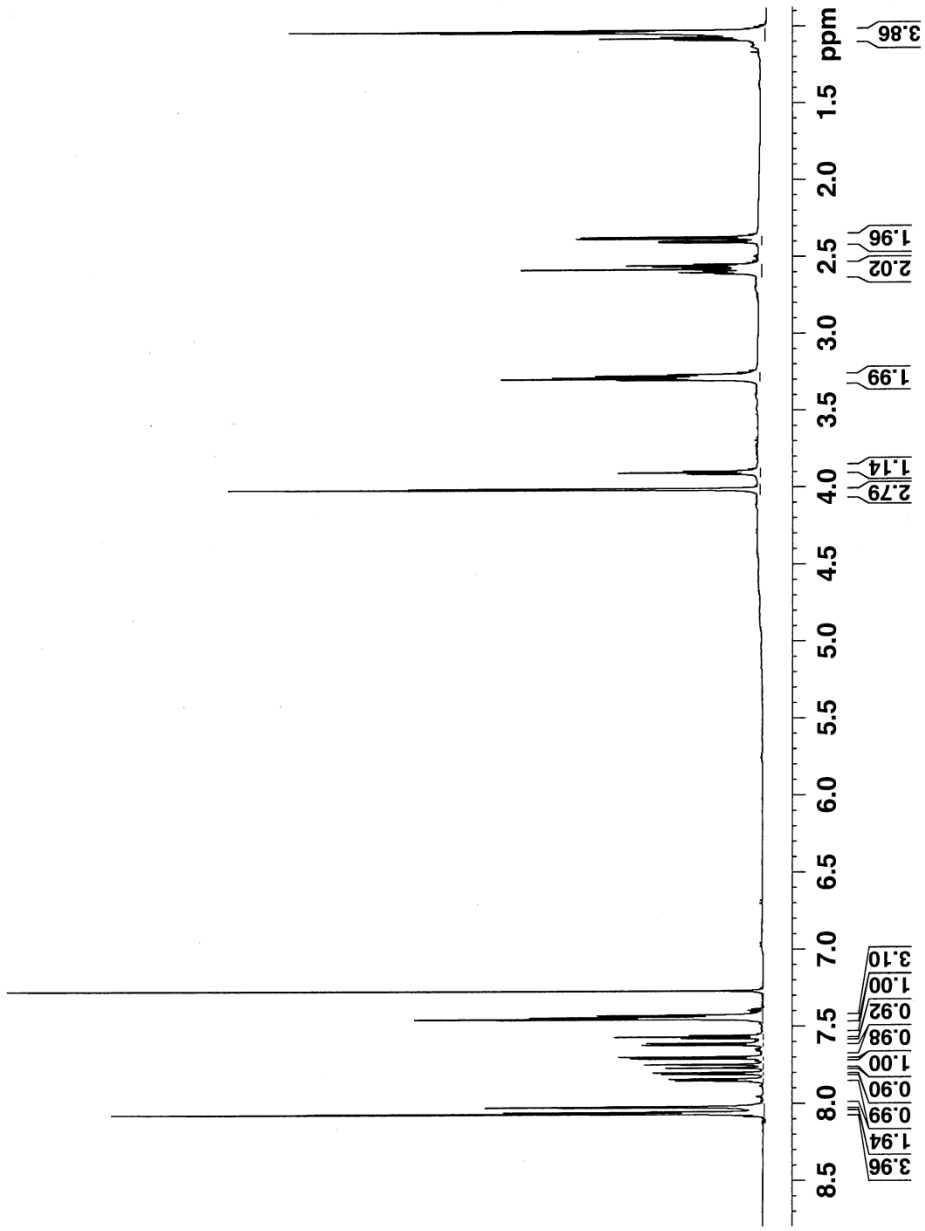
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	20.655	BB	1.3973	3708.29371	84.97341	98.7746
2	27.347	BB	0.6496	46.00518	3.89633	1.2254

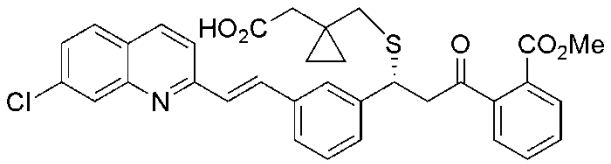


21

```
NAME              SS-05-91
EXPNO                    1
PROCNO                   1
Date_             20130918
Time                 11.56
INSTRUM              spect
PROBHD   5 mm CPDCH 13C
PULPROG                zg30
TD                   95236
SOLVENT              CDCl3
NS                      10
DS                       2
SWH              11904.762 Hz
FIDRES               0.125003 Hz
AQ               3.9999621 sec
RG                    11.3
DW                   42.000 use
DE                    6.50 use
TE                   298.3 K
D1               2.00000000 sec
TD0                      1

======== CHANNEL f1 =======
NUC1                   1H
P1                   9.40 use
PL1                  -3.20 dB
PL1W            33.59817505 W
SFO1            700.1516910 MHz
SI                  131072
SF              700.1471400 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```





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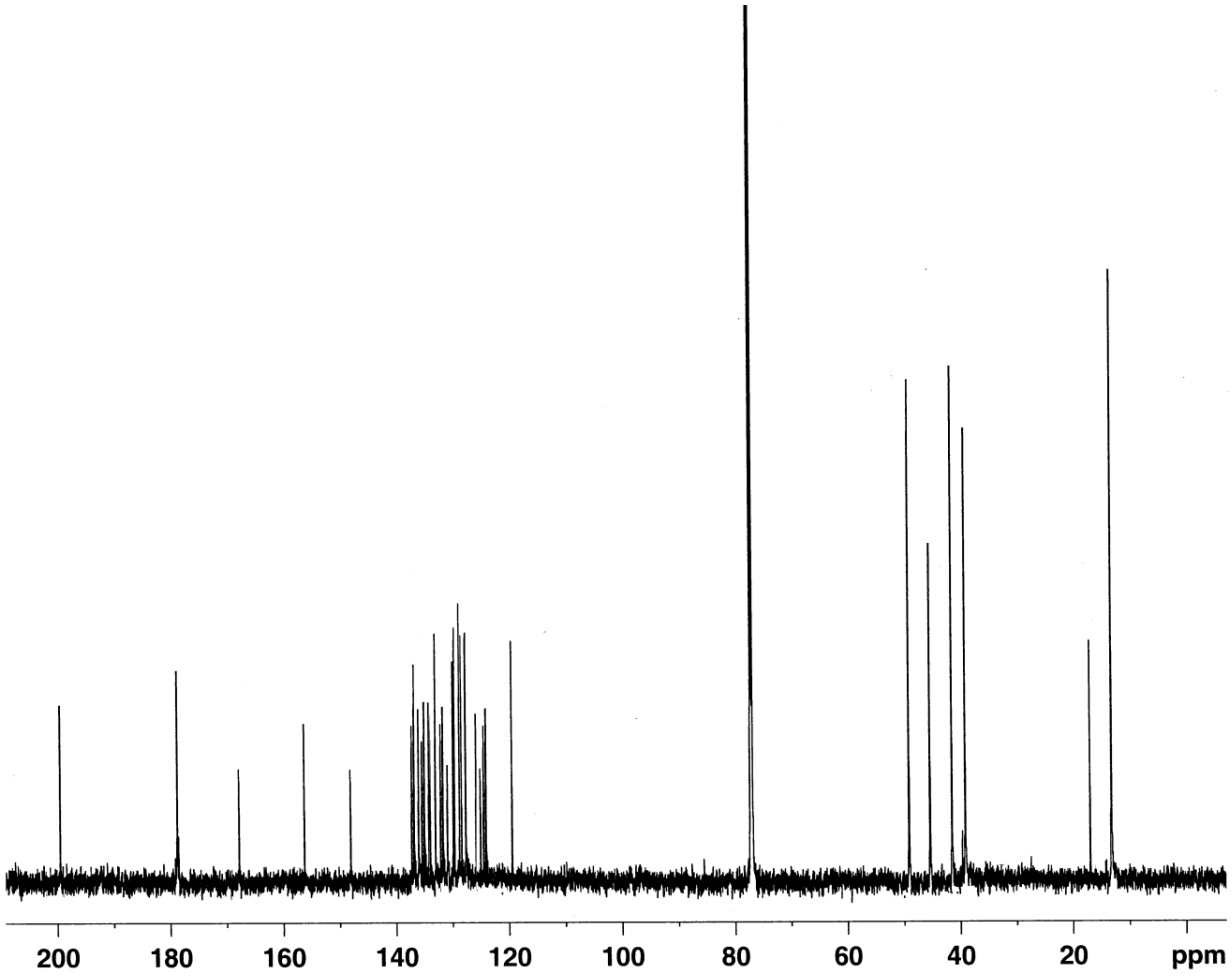
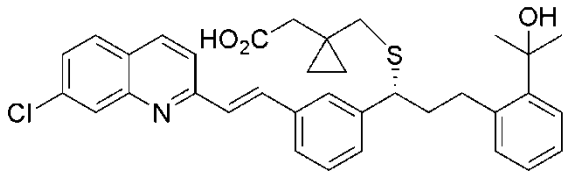
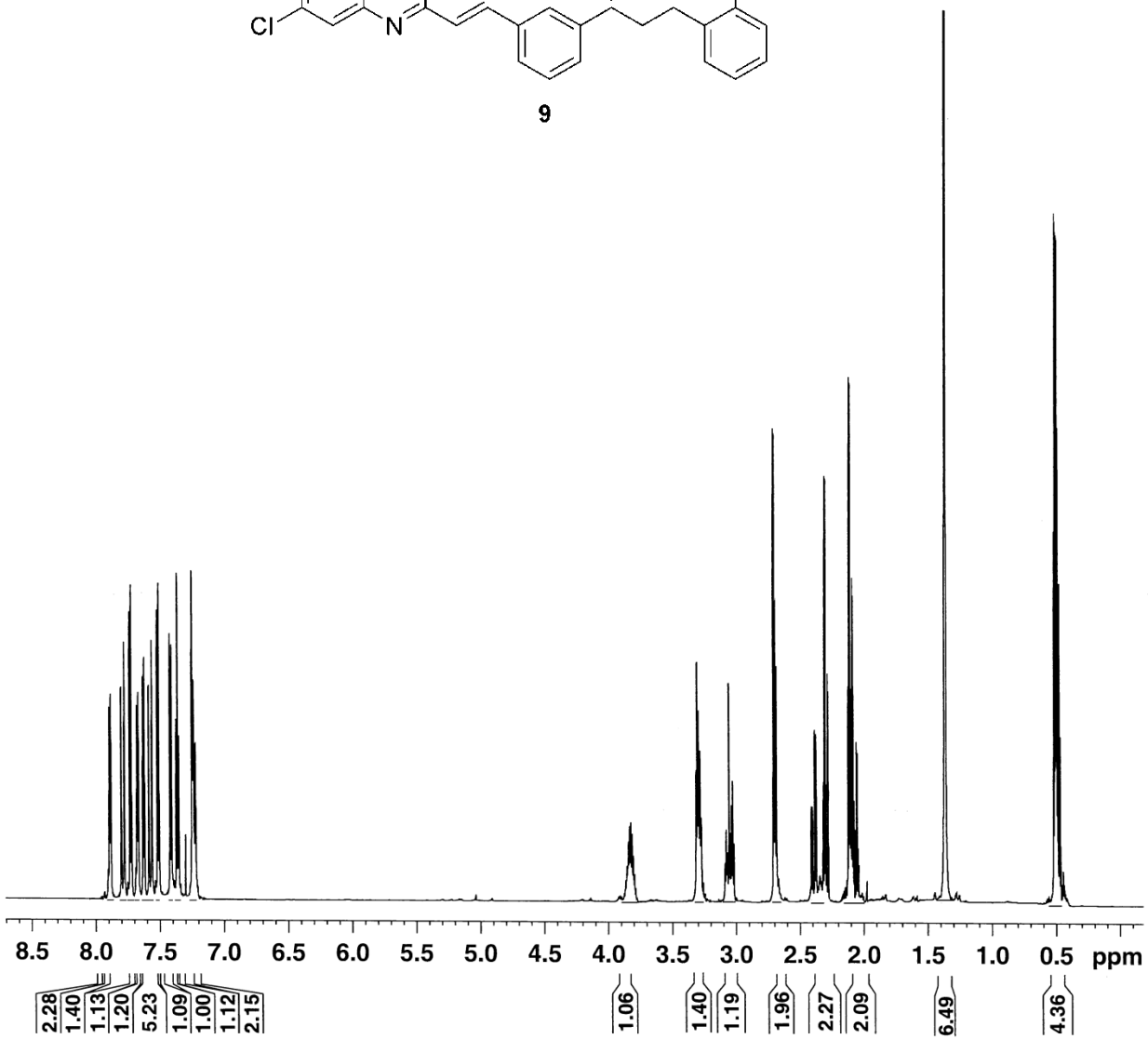


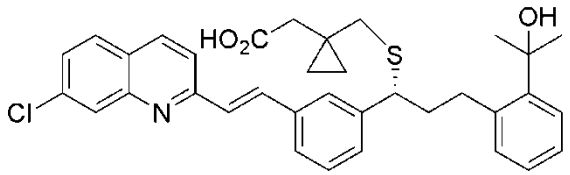
NAME	SS-05-91
EXPNO	4
PROCNO	1
Date_	20130919
Time	12.35
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	51
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



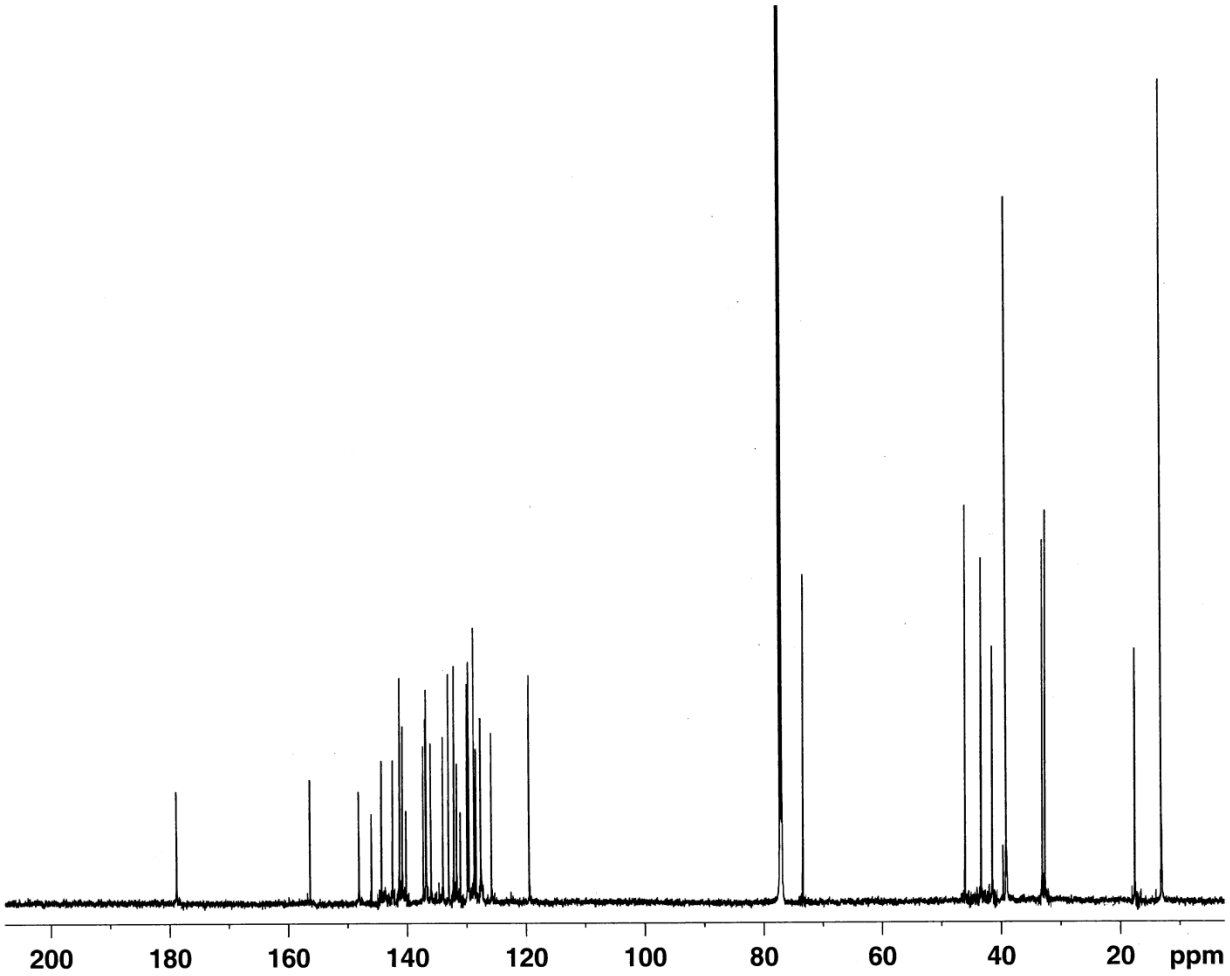
9



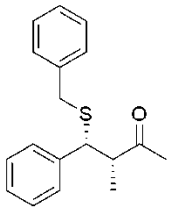
NAME	SS-05-102
EXPNO	1
PROCNO	1
Date_	20130918
Time	12.20
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	12
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	12.7
DW	42.000 use
DE	6.50 use
TE	298.1 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



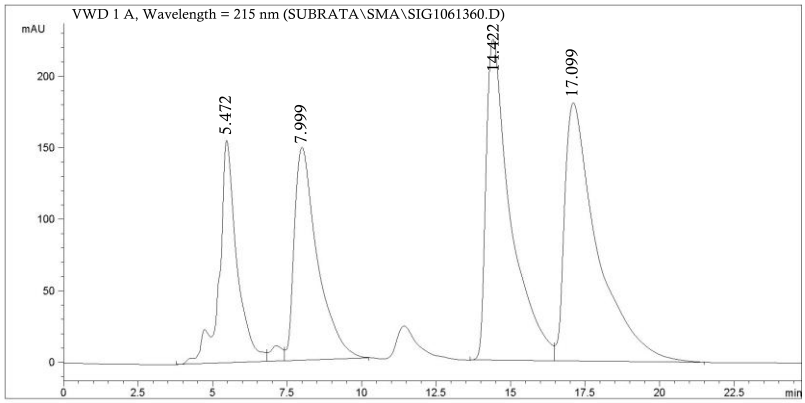
9



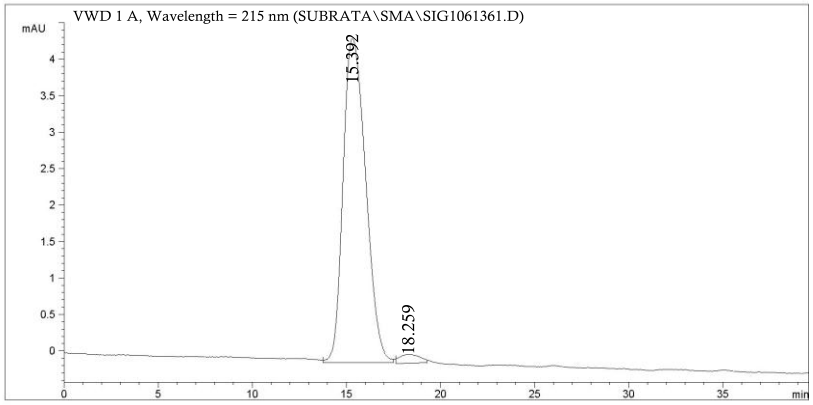
NAME	SS-05-102
EXPNO	3
PROCNO	1
Date_	20130919
Time	12.44
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	124
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



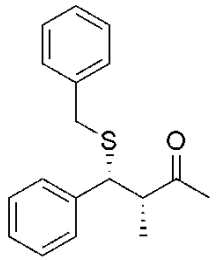
25a



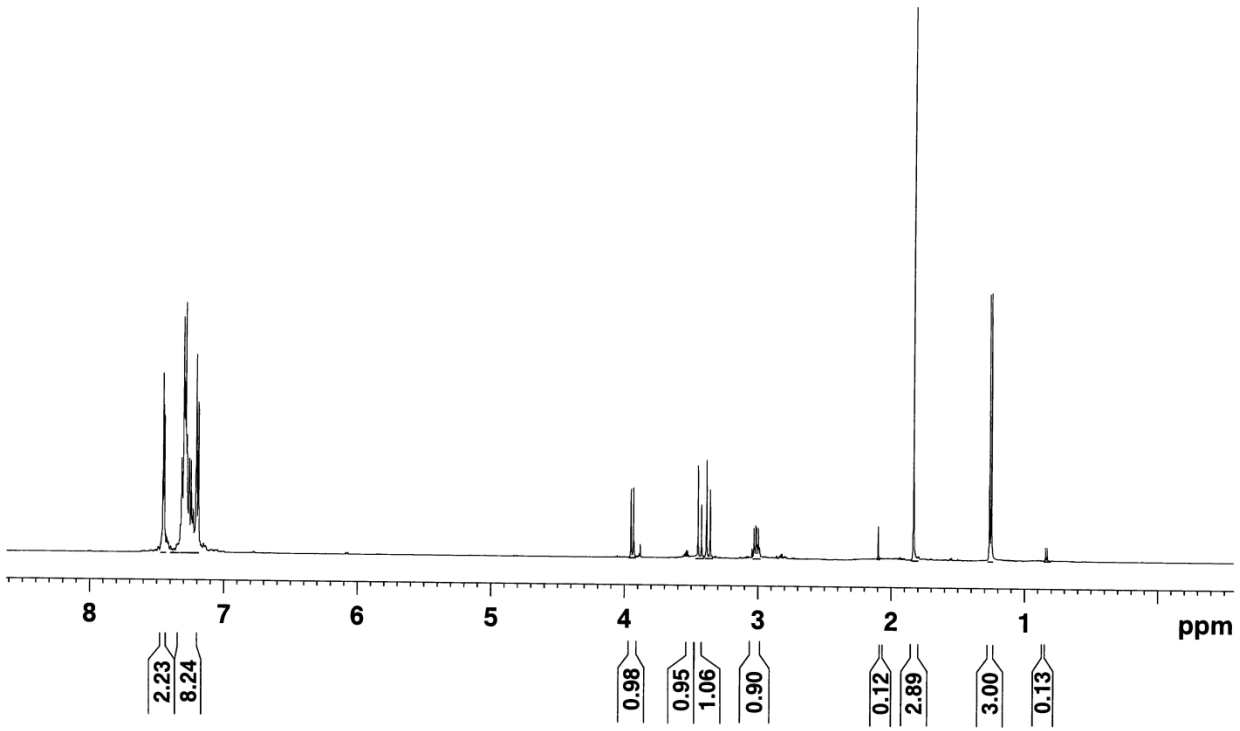
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.472	VV	0.5344	5876.37256	155.39836	14.4836
2	7.999	VV	0.7982	8051.19287	148.90695	19.8438
3	14.422	BV	0.8241	1.28537e4	224.39852	31.6806
4	17.099	VB	1.0900	1.37836e4	180.58675	33.9920



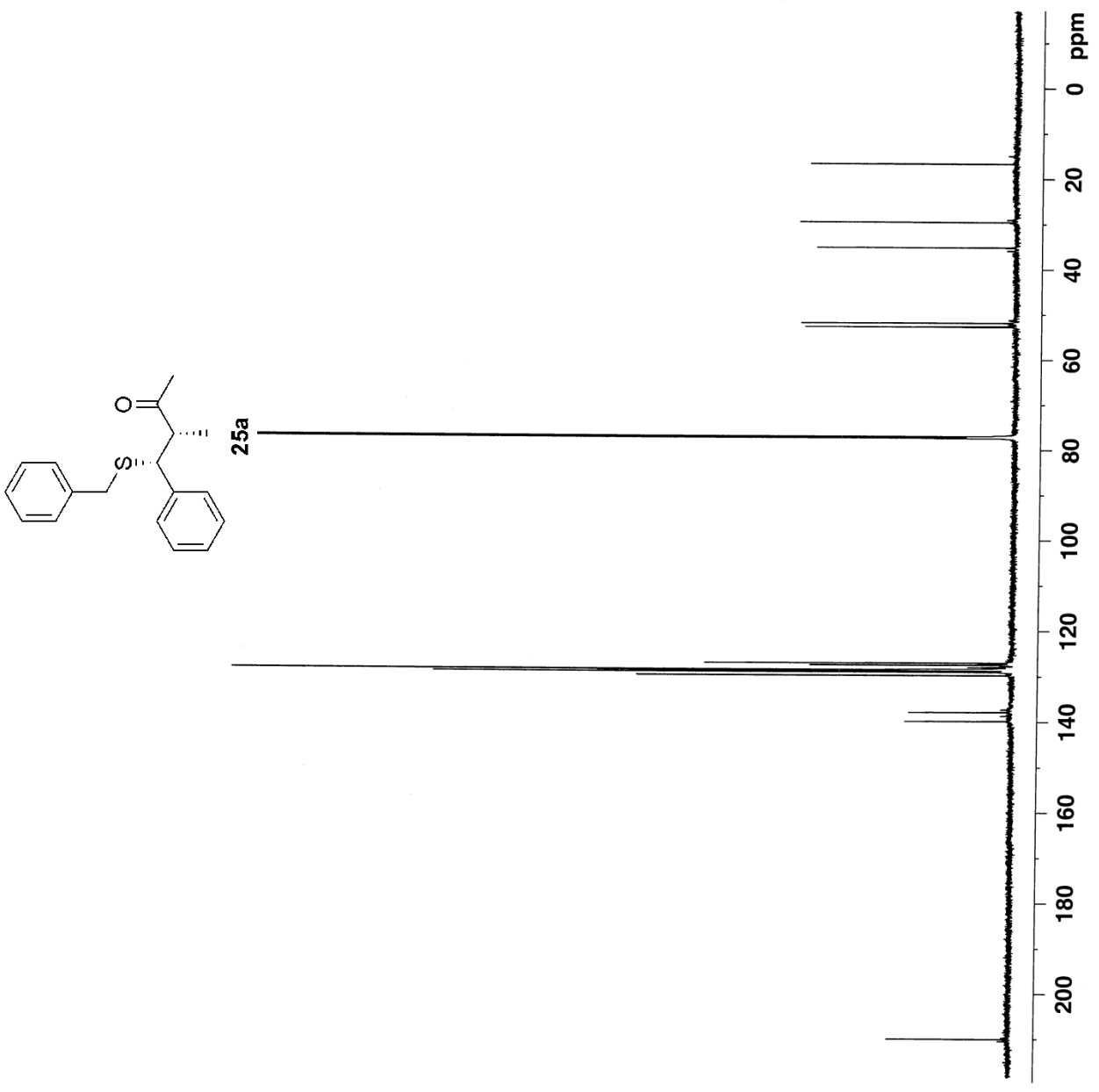
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.392	MM	1.3952	1069.99026	4.45072	98.7522
2	18.259	MM	1.2293	13.52114	1.24761e-1	1.2478



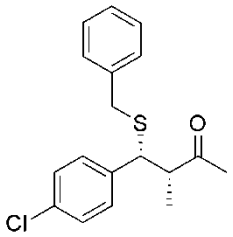
25a



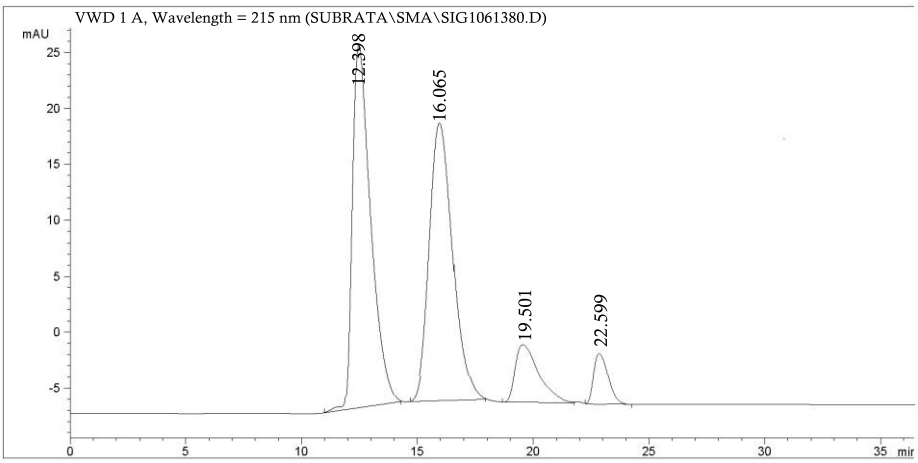

```
Current Data Parameters
NAME                  SS-6-136
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130316
Time                     18.08
INSTRUM                  spect
PROBHD    5 mm PATXI 1H/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       67.68
DW                     62.400 usec
DE                      6.50 usec
TE                      297.9 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             500.1330008 MHz
NUC1                       1H
P1                       7.80 usec
PLW1            12.00000000 W

F2 - Processing parameters
SI                       65536
SF               500.1300000 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```



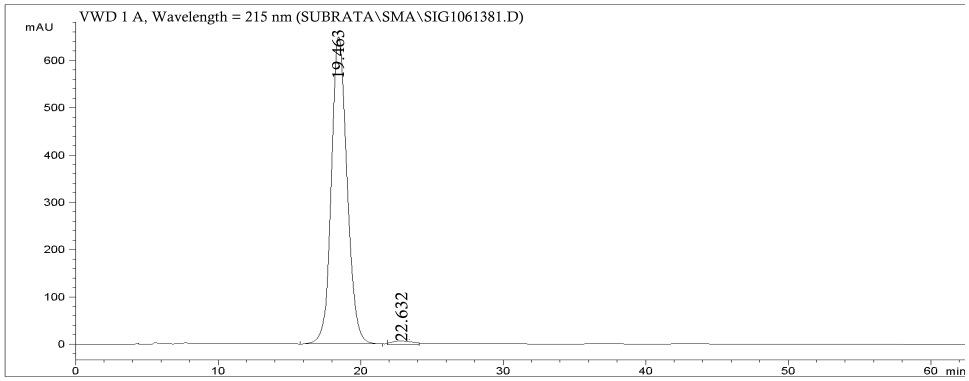

```
NAME                SS-06-136
EXPNO                       2
PROCNO                      1
Date_                20130323
Time                    19.22
INSTRUM                  spect
PROBHD     5 mm CPDCH 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          15
DS                           4
SWH                  41666.668 Hz
FIDRES               0.635783 Hz
AQ                   0.7864820 sec
RG                         203
DW                      12.000 use
DE                      16.50 use
TE                      298.1 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 =======
NUC1                       13C
P1                      9.00 use
PL1                     4.50 dB
PL1W                38.14553833 W
SFO1                176.0697436 MHz

======== CHANNEL f2 =======
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                   65.00 use
PL2                     -3.20 dB
PL12                    13.60 dB
PL13                   120.00 dB
PL2W                33.59817505 W
PL12W                0.70196527 W
PL13W                0.00000000 W
SFO2                700.1499406 MHz
SI                       32768
SF                  176.0521380 MHz
WDW                         EM
SSB                          0
LB                      3.00 Hz
GB                           0
PC                      1.00
```



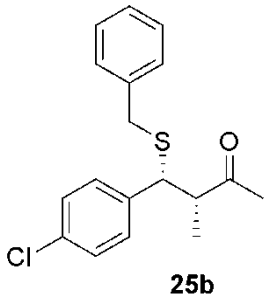
25b



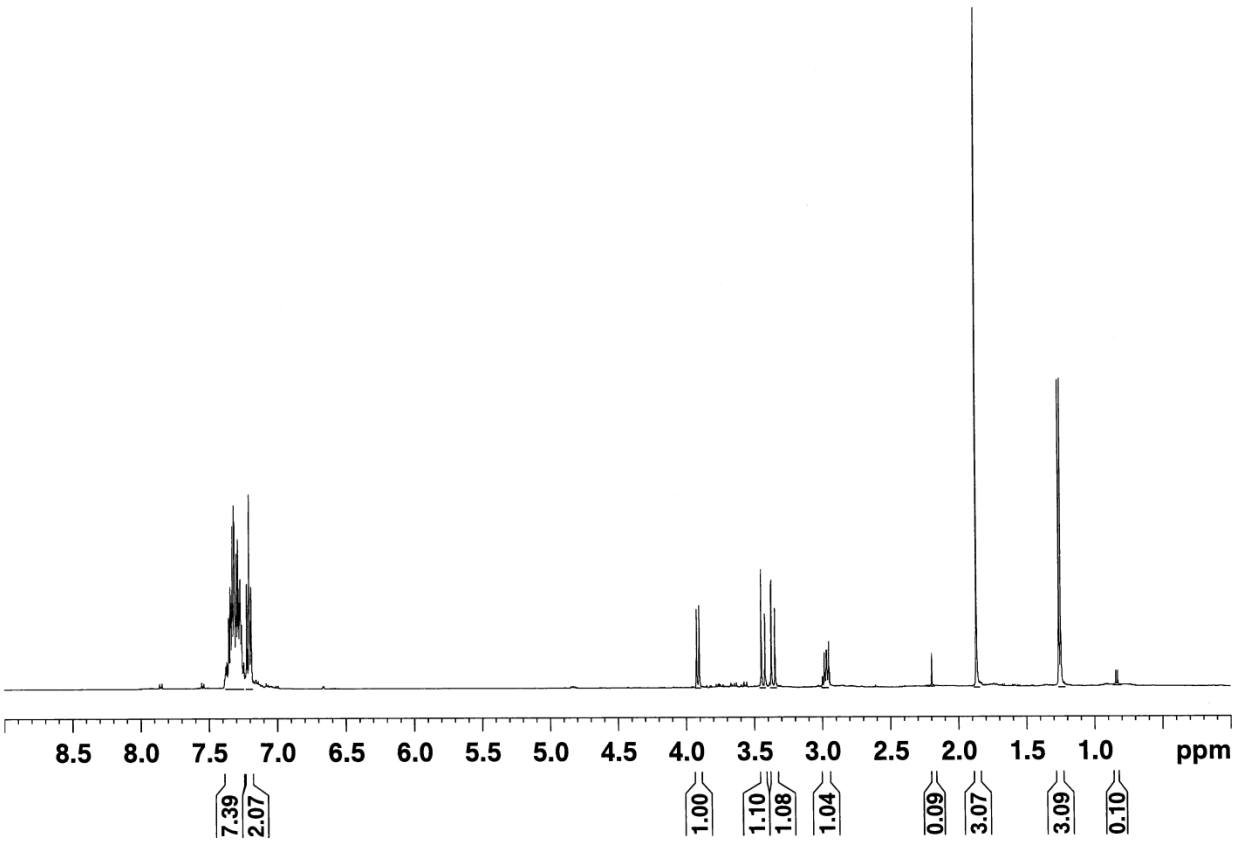
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	12.398	BB	0.8174	1824.29565	32.74717	48.2617
2	16.065	BB	1.0487	1747.72729	24.86211	46.2362
3	19.501	BB	1.0083	128.50039	6.82813	3.3995
4	22.599	VB	0.6398	79.18955	5.16049	2.1026



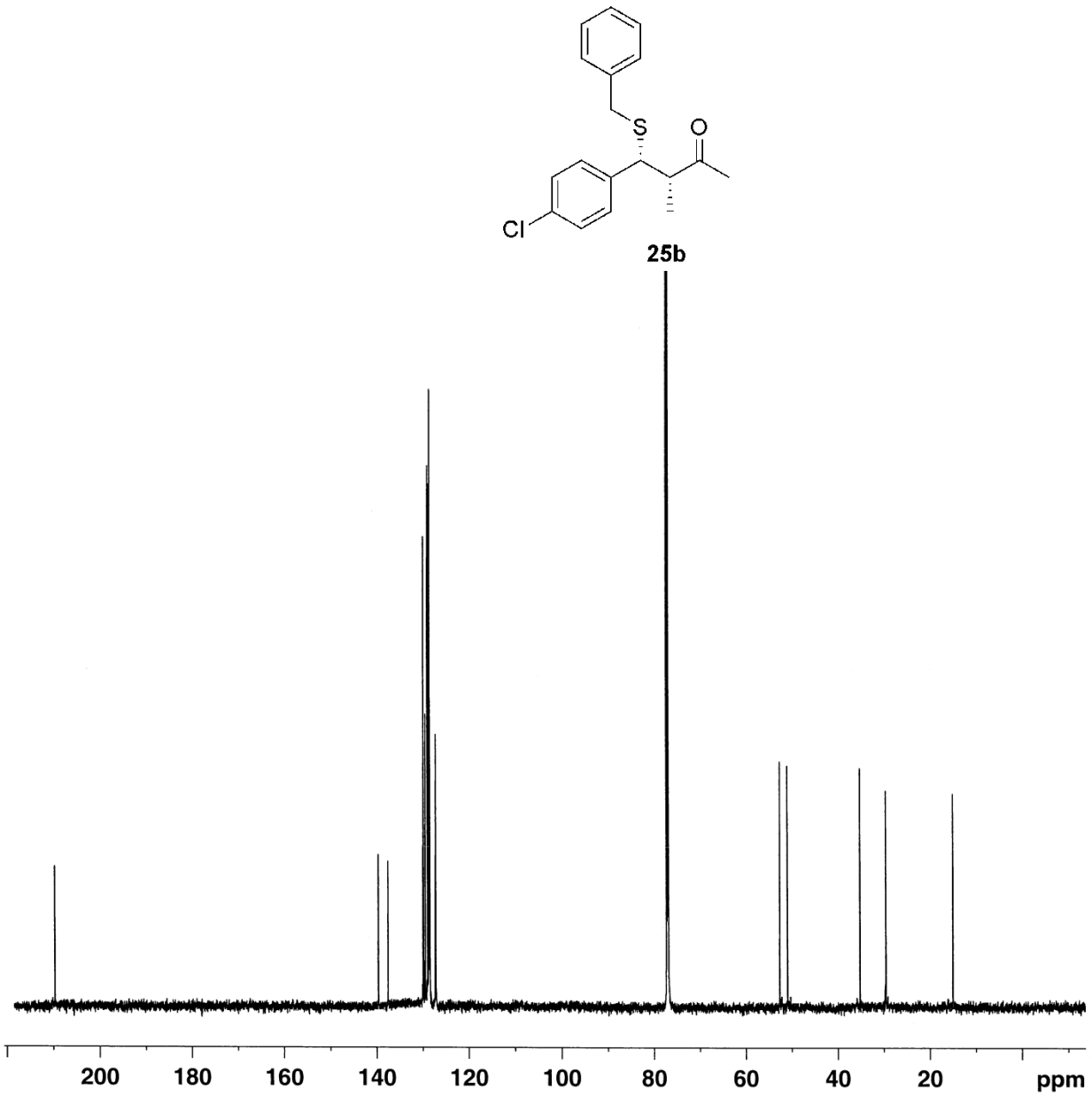
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	19.463	BV	1.1863	1.54399e4	647.09675	98.1598
2	22.632	BB	0.8675	289.45151	8.98441	1.8402



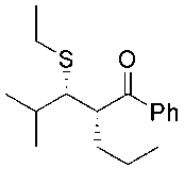
25b



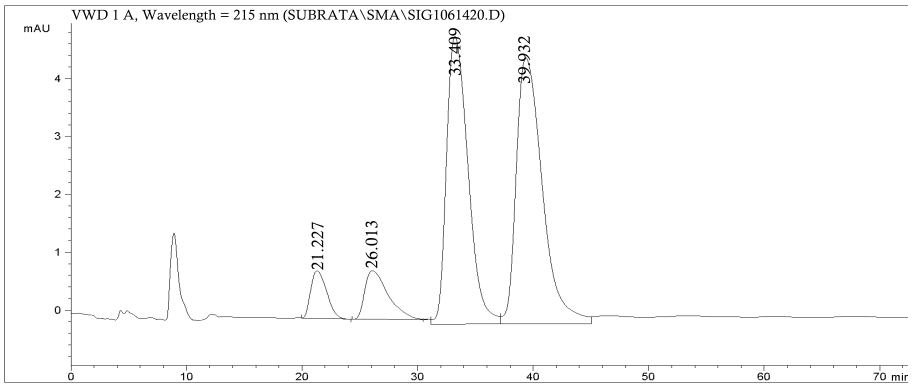

```
Current Data Parameters
NAME            SS-6-137
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130316
Time               18.26
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 46.39
DW                 62.400 use
DE                  6.50 use
TE                297.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1          500.1330008 MHz
NUC1                   1H
P1                  7.80 use
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300000 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



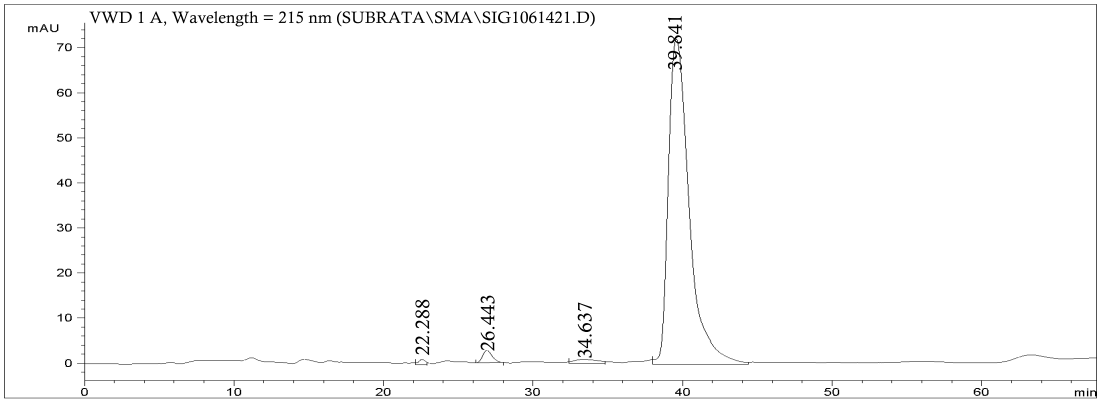
NAME	SS-06-137
EXPNO	1
PROCNO	1
Date_	20130323
Time	19.26
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	20
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00



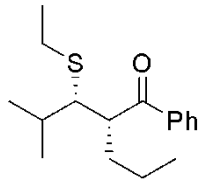
25c



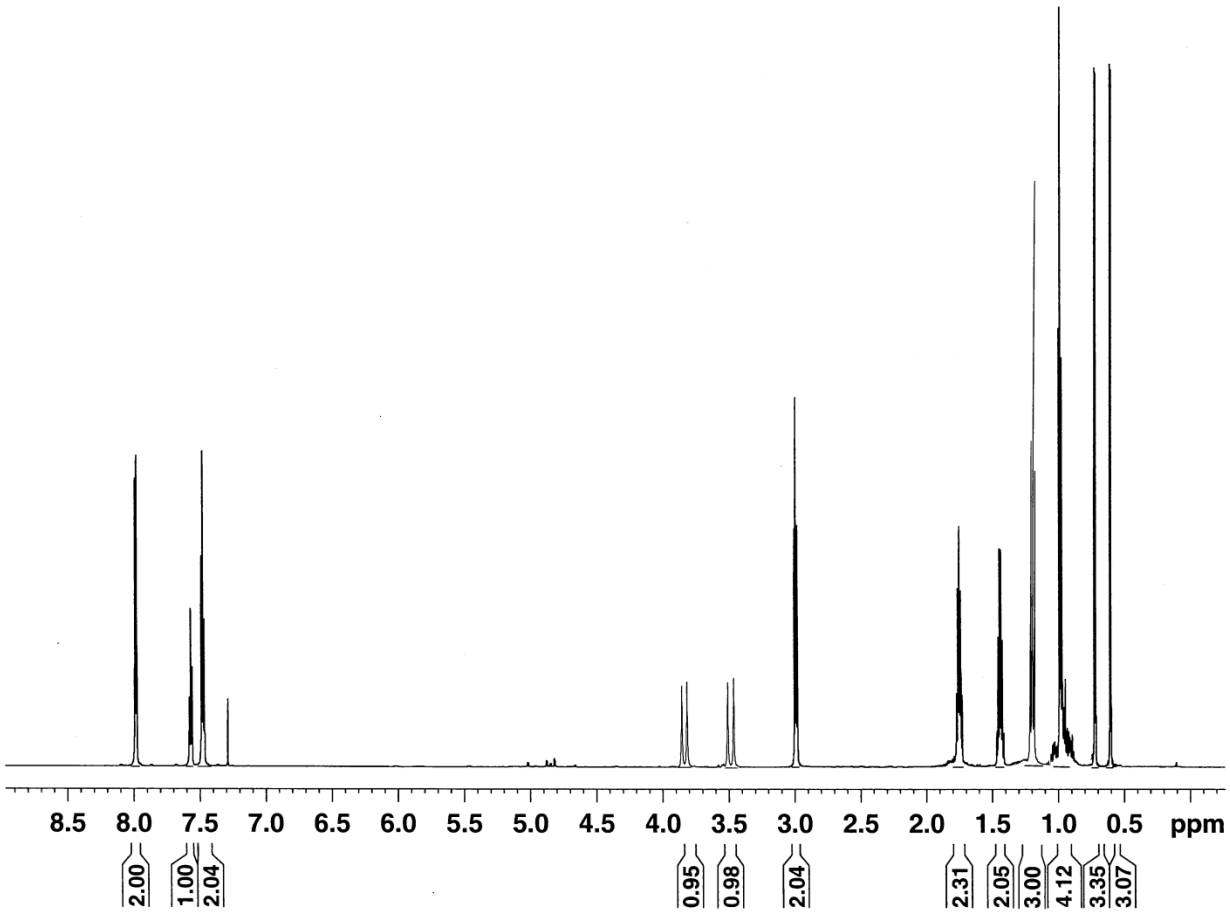
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.227	BV	0.3198	49.98108	0.71471	12.2365
2	26.013	BB	0.3508	58.04732	0.71229	14.5933
3	33.409	BV	0.3107	149.95503	4.76512	35.1783
4	39.932	VB	0.3199	153.98827	4.39991	37.9919



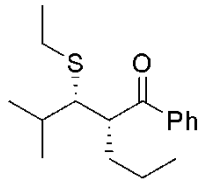
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	22.288	VB	0.1186	4.62785	1.02493	1.1255
2	26.443	BBA	0.2933	28.26716	3.92412	6.8746
3	34.637	BB	0.3594	6.27177	0.77961	1.5253
4	39.841	VB	1.6972	372.01769	73.46691	90.4746



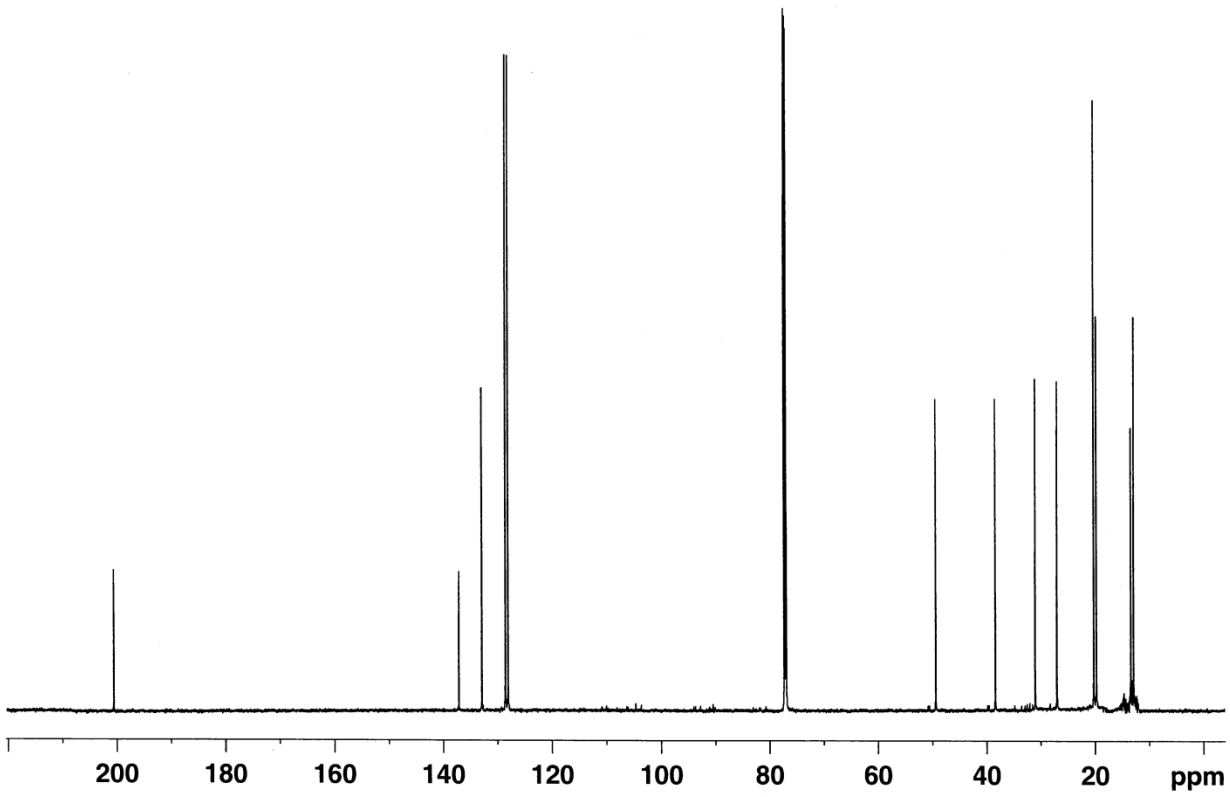
25c



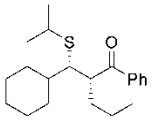
NAME	SS-06-142
EXPNO	1
PROCNO	1
Date_	20130916
Time	13.29
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	24
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	18
DW	42.000 use
DE	6.50 use
TE	298.1 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



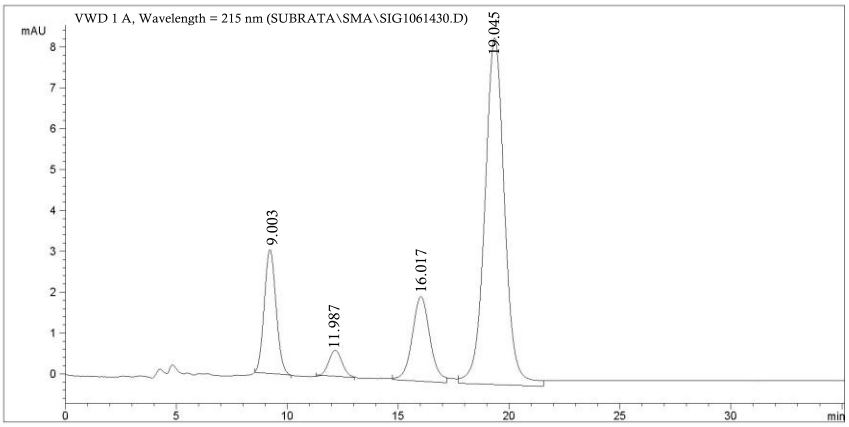
25c



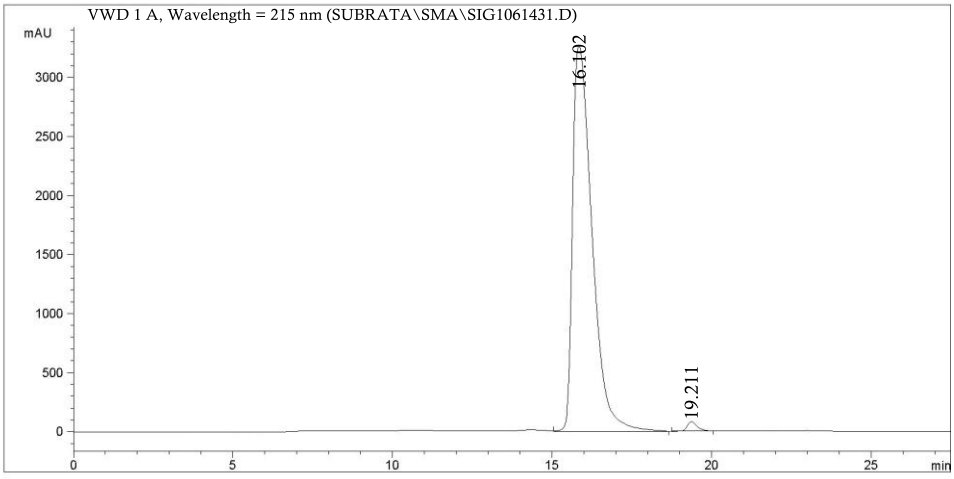
NAME	SS-06-142	
EXPNO	2	
PROCNO	1	
Date_	20130916	
Time	13.33	
INSTRUM	spect	
PROBHD	5 mm CPDCH 13C	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	29	
DS	4	
SWH	41666.668	Hz
FIDRES	0.635783	Hz
AQ	0.7864820	sec
RG	203	
DW	12.000	use
DE	16.50	use
TE	298.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.00	use
PL1	4.50	dB
PL1W	38.14553833	W
SFO1	176.0697436	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	65.00	use
PL2	-3.20	dB
PL12	13.60	dB
PL13	120.00	dB
PL2W	33.59817505	W
PL12W	0.70196527	W
PL13W	0.00000000	W
SFO2	700.1499406	MHz
SI	32768	
SF	176.0521380	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.40	



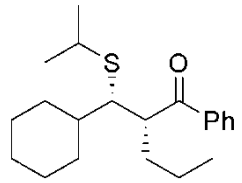
25d



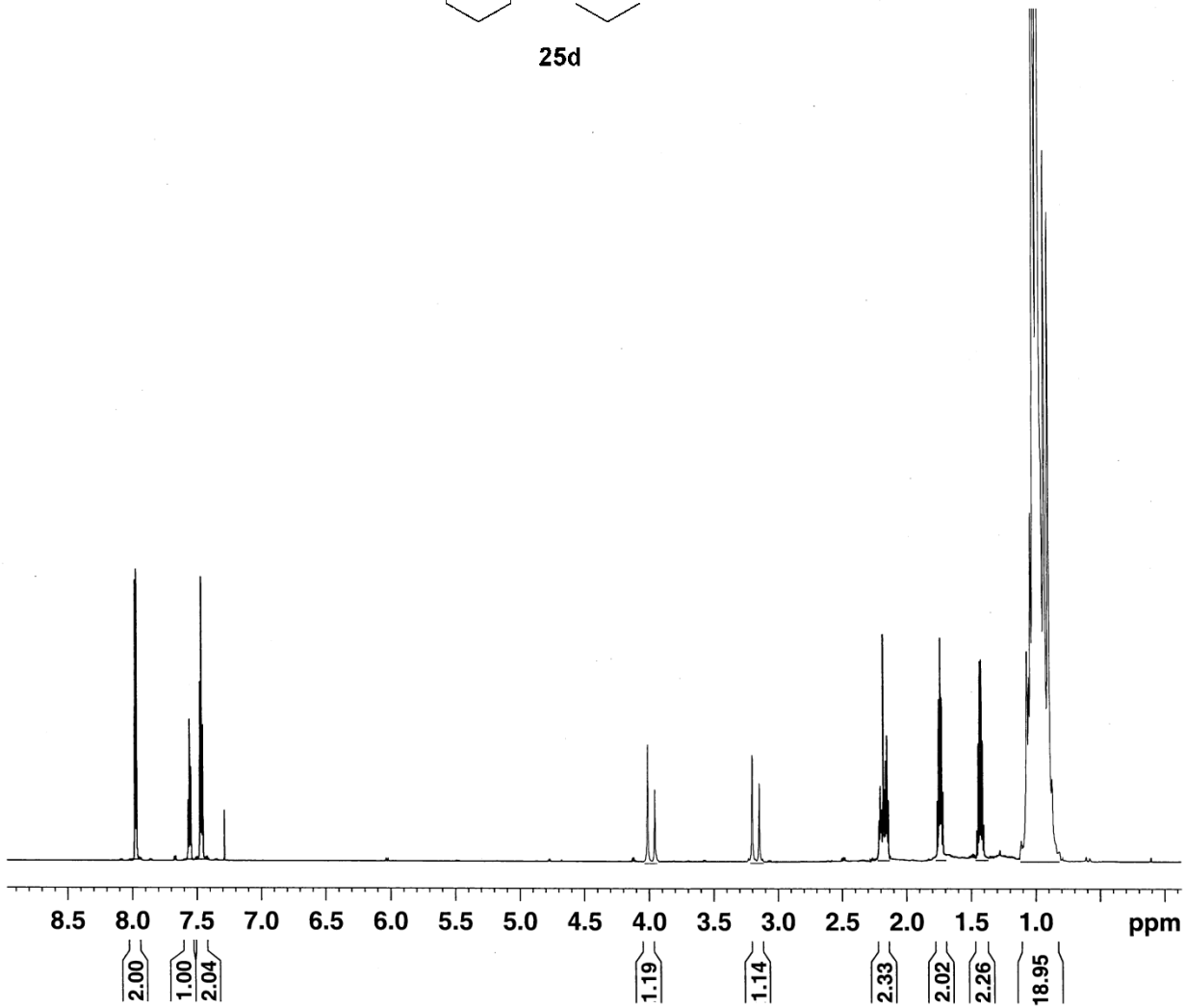
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.003	BV	0.2619	172.88273	3.19409	14.5639
2	11.987	BB	0.2973	41.63982	0.70072	3.5078
3	16.017	BV	0.9361	173.10049	1.95992	14.5825
4	19.045	VB	1.2639	799.41939	8.37319	67.3458



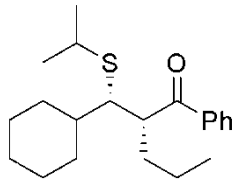
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	16.102	VB	0.7989	4.50028e5	3228.99631	98.1463
2	19.211	BB	0.0761	8499.72833	91.15482	1.8537



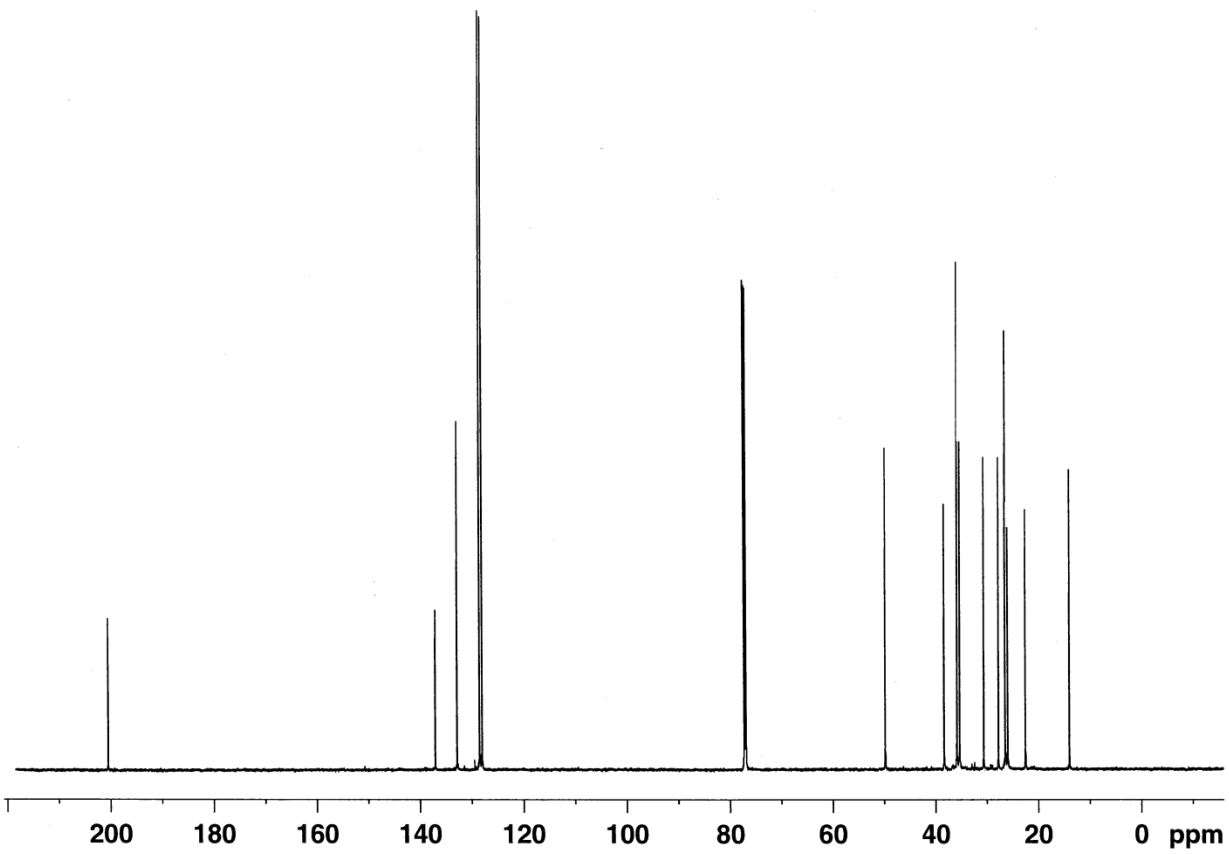
25d



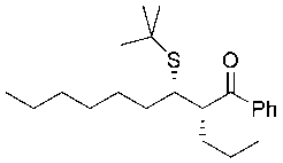
NAME	SS-06-143
EXPNO	1
PROCNO	1
Date_	20130916
Time	13.44
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDC13
NS	14
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	14.2
DW	42.000 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 usec
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



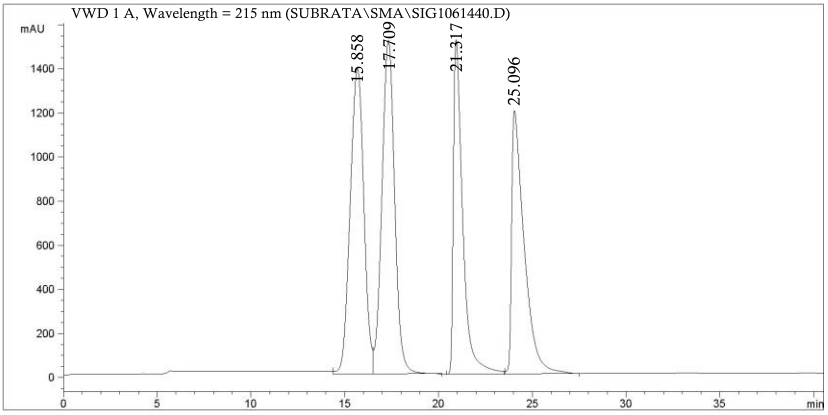
25d



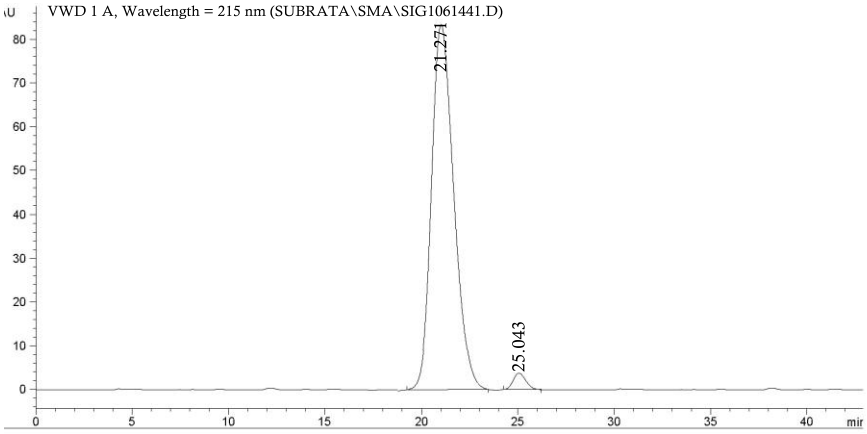
NAME	SS-06-143
EXPNO	2
PROCNO	1
Date_	20130916
Time	13.48
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	13
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 usec
DE	16.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 usec
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 usec
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



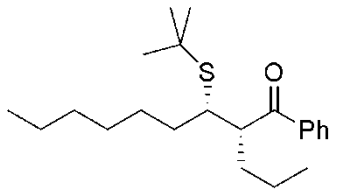
25e



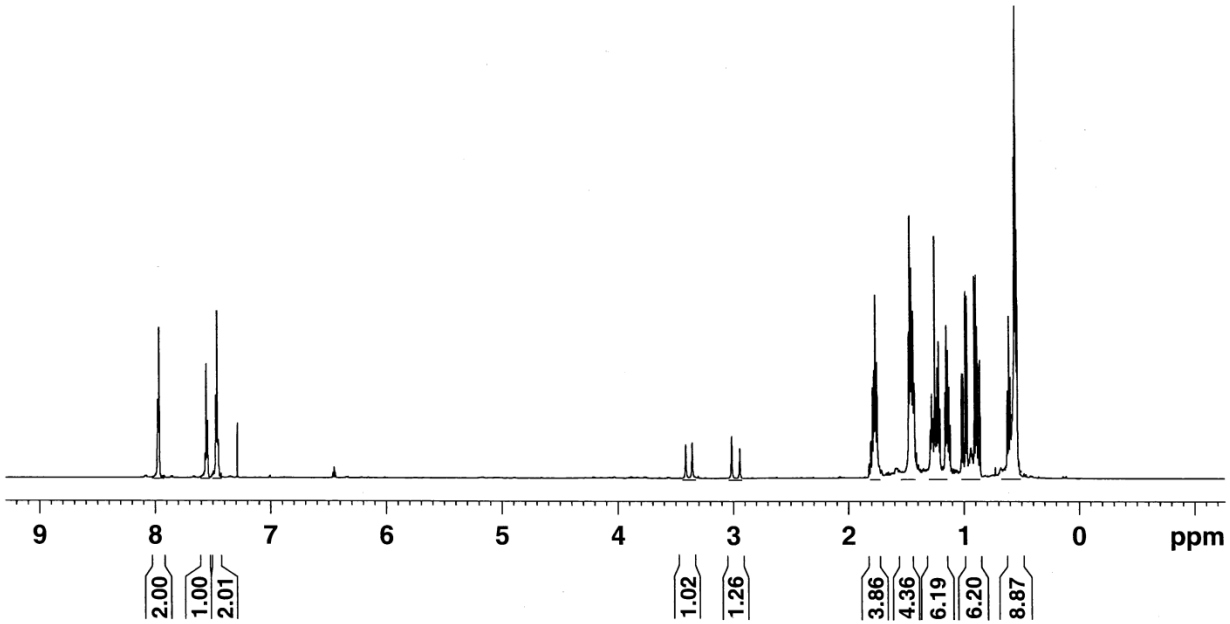
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.858	BB	0.4311	4.30892e5	1473.37919	25.2347
2	17.709	BV	0.4016	4.32818e5	1569.50731	25.3996
3	21.317	BV	0.3718	4. 49731e5	1585.34506	26.3926
4	25.096	VB	0.4439	3.92036e5	1259.64024	22.9731



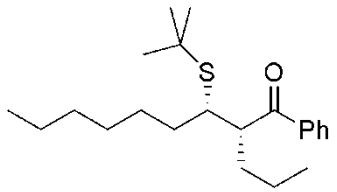
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	21.271	BV	0.9727	8069.37516	82.72091	97.3490
2	25.043	BB	0.1782	219.74456	4.19967	2.6510



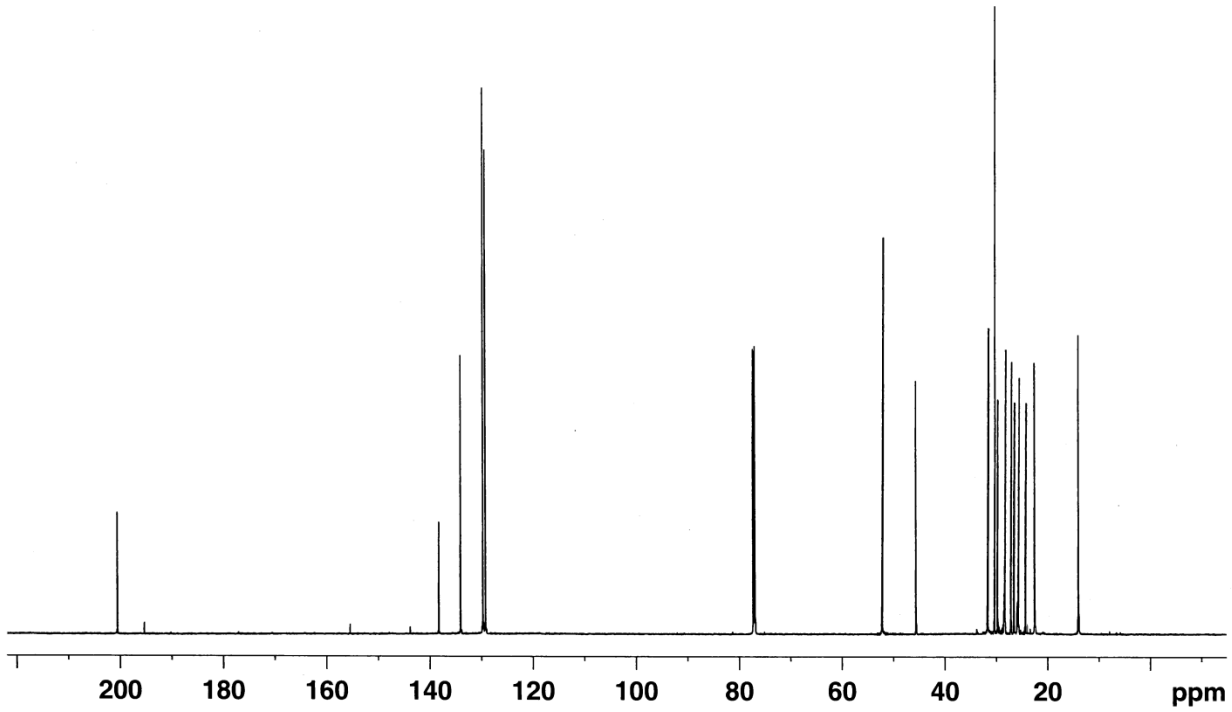
25e



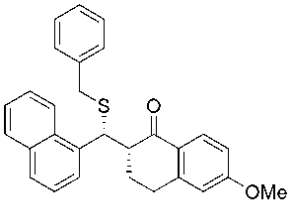
NAME	SS-06-144
EXPNO	1
PROCNO	1
Date_	20130916
Time	13.56
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	15
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	14.2
DW	42.000 use
DE	6.50 use
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



25e



NAME	SS-06-144
EXPNO	2
PROCNO	1
Date_	20130916
Time	14.01
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	45
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



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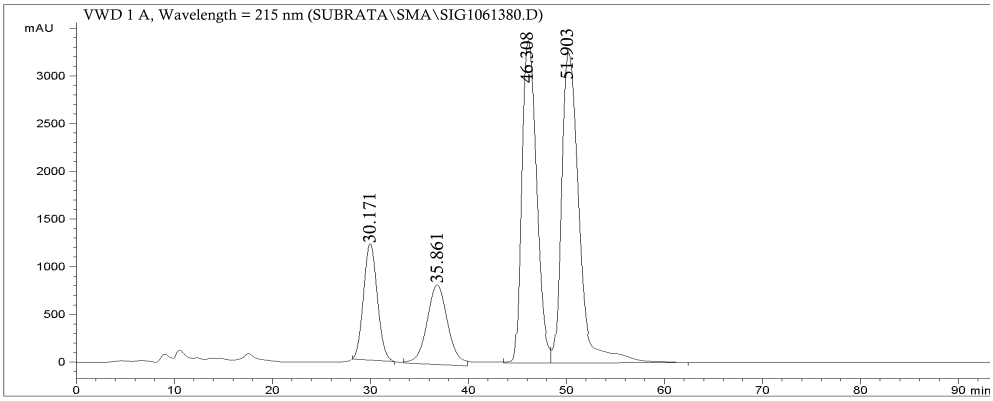
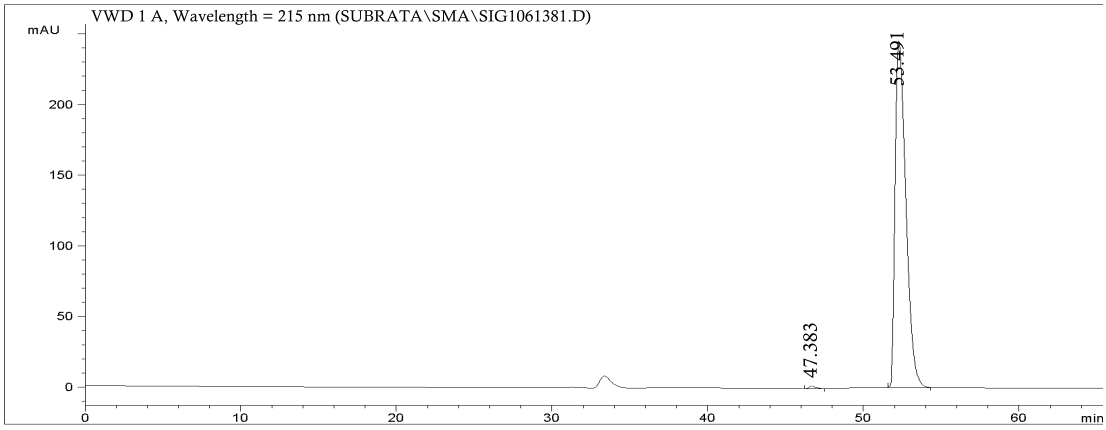
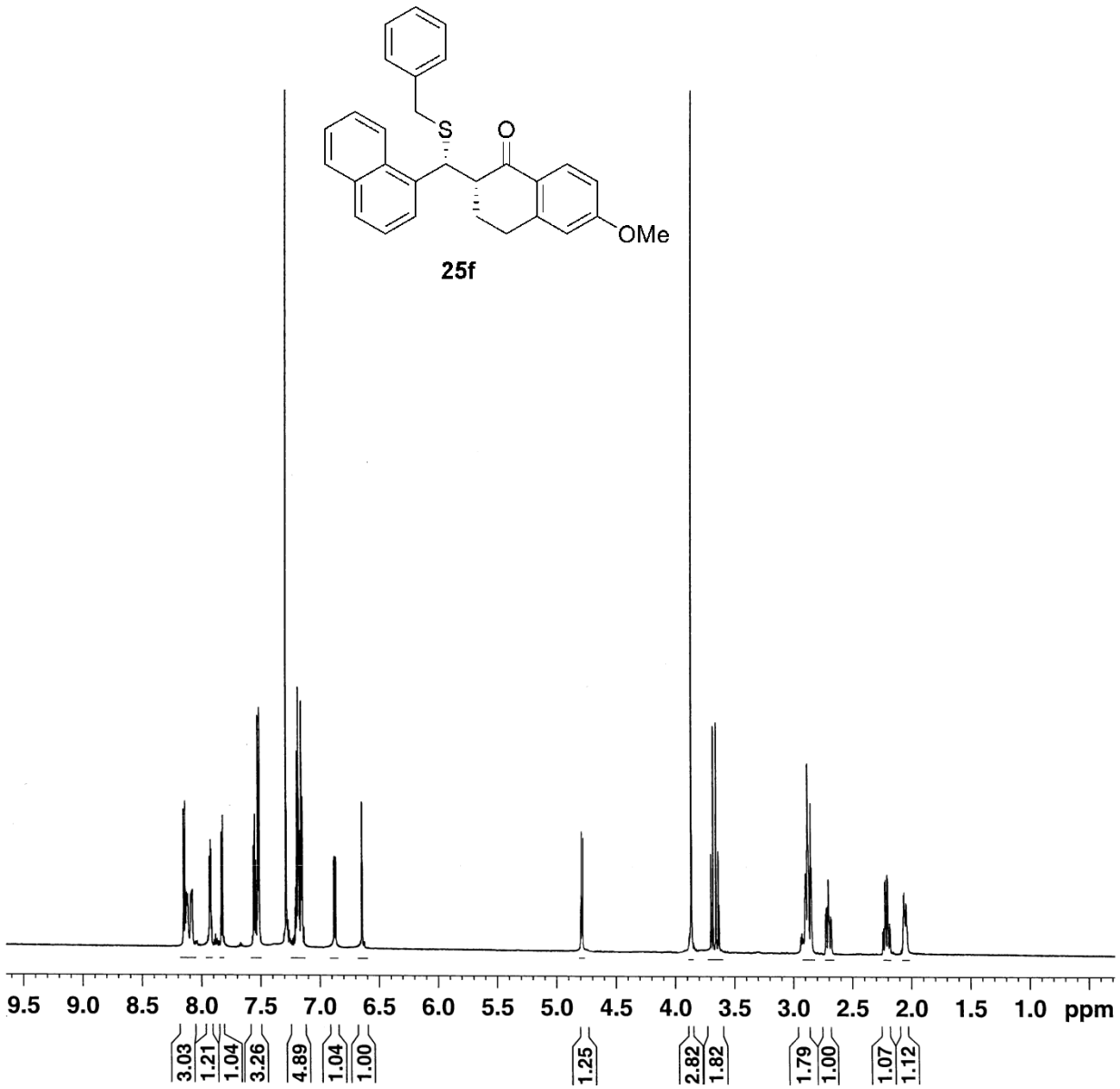


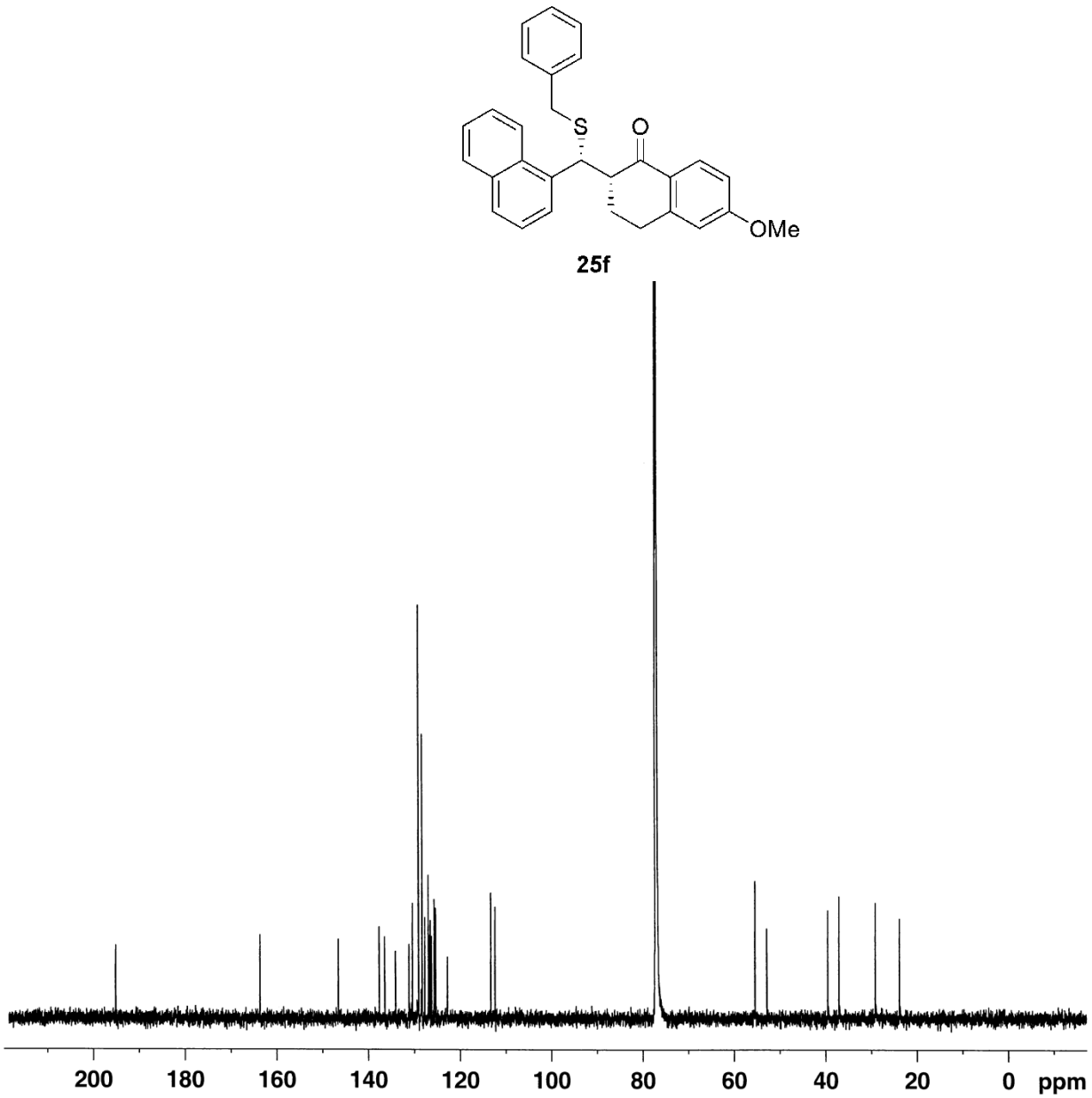
Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	30.171	MM	0.9013	3200.49912	1353.98101	12.1877
2	35.861	MM	1.1275	3208.55372	812.29176	12.2184
3	46.308	BB	0.3782	9863.82011	3412.02338	37.5621
4	51.903	VB	0.3869	9987.13170	3115.06744	38.0318



Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	47.383	MM	0.1075	11.79156	3.07795	0.9014
2	53.491	VV	0.3011	1296.35991	248.83851	99.0986



NAME	SS-06-138
EXPNO	1
PROCNO	1
Date_	20130323
Time	19.47
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zg30
TD	95236
SOLVENT	CDCl3
NS	13
DS	2
SWH	11904.762 Hz
FIDRES	0.125003 Hz
AQ	3.9999621 sec
RG	20.2
DW	42.000 use
DE	6.50 use
TE	298.2 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	1H
P1	9.40 use
PL1	-3.20 dB
PL1W	33.59817505 W
SFO1	700.1516910 MHz
SI	131072
SF	700.1471400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



NAME	SS-06-138
EXPNO	2
PROCNO	1
Date_	20130323
Time	19.49
INSTRUM	spect
PROBHD	5 mm CPDCH 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	334
DS	4
SWH	41666.668 Hz
FIDRES	0.635783 Hz
AQ	0.7864820 sec
RG	203
DW	12.000 use
DE	16.50 use
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.00 use
PL1	4.50 dB
PL1W	38.14553833 W
SFO1	176.0697436 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	65.00 use
PL2	-3.20 dB
PL12	13.60 dB
PL13	120.00 dB
PL2W	33.59817505 W
PL12W	0.70196527 W
PL13W	0.00000000 W
SFO2	700.1499406 MHz
SI	32768
SF	176.0521380 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00