$NaHSO_3$-Promoted Ring Opening of Aziridines and Epoxides with H_2O

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Supporting Information

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1. General Information

^{1}H NMR spectra were taken with a Bruker AVANCE III 600 MHz NMR spectrometers. The chemical shifts are reported in ppm downfield to the $CDCl_3$ resonance (δ = 7.27) and d_6-DMSO (δ = 2.50). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz), integration, and assignment. ^{13}C NMR data were collected at 150 MHz with complete proton decoupling. The chemical shifts are reported in ppm downfield to the central $CDCl_3$ resonance (δ = 77.0) and d_6-DMSO (δ =39.5). Coupling constants in ^{1}H NMR spectra are given in Hz. High-resolution mass spectra were performed on a micrOTOF-Q II instrument with an ESI source. Melting points were measured with a RD-II melting point apparatus and are uncorrected. A variety of aziridines were synthesized from the corresponding alkenes according the literatures[1-2]. The commercially available reagents were used without further purification. All solvents were purchased from commercial sources and used without further purification. Deuterated solvents were purchased from aladdin. All reactions were performed under atmosphere using oven-dried glassware. Column chromatography was performed on silica gel (200-300 mesh).

2. General procedure for the ring openings of aziridines

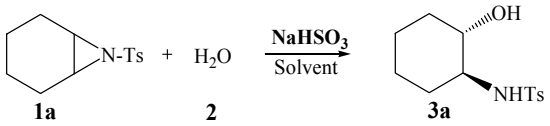
A glasstesttube was charged with *N*-tosylazirdines **1** (0.2 mmol), $NaHSO_3$ (41.9 mg, 2.0 equiv.), acetone (1.5 mL) and H_2O (1.5 mL). The reaction mixture was stirred under air atmosphere at the specified temperature for a period of time. After completion of the reaction, as indicated by TLC, the reaction mixture was evaporated under vacuum. Subsequently, the remainder was extracted with CH_2Cl_2 (2×5 mL) and the $NaHSO_3$ was filtered. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford **3** or **4**.

3. Screening of the reaction condition

Subsequently, the effect of the amount of $NaHSO_3$ was investigated. Trace product was detected in the absence of $NaHSO_3$ (Table 1, entry 1). With the increase of its amount, the yield improved gradually (Table 1, entries 2-4) and the best yield was obtained when 2.0 equiv of $NaHSO_3$ was used (Table 1, entry 4). Screening of the volume of mixture solvent revealed that higher amount led to higher yield (Table 1,

entry 9 *vs.* 4, 6-8). The best 70% yield was obtained when 3.0 mL of mixture solvent was utilized, which was probably due to the solubility and ionization of $NaHSO_3$ (Table 1, entry 9). It was also found that the reaction temperature had a significant influence on the reaction rate. The yield rose following the increase of the temperature and the most suitable temperature was 55 ^oC (Table 1, entry 12). At last, extensive screening showed that the optimal reaction conditions were 0.2 mmol *N*-tosylcyclohexylaziridine **1a** and 2.0 equiv of $NaHSO_3$ in 3.0 mL of acetone/H_2O (1:1) mixture system under air atmosphere at 55 ^oC for 24 h, which provided the ring-opening product with the quantitative transformation and 100% regioselectivity (Table 1, entry 12).

Table 1. Screening of reaction conditions for ring opening of *N*-tosylcyclohexylaziridine **1a** with H_2O[a]



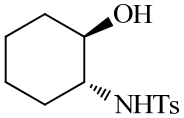
1a **2** **3a**

Entry	Solvent	Amount of $NaHSO_3$ (equiv.)	Solvent dosage (mL)	T (^oC)	Yield[b] (%)
1	Acetone/H_2O=1:1	0	1.0	25	Trace
2	Acetone/H_2O=1:1	0.5	1.0	25	17
3	Acetone/H_2O=1:1	1.5	1.0	25	34
4	Acetone/H_2O=1:1	2.0	1.0	25	37
5	Acetone/H_2O=1:1	2.5	1.0	25	35
6	Acetone/H_2O=1:1	2.0	0.5	25	19
7	Acetone/H_2O=1:1	2.0	1.5	25	48
8	Acetone/H_2O=1:1	2.0	2.0	25	53
9	Acetone/H_2O=1:1	2.0	3.0	25	70
10	Acetone/H_2O=1:1	2.0	3.0	35	84
11	Acetone/H_2O=1:1	2.0	3.0	45	91
12	Acetone/H_2O=1:1	2.0	3.0	55	99

[a] Unless otherwise noted, all reactions were carried out with *N*-tosylcyclohexylaziridine **1a** (50 mg, 0.2 mmol) and $NaHSO_3$ under identified conditions for 24 h. [b] Isolated yield.

3. Characterization of products

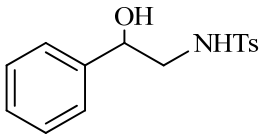
trans-2-(*N*-Tosylamino)-1-cyclohexanol 3a[3]



White solid; mp 128-130 ^oC; ^1H NMR (600 MHz, $CDCl_3$): δ 1.21-1.26 (m, 4H), 1.57-1.59 (m, 1H), 1.64-1.67 (m, 1H), 1.72-1.74 (m, 1H), 1.99-2.02 (m, 1H), 2.43 (s,

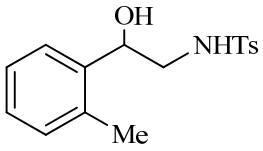
3H), 2.68 (d, J = 3.2 Hz, 1H), 2.84-2.88 (m, 1H), 3.28-3.32 (m, 1H), 5.02 (d, J = 7.1 Hz, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.80 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3481, 3273, 2934, 2861, 1519, 1450, 1322, 1283, 1156 cm^{-1}.

2-(*N*-Tosylamino)-1-phenyl-1-ethanol 3b [4-5]



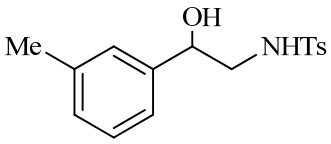
White solid; mp 109-111 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.41 (s,3H), 2.69 (br,1H), 3.01 (dd, J = 12.7, 9.1 Hz, 1H), 3.22 (d, J = 12.0 Hz, 1H), 4.79 (dd, J = 8.8, 3.5 Hz,1H), 5.32 (brs,1H), 7.26-7.32 (m, 7H), 7.72 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3402, 3169, 2921, 2856, 1588, 1486, 1442, 1318, 1151 cm^{-1}.

2-(*N*-Tosylamino)-1-(2-methylphenyl)-1-ethanol 3c



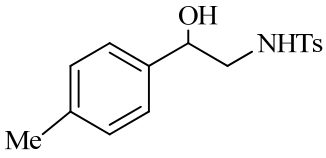
White solid; mp 116-118 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.20 (s, 3H), 2.38 (s, 3H), 2.88-2.93 (m, 1H), 3.11-3.15 (m, 1H), 3.31 (br, 1H), 4.99 (dd, J = 9.2, 2.8 Hz, 1H), 5.76 (brs, 1H), 7.06 (dd, J = 5.3, 3.6 Hz, 1H), 7.12 (dd, J = 5.6, 3.4 Hz, 1H), 7.24 (d, J = 8.2 Hz, 2H), 7.36 (dd, J = 5.5, 2.7 Hz, 1H), 7.71 (d, J = 8.3 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 18.9, 21.5, 49.2, 69.7, 125.4, 126.3, 127.1, 127.8, 129.8, 130.4, 134.6, 136.8, 139.0, 143.5 ppm; MS (ESI): Calcd for $C_{16}H_{19}NO_3S$ [M + Na+] 328.0983, Found 328.0980; IR (neat): 3448, 3145, 2929, 2865, 1609, 1493, 1260, 1217 cm^{-1}.

2-(*N*-Tosylamino)-1-(3-methylphenyl)-1-ethanol 3d



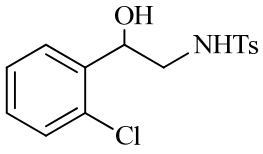
White solid; mp 97-99 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.30 (s, 3H), 2.40 (s, 3H), 2.98-3.02 (m, 1H), 3.12 (br, 1H), 3.17-3.22 (m, 1H), 4.74 (dd, J = 8.8, 3.0 Hz, 1H), 5.45 (br, 1H),7.04-7.07 (m, 3H), 7.18 (td, J = 7.8, 1.4 Hz, 1H), 7.26 (dd, J = 8.5, 0.6 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.4, 21.5, 50.3, 72.8, 122.9, 126.6, 127.1, 128.5, 128.9, 129.8, 136.8, 138.3, 140.9, 143.5 ppm; MS (ESI): Calcd for $C_{16}H_{19}NO_3S$ [M + Na+] 328.0983, Found 328.0981; IR (neat): 3513, 3281, 3032, 2924, 2870, 1601, 1493, 1330, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(4-methylphenyl)-1-ethanol 3e



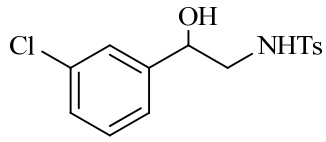
White solid; mp 132-134 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.31 (s, 3H), 2.41 (s,3H),2.96 (br, 1H), 2.97-3.01 (m, 1H), 3.16-2.20 (m, 1H), 4.74 (dd, J = 8.9, 3.4 Hz, 1H), 5.44 (br, 1H), 7.10 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.1 Hz, 2H), 7.27 (d, J = 7.9 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3502, 3264, 3054, 2924, 2854, 1601, 1493, 1325, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(2-chlorophenyl)-1-ethanol 3f



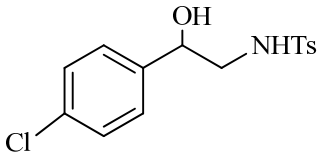
White solid; mp 105-107 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.40 (s, 3H), 2.93-2.98 (m, 1H), 3.25 (d, J = 4.0 Hz, 1H), 3.33-3.37 (m, 1H), 5.14-5.17 (m, 1H), 5.44 (dd, J = 7.6, 5.0 Hz, 1H), 7.18 (td, J = 7.6, 1.7 Hz, 1H), 7.23 (dd, J = 7.6, 1.3 Hz, 1H), 7.25-7.27 (m, 3H), 7.52 (dd, J = 7.6, 1.7 Hz, 1H), 7.73 (d, J = 8.3 Hz, 1H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 48.4, 69.5, 127.2, 127.5, 129.1, 129.4, 129.8, 131.6, 136.6, 138,2, 143.6 ppm; MS (ESI): Calcd for $C_{15}H_{16}ClNO_3S$ [M + Na+] 348.0437, Found 348.0433; IR (neat): 3502, 3281, 3064, 2929, 2854, 1601, 1498, 1331, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(3-chlorophenyl)-1-ethanol 3g[6]



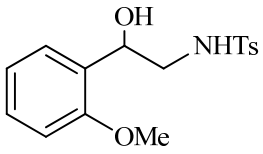
White solid; mp 126-129 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.41 (s, 3H), 2.95-2.99 (m, 1H), 3.16-3.20 (m, 1H), 4.79 (dd, J = 8.6, 3.4 Hz, 1H), 5.41 (dd, J = 7.4, 5.2 Hz, 1H), 7.19 (d, J = 8.5 Hz, 2H), 7.25 (dd, J = 6.5, 1.8 Hz, 2H), 7.27 (d, J = 8.6 Hz, 2H), 7.69 (J = 8.3 Hz, 2H) ppm; IR (neat): 3428, 3314, 2942, 2861, 1598, 1486, 1335, 1156 cm^{-1}.

2-(*N*-Tosylamino)-1-(4-chlorophenyl)-1-ethanol 3h



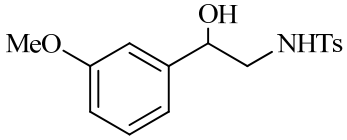
White solid; mp 135-137 °C; ^{1}HNMR (600 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.94-2.97 (m, 1H), 3.15-3.18 (m, 1H), 3.34 (br, 1H), 4.76-4.79 (m, 1H), 5.65 (br, 1H), 7.12-7.26 (m, 6H), 7.68 (dd, J = 8.2, 6.5 Hz, 2H); IR(neat): 3502, 3286, 3070, 2924, 2854, 1601, 1493, 1325, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(2-methoxyphenyl)-1-ethanol 3i



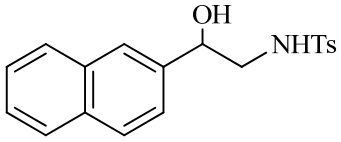
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.41 (s, 3H), 3.02 (br, 1H), 3.04-3.09 (m, 1H), 3.31-3.35 (m, 1H), 3.78 (s, 3H), 4.94 (dd, J = 8.4, 3.5 Hz, 1H), 5.16 (dd, J = 8.0, 4.3 Hz, 1H), 6.82 (d, J = 7.4 Hz, 1H), 6.93 (t, J = 7.4 Hz, 1H), 7.24 (td, J = 7.9, 1.7 Hz, 1H), 7.27 (d, J =7.9 Hz, 3H), 7.72 (d, J = 8.3 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 48.4, 55.3, 69.1, 110.4, 120.9, 127.0, 127.2, 128.6, 129.1, 129.7, 137.0, 143.4, 156.2 ppm; MS (ESI): Calcd for $C_{16}H_{19}NO_4S$ [M + Na+] 344.0932, Found 344.0928; IR (neat): 3502, 3286, 3064, 2924, 2853, 1601, 1493, 1325, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(3-methoxyphenyl)-1-ethanol 3j



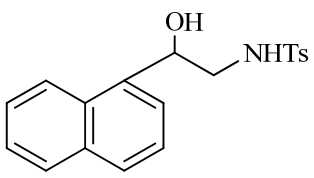
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.40 (s, 3H), 2.97 (br, 1H), 2.99-3.03 (m, 1H), 3.20-3.24 (m, 1H), 3.76 (s, 3H), 4.76 (dd, J = 8.7, 3.3 Hz, 1H), 5.29 (dd, J = 8.0, 4.7 Hz, 1H), 6.80 (dd, J = 8.2, 2.5 Hz, 1H), 6.83-6.84 (m, 2H), 7.21 (t, J = 8.0 Hz, 1H), 7.27 (d, J = 8.1 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.5, 50.2, 55.3, 72.7, 111.4, 113.7, 118.1, 127.1, 129.7, 129.8, 136.7, 142.6, 143.6, 159.8 ppm; MS (ESI): Calcd for $C_{16}H_{19}NO_4S$ [M + Na+] 344.0932, Found 344.0930; IR (neat): 3502, 3286, 3064, 2924, 2854, 1601, 1493, 1325, 1158 cm^{-1}.

2-(*N*-Tosylamino)-1-(Naphthalene-2-yl)-1-ethanol 3k[6]



White solid; mp 125-127 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.62 (br, 1H), 3.09-3.13 (m, 1H), 3.31-3.35 (m, 1H), 4.96 (dd, J = 8.4, 3.6 Hz, 1H), 5.17 (br, 1H), 7.23 (d, J = 8.0 Hz, 2H), 7.35 (dd, J = 8.5, 1.6 Hz, 1H), 7.46-7.49 (m, 2H), 7.70 (d, J = 8.3 Hz, 2H), 7.74 (s, 1H), 7.77-7.81 (m, 3H) ppm; IR (neat): 3465, 3313, 2951, 2923, 2839, 1601, 1489, 1331, 1147 cm^{-1}.

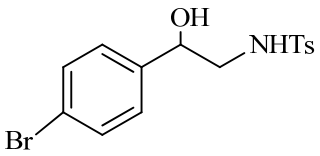
2-(*N*-Tosylamino)-1-(Naphthalene-1-yl)-1-ethanol 3l



White solid; mp 160-162 ^{o}C; ^{1}HNMR (600 MHz, d_6-DMSO): δ 2.31 (s, 3H), 2.86-2.90 (m, 1H), 3.08 (m, 1H), 3.39 (s, 1H), 5.38-5.39 (m, 1H), 5.71 (d, J = 4.1 Hz, 1H), 7.31 (d, J = 8.0 Hz, 2H), 7.46-7.49 (m, 2H), 7.64 (d, J = 7.1 Hz, 1H), 7.68 (d, J = 8.2 Hz, 2H), 7.80 (d, J = 8.1 Hz, 1H), 7.84 (s, 1H), 7.90 (d, J = 7.9 Hz, 1H), 8.01 (d , J = 8.3 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6): δ 21.4, 50.4, 69.3, 123.3, 124.0,

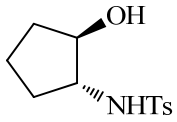
125.9, 126.0, 126.5, 127.0, 128.1, 129.2, 130.0, 130.4, 133.7, 138.1, 139.1, 143.0 ppm; MS (ESI): Calcd for $C_{19}H_{19}NO_3S$ [M + Na+] 364.0983, Found 364.0979; IR (neat): 3416, 3183, 3064, 2940, 2919, 2854, 1601, 1493, 1320, 1142 cm^{-1}.

2-(*N*-Tosylamino)-1-(4-bromophenyl)-1-ethanol 3m



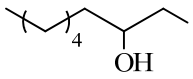
White solid; mp 145-147 °C; ^{1}H NMR (600 MHz,$CDCl_3$): δ 2.42 (s, 3H), 2.93 (br, 1H), 2.95-3.00(m, 1H), 3.18-3.22 (m, 1H), 4.78 (dd, J = 8.5, 3.4 Hz, 1H), 5.24 (m, 1H), 7.15(d, J = 8.4 Hz, 2H), 7.28 (d, J = 8.1 Hz, 2H), 7.42 (d , J = 8.4 Hz, 2H), 7.69 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3524, 3243, 3048,2924, 2854, 1601, 1493, 1320, 1158 cm^{-1}.

trans- 2-(*N*-Tosylamino)-1-cyclopentanol 3o[7-8]



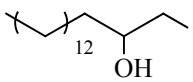
White solid; mp 86-88 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.28-1.35 (m, 1H), 1.45-1.60 (m, 3H), 1.78-1.84 (m, 1H), 1.90-1.95 (m, 1H), 2.40 (s, 3H), 3.06 (br, 1H), 3.22 (dd, J = 8.0, 6.2 Hz, 1H), 4.01 (q, J = 6.8 Hz, 1H), 5.64 (br, 1H), 7.28 (d, J = 8.3 Hz, 2H), 7.77 (d, J = 8.3 Hz, 2H) ppm; IR (neat): 3465, 3186, 3067, 2951, 2843, 1612, 1599, 1510, 1493, 1261, 1127 cm^{-1}.

2-(*N*-Tosylamino)octan-1-ol 3p



Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.82-0.88 (m, 3H), 1.08-1.09 (m, 3H), 1.16-1.19 (m, 1H), 1.24-1.27 (m, 2H), 1.32-1.34 (m, 1H), 1.39-1.43 (m, 1H), 1.77 (s, 2H), 2.43 (s, 3H), 3.22 (br, 1H), 3.47-3.50 (m, 1H), 3.56-3.58 (m, 1H), 4.69 (d, J = 7.6 Hz, 1H), 5.30 (s, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.77 (d, J = 8.2 Hz, 2H) ppm; IR (neat): 3507, 3286, 2950, 2919, 2854, 1601, 1514, 1330, 1158 cm^{-1}.

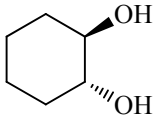
2-(*N*-Tosylamino) hexadecan-1-ol 3q



White solid; mp 43-45 °C; ^{1}H NMR (600 MHz, $CDCl_3$): δ 0.86-0.90 (m, 3H), 1.16-1.28 (m, 24H),1.38-1.45 (m, 3H), 1.66 (s, 1H), 2.43 (s, 3H), 2.86 (d, J = 6.4 Hz, 2H), 4.91 (t, J = 6.4 Hz, 1H), 7.31 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$): δ 14.0, 14.1, 21.5, 23.1, 23.3, 25.5, 29.3, 29.5, 29.7, 30.1, 31.7, 31.9, 36.5, 36.8, 50.3, 73.9,

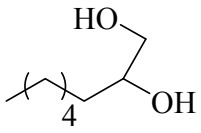
137.1, 129.7, 136.8, 143.3 ppm; MS (ESI): Calcd for $C_{23}H_{41}NO_3S$ [M + Na+] 434.2705, Found 434.2703; IR (neat): 3443, 3145, 2962, 2929, 2865, 1601, 1493, 1320, 1153 cm^{-1}.

trans-1,2-Cyclohexanediol 3r[9]



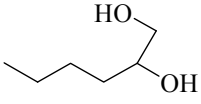
White solid; mp 103-104 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 1.25-1.27 (m, 4H), 1.17 (s, 2H), 1.97-1.98 (m, 2H), 2.21 (br, 2H), 3.36 (s, 2H) ppm; IR (neat): 3369, 3271, 2933, 2869, 2627, 1606, 1468, 1364 cm^{-1}.

octane-1,2-diol



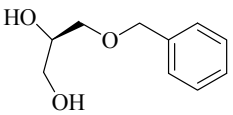
^1H NMR (600 MHz, $CDCl_3$): δ 0.87-0.90 (t, 3H), 1.28-1.44 (m, 10H), 2.82 (s, 2H), 3.41-3.44 (m, 1H), 3.63-3.70 (m, 2H) ppm.

hexane-1,2-diol



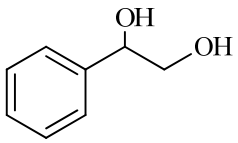
^1H NMR (600 MHz, $CDCl_3$): δ 0.89-0.93 (t, 3H), 1.31-1.44 (m, 6H), 2.97 (s, 2H), 3.40-3.45 (m, 1H), 3.63-3.70 (m, 2H) ppm.

(R)-3-(benzyloxy)propane-1,2-diol



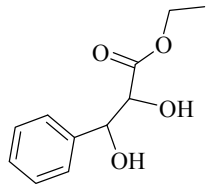
^1H NMR (600 MHz, $CDCl_3$): δ 2.34 (s, 1H), 2.81 (s, 1H), 3.52-3.59 (m, 2H), 3.61-3.72 (m, 2H), 3.88-3.92 (m, 1H), 4.55 (s, 2H), 7.30-7.38 (m, 5H) ppm.

1-Phenyl-1, 2-ethanediol 3s[10]



White solid; mp 66-67 °C; ^1H NMR (600 MHz, $CDCl_3$): δ 3.01 (brs, 2H), 3.62-3.65 (m, 1H), 3.73 (s, 1H), 4.79 (s, 1H), 7.27-7.36 (m, 5H) ppm; IR (neat): 3316, 3204, 3085, 3062, 2966, 1636, 1490 cm^{-1}.

ethyl 2,3-dihydroxy-3-phenylpropanoate



^1H NMR (600 MHz, $CDCl_3$): δ 1.14-1.16 (t, 3H), 2.95-2.97 (d, 1H), 3.26-3.27 (d, 1H), 4.11-4.12 (d, 1H), 4.24-4.25 (d, 2H), 4.90-5.10 (d, 1H), 7.29-7.40 (m, 5H) ppm.

4. Reference

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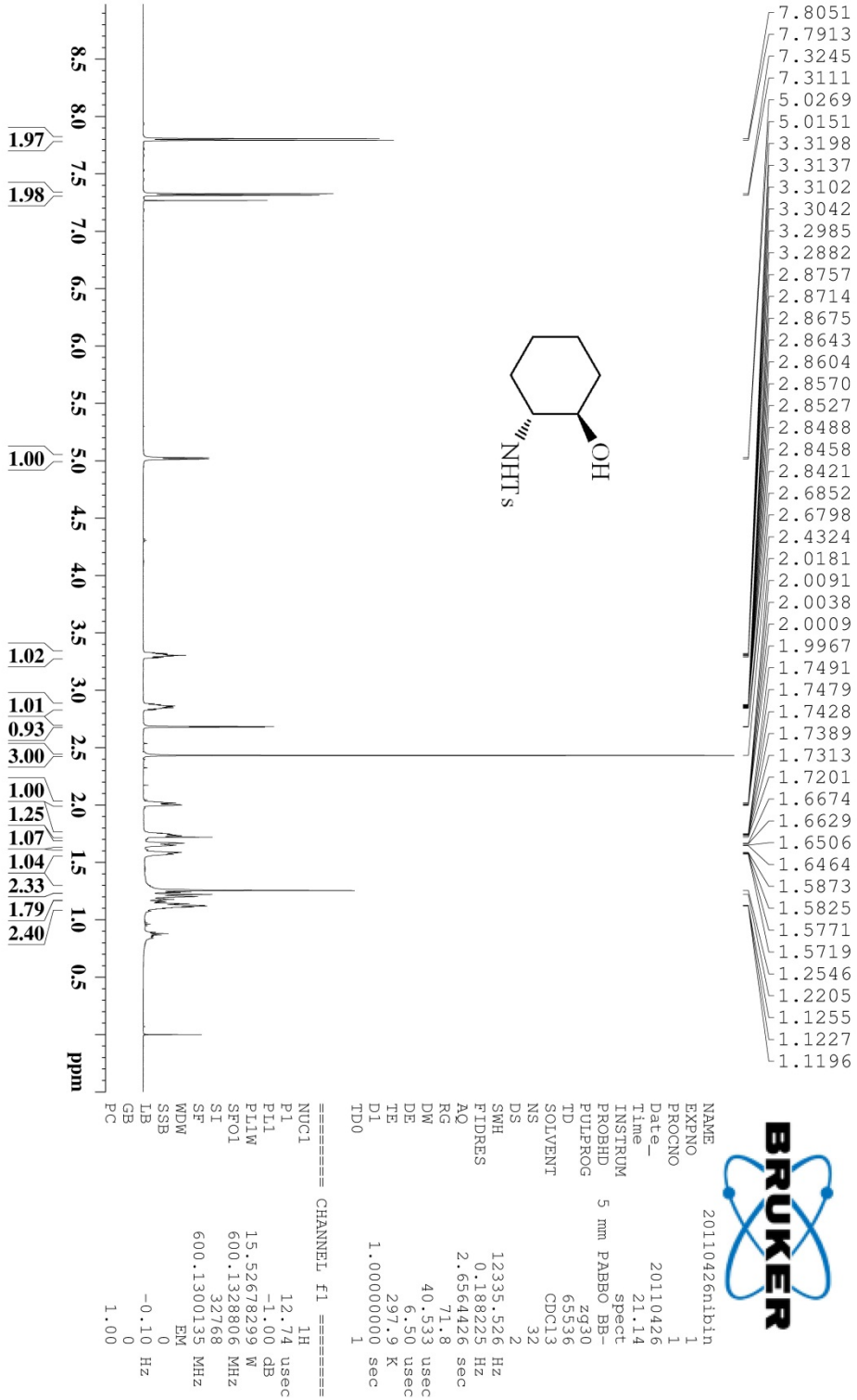
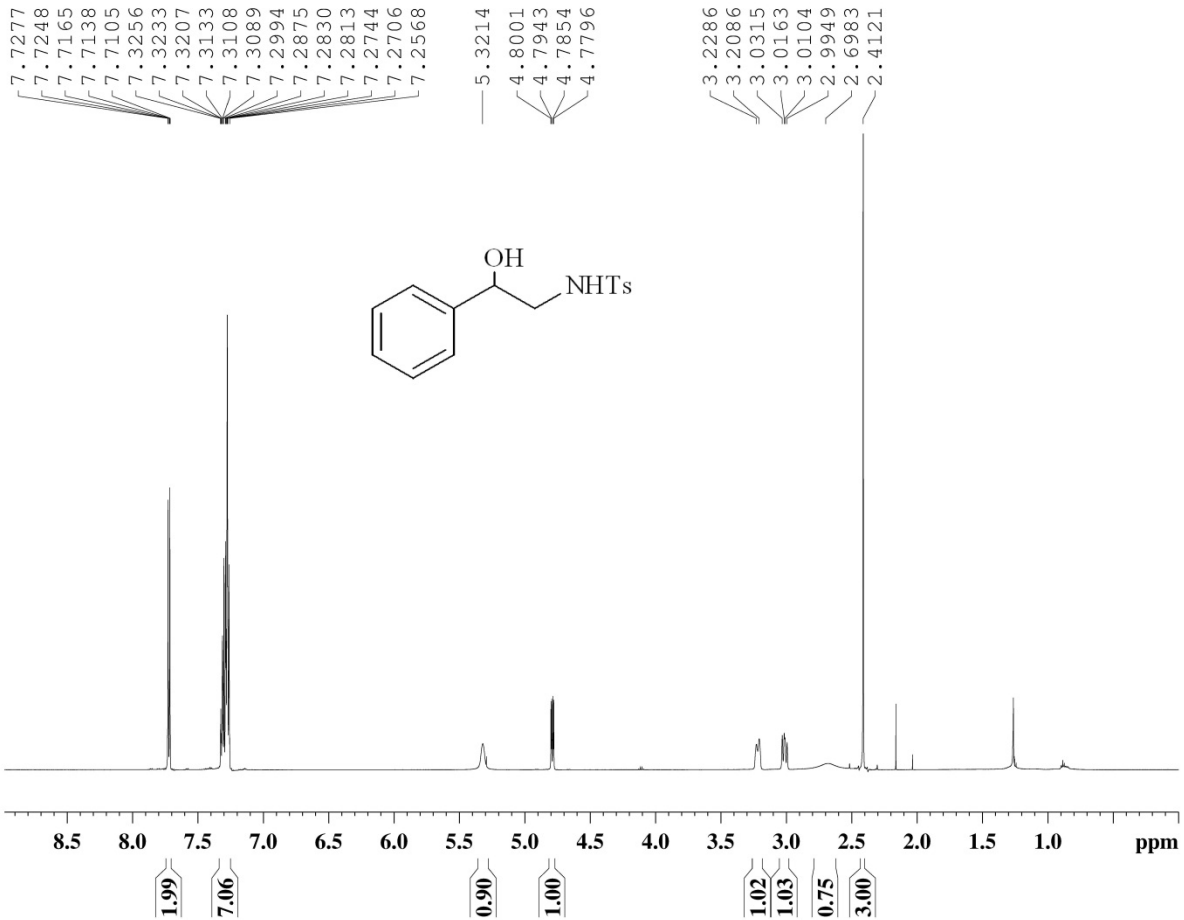
5. NMR spectrum of products





BRUKER

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EXPNO	6
PROCNO	1
Date_	20110822
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TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	57
DW	40.533 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
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P1	12.60 usec
SI	32768
SF	600.1300154 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00

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7.7048
7.7022
7.3685
7.3624
7.3594
7.3532
7.2450
7.2314
7.1299
7.1243
7.1205
7.1148
7.0640
7.0578
7.0551
7.0491
5.7548
5.0028
4.9981
4.9875
4.9827
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2.9200
2.9105
2.9040
2.8975
2.8879
2.8820
2.3749
2.1995
2.9262
3.1088
OH
Me
NHTs
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1.03
2.10
2.02
1.00
1.02
1.04
1.01
1.04
1.04
3.06
3.00
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
BRUKER
NAME 20110809nibin
EXPNO 3
PROCNO 1
Date_ 20110809
Time_ 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 16
DW 40.533 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
======== CHANNEL f1 ========
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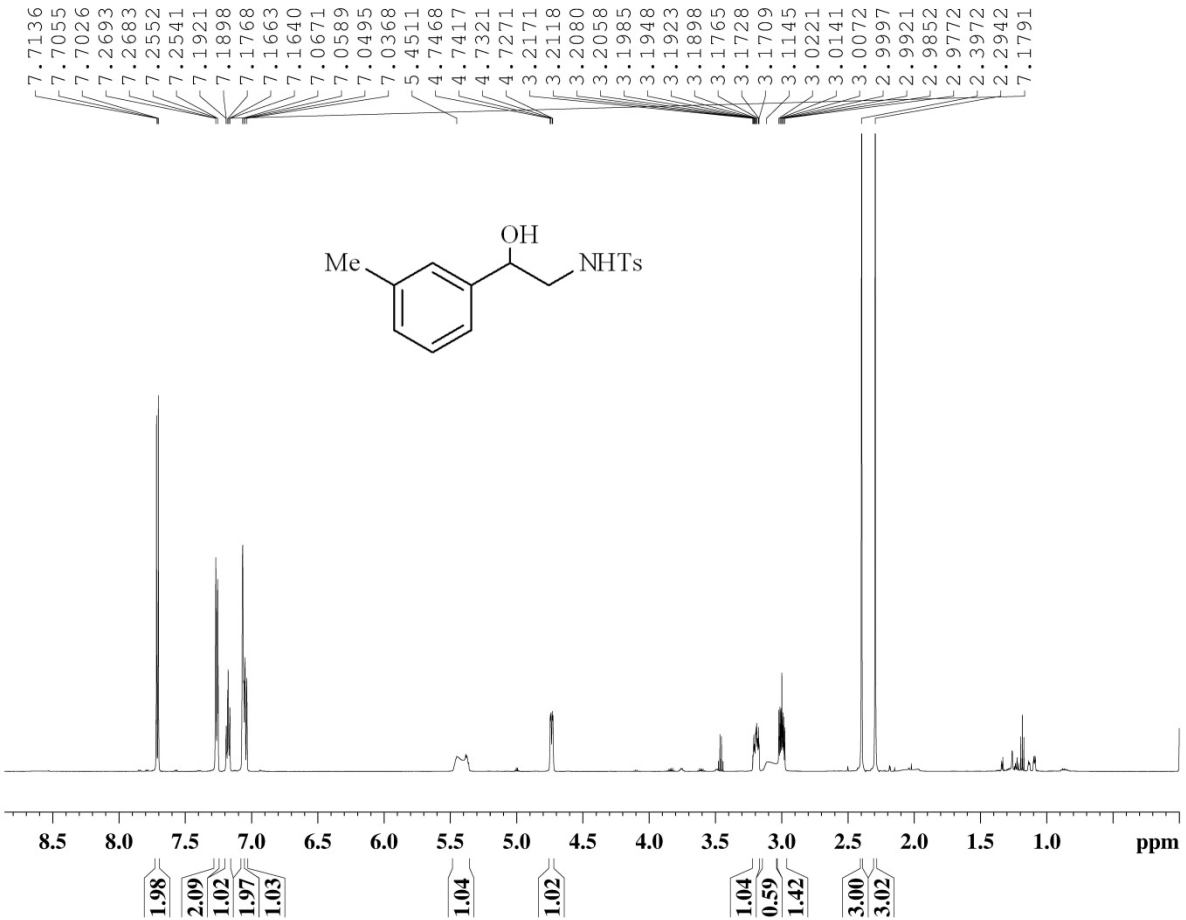
SI 32768
SF 600.1300326 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



BRUKER

NAME	20110726nibin
EXPNO	1
PROCNO	1
Date_	20110726
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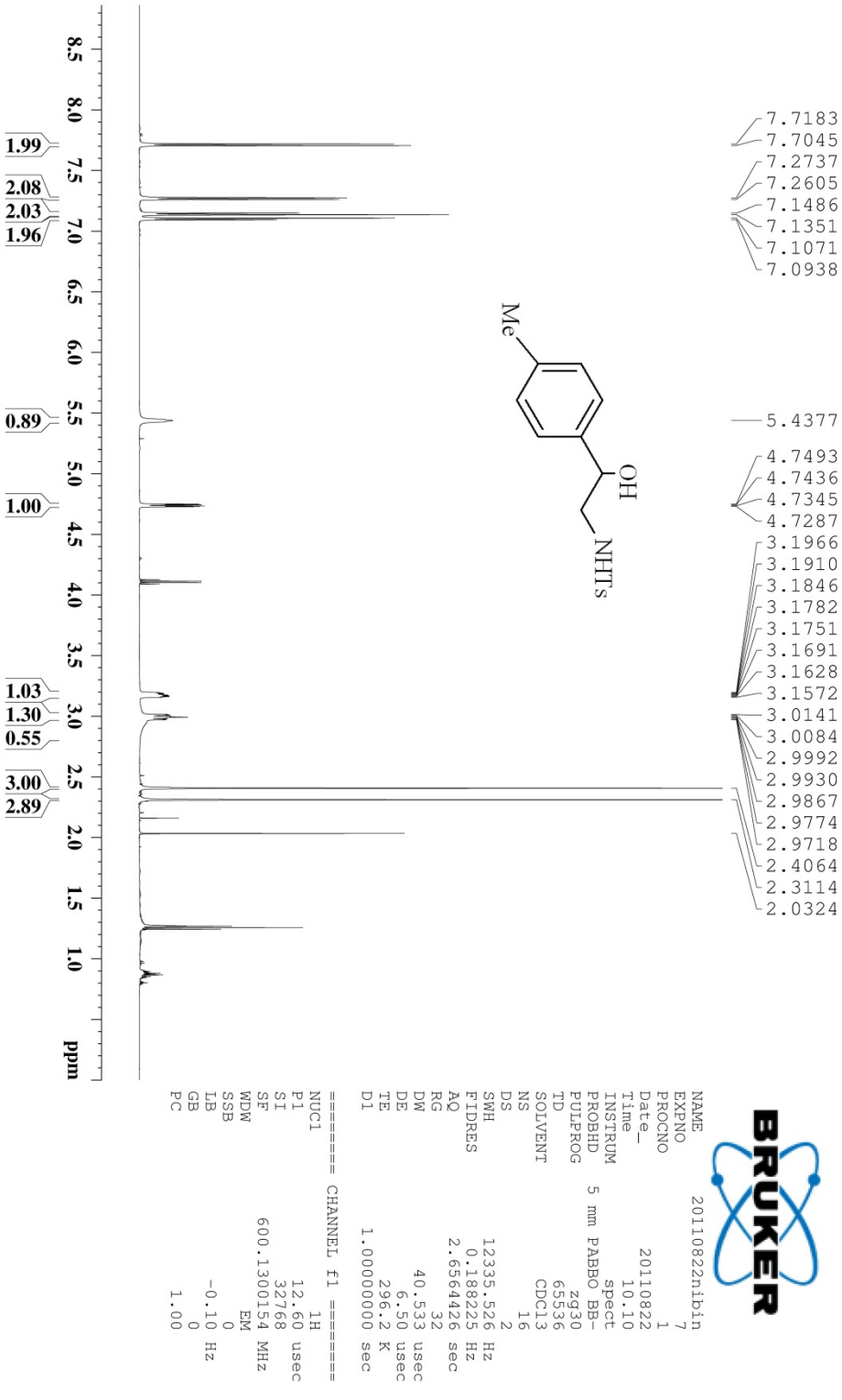
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	40.3
DW	40.533 usec
DE	6.50 usec
TE	299.5 K
D1	1.00000000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300224 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00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7.1071
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5.4377
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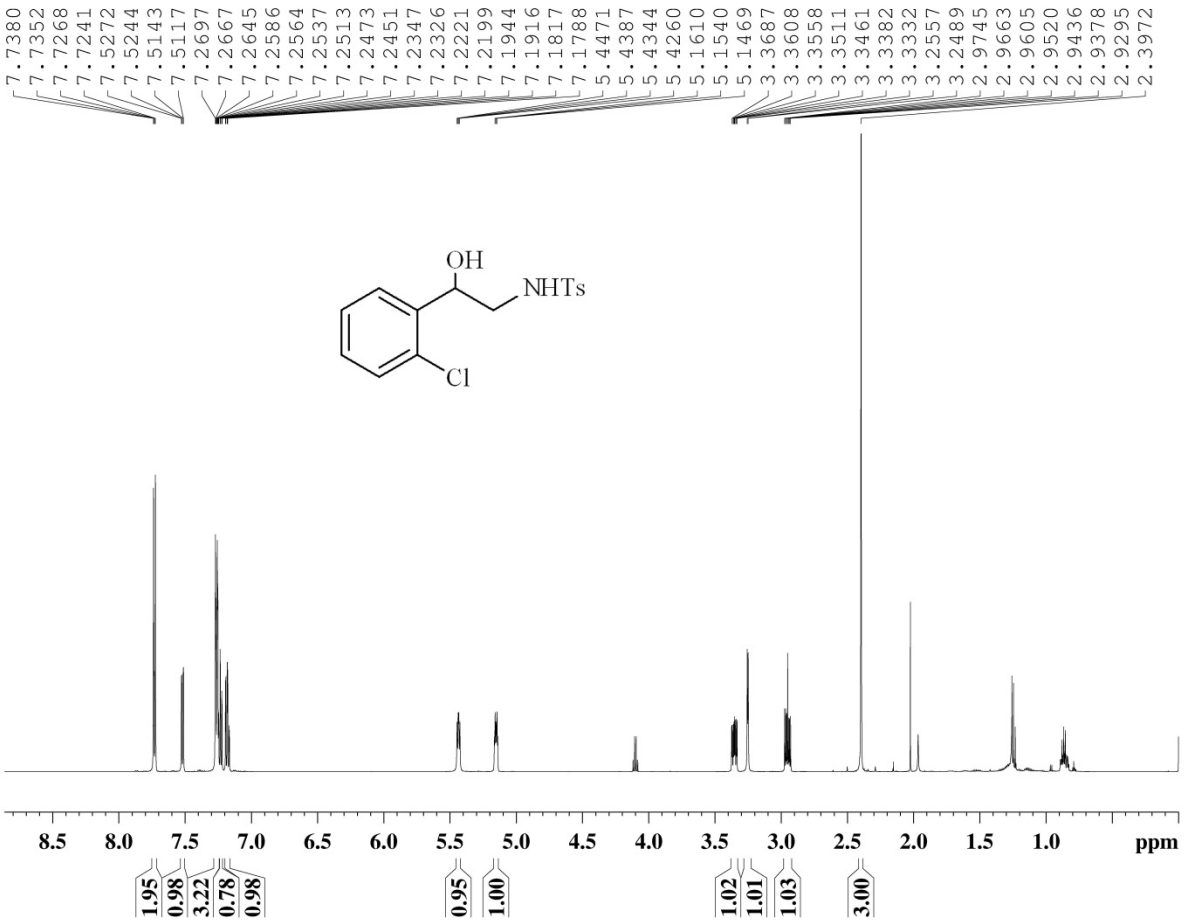
4.7436
4.7345
4.7287
3.1966
3.1910
3.1846
3.1782
3.1751
3.1691
3.1628
3.1572
3.0141
3.0084
2.9992
2.9930
2.9867
2.9774
2.9718
2.4064
2.3114
2.0324
Me
OH
NHTs
1.99
2.08
2.03
1.96
0.89
1.00
1.03
1.30
0.55
3.00
2.89
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
ppm
BRUKER
NAME 20110822nibin
EXPNO 7
PROCNO 1
Date_ 20110822
Time 10.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 32
DW 40.533 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
SI 32768
SF 600.1300154 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



BRUKER

NAME	20110809nibin
EXPNO	4
PROCNO	1
Date_	20110809
Time	15.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	40.3
DW	40.533 usec
DE	6.50 usec
TE	299.3 K
D1	1.00000000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300172 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00

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5.4104
5.4018
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4.7924
4.7837
4.7780
3.2026
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3.1804
3.1746
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2.9798
2.9717
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Cl
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NHTs
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
BRUKER
NAME 20110822nibin
EXPNO 10
PROCNO 1
Date_ 20110822
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 45.2
DW 40.533 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
======== CHANNEL f1 ========
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SSB 0
LB -0.10 Hz
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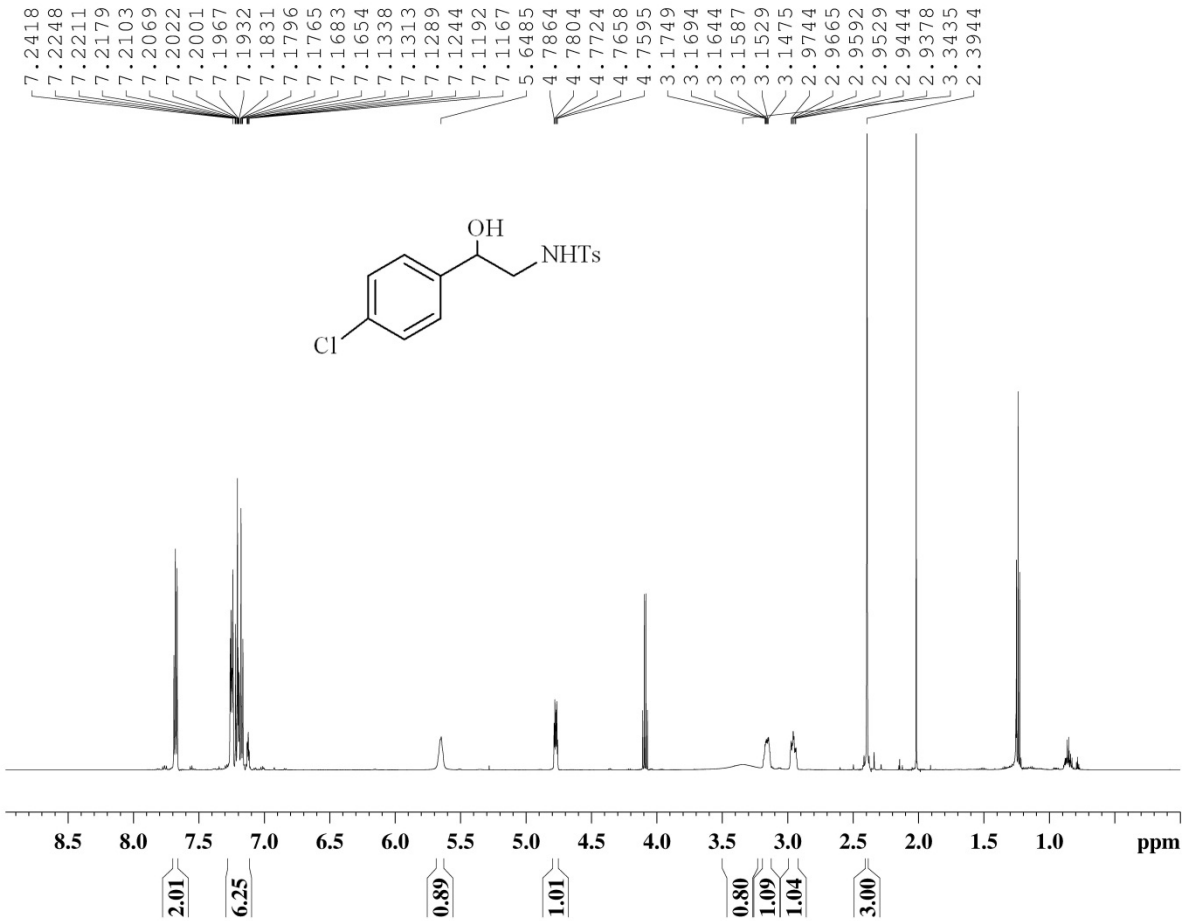
PC 1.00



BRUKER

NAME	20110822nibin
EXPNO	5
PROCNO	1
Date_	20110822
Time	10.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	28.5
DW	40.533 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300154 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00

7.7181
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7.2278
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5.1466
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4.9297
3.7758
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3.3126
3.0871
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3.0729
3.0656
3.0582
3.0513
3.0441
2.4099
3.0234
OMe
OH
NHTs
1.94
2.90
1.04
0.99
0.99
0.97
0.99
3.08
1.05
1.31
0.63
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
NAME 20110726nibin
EXPNO 4
PROCNO 1
Date_ 20110726
Time 16.23
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
======== CHANNEL f1 ========
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SI 32768
SF 600.1300158 MHz
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SSB 0
LB -0.10 Hz
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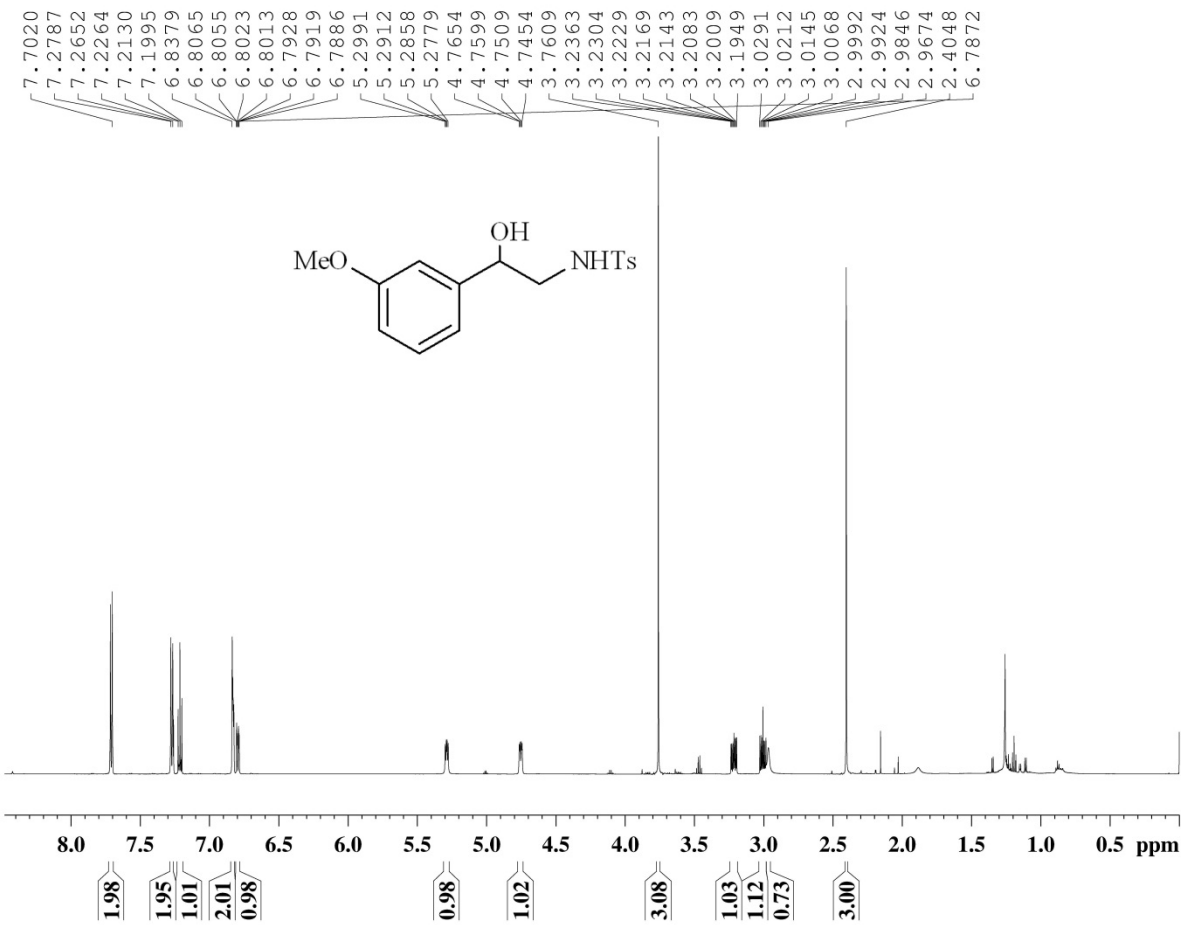
PC 1.00



BRUKER

NAME	20110726nibin
EXPNO	3
PROCNO	1
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INSTRUM	spect
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PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	40.3
DW	40.533 usec
DE	6.50 usec
TE	299.6 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300171 MHz
WDW	GM
SSB	0
LB	-0.10 Hz
GB	0.1
PC	1.00

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5.0
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3.0
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ppm
BRUKER
NAME 20110822nibin
EXPNO 8
PROCNO 1
Date_ 20110822
Time 10.16
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 80.6
DW 40.533 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
SI 32768
SF 600.1300154 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

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7.6310
7.5280
7.5264
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2.8627
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OH
NHTs
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2.03
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1.43
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1.03
3.00
8.5
8.0
7.5
7.0
6.5
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4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
BRUKER
NAME 20110726nibin
EXPNO 5
PROCNO 1
Date_ 20110726
Time 16.28
INSTRUM spect
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PULPROG zg30
TD 65536
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DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
======== CHANNEL f1 ========
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SI 32768
SF 600.1300132 MHz
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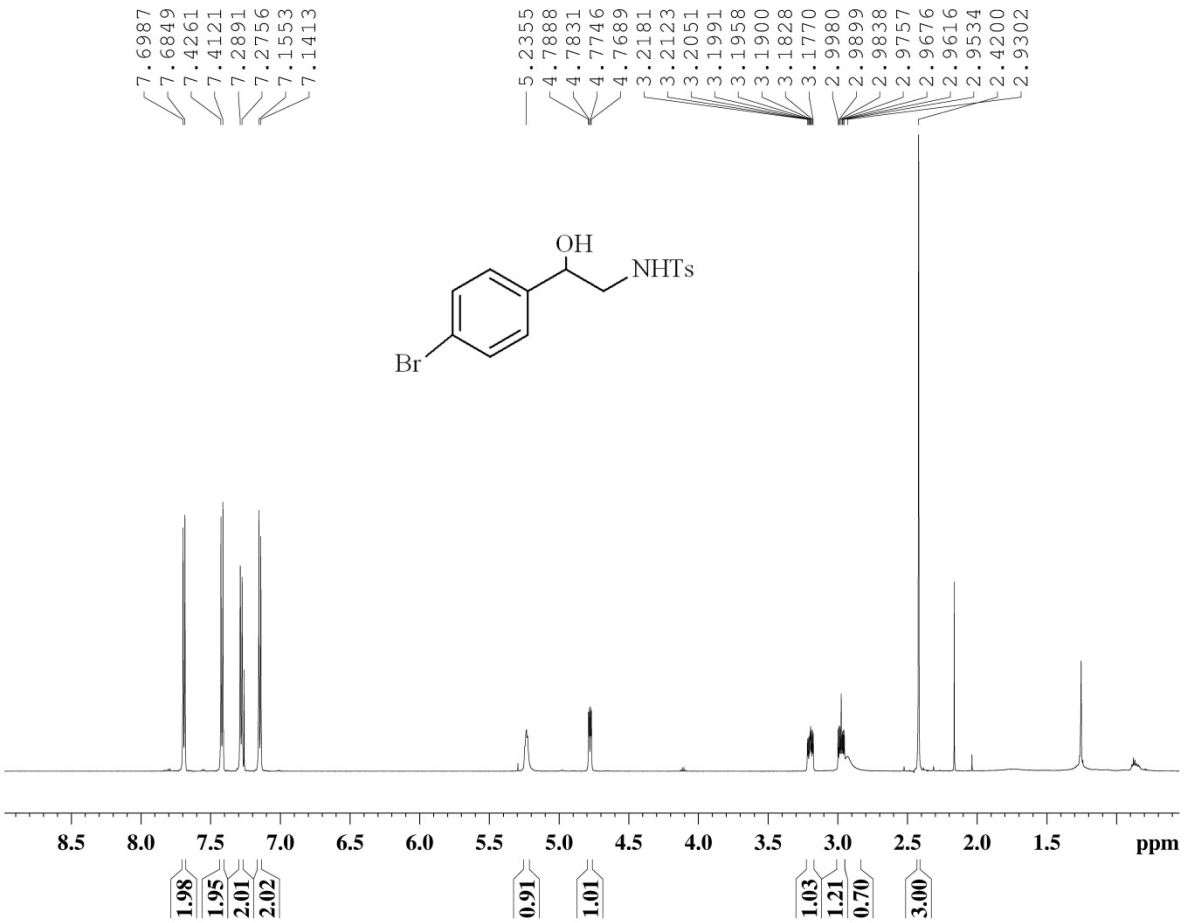
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

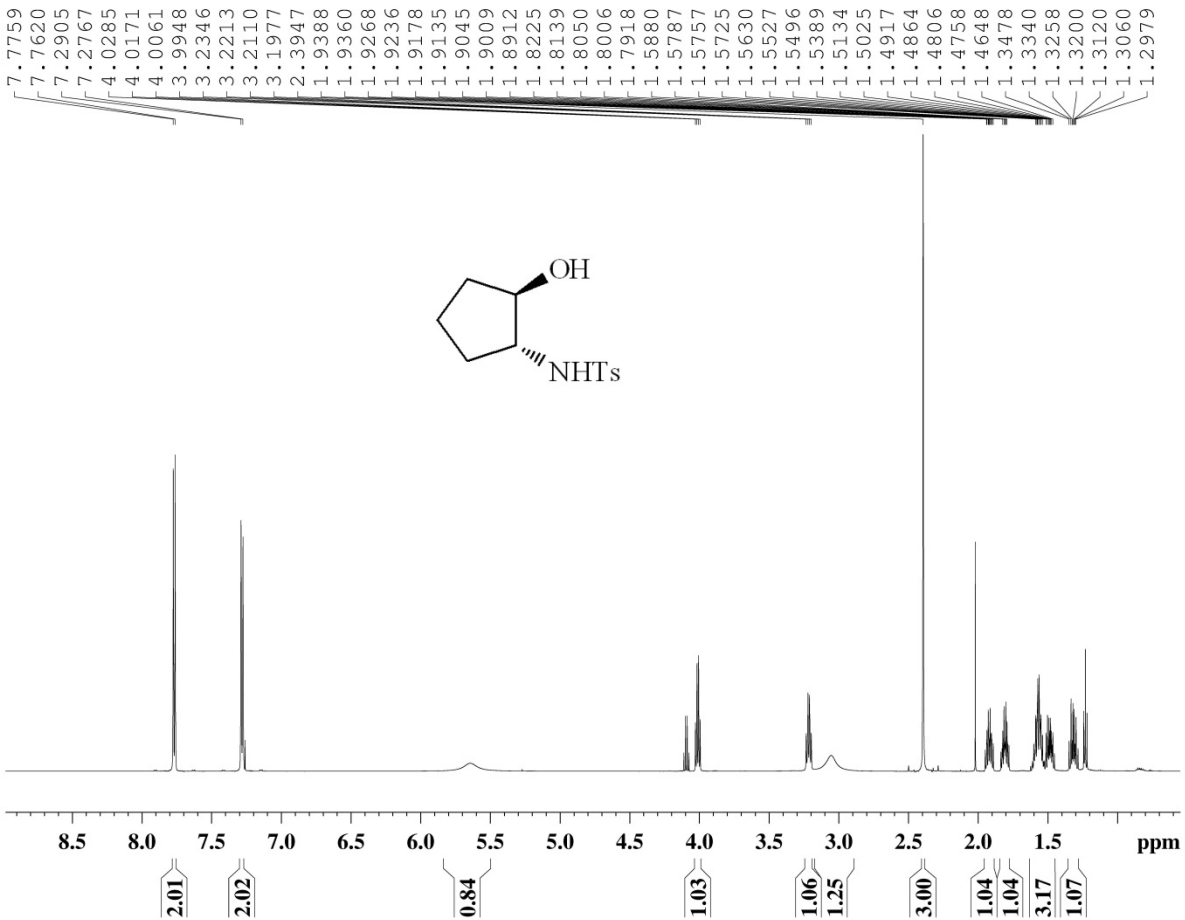


BRUKER

NAME	20110822nibin
EXPNO	9
PROCNO	1
Date_	20110822
Time	10.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	80.6
DW	40.533 usec
DE	6.50 usec
TE	296.3 K
D1	1.00000000 sec

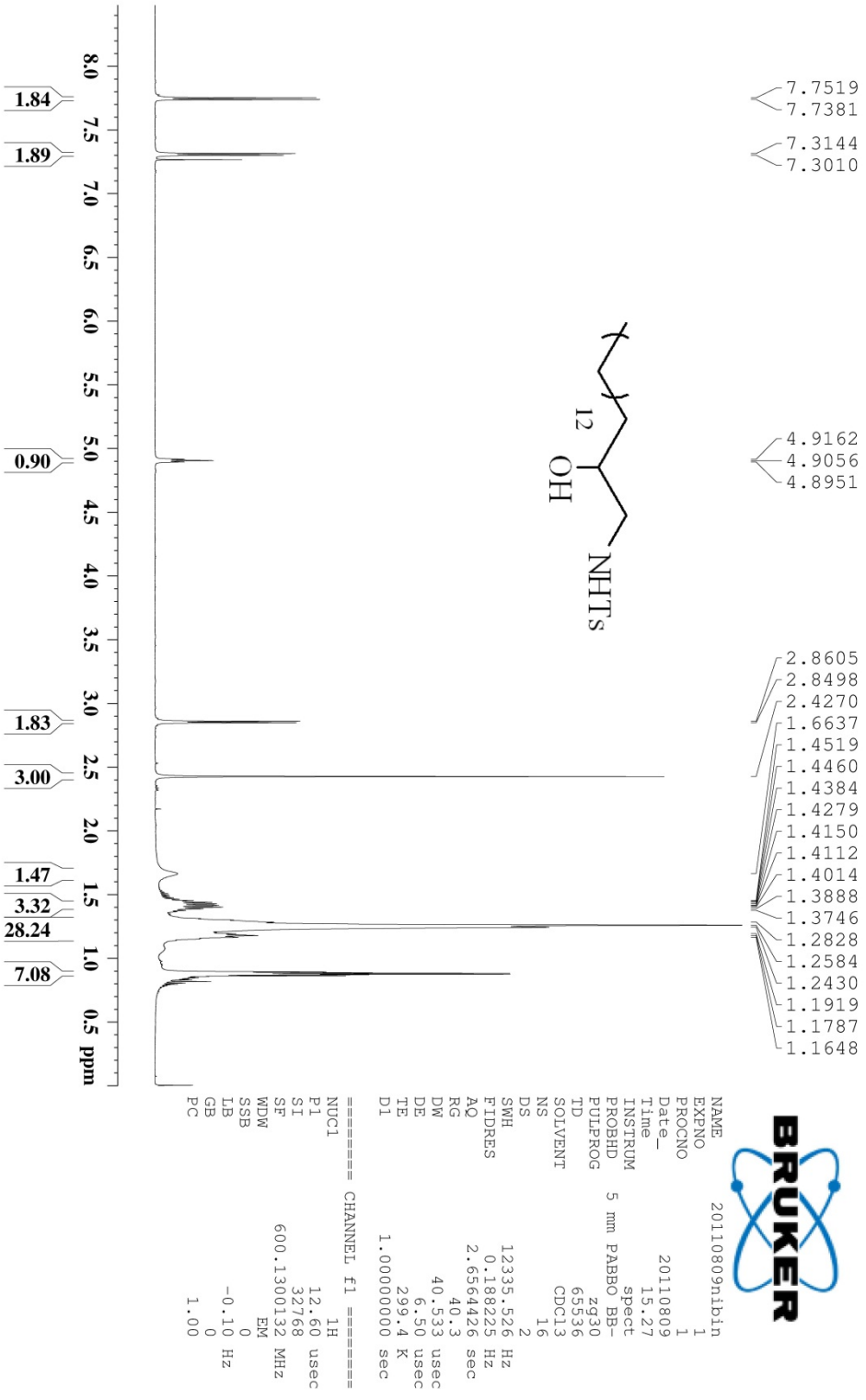
======== CHANNEL f1 ========

NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300154 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00



BRUKER

NAME	20110822nibin
EXPNO	1
PROCNO	1
Date_	20110822
Time	9.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	18
DW	40.533 usec
DE	6.50 usec
TE	296.0 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300154 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00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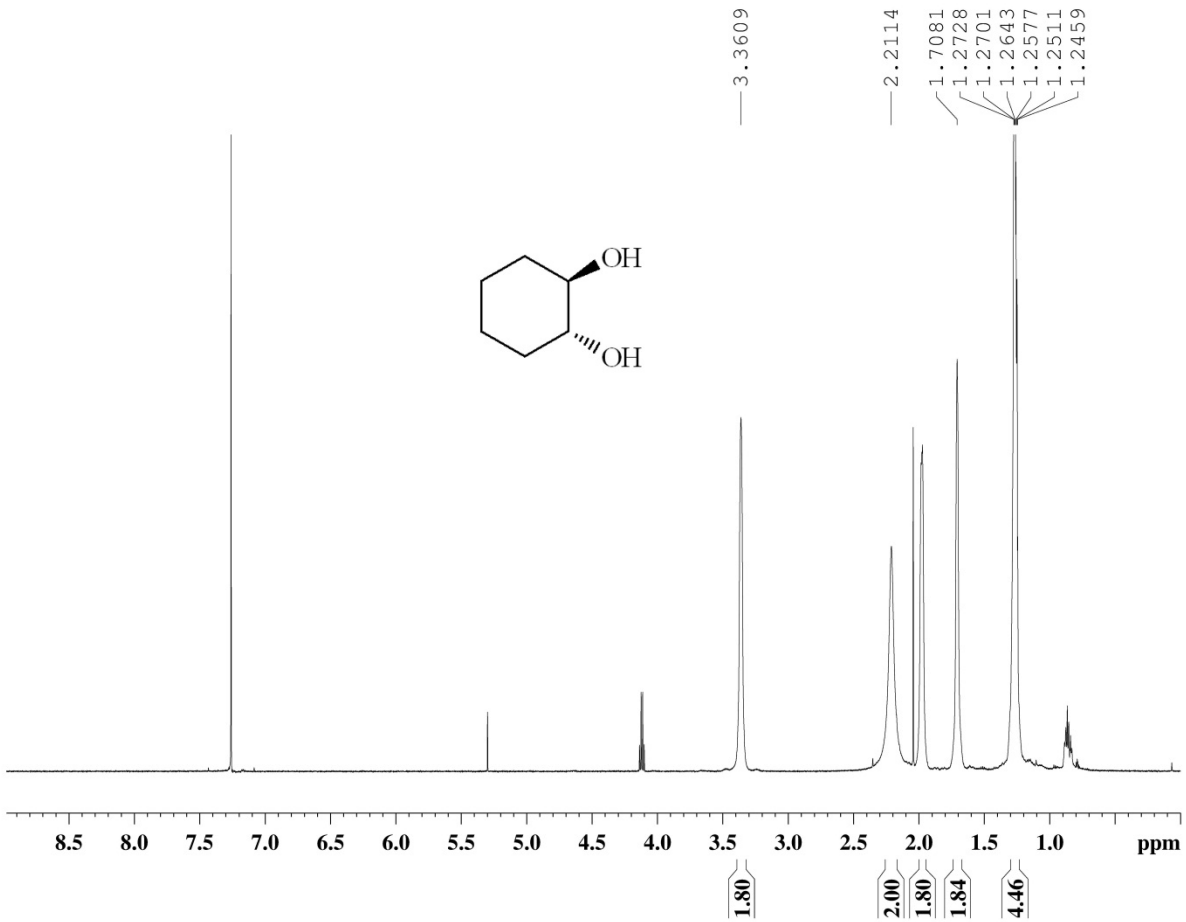
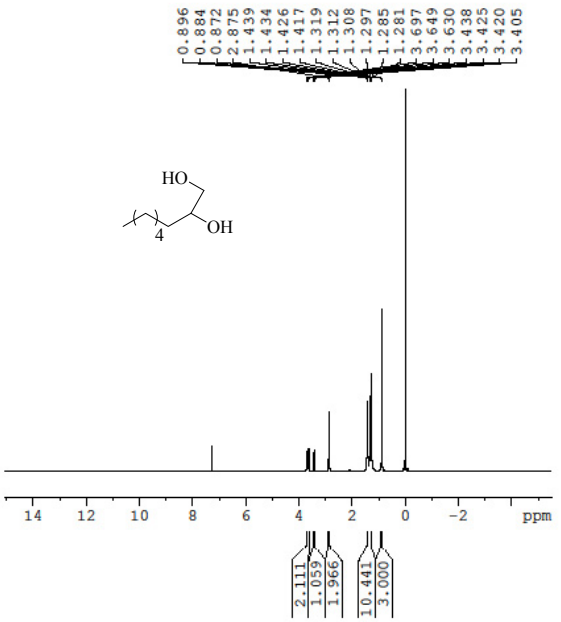
7.7381
7.3144
7.3010
4.9162
4.9056
4.8951
2.8605
2.8498
2.4270
1.6637
1.4519
1.4460
1.4384
1.4279
1.4150
1.4112
1.4014
1.3888
1.3746
1.2828
1.2584
1.2430
1.1919
1.1787
1.1648
1.84
1.89
0.90
1.83
3.00
1.47
3.32
28.24
7.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
OH
12
NHTs
BRUKER
NAME 20110809nibin
EXPNO 1
PROCNO 1
Date_ 20110809
Time 15.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 40.3
DW 40.533 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
SI 32768
SF 600.1300132 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00

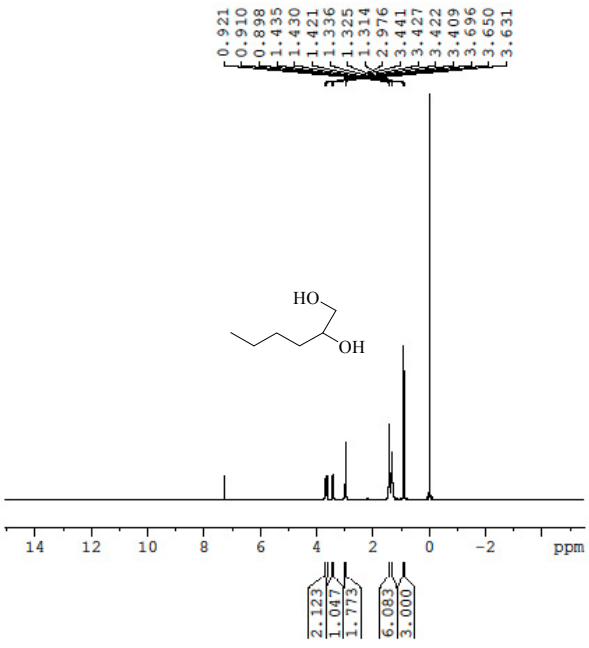


BRUKER

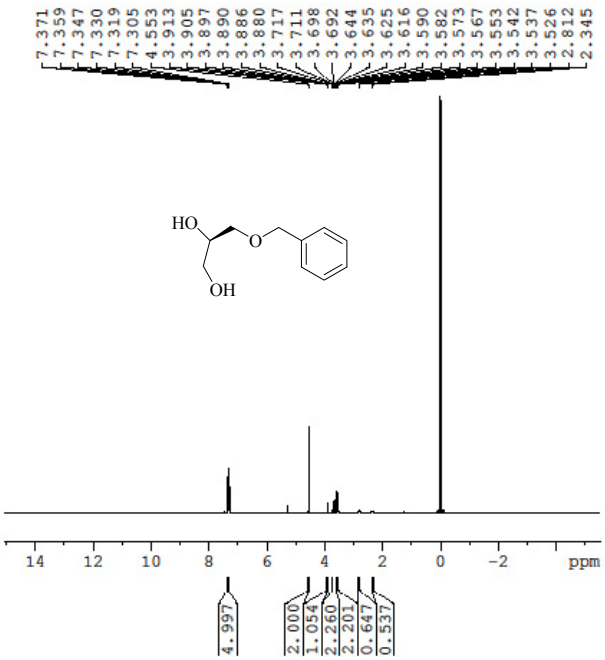
NAME	20110822nibin
EXPNO	2
PROCNO	1
Date_	20110822
Time	9.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	114
DW	40.533 usec
DE	6.50 usec
TE	296.0 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.60 usec
SI	32768
SF	600.1300154 MHz
WDW	EM
SSB	0
LB	-0.10 Hz
GB	0
PC	1.00




```
NAME        20140110zhangrui
EXPNO                      6
PROCNO                     1
Date_               20140110
Time                   15.12
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               12335.526 Hz
FIDRES             0.188225 Hz
AQ                2.6564426 sec
RG                     71.8
DW                   40.533 usec
DE                     6.50 usec
TE                    292.2 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.00 usec
SI                     32768
SF              600.1300104 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```



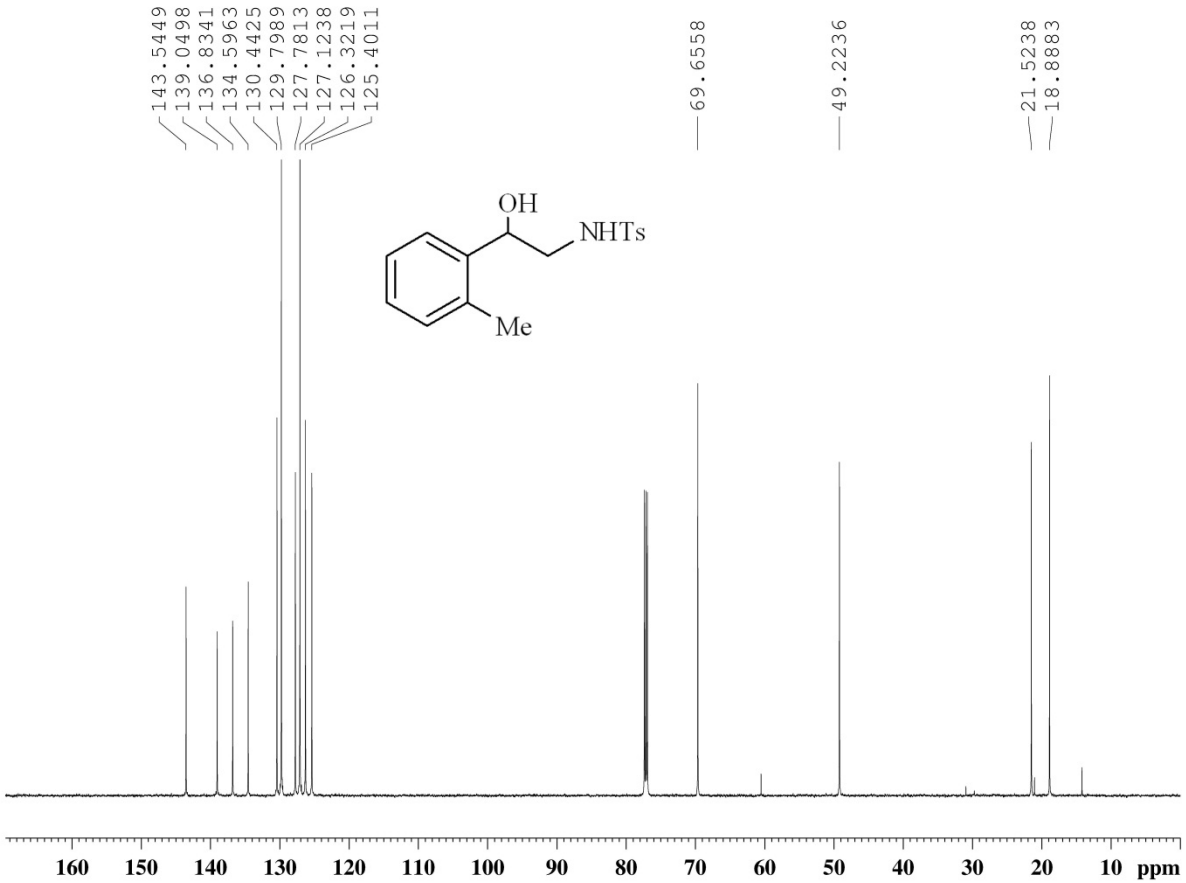

```
NAME        20140110zhangrui
EXPNO                      5
PROCNO                     1
Date_               20140110
Time                   15.06
INSTRUM                spect
PROBHD    5 mm PADUL 13C
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               12335.526 Hz
FIDRES             0.188225 Hz
AQ                2.6564426 sec
RG                     80.6
DW                   40.533 usec
DE                     6.50 usec
TE                    292.2 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.00 usec
SI                     32768
SF              600.1300096 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```



BRUKER

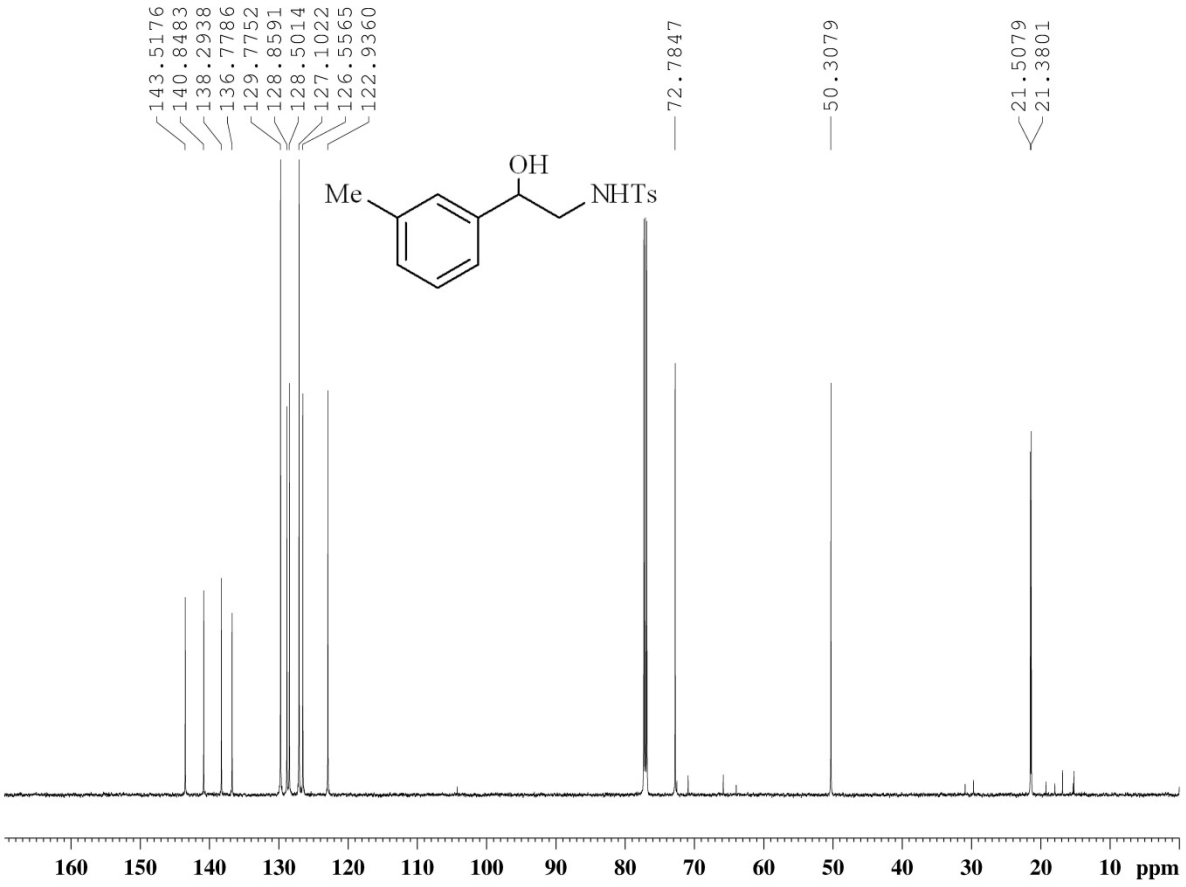
NAME	20140110zhangrui
EXPNO	9
PROCNO	1
Date_	20140110
Time	15.29
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12335.526 Hz
FIDRES	0.188225 Hz
AQ	2.6564426 sec
RG	114
DW	40.533 usec
DE	6.50 usec
TE	292.6 K
D1	1.00000000 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
SI	32768
SF	600.1300171 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

7.3581
7.3450
7.3406
7.3357
7.3028
7.2987
7.2889
7.2792
7.2747
4.7886
3.7245
3.6514
3.6389
3.0866
1.2618
OH
OH
5.38
1.00
1.00
1.11
1.90
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
BRUKER
NAME 20110822nibin
EXPNO 4
PROCNO 1
Date_ 20110822
Time 9.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 57
DW 40.533 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
SI 32768
SF 600.1300154 MHz
WDW EM
SSB 0
LB -0.10 Hz
GB 0
PC 1.00



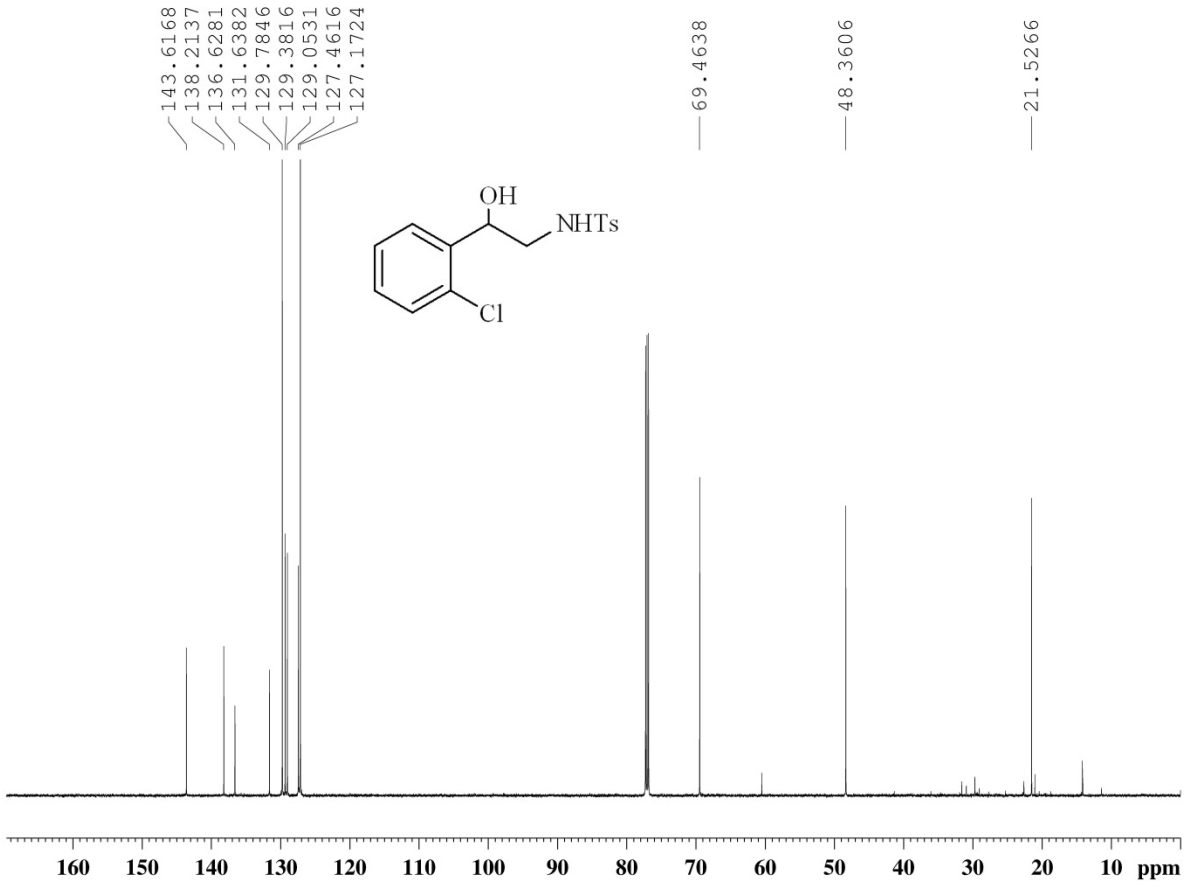
BRUKER

NAME	20110810nibin
EXPNO	2
PROCNO	1
Date_	20110810
Time	9.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	655
DS	2
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	6.50 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.30 usec
SI	32768
SF	150.9028096 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



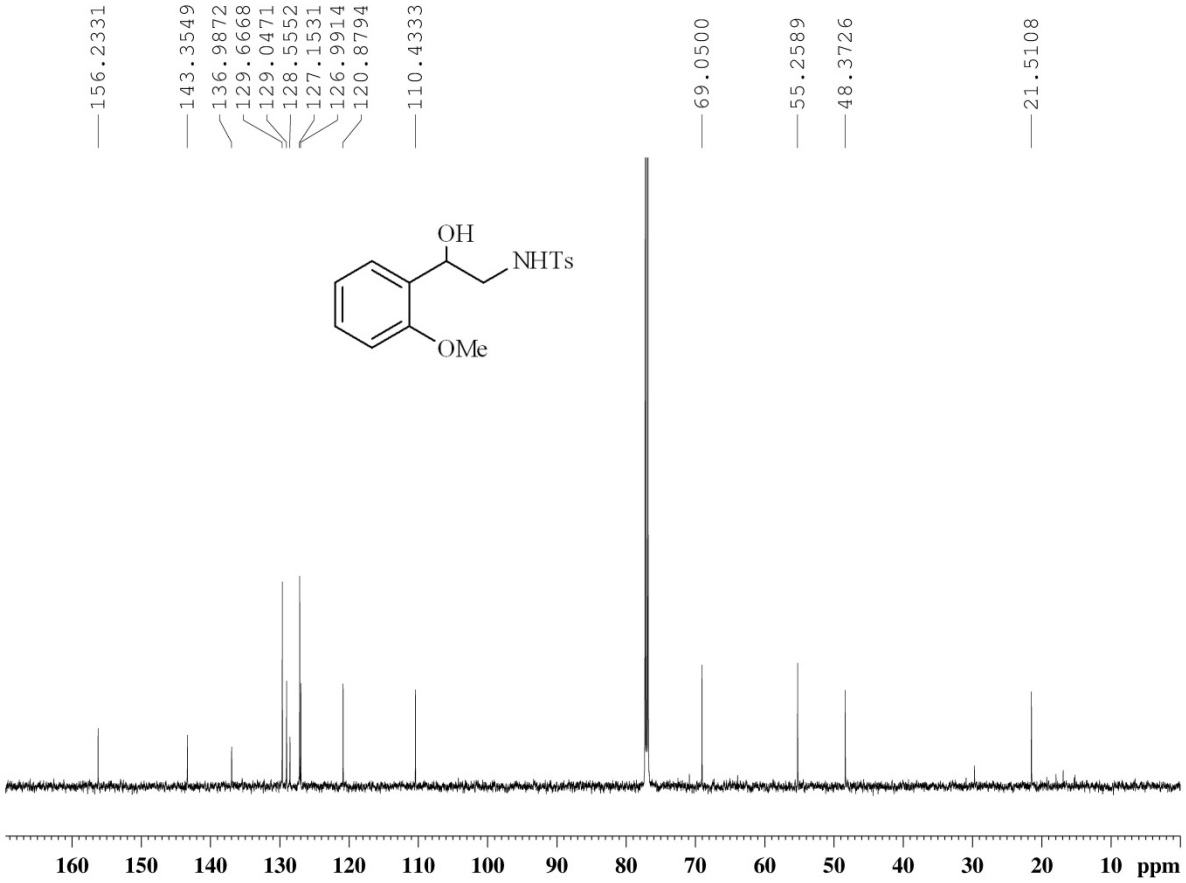
BRUKER

NAME	20110802nibin
EXPNO	2
PROCNO	1
Date_	20110802
Time	14.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	805
DS	2
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	6.50 usec
TE	300.3 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.30 usec
SI	32768
SF	150.9028096 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



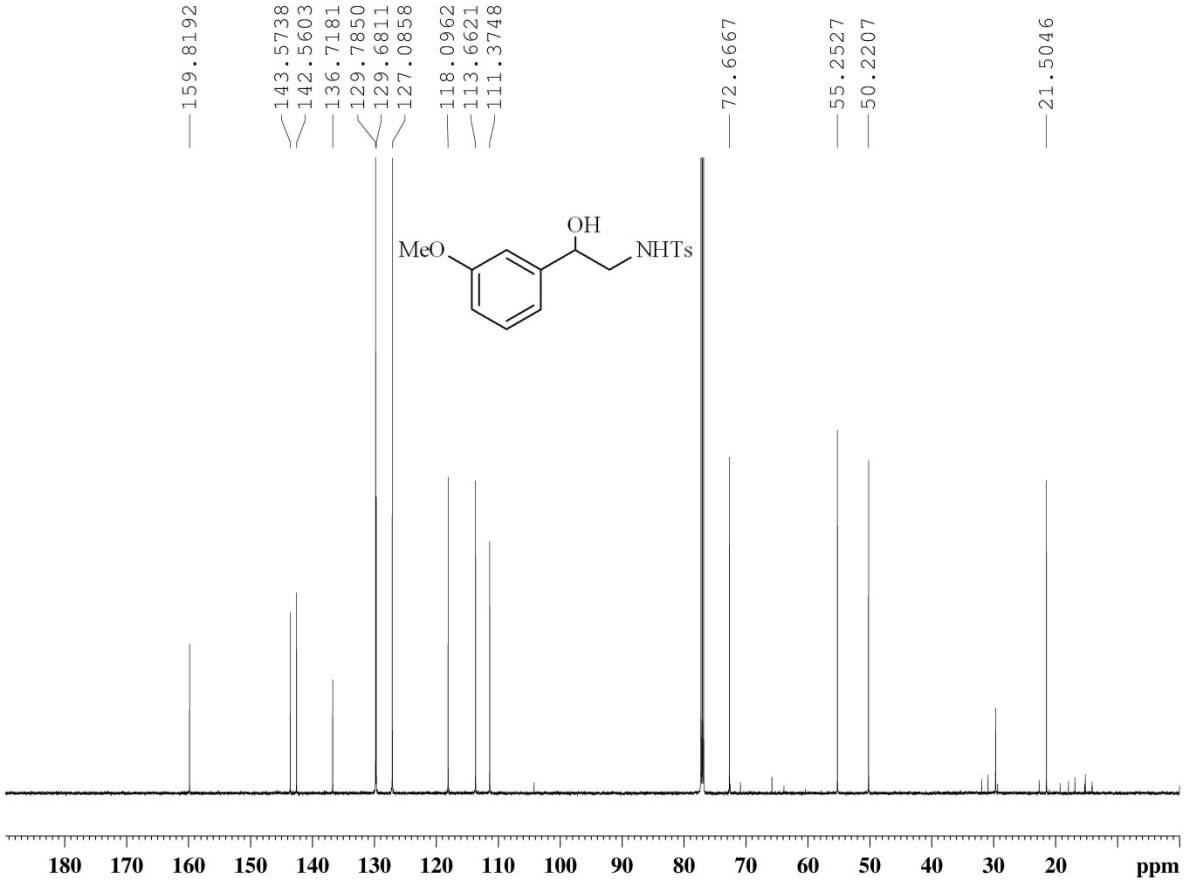
BRUKER

NAME	20110810nibin
EXPNO	1
PROCNO	1
Date_	20110810
Time	8.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	992
DS	2
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.30 usec
SI	32768
SF	150.9028096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



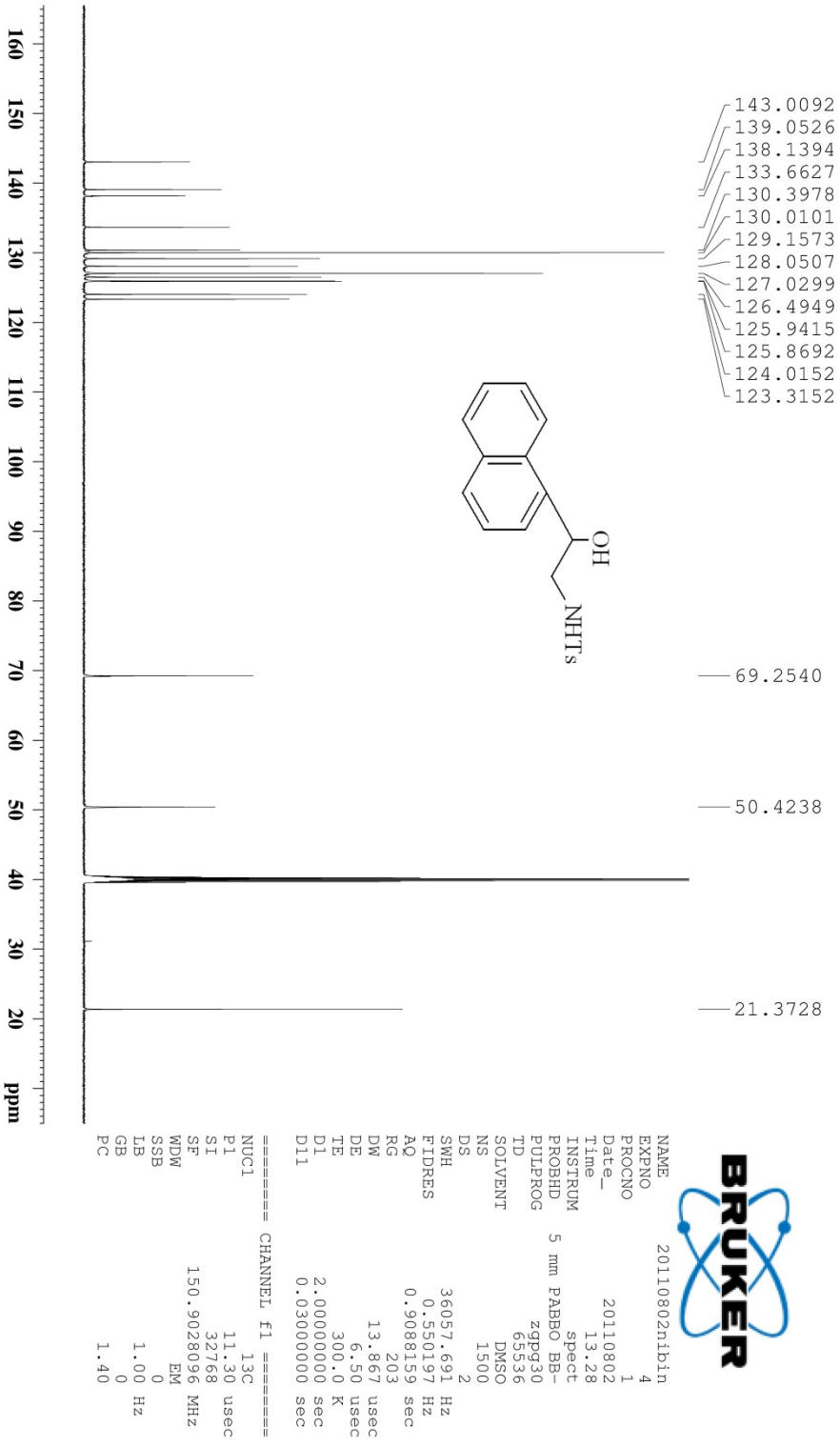
BRUKER

NAME	20110802nibin
EXPNO	1
PROCNO	1
Date_	20110802
Time	8.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3347
DS	2
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	6.50 usec
TE	296.4 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.30 usec
SI	32768
SF	150.9028096 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40



BRUKER

NAME	20110802nibin
EXPNO	3
PROCNO	1
Date_	20110802
Time	12.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	1577
DS	2
SWH	36057.691 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	203
DW	13.867 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	11.30 usec
SI	32768
SF	150.9028096 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40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138.1394
133.6627
130.3978
130.0101
129.1573
128.0507
127.0299
126.4949
125.9415
125.8692
124.0152
123.3152
OH
NHTs
69.2540
50.4238
21.3728
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
NAME 20110802nibin
EXPNO 4
PROCNO 1
Date_ 20110802
Time 13.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

143.3757
136.8048
129.7124
127.1083
73.9711
50.3021
36.8220
36.5125
31.8986
31.7056
30.0584
29.6981
29.5982
29.5246
29.3237
25.4849
23.3025
23.1039
22.6751
21.5029
14.1034
NHTs
OH
12
150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
NAME 20110810nibin
EXPNO 3
PROCNO 1
Date_ 20110811
Time 9.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2188
DS 2
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 13.867 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.30 usec
SI 32768
SF 150.9028096 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

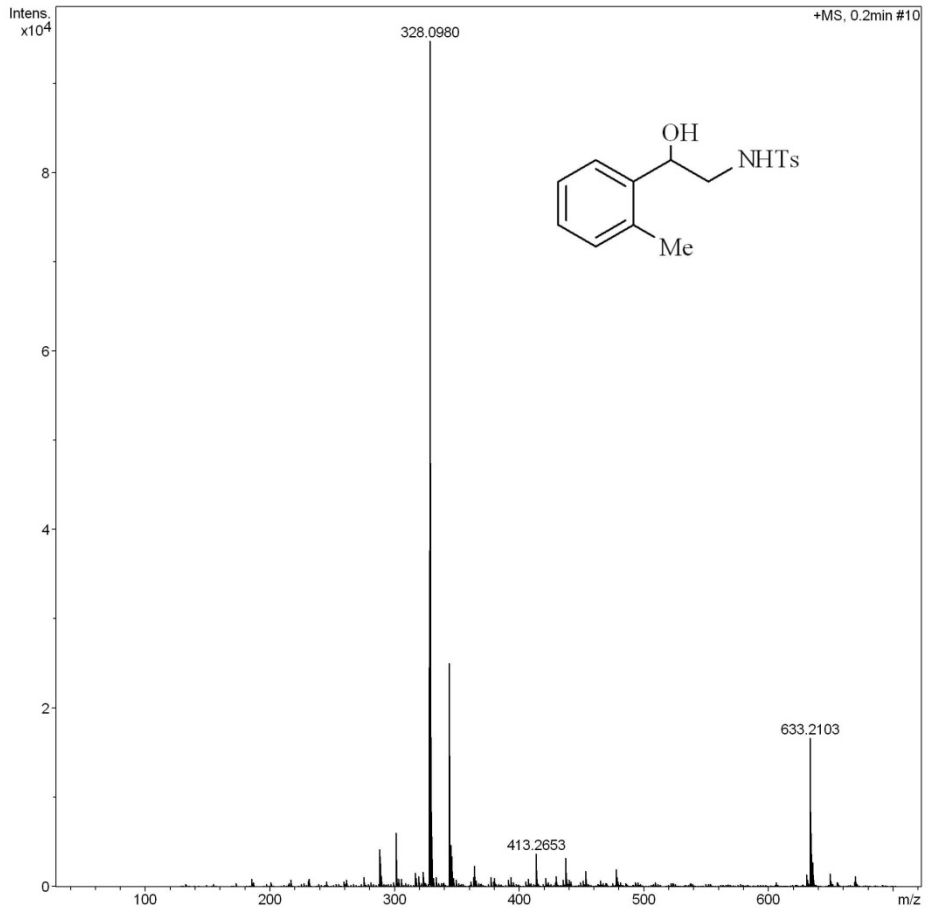
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-5.d	Acquisition Date	8/15/2011 4:08:49 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



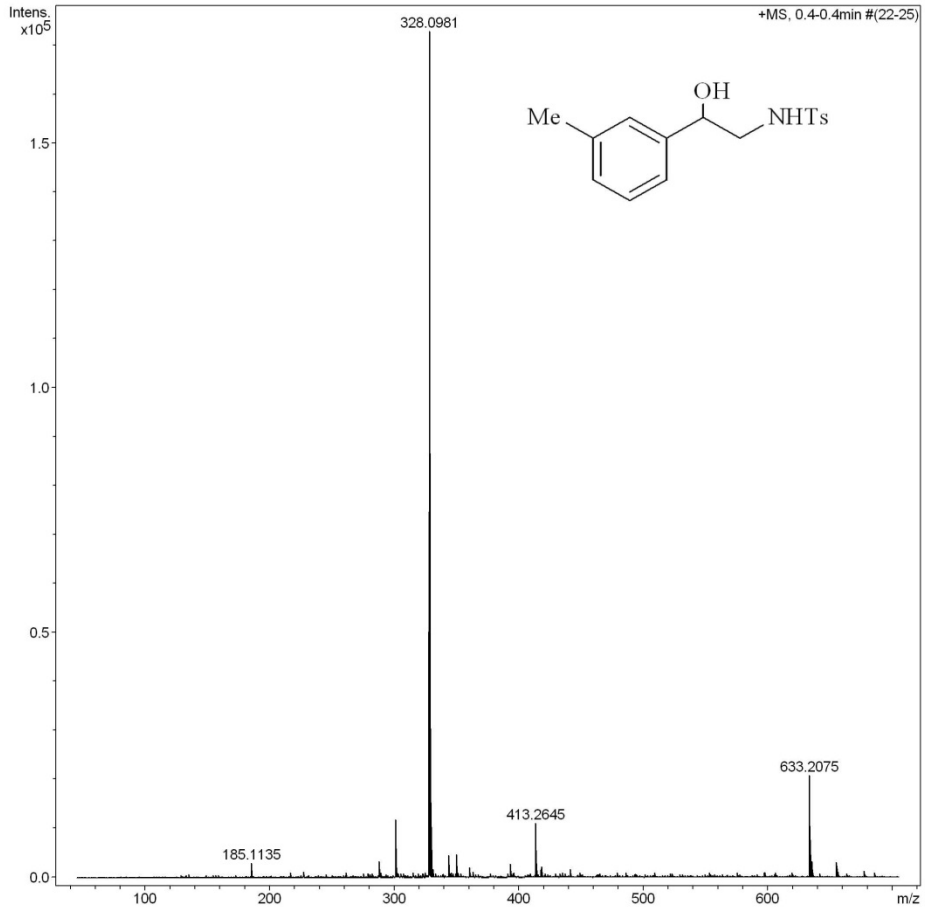
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-1.d	Acquisition Date	8/15/2011 3:53:14 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



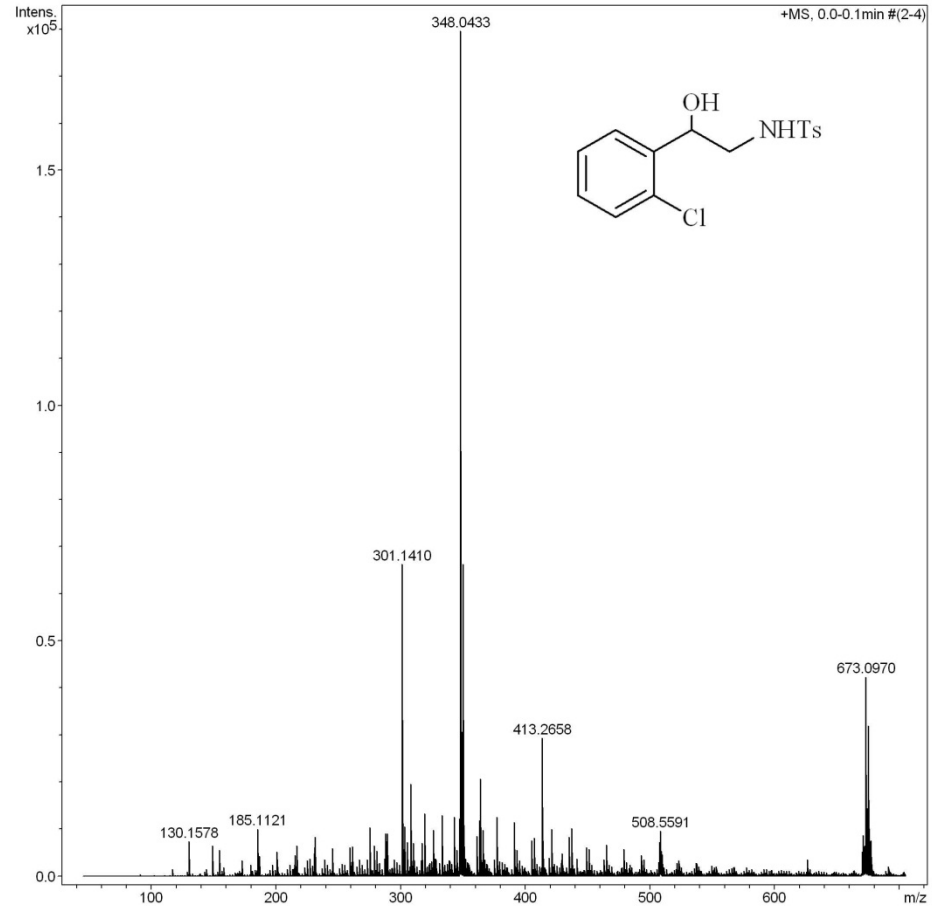
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-6.d	Acquisition Date	8/15/2011 4:15:22 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Bruker Compass DataAnalysis 4.0 printed: 8/15/2011 6:01:55 PM Page 1 of 1

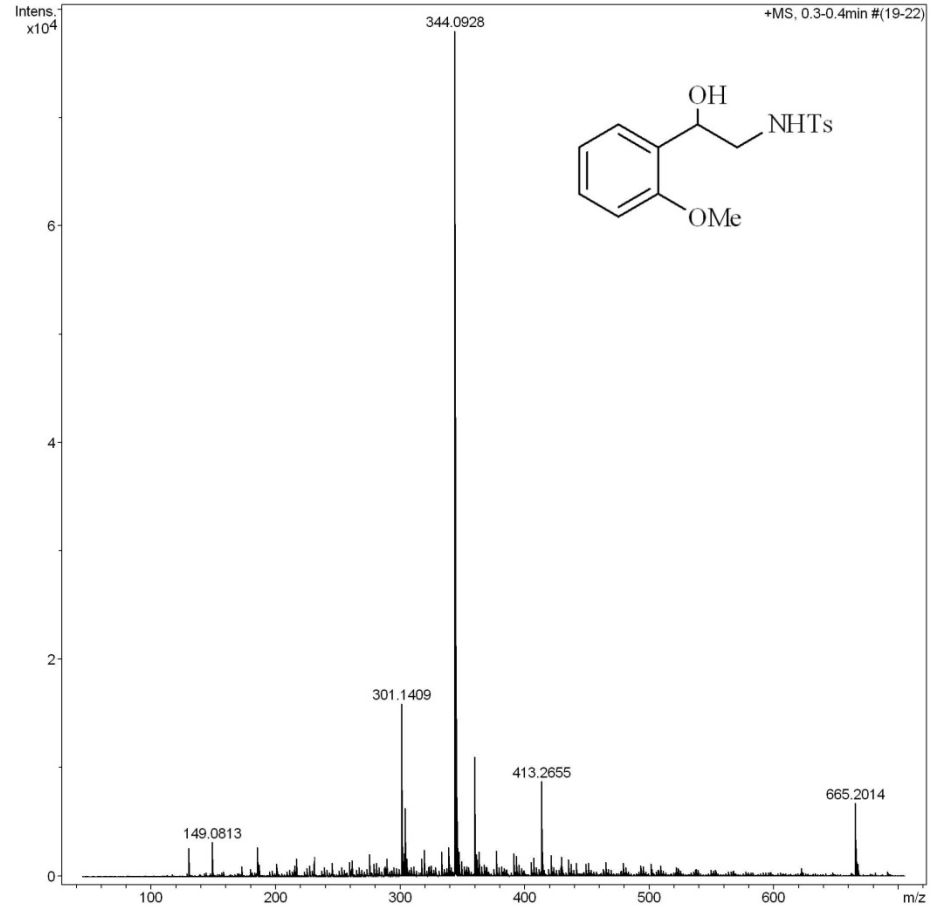
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-2.d	Acquisition Date	8/15/2011 3:56:45 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



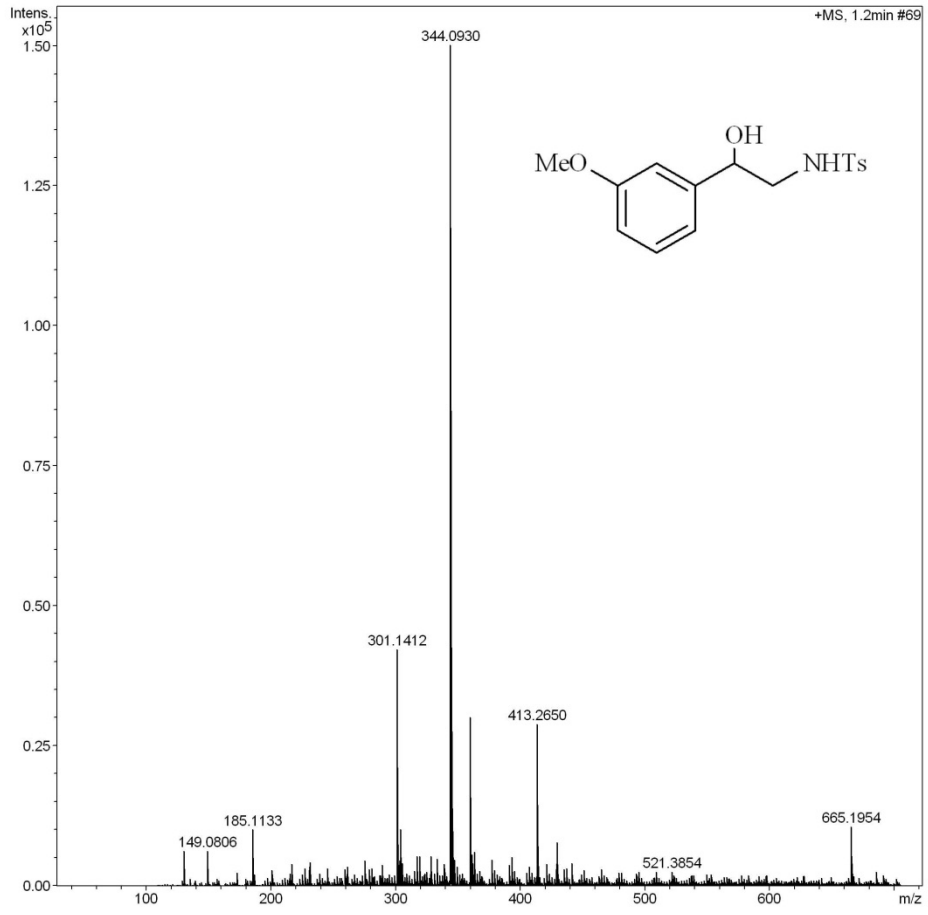
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-3.d	Acquisition Date	8/15/2011 3:58:50 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



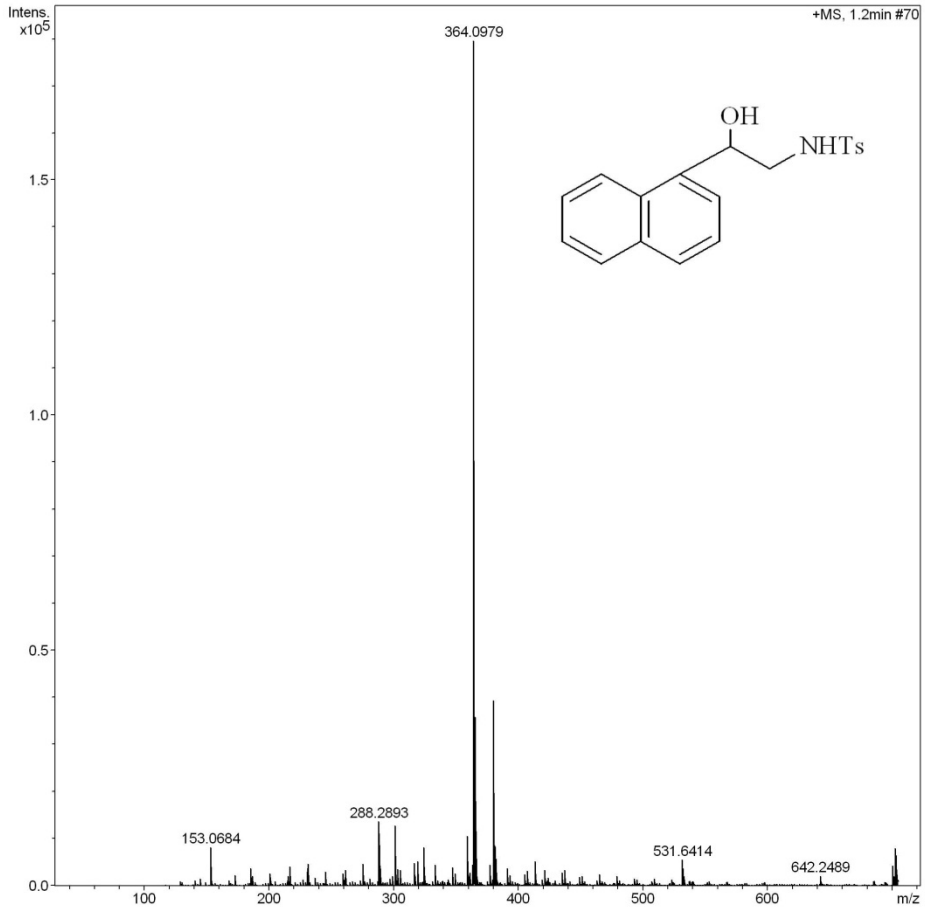
Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-4.d	Acquisition Date	8/15/2011 4:04:46 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Display Report

Analysis Info

Analysis Name	D:\Data\Chang-HongHong\20110815-7.d	Acquisition Date	8/15/2011 4:17:18 PM
Method	tune_low.m	Operator	TJU
Sample Name		Instrument	micrOTOF-Q II 10204
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source