Supporting Information

Enantioselective Pd-Catalyzed Hydrogenation of Enesulfonamides

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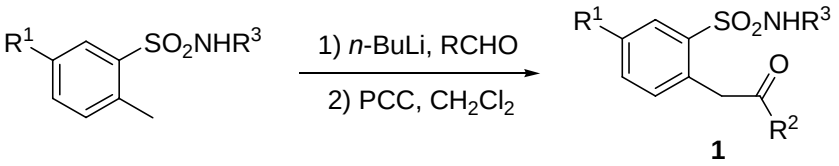
1. General and Materials

General: All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques or in a nitrogen-filled glovebox, unless otherwise noted. The chemical shifts for ^{1}H NMR were recorded in ppm downfield from tetramethylsilane (TMS) with the solvent resonance as the internal standard. The chemical shifts for ^{13}C NMR were recorded in ppm downfield using the central peak of d-chloroform (77.23 ppm) as the internal standard. Coupling constants (*J*) are reported in Hz and refer to apparent peak multiplications. Flash column chromatography was performed on silica gel (200-300 mesh). Optical rotations were measured with JASCO P-1010 polarimeter.The configuration was determined by comparison of rotation sign with the literature data or by analogue.

Materials: Commercially available reagents were used throughout without further purification. Acetone was distilled from anhydrous $CaSO_4$. The other solvents for asymmetric hydrogenation reaction were purchased without further purification. (*S*,*S*)-f-Binaphane was prepared according to the literature.[1]

2. Typical Procedure for Synthesis of Intermediate Ketones (1)

Intermediate ketones **1** were prepared from the corresponding substituted starting materials according to the procedures reported in the literature.[2,3]



1

To a solution of the intermediate alcohol (2.1 mmol) in CH_2Cl_2 (15 mL) was added PCC (888 mg, 4.1 mmol). The resulting dark-brown solution was stirred for overnight at ambient temperature. After addition of Et_2O (50 mL) and additional stirring (30 min), the mixture was filtered (Et_2O) through a short pad of silica gel. Concentration in vacuo afforded the analytically pure ketones **1.**

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-phenylethanone (1a). Yield: 81%, mp = 129-131 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.38 (s, 9H), 4.84 (s, 2H), 7.16 (br, 1H), 7.32-7.33 (m, 1H), 7.49-7.53 (m, 3H), 7.59-7.63 (m, 2H), 8.05 (d, *J* = 8.2 Hz, 1H), 8.23 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.0, 43.6, 84.4, 126.1, 127.8, 128.6, 129.0, 131.7, 133.7, 133.8, 134.0, 134.6, 136.6, 137.6, 148.9, 196.8. HRMS Calculated for $C_{19}H_{21}NO_5SNa$ $(M+Na)^+$ 398.1038, found: 398.1049.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*o*-tolylethanone (1b). Yield: 97%, mp = 131-132 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.35 (s, 9H), 2.49 (s, 3H), 4.74 (s, 2H), 7.25-7.31 (m, 1H), 7.38-7.39 (m, 1H), 7.45-7.49 (m, 1H), 7.58-7.60 (m, 1H), 7.72 (br, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 8.19 (d, *J* = 7.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 28.0, 46.2, 84.4, 126.1, 127.7, 129.2, 131.6, 132.1, 132.4, 133.7, 133.9, 134.8, 136.9, 137.7, 139.2, 149.3. HRMS Calculated for $C_{20}H_{23}NO_5SNa$ $(M+Na)^+$ 412.1195, found: 412.1201.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*m*-tolylethanone (1c). Yield: 99%, mp = 121-123 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.35 (s, 9H), 2.39 (s, 3H), 4.79 (s, 2H), 7.28-7.30 (m, 1H), 7.35-7.38 (m, 2H), 7.46-7.48 (m, 1H), 7.57-7.59 (m, 1H), 7.82-7.84 (m, 2H), 8.20 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 28.0, 43.6, 84.3, 125.8, 127.6, 128.9, 129.1, 131.6, 133.7, 133.9, 134.5, 134.8, 136.6, 137.6, 138.8, 149.2. 197.1. HRMS Calculated for $C_{20}H_{23}NO_5SNa$ $(M+Na)^+$ 412.1195, found: 412.1181.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*p*-tolylethanone (1d). Yield: 77%, mp = 142-143 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.37 (s, 9H), 2.43 (s, 3H), 4.79 (s, 2H), 7.28-7.33 (m, 4H), 7.46-7.49 (m, 1H), 7.58-7.62 (m, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 8.22 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.9, 28.0, 43.4, 84.3, 127.7, 128.7, 129.7, 131.6, 133.7, 133.9, 134.8, 144.7, 196.5. HRMS Calculated for $C_{20}H_{23}NO_5SNa$ $(M+Na)^+$ 412.1195, found: 412.1201.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*p*-methoxyphenylethanone (1e). Yield: 83%, mp = 142-143 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.37 (s, 9H), 3.88 (s, 3H), 4.77 (s, 2H), 6.95 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.45-7.49 (m, 2H), 7.57-7.59 (m, 1H), 8.02 (d, *J* = 8.6 Hz, 2H), 8.21 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.0, 43.1, 55.7, 84.3, 114.2, 127.6, 129.6, 130.9, 131.6, 133.6, 133.9, 134.9, 137.5, 149.0, 164.1, 195.4. HRMS Calculated for $C_{20}H_{23}NO_6SNa$ $(M+Na)^+$ 428.1144, found: 428.1138.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*p*-fluorophenylethanone (1f). Yield: 77%, mp = 141-142 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.36 (s, 9H), 4.79 (s, 2H), 7.13-7.17 (m, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.47-7.51 (m, 2H), 7.59-7.63 (m, 1H), 8.05-8.07 (m, 2H), 8.20 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.9, 43.4, 84.5, 115.9, 116.2, 127.7, 131.2, 131.3, 131.6, 132.9, 133.6, 134.0, 134.5, 137.5, 149.3, 164.9, 167.4, 195.4. HRMS Calculated for $C_{19}H_{20}FNO_5FSNa$ $(M+Na)^+$ 416.0944, found: 416.0928.

2-(*o*-*tert*-Butyl phenylsulfonylcarbamate)-1-*p*-chlorophenylethanone (1g). Yield: 92%, mp = 153-155 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.36 (s, 9H), 4.78 (d, *J* = 3.2 Hz, 2H), 7.29-7.32 (m, 1H), 7.44-7.51 (m, 3H), 7.59-7.61 (m, 1H), 7.96-7.99 (m, 2H), 8.19-8.22 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.0, 43.6, 84.5, 127.9, 129.3, 130.0, 131.6, 133.6, 134.0, 134.3, 134.9, 137.6, 140.2, 149.1, 195.8. HRMS Calculated for $C_{19}H_{20}NO_5SClNa$ $(M+Na)^+$ 432.0648, found: 432.0661.

***tert*-Butyl 2-(2-oxopropyl)phenylsulfonylcarbamate (1h).** Yield: 85%, mp = 146-147 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.38 (s, 9H), 2.26 (s, 3H), 4.22 (s, 2H), 7.45-7.49 (m, 1H), 7.57-7.61 (m, 2H), 8.18 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.0, 30.0, 48.5, 84.5, 127.8, 131.5, 133.6, 134.0, 134.2, 137.5, 149.4, 205.7. HRMS Calculated for $C_{14}H_{19}NO_5NaS$ $(M+Na)^+$ 336.0882, found: 336.0896.

***tert*-Butyl 2-(2-oxopentyl)phenylsulfonylcarbamate (1i).** Yield: 88%, mp = 120-121 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (t, *J* = 7.4 Hz, 3H), 1.37 (s, 9H), 1.59-1.65 (m, 2H), 2.52 (t, *J* = 7.4 Hz, 2H), 4.19 (s, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.43-7.47 (m, 1H), 7.57-7.60 (m, 1H), 8.16 (d, *J* = 7.9 Hz, 1H), 8.28 (br, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.8, 17.2, 28.0, 44.6, 47.6, 84.5, 127.6, 131.5, 133.7, 133.9, 134.3, 137.4, 149.6. 207.7. HRMS Calculated for $C_{16}H_{23}NO_5SNa$ $(M+Na)^+$ 364.1195,

found: 364.1190.

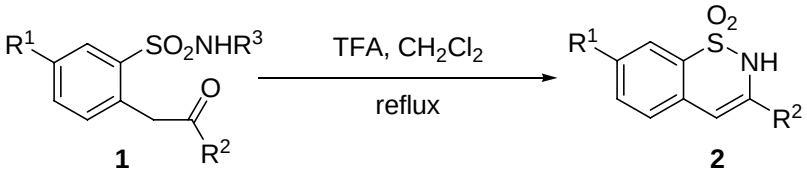
***tert*-Butyl 2-(2-oxoheptyl)phenylsulfonylcarbamate (1j).** Yield: 88%, mp = 106-107 °C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87-0.90 (m, 3H), 1.25-1.34 (m, 4H), 1.38 (s, 9H), 1.59-1.63 (m, 2H), 2.52-2.55 (m, 2H), 4.19 (s, 2H), 7.26-7.28 (m, 1H), 7.46-7.48 (m, 1H), 7.57-7.58 (m, 1H), 7.62 (br, 1H), 8.17-8.19 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.6, 23.5, 28.0, 31.5, 42.8, 47.8, 84.4, 127.7, 131.5, 133.6, 133.9, 134.2, 207.8. HRMS Calculated for $C_{21}H_{23}NO_5SNa$ $(M+Na)^+$ 392.1474, found: 392.1493.

***tert*-Butyl 2-(2-oxo-4-phenylbutyl)phenylsulfonylcarbamate (1k).** Yield: 88%, mp = 117-119 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.38 (s, 9H), 2.88-2.94 (m, 4H), 4.17 (s, 2H), 7.18-7.21 (m, 5H), 7.27-7.29 (m, 2H), 7.45 (m, 1H), 7.56 (m, 1H), 8.17 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.9, 29.7, 43.9, 47.6, 84.4, 126.2, 127.5, 128.5, 128.6, 131.4, 133.6, 133.9, 134.0, 137.3, 140.9, 149.6，206.7. HRMS Calculated for $C_{21}H_{25}NO_5SNa$ $(M+Na)^+$ 426.1351, found: 426.1364.

2-(*o*-*tert*-Butyl –*m*-tolylsulfonylcarbamate)-1-phenylethanone (1l). Yield: 98%, mp = 133-135 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.17 (s, 9H), 2.39 (s, 3H), 4.68 (s, 1H), 4.75 (m, 2H), 7.14-7.16 (m, 1H), 7.29-7.31 (m, 1H), 7.45-7.49 (m, 2H), 7.56-7.58 (m, 1H), 7.91 (br, 1H), 8.05 (d, J = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.2, 30.1, 42.9, 55.5, 128.7, 129.0, 130.2, 130.7, 133.4, 133.7, 136.7, 137.7, 141.1, 197.9. HRMS Calculated for $C_{19}H_{23}NO_3SNa$ $(M+Na)^+$ 368.1296, found: 368.1309.

***tert*-Butyl 2-(2-(furan-2-yl)-2-oxoethyl)phenylsulfonylcarbamate (1m).** Yield: 77%, mp = 133-134 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.35 (s, 9H), 4.69 (s, 2H), 6.58 (br, 1H), 7.31-7.32 (m, 1H), 7.36-7.38 (m, 1H), 7.46-7.50 (m, 1H), 7.58-7.64 (m, 2H), 8.22 (d, J = 0.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.0, 43.0, 112.8, 118.3, 127.9, 131.6, 133.7, 133.9, 147.0. HRMS Calculated for $C_{17}H_{19}NO_6SNa$ $(M+Na)^+$ 388.0831, found: 388.0836.

3. Typical Procedure for Synthesis of Cyclic Enesulfonamides (2)



1 **2**

TFA (0.24 mL, 3.0 mmol) were added to a solution of ketone compound **1** (1.0 mmol) in CH_2Cl_2 (20 mL). The resulting solution was heated to reflux for overnight, then cooled to ambient temperature and filtered through a pad of silica gel. Concentration in vacuo and purification by flash chromatography afforded cyclic enesulfonamides **2**.

3-Phenyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2a) (known compound[4]). Yield: 90%, mp = 202-204 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 6.68 (s, 1H), 6.87 (s, 1H), 7.48-7.51 (m, 5H), 7.60-7.64 (m, 1H), 7.70-7.72 (m, 2H), 7.91 (d, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 106.9, 121.6, 126.8, 127.8, 129.4, 130.5, 132.4, 134.4.

3-*o*-Tolyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2b). Yield: 77%, mp = 155-156 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.46 (s, 3H), 6.24 (s, 1H), 7.02 (s, 1H), 7.21-7.46 (m, 6H), 7.56-7.58 (m, 1H), 7.82 (d, J = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.2, 108.5, 121.5, 126.3, 127.4, 127.6, 129.8, 130.1, 131.3, 132.4, 133.7, 134.6, 137.8, 139.7. HRMS Calculated for $C_{15}H_{13}NO_2SNa$ $(M+Na)^+$ 294.0565, found: 294.0561.

3-*m*-Tolyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2c). Yield: 90%, mp = 218-219 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H), 6.64-6.66 (m, 1H), 6.89 (br, 1H), 7.25-7.29 (m, 1H),

7.35-7.38 (m, 1H), 7.48-7.50 (m, 4H), 7.58-7.61 (m, 1H), 7.90 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 106.7, 121.6, 123.9, 127.4, 127.7, 129.2, 131.3, 132.4. HRMS Calculated for $C_{15}H_{13}NO_2SNa$ $(M+Na)^+$ 294.0565, found: 294.0555.

3-*p*-Tolyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2d). Yield: 77%, mp = 270-271 °C，^{1}H NMR (400 MHz, d^6-DMSO): δ 2.37(s, 3H), 6.94 (s, 1H), 7.32 (d, *J* = 0.8 Hz, 2H), 7.52-7.55 (m, 1H), 7.66-7.68 (m, 4H), 7.82 (d, *J* = 0.8 Hz, 1H), 11.00 (br, 1H). ^{13}C NMR (100 MHz, d^6-DMSO): δ 21.5, 105.7, 121.2, 127.2, 128.0, 128.2, 130.0, 131.9, 132.6, 134.2, 139.8, 140.3. HRMS Calculated for $C_{15}H_{13}NO_2SNa$ $(M+Na)^+$ 294.0565, found: 294.0551.

3-*p*-Methoxyphenyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2e). Yield: 78%, mp = 209-211 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.86 (s, 3H), 6.58 (s, 1H), 6.84 (m, 1H), 6.96-6.99 (m, 2H), 7.46-7.48 (m, 2H), 7.58-7.65 (m, 3H), 7.89 (d, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.7, 105.6, 114.7, 121.6, 127.5, 127.6, 128.3, 132.4. HRMS Calculated for $C_{15}H_{13}NO_3SNa$ $(M+Na)^+$ 310.0514, found: 310.0504.

3-*p*-Fluorophenyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2f). Yield: 77%, mp = 236-237 °C，^{1}H NMR (400 MHz, d^6-DMSO): δ 6.96-6.99 (m, 1H), 7.31-7.39 (m, 2H), 7.54-7.58 (m, 1H), 7.65-7.71 (m, 2H), 7.82-7.85 (m, 3H), 10.08 (br, 1H). ^{13}C NMR (100 MHz, d^6-DMSO): δ 106.4, 116.1, 116.4, 121.0, 128.1, 129.4, 129.5, 131.1, 131.9, 132.5, 133.9, 138.6, 162.3, 164.7. HRMS Calculated for $C_{14}H_{10}FNO_2SNa$ $(M+Na)^+$ 298.0314, found: 298.0301.

3-*p*-Chlorophenyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2g). Yield: 93%, mp = 273-275 °C，^{1}H NMR (400 MHz, DMSO): δ 7.05 (s, 1H), 7.55-7.59 (m, 3H), 7.68-7.73 (m, 2H), 7.79-7.85 (m, 3H), 11.1 (br, 1H). ^{13}C NMR (100 MHz, DMSO): δ 107.2, 121.2, 128.4, 128.5, 128.9, 129.5, 132.2, 132.8, 133.6, 133.9, 135.1, 138.5. HRMS Calculated for $C_{14}H_{10}NO_2SClNa$ $(M+Na)^+$ 314.0018, found: 314.0013.

3-Methyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2h) (known compound[5]). Yield: 89%, mp = 106-107 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.16 (s, 3H), 6.04 (s, 1H), 7.17 (br, 1H), 7.29-7.31 (m, 1H), 7.41-7.42 (m, 1H), 7.52-7.54 (m, 1H), 7.86 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.2, 105.6, 121.5, 126.6, 126.9, 132.4.

3-Propyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2i). Yield: 95%, mp = 78-80 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 0.97-1.00 (m, 3H), 1.65-1.71 (m, 2H), 2.36-2.39 (m, 2H), 6.06 (s, 1H), 7.14 (br, 1H), 7.30-7.32 (m, 1H), 7.38-7.42 (m, 1H), 7.52-7.56 (m, 1H), 7.86 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.5, 20.5, 36.8, 105.4, 121.4, 126.8, 126.9, 132.3, 133.8, 140.9. HRMS Calculated for $C_{11}H_{13}NO_2SNa$ $(M+Na)^+$ 274.0878, found: 274.0881.

3-Amyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2j). Yield: 73%, mp = 81-83 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89-0.93 (m, 3H), 1.34-1.59 (m, 4H), 1.63-1.67 (m, 2H), 2.37-2.41 (m, 2H), 6.07 (s, 1H), 6.72(br, 1H), 7.31-7.33 (m, 1H), 7.39-7.43 (m, 1H), 7.53-7.57 (m, 1H), 7.86 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.1, 22.5, 26.9, 31.2, 34.9, 105.0, 121.4, 126.8, 126.9, 130.7, 132.3, 133.9, 141.2. HRMS Calculated for $C_{11}H_{13}NO_2SNa$ $(M+Na)^+$ 246.0565, found: 246.0556.

3-(2-Phenylethyl)-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2k). Yield: 88%, mp = 65-67 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.63-2.67 (m, 2H), 2.92-2.96 (m, 2H), 5.96 (s, 1H), 7.18-7.35 (m, 6H), 7.48-7.49 (m, 1H), 7.65 (s, 1H), 7.84 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 33.8, 36.9, 105.5, 121.4, 126.6, 126.9, 127.1, 128.7, 128.8, 130.6, 132.4, 133.7, 140.4. HRMS Calculated for $C_{16}H_{16}NO_2S$ $(M+H)^+$ 286.0902, found: 286.0900.

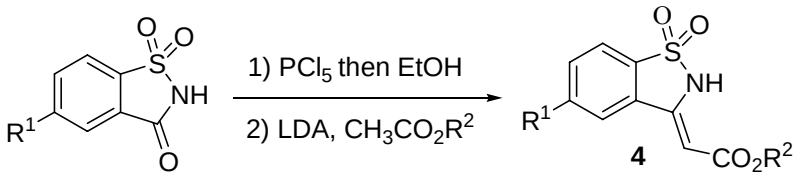
3-Phenyl-2*H*-1λ^6-*m*-methyl-benzo[*e*][1,2]thiazine 1,1-Dioxide (2l). Yield: 77%, mp = 207-209

°C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.47 (s, 3H), 6.65 (s, 1H), 6.87 (s, 1H), 7.38-7.47 (m, 5H), 7.68-7.71 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 106.9, 121.5, 126.6, 127.8, 129.3, 130.3, 133.4, 138.5. HRMS Calculated for $C_{15}H_{13}NO_2SNa$ $(M+Na)^+$ 294.0565, found: 294.0553.

3-Fural-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-Dioxide (2m). Yield: 82%, mp = 181-183 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 6.54 (s, 1H), 6.75 (s, 1H), 6.78 (d, *J* = 3.3 Hz, 1H), 7.19 (br, 1H), 7.45-7.48 (m, 2H), 7.53 (s, 1H), 7.57-7.61 (m, 1H), 7.89(d, *J* = 7.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 104.5, 109.7, 112.5, 121.7, 127.8, 127.9, 132.5, 144.4. HRMS Calculated for $C_{12}H_{10}NO_3S$ $(M+H)^+$ 248.0381, found: 248.0382.

4. Typical Procedure for Synthesis of Cyclic Enesulfonamides (4)

Cyclic enesulfonamides **4** were prepared from saccharin according to the procedures reported in the literature.[9]



3-Ethoxy-1,2-benzisothiazole 1,l –Dioxide: In a dry 250-mL singleneck, round-bottomed flask equipped with magnetic stir bar and air condenser were placed 1.83 g (10 mmol) of saccharin and 2.71 g (13 mmol, 1.3 equiv) of PCl_5. The contents were gently heated until the reaction had subsided, at which time the temperature was raised to 175 °C for an additional 1.6 h. The $POC1_3$ was removed by suction to give crude 3-chloro-1,2-benzisothiazole 1,l-dioxide, which was treated with 90 mL of absolute ethanol. After the reaction mixture was refluxed for 1 h, the solution was filtered, the filtrate was cooled in an ice bath, and the resulting solid was collected by filtration to give 3-ethoxy-1,2-benzisothiazole 1,l –dioxide 0.82 g (39%).

In a dry 100-mL two-necked round-bottom flask equipped with a magnetic stirring bar, argon, and syringe inlets was placed 422 mg (2.0 mmol) of 3-ethoxy-l,2-benzisothiazole 1,l-dioxide in 20 mL of dry THF. After the reaction mixture was cooled to -78 °C in a dry ice-acetone bath, 1.1 equiv of the appropriate organolithium reagent of the ethyl acetate was added via syringe. The reaction mixture was stirred for 4 h at this temperature, and quenched at -78 °C by addition of 40 mL of saturated NH_4Cl solution. The aqueous layer was extracted three times with EtOAc (3 X 20 mL), and the organic extracts were dried over anhydrous Na_2SO_4. After concentration in vacuo, the residue was finally purified by flash chromatography to give **4**.

(1,1-Dioxo-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid methyl ester (**4a**). Yield: 67%, mp = 184-187 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.82 (s, 3H), 5.71 (s, 1H), 7.72-7.77 (m, 3H), 7.88-7.90 (m, 1H), 10.1 (br, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 52.1, 88.4, 121.8, 122.6, 128.9, 132.9, 133.8, 143.8, 168.9. $C_{10}H_9NO_4SNa$ $(M+Na)^+$ 262.0150, found: 262.0146.

(1,1-Dioxo-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid ethyl ester (4b) (Known compound [6]). Yield: 67%, mp = 174-176 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.32-1.36 (m, 3H), 4.24-4.29 (m, 2H), 5.71 (s, 1H), 7.72-7.76 (m, 3H), 7.88-7.90 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.5, 61.1, 88.9, 121.8, 122.6, 128.9, 132.9, 133.8, 134.3, 143.7, 168.6.

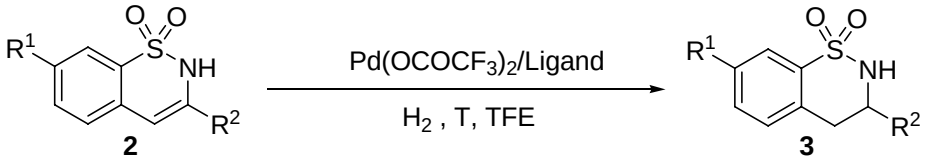
(1,1-Dioxo-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid *t*-butyl ester (4c). Yield: 67%, mp =

155-156 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.53 (s, 9H), 5.64 (s, 1H), 7.69-7.73 (m, 3H), 7.87-7.88 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.4, 81.8, 90.7, 121.8, 122.4, 129.1, 132.7, 133.7, 134.2, 142.9, 168.2. HRMS Calculated for $C_{13}H_{15}NO_4SNa$ $(M+Na)^+$ 304.0619, found: 304.0630.

(1,1-Dioxo-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid benzyl ester (4d). Yield: 77%, mp = 169-171 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 5.25 (s, 2H), 5.76 (s, 1H), 7.36-7.41 (m, 5H), 7.71-7.74 (m, 3H), 7.87-7.89 (m, 1H), 10.14 (br, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 66.7, 88.3, 121.7, 122.4, 128.4, 128.5, 128.7, 132.8, 133.7, 135.6, 143.9, 168.3. HRMS Calculated for $C_{16}H_{13}NO_4SNa$ $(M+Na)^+$ 338.0463, found: 338.0465.

(1,1-Dioxo-1*H*-1λ^6-*p*-methyl-benzo[*d*]isothiazol-3-yl)-acetic acid ethyl ester (4e). Yield: 77%, mp = 215-217 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.31-1.35 (m, 3H), 2.51 (s, 3H), 4.24-4.29 (m, 2H), 5.68 (s, 1H), 7.50-7.53 (m, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 10.08 (br, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.5, 22.1, 60.9, 88.5, 121.5, 122.7, 131.7, 133.8, 143.9, 144.9, 168.7. HRMS Calculated for $C_{12}H_{13}NO_4SNa$ $(M+Na)^+$ 290.0463, found: 290.0450.

5. Typical Procedure for Asymmetric Hydrogenation of Enesulfonamides (2)



2a-**2g**, **2l**, **2m**: L = (*R*,*S*$_p$)-JosiPhos
2h-**2k**: L = (*R*,*R*$_p$)-WalPhos

Typical procedure for asymmetric hydrogenation of Cyclic Enamines: Ligand (0.003 mmol) and Pd(OCO CF_3)$_2$ (0.85 mg, 0.0025 mmol) were placed in a dried Schlenk tube under nitrogen atmosphere, and degassed anhydrous acetone was added. The mixture was stirred at rt for 1 h. The solvent was removed under vacuum to give the catalyst. This catalyst was taken into a glove box filled with nitrogen and dissolved in dry TFE (3.0 mL). To the enammine (0.125 mmol) was added this catalyst solution, and then the mixture was transferred to an autoclave. The autoclave was stirred under 70 °C (oil bath temperature was showed). After releasing of the hydrogen, the autoclave was opened and the reaction mixture was evaporated. Conversion was determined by ^{1}H NMR analysis. The enantiomeric excess was determined by HPLC after purification on silica gel using petroleum ether and EtOAc. (Notes: for substrates **2a**-**2g**, **2l**, **2m**, (*R*,*S*$_p$)-JosiPhos was used; substrates **2h**-**2k**, (*R*,*R*$_p$)-WalPhos was used).

Racemates of **3** were prepared by the reduction of the corresponding enamines using Pd/C in MeOH or hydrogenation of corresponding substrates with racemic ligands.

3,4-Dihydro-3-phenyl-2*H*-1λ^6-benzo[*e*][1,2]thiazine 1,1-dioxide (3a) (known compound[4]**).** Yield: 96%, 98% ee (*R*), $[\alpha]^{25}_D$ = + 51.7 (c 0.93, $CHCl_3$); mp = 126-128 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.16-3.27 (m, 2H), 4.90-4.97 (m, 1H), 5.03 (d, *J* = 10.4 Hz, 1H), 7.22-7.25 (m, 1H), 7.32-7.47 (m, 7H), 7.76 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.8, 56.9, 123.9, 126.4, 127.9, 128.6, 129.2, 129.6, 132.4, 135.2, 137.9, 139.8. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 16.1 min (minor), t_2 = 19.9 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*o*-methyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3b). Yield: 97%, 98% ee (*R*), $[\alpha]^{24}_D$ = + 11.4 (c 0.77, $CHCl_3$); mp = 182-183 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.46 (s, 3H), 3.13 (dd, *J* = 16.6, 3.6 Hz, 1H), 3.34-3.41 (m, 1H), 4.67 (d, *J* = 10.4 Hz, 1H), 5.15-5.22 (m, 1H),

7.25-7.29 (m, 4H), 7.40-7.43 (m, 2H), 7.46-7.49 (m, 1H), 7.84 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.4, 34.5, 53.6, 124.2, 125.2, 126.8, 128.1, 128.6, 129.7, 131.3, 132.4, 135.3, 136.4, 137.3. HRMS Calculated for $C_{15}H_{15}NO_2SNa$ $(M+Na)^+$ 296.0721, found: 296.0728. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 12.0 min (minor), t_2 = 14.8 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*m*-methyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3c). Yield: 97%, 97% ee (*R*), $[\alpha]^{24}_D$ = + 46.2 (c 0.63, $CHCl_3$); mp = 147-149 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3H), 3.21-3.24 (m, 2H), 4.86-4.94 (m, 2H), 7.16-7.17 (m, 1H), 7.21-7.32 (m, 4H), 7.35-7.39 (m, 1H), 7.44-7.47 (m, 1H), 7.79-7.81 (d, *J* = 0.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.7, 35.8, 56.9, 123.3, 123.9, 127.2, 127.9, 129.1, 129.3, 129.6, 132.4, 135.2, 137.9, 138.9, 139.7. HRMS Calculated for $C_{15}H_{15}NO_2SNa$ $(M+Na)^+$ 296.0721, found: 296.0717. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 11.3 min (minor), t_2 = 13.4 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*p*-methyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3d). Yield: 99%, 97% ee (*R*), $[\alpha]^{24}_D$ = + 18.7(c 0.47, $CHCl_3$); mp = 151-152 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.37 (s, 3H), 3.24 (d, *J* = 6.6 Hz, 2H), 4.70 (d, *J* = 9.8 Hz, 1H), 4.92-4.96 (m, 1H), 7.21-7.33 (m, 5H), 7.39-7.43 (m, 1H), 7.47-7.50 (m, 1H), 7.85 (d, *J* = 7.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 35.8, 56.7, 123.9, 126.3, 128.0, 129.7, 129.8, 132.4. HRMS Calculated for $C_{15}H_{15}NO_2SNa$ $(M+Na)^+$ 296.0721, found: 296.0711. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 13.7 min (minor), t_2 = 18.4 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*p*-methoxyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3e) (known compound[3]). Yield: 97%, 95% ee (*R*), $[\alpha]^{24}_D$ = + 28.6 (c 0.77, $CHCl_3$); mp = 123-125 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.19-3.23 (m, 2H), 3.82 (s, 3H), 4.84-4.87 (m, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 7.24 (m, 1H), 7.34-7.37 (m, 3H), 7.44-7.46 (m, 1H), 7.79-7.81 (d, *J* = 7.6Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.8, 55.6, 56.5, 114.5, 123.9, 127.7, 127.9, 129.7, 131.9, 132.4, 135.2, 137.9, 159.7. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 14.9 min (minor), t_2 = 20.6 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*p*-fluoro-benzo[*e*][1,2]thiazine 1,1-dioxide (3f) (known compound[3])**.** Yield: 99%, 98% ee (*R*), $[\alpha]^{24}_D$ = + 59.2 (c 0.50, $CHCl_3$); mp = 141-143 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.17-3.27 (m, 2H), 4.88-4.95 (m, 1H), 5.02 (d, *J* = 10.3 Hz, 2H), 7.07-7.12 (m, 2H), 7.24-7.26 (m, 1H), 7.35-7.48 (m, 4H), 7.77-7.79 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.7, 56.4, 115.9, 116.2, 123.8, 128.1, 128.2, 128.3, 129.6, 132.5, 134.9, 135.7, 137.9, 163.9. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 13.1 min (minor), t_2 = 17.2 min (major).

3,4-Dihydro-3-phenyl-2*H*-1λ^6-*p*-chloro-benzo[*e*][1,2]thiazine 1,1-dioxide (3g) (known compound[3]**)**. Yield: 97%, 98% ee (*R*), $[\alpha]^{24}_D$ = + 26.9 (c 1.00, $CHCl_3$); mp = 148-150 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.23-3.29 (m, 2H), 4.78 (br, 1H), 4.90-4.94 (m, 1H), 7.29-7.31 (m, 1H), 7.38-7.44 (m, 5H), 7.48-7.52 (m, 1H), 7.83-7.86 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.6, 56.5, 123.9, 126.4, 127.8, 128.2, 128.6, 129.2, 129.4, 129.6, 132.6. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 12.7 min (minor), t_2 = 16.4 min (major).

3-Methyl-3,4-dihydro-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (3h) (known compound[7])**.**Yield: 99%, 98% ee (*R*), $[\alpha]^{24}_D$ = - 69.4 (c 0.53, $CHCl_3$); mp = 181-183 ^{o}C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.40 (d, *J* = 6.5 Hz, 3H), 2.77-2.84 (m, 1H), 2.97 (dd, *J* = 17.1, 3.2 Hz, 1H), 4.02-4.12 (m, 1H), 4.28 (br, 1H), 7.20-7.22 (m, 1H), 7.36-7.39 (m, 1H), 7.43-7.47 (m, 1H), 7.90 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.0, 36.5, 49.7, 124.3, 127.9, 129.6, 132.3. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 8.3 min (major), t_2 = 14.4 min (minor).

3-Propyl-3,4-dihydro-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (3i). Yield: 92%, 96% ee (*R*), $[\alpha]^{24}_{D}$ = - 60.4 (c 0.87, $CHCl_3$); mp = 80-82 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 0.96-0.99 (m, 3H), 1.49-1.65 (m, 4H), 2.71-2.79 (m, 1H), 2.90 (dd, *J* = 17.1, 3.9 Hz, 1H), 3.85-3.90 (m, 1H), 4.45 (br, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.29-7.41 (m, 2H), 7.74 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.9, 18.8, 34.8, 38.1, 53.4, 124.2, 127.8, 129.7, 132.2, 135.5, 137.7. HRMS Calculated for $C_{11}H_{15}NO_2SNa$ $(M+Na)^+$ 248.0721, found: 248.0714. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 8.9 min (major), t_2 = 18.6 min (minor).

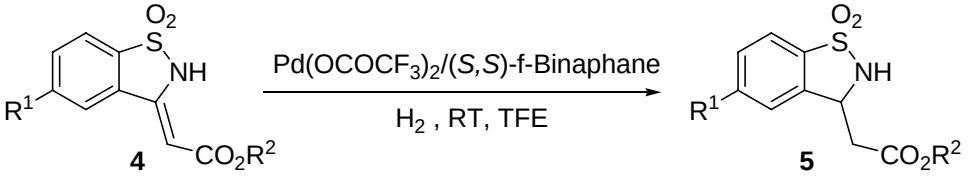
3-Amyl -3,4-dihydro-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (3j). Yield: 90%, 90% ee (*R*), $[\alpha]^{24}_{D}$ = - 30.52 (c 0.83, $CHCl_3$); mp = 93-94 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 0.89-0.93 (m, 3H), 1.32-1.37 (m, 4H), 1.58-1.62 (m, 2H), 1.63-1.66 (m, 2H), 2.75-2.83 (m, 1H), 2.95 (dd, *J* = 17.0, 3.9 Hz, 1H), 3.89 (m, 1H), 4.25 (d, *J* = 11.5 Hz, 1H), 7.19-7.22 (d, *J* = 7.6 Hz, 1H), 7.34-7.38 (m, 1H), 7.41-7.45 (m, 1H), 7.80 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.2, 22.7, 25.2, 31.6, 34.9, 36.2, 53.8, 124.3, 127.9, 129.7, 132.2, 135.4, 137.8. HRMS Calculated for $C_{13}H_{19}NO_2SNa$ $(M+Na)^+$ 276.1034, found: 276.1023. HPLC (AD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 7.0 min (major), t_2 = 9.1 min (minor).

3-2-Phenylethyl-3,4-dihydro-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (3k). Yield: 75%, 96% ee (*R*), $[\alpha]^{24}_{D}$ = - 5.74 (c 0.73, $CHCl_3$); mp = 65-67 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 1.92-1.98 (m, 2H), 2.79-2.95 (m, 4H), 3.85-3.88 (m, 1H), 4.37 (br, 1H), 7.17-7.26 (m, 4H), 7.28-7.39 (m, 3H), 7.40-7.42 (m, 1H), 7.79 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 31.7, 34.9, 37.9, 53.1, 124.3, 126.5, 127.9, 128.8, 129.7, 132.3, 135.2, 137.8, 140.9. HRMS Calculated for $C_{16}H_{17}NO_2SNa$ $(M+Na)^+$ 310.0878, found: 310.0868. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 13.6 min (major), t_2 = 32.5 min (minor).

3-Phenyl-3,4-dihydro-2*H*-*m*-methyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3l). Yield: 97%, 96% ee (*R*), $[\alpha]^{24}_{D}$ = + 49.3 (c 0.60, $CHCl_3$); mp = 197-198 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3H), 3.19 (d, *J* = 7.8 Hz, 2H), 4.79 (d, *J* = 10.4 Hz, 1H), 4.93-4.97 (m, 1H), 7.14-7.16 (d, *J* = 7.9 Hz, 1H), 7.25-7.28 (m, 1H), 7.34-7.45 (m, 5H), 7.64 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 35.5, 57.0, 124.1, 126.4, 128.6, 129.2, 129.5, 132.0, 133.3, 137.6, 138.2, 139.8. HRMS Calculated for $C_{15}H_{15}NO_2SNa$ $(M+Na)^+$ 296.0721, found: 296.0721. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 12.6 min (minor), t_2 = 16.0 min (major).

3-Fural-3,4-dihydro-2*H*- *m*-methyl-benzo[*e*][1,2]thiazine 1,1-dioxide (3m). Yield: 99%, 81% ee (*R*)), $[\alpha]^{15}_{D}$ = + 138.6 (c 0.20, $CHCl_3$); mp = 109-111 °C，^{1}H NMR (400 MHz, $CDCl_3$): δ 3.24 (dd, *J* = 17.1, 4.2 Hz, 1H), 3.32-3.40 (m, 1H), 4.77 (d, *J* = 11.1 Hz, 1H), 5.09-5.15 (m, 1H), 6.39 (m, 2H), 7.26-7.28 (m, 1H), 7.38-7.43 (m, 2H), 7.46-7.49 (m, 1H), 7.82 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 33.2, 51.1, 107.4, 110.8, 124.3, 128.2, 129.8, 132.5, 134.4, 137.7, 143.0, 151.7. HRMS Calculated for $C_{12}H_{11}NO_3SNa$ $(M+Na)^+$ 272.0357, found: 272.0361. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 11.9 min (minor), t_2 = 14.0 min (major).

6. Typical Procedure for Asymmetric Hydrogenation of Enesulfonamides (4)



Typical procedure for asymmetric hydrogenation of Cyclic Enamines: (*S*,*S*)-f-Binaphane (2.4 mg, 0.003 mmol) and Pd(OCO CF_3)$_2$ (0.85 mg, 0.0025 mmol) were placed in a dried Schlenk tube under nitrogen atmosphere, and degassed anhydrous acetone was added. The mixture was stirred at rt for 1 h. The solvent was removed under vacuum to give the catalyst. This catalyst was taken into a glove box filled with nitrogen and dissolved in dry TFE (3.0 mL). To the enammine (0.125 mmol) was added this catalyst solution, and then the mixture was transferred to an autoclave. The autoclave was stirred under room temperature. After release of the hydrogen, the autoclave was opened and the reaction mixture was evaporated. Conversion was determined by ^{1}H NMR analysis. The enantiomeric excess was determined by HPLC after purification on silica gel using petroleum ether and EtOAc.

Racemates of **5** were prepared by the reduction of the corresponding enamines using Pd/C in MeOH or hydrogenation of corresponding substrates with racemic ligands.

(1,1-Dioxo-2,3-dihydro-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid methyl ester (5a) (known compound[8]). Yield: 97%, 86% ee (*S*), $[\alpha]^{24}_D$ = - 112.5 (c 0.7, $CHCl_3$), mp = 139-141 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.77-2.84 (m, 1H), 2.97-3.02 (dd, *J* = 17.0, 3.4 Hz, 1H), 2.97 (s, 3H), 5.09-5.13 (m, 1H), 5.56 (br, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.55-7.65 (m, 2H), 7.81 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.2, 52.4, 53.6, 121.6, 123.9, 129.8, 133.3, 138.0, 171.3. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 12.3 min (major), t_2 = 15.5 min (minor).

(1,1-Dioxo-2,3-dihydro-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid ethyl ester (5b) (known compound[8]). Yield: 97%, 92% ee (*S*), $[\alpha]^{24}_D$ = - 112.5 (c 0.7, $CHCl_3$); mp = 116-117 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.25-1.30 (m, 3H), 2.80-2.83 (m, 1H), 2.97 (m, 1H), 4.19-4.23 (m, 2H), 5.12 (m, 1H), 5.43 (br, 1H), 7.38-7.40 (m, 1H), 7.57-7.65 (m, 2H), 7.81 (d, *J* = 7.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ14.3, 40.5, 53.8, 61.7, 121.8, 124.1, 129.9, 133.5, 138.2. HPLC (OJ-H column, ^{i}PrOH/hexane 30/70, 0.8 mL min^{-1}, 254 nm): t_1 = 22.1 min (minor), t_2 = 24.2 min (major).

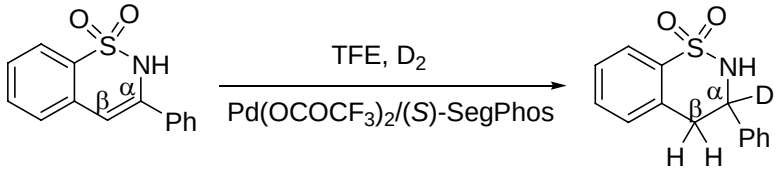
(1,1-Dioxo-2,3-dihydro-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid *t*-butyl ester (5c). Yield: 97%, 96% ee (*R*), $[\alpha]^{24}_D$ = + 1.17 (c 0.84, $CHCl_3$); mp = 114-115 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.46 (s, 9H), 2.69-2.76 (m, 1H), 2.92 (dd, *J* = 16.8, 3.4 Hz, 1H), 5.02-5.07 (m, 1H), 5.47 (br, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.54-7.58 (m, 1H), 7.62-7.66 (m, 1H), 7.79-7.82 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.2, 41.2, 53.9, 82.6, 121.7, 124.1, 129.9, 133.4, 138.5, 163.2, 170.1. HRMS Calculated for $C_{13}H_{17}NO_4SNa$ $(M+Na)^+$ 306.0776, found: 306.0772. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 9.1 min (major), t_2 = 10.0 min (minor).

(1,1-Dioxo-2,3-dihydro-1*H*-1λ^6-benzo[*d*]isothiazol-3-yl)-acetic acid benzyl ester (5d). Yield: 97%, 87% ee (*S*), $[\alpha]^{24}_D$ = - 48.95 (c 0.84, $CHCl_3$); mp = 132-133 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.82-2.88 (m, 1H), 3.04 (m, 1H), 5.09-5.29 (m, 3H), 5.45 (br, 1H), 7.34-7.38 (m, 6H), 7.54-7.62 (m, 2H), 7.80 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.4, 53.6, 67.3, 121.7, 123.9, 128.5, 128.6, 128.7, 129.8, 133.3, 137.9, 170.6. HRMS Calculated for $C_{16}H_{15}NO_4SNa$ $(M+Na)^+$ 340.0619, found: 340.0633. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 17.8 min (major), t_2 = 24.6 min (minor).

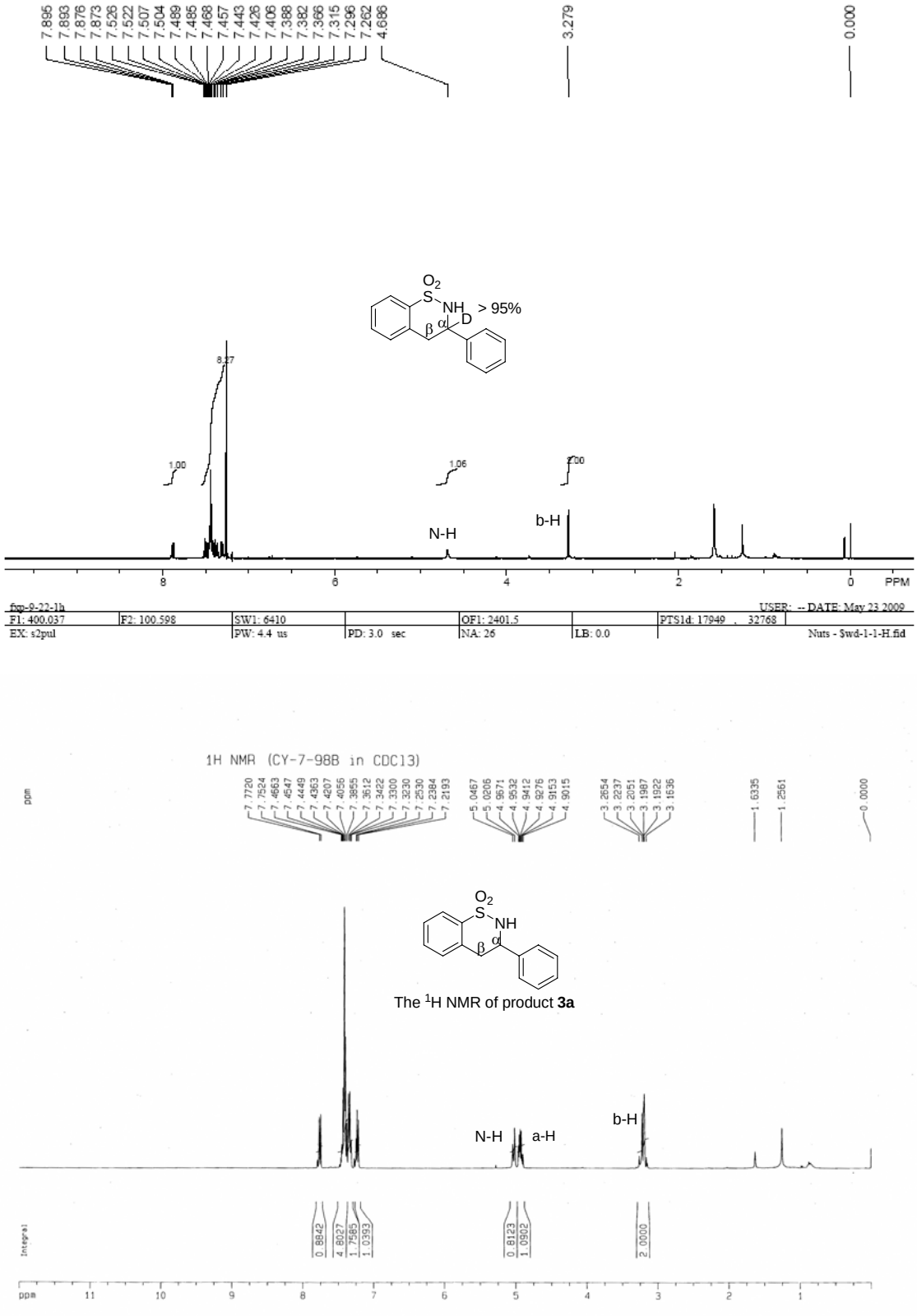
(1,1-Dioxo-2,3-dihydro-1*H*-1λ^6-*p*-methyl-benzo[*d*]isothiazol-3-yl)-acetic acid ethyl ester (5e). Yield: 99%, 87% ee (*S*), $[\alpha]^{24}_D$ = -105.79 (c 0.42, $CHCl_3$); mp = 161-162 ^oC, ^1H NMR (400 MHz, $CDCl_3$): δ 1.25-1.30 (m, 3H), 2.46 (s, 3H), 2.76 (dd, *J* = 16.9, 10.0 Hz, 1H), 2.95 (dd, *J* = 16.9, 3.4 Hz, 1H), 4.19-4.25 (m, 2H), 5.03-5.07 (m, 1H), 5.51 (br, 1H), 7.17 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.4, 22.0, 40.6, 53.7, 61.7, 121.6, 124.4, 130.9, 138.6, 144.5, 170.9. HRMS Calculated for $C_{12}H_{15}NO_4SNa$ $(M+Na)^+$ 292.0619, found: 292.0609. HPLC (OD-H column, ^{i}PrOH/hexane 30/70, 0.7 mL min^{-1}, 254 nm): t_1 = 32.7 min (minor), t_2 = 35.0 min (major).

7. Isotopic Labeling Experiments Using D_2 and CF_3CH_2OD

Deuteration with D_2:



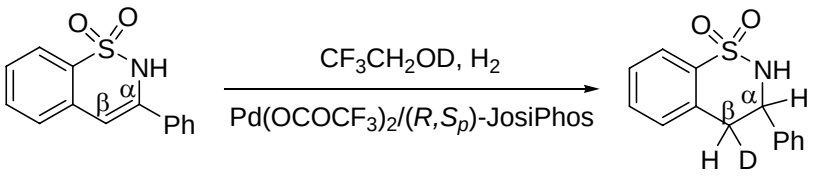
(*S*)-SegPhos (3.7 mg, 0.006 mmol) and $Pd(OCOCF_3)_2$ (1.7 mg, 0.005 mmol) were placed in a dried Schlenk tube under nitrogen atmosphere, and degassed anhydrous acetone was added. The mixture was stirred at rt for 1 h. The solvent was removed under vacuum to give the catalyst. This catalyst was taken into a glove box filled with nitrogen and dissolved in dry TFE (3.0 mL). To the enesulfonamide **3a** (64 mg, 0.25 mmol) was added this catalyst solution, and then the mixture was transferred to an autoclave. The autoclave was filled with D_2 of 10 atm, and stirred under 70 ^oC (oil bath temperature was showed) for 24 h. The product was obtained after purification on silica gel using petroleum ether and EtOAc. ^1H NMR analysis of the crude hydrogenated product showed that one deuterium atom was incorporated to the α-position, and deuterium at the β-position was not observed, which suggested that the hydrogenation of enesulfonamides was conducted *via N*-sulfonylimine intermediates (Figure 1).



The ^{1}H NMR of product **3a**

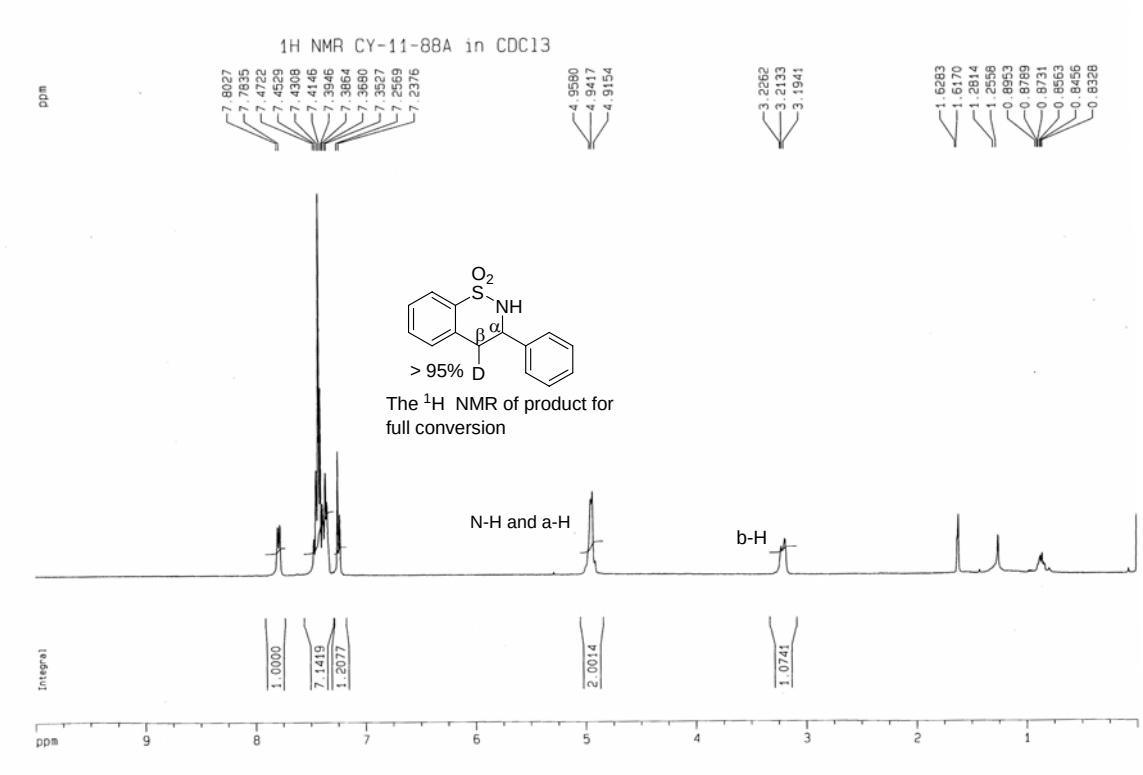
Figure 1

Deuteration with CF_3CH_2OD:



For the full conversion experiment: (R,S_p)-Josiphos (1.9 mg, 0.003 mmol) and $Pd(OCOCF_3)_2$ (0.9 mg, 0.0025 mmol) were placed in a dried Schlenk tube under nitrogen atmosphere, and degassed anhydrous acetone was added. The mixture was stirred at rt for 1 h. The solvent was removed under vacuum to give the catalyst. This catalyst was taken into a glove box filled with nitrogen and dissolved in dry CF_3CH_2OD (3.0 mL). To the enesulfonamide **3a** (32 mg, 0.125 mmol) was added this catalyst solution, and then the mixture was transferred to an autoclave. The autoclave was filled with H_2 of 28 atm, and stirred under 70 ^oC (oil bath temperature was showed) for 18 h. The product and the starting material were obtained after purification on silica gel using petroleum ether and EtOAc. ^1H NMR analysis of the crude hydrogenated product showed that one deuterium atom was incorporated to the β-position.

For the incomplete conversion experiment: Under the above conditions with H_2 pressure was 1 atm and stirred under 65 ^oC (oil bath temperature was showed) for 3 h. ^1H NMR analysis of the crude hydrogenated product showed that one deuterium atom was incorporated to the β-position, while no deuterium atom was observed in the recovered starting materials (Figure 2).



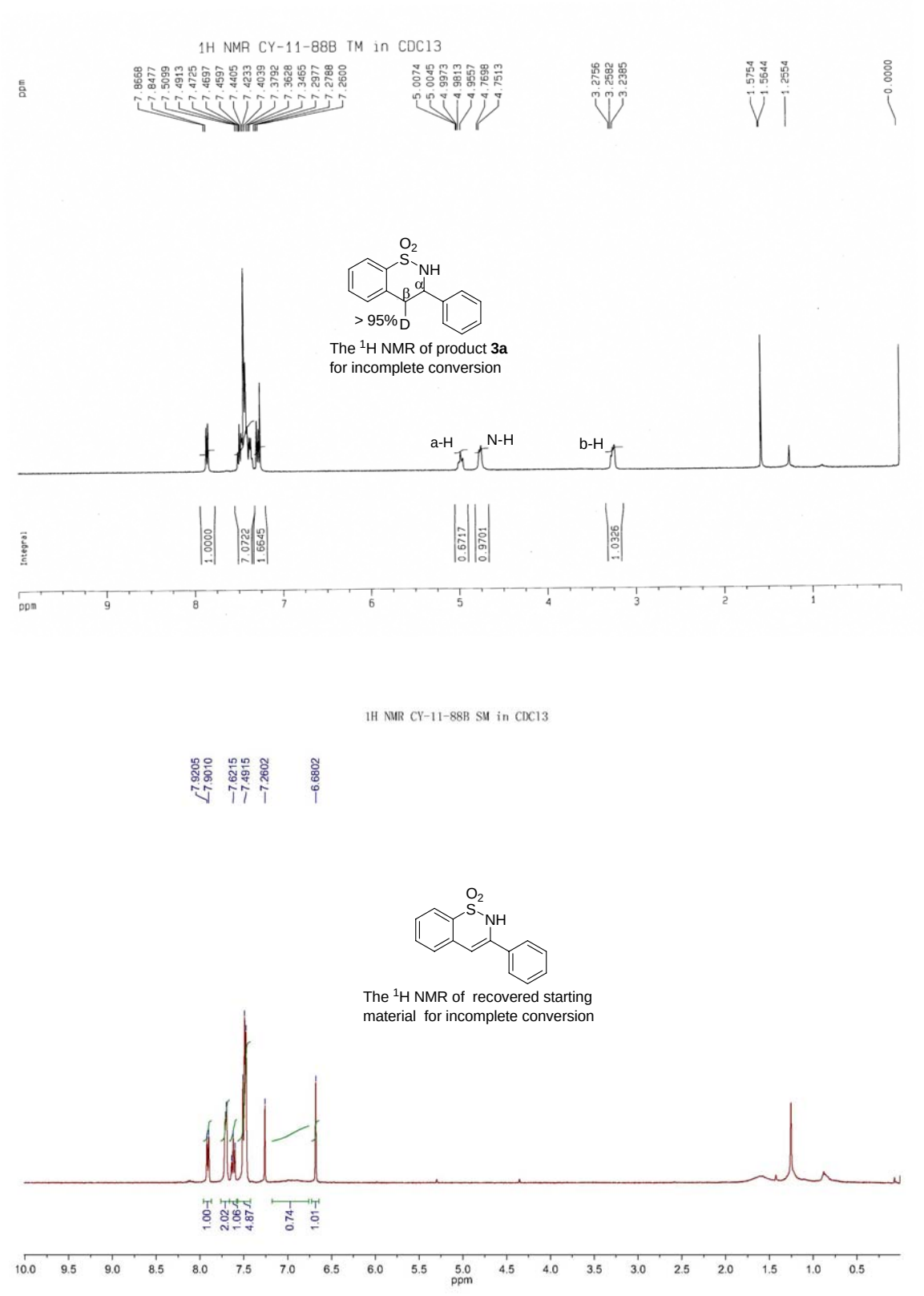
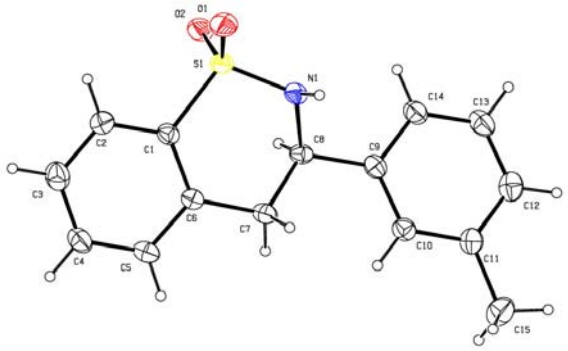


Figure 2

The above experiments confirmed that the hydrogenation of enesulfonamides was conducted *via* *N*-sulfonylimine intermediates, and the tautomerization process of enesulfonamides to *N*-sulfonylimine intermediates was slower than the hydrogenation.

8. Determination of Absolute Configuration of Hydrogenated Product 3.

Recrystallization from DCM/hexane gave sulfonamide **3c** (>99% ee) as a colorless crystal, and its absolute configuration was assigned as (*R*)-**3c** by X-ray diffraction analysis.



Crystal data and structure refinement for **3c**.

Identification code	p212121
Empirical formula	C15 H15 N O2 S
Formula weight	273.34
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 4.972(4) A alpha = 90 deg. b = 13.870(10) A beta = 90 deg. c = 19.934(14) A gamma = 90 deg.
Volume	1374.5(16) A^3
Z, Calculated density	4, 1.321 Mg/m^3
Absorption coefficient	0.232 mm^-1
F(000)	576
Crystal size	0.21 x 0.18 x 0.15 mm
Theta range for data collection	2.52 to 25.99 deg.
Limiting indices	-6<=h<=6, -17<=k<=14, -20<=l<=24
Reflections collected / unique	6867 / 2682 [R(int) = 0.0773]
Completeness to theta = 25.99	99.4 %
Absorption correction	None
Max. and min. transmission	0.9660 and 0.9528
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2682 / 0 / 177
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1139
R indices (all data)	R1 = 0.0907, wR2 = 0.1275
Absolute structure parameter	-0.07(14)
Largest diff. peak and hole	0.184 and -0.228 e.A^-3

Bond lengths [A] and angles [deg] for **3c**.

C(1)-C(2)	1.366(5)
C(1)-C(6)	1.400(4)
C(1)-S(1)	1.763(4)
C(2)-C(3)	1.383(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.372(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.373(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.515(5)
C(7)-C(8)	1.521(4)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-N(1)	1.497(4)
C(8)-C(9)	1.520(5)
C(8)-H(8)	0.9800
C(9)-C(10)	1.370(5)
C(9)-C(14)	1.400(5)
C(10)-C(11)	1.393(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.392(6)
C(11)-C(15)	1.506(6)
C(12)-C(13)	1.388(6)
C(12)-H(12)	0.9300
C(13)-C(14)	1.367(5)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
N(1)-S(1)	1.598(3)
N(1)-H(1N)	0.79(3)
O(1)-S(1)	1.437(3)
O(2)-S(1)	1.432(3)
C(2)-C(1)-C(6)	121.6(3)
C(2)-C(1)-S(1)	117.9(3)
C(6)-C(1)-S(1)	120.4(3)
C(1)-C(2)-C(3)	120.1(4)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	119.4(4)
C(4)-C(3)-H(3)	120.3

C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	120.6(4)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	121.2(4)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	117.1(3)
C(5)-C(6)-C(7)	119.7(3)
C(1)-C(6)-C(7)	123.2(3)
C(6)-C(7)-C(8)	114.3(3)
C(6)-C(7)-H(7A)	108.7
C(8)-C(7)-H(7A)	108.7
C(6)-C(7)-H(7B)	108.7
C(8)-C(7)-H(7B)	108.7
H(7A)-C(7)-H(7B)	107.6
N(1)-C(8)-C(9)	109.1(3)
N(1)-C(8)-C(7)	110.0(3)
C(9)-C(8)-C(7)	114.6(3)
N(1)-C(8)-H(8)	107.6
C(9)-C(8)-H(8)	107.6
C(7)-C(8)-H(8)	107.6
C(10)-C(9)-C(14)	118.4(4)
C(10)-C(9)-C(8)	122.6(3)
C(14)-C(9)-C(8)	119.0(3)
C(9)-C(10)-C(11)	122.7(4)
C(9)-C(10)-H(10)	118.7
C(11)-C(10)-H(10)	118.7
C(12)-C(11)-C(10)	118.2(4)
C(12)-C(11)-C(15)	121.2(4)
C(10)-C(11)-C(15)	120.6(4)
C(13)-C(12)-C(11)	119.2(4)
C(13)-C(12)-H(12)	120.4
C(11)-C(12)-H(12)	120.4
C(14)-C(13)-C(12)	121.8(4)
C(14)-C(13)-H(13)	119.1
C(12)-C(13)-H(13)	119.1
C(13)-C(14)-C(9)	119.7(4)
C(13)-C(14)-H(14)	120.2
C(9)-C(14)-H(14)	120.2
C(11)-C(15)-H(15A)	109.5
C(11)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(11)-C(15)-H(15C)	109.5

H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(8)-N(1)-S(1)	117.0(2)
C(8)-N(1)-H(1N)	114(3)
S(1)-N(1)-H(1N)	116(2)
O(2)-S(1)-O(1)	117.34(17)
O(2)-S(1)-N(1)	108.69(18)
O(1)-S(1)-N(1)	107.63(18)
O(2)-S(1)-C(1)	105.57(17)
O(1)-S(1)-C(1)	111.24(17)
N(1)-S(1)-C(1)	105.78(17)

9. References

(1) Xiao, D.; Zhang, X. *Angew. Chem., Int. Ed*. **2001,** *40*, 3425.

(2) (a) Neustadt, B. R. *Tetrahedron Lett*. **1994**, *35*, 379.
(b) Freitag, D.; Metz, P. *Tetrahedron* **2006**, *62*, 1799.

(3) (a) Fang, F.; Wng, R.; Liu, Z.-P.; Ji, A.-G. *Heterocycles* **2007**, *71*, 2377.
(b) Wang, Y.-Q; Lu, S.-M.; Zhou, Y.-G. *J. Org. Chem*. **2007**, *72*, 3729.

(4) Takeuchi, Y.; Liu, Z.-P.; Satoh, A.; Shiragami, T.; Shibata, N. *Chem. Pharm. Bull.* **1999**, *47*, 1730.

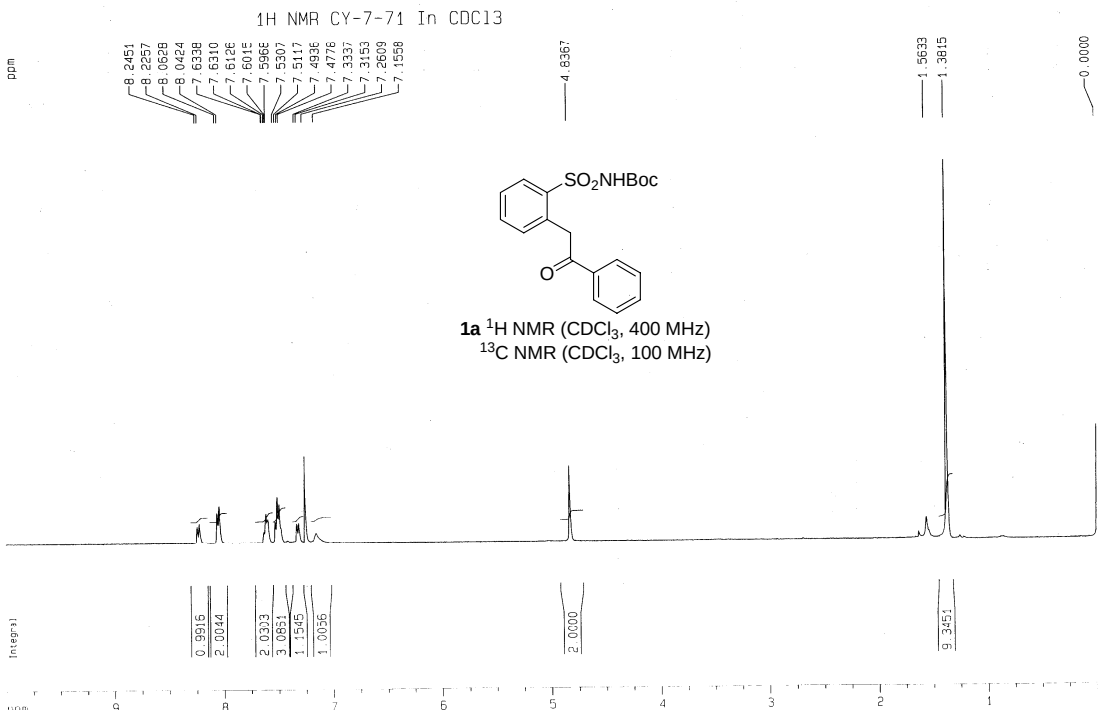
(5) William, L. J. Thomas, D. G.; Aaron, L.D.; James, F. W. *J. Org. Chem*. **2005**, *70*, 9147.

(6) Melchiorre. *et al. Annadi di Chimical(Rome, Italy)*. **1971**, *61*, 399.

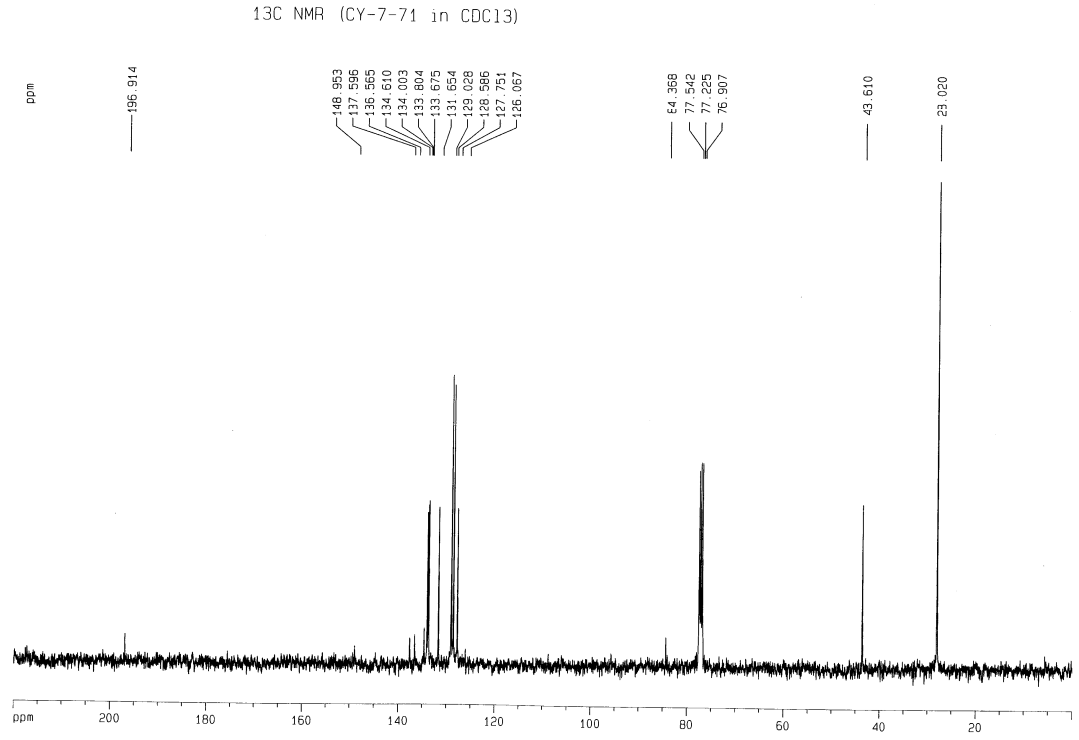
(7) Liu, X.-Y.; Li, C.-, H.; Che, C.-M. *Org. Lett*. **2006**, *8*, 2707.

(8) Rao, B. K.; Hamor, G. H. *J. Pharm.Sciences*. **1969**, *58*, 1969.

(9) Davis, F. A.; Towson, J. C.; Vashi, D, A.; Thimmareddy, R.; McCauley, J. P.; Harakal, M. E.; Gosciniak, D. J. *J. Org.Chem*. **1990**, *55*, 1254.



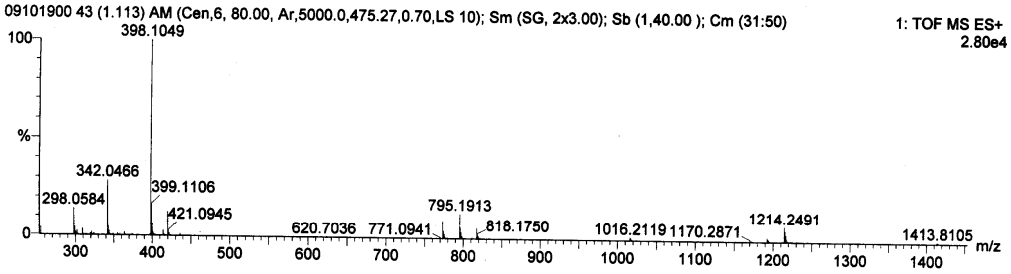
1a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-4 O: 2-5 Na: 1-1 S: 1-1
CY-7-71
09101900 43 (1.113) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (31:50) 1: TOF MS ES+ 2.80e4



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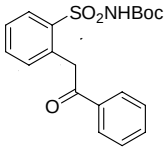
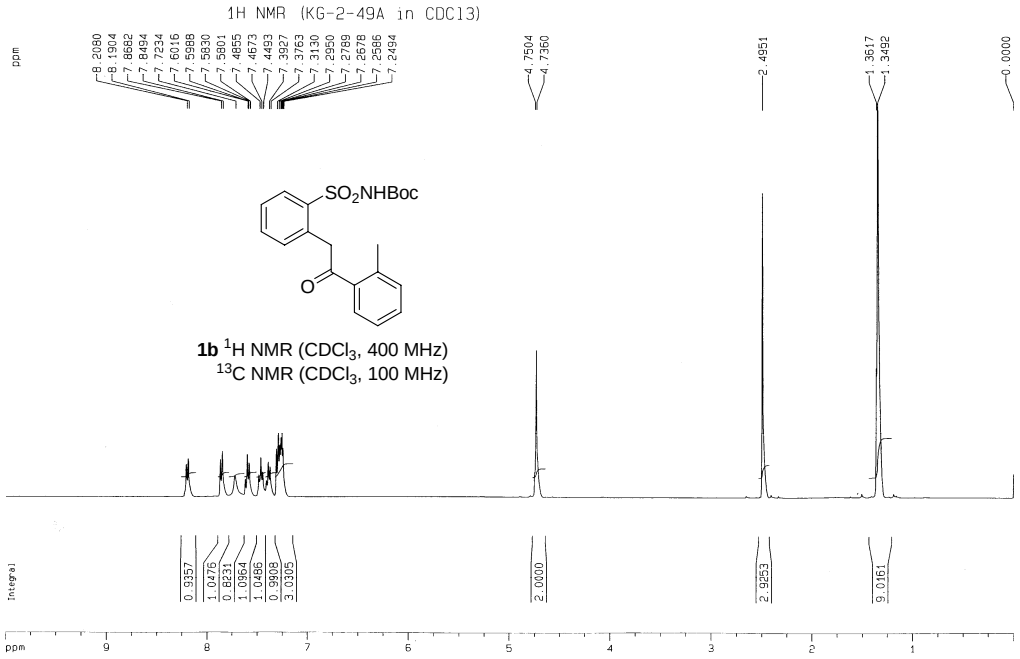
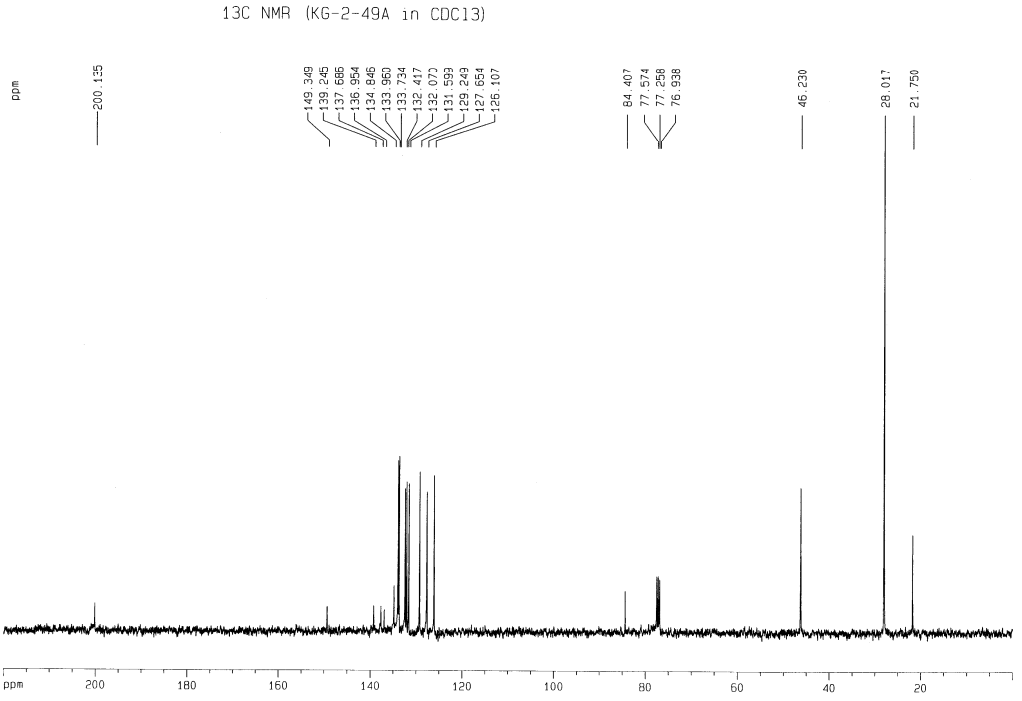


1a HRMS



1b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



Elemental Composition Report **Page 1**

Single Mass Analysis
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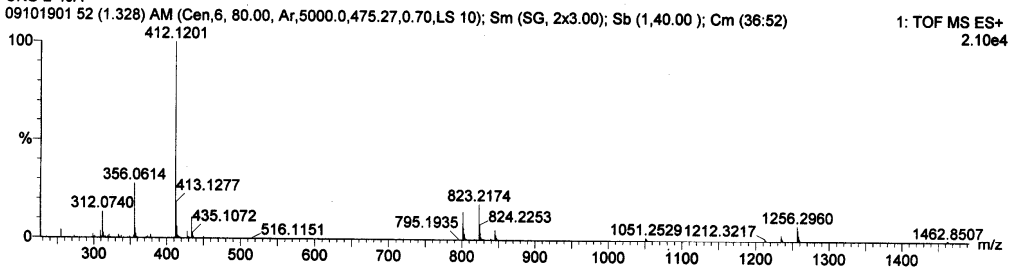
Selected filters: None

Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-4 O: 5-5 Na: 1-1 S: 1-1
CKG-2-49A
09101901 52 (1.328) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (36:52) 1: TOF MS ES+ 2.10e4



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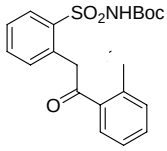
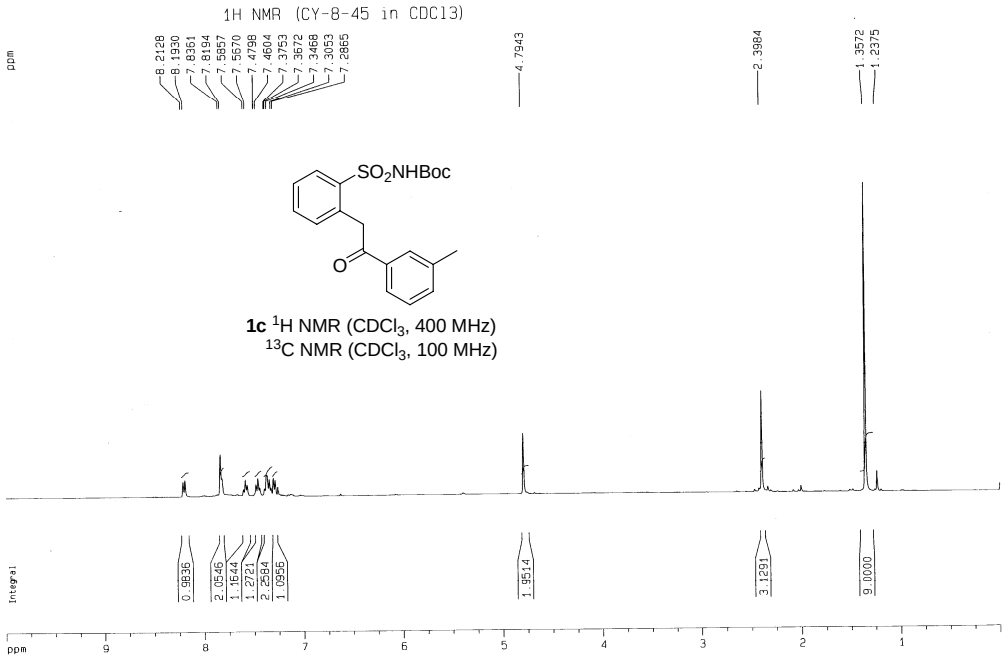
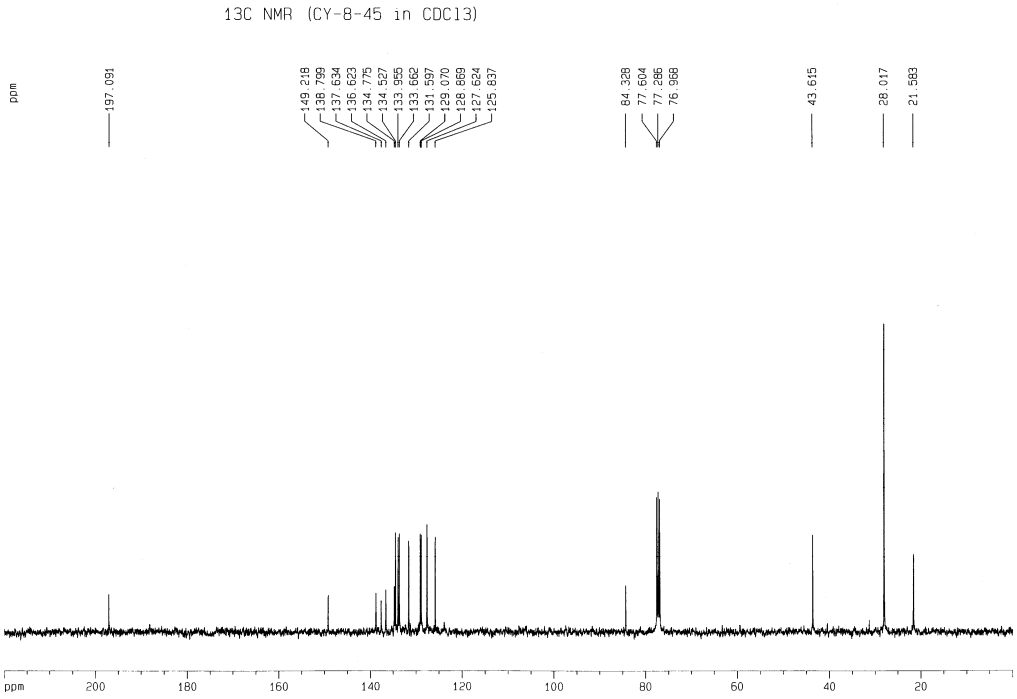


1b HRMS



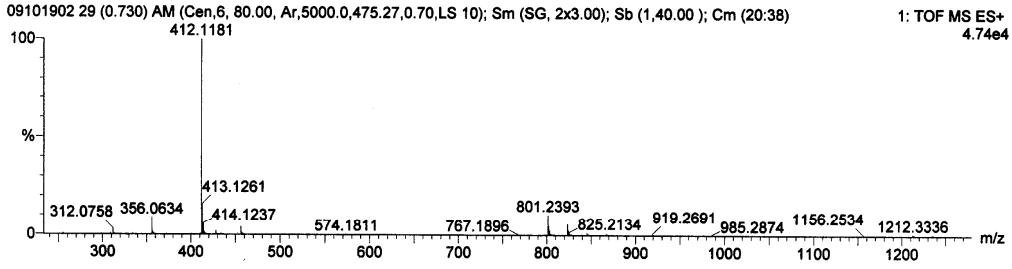
1c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



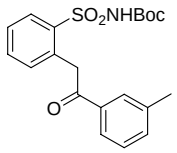
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

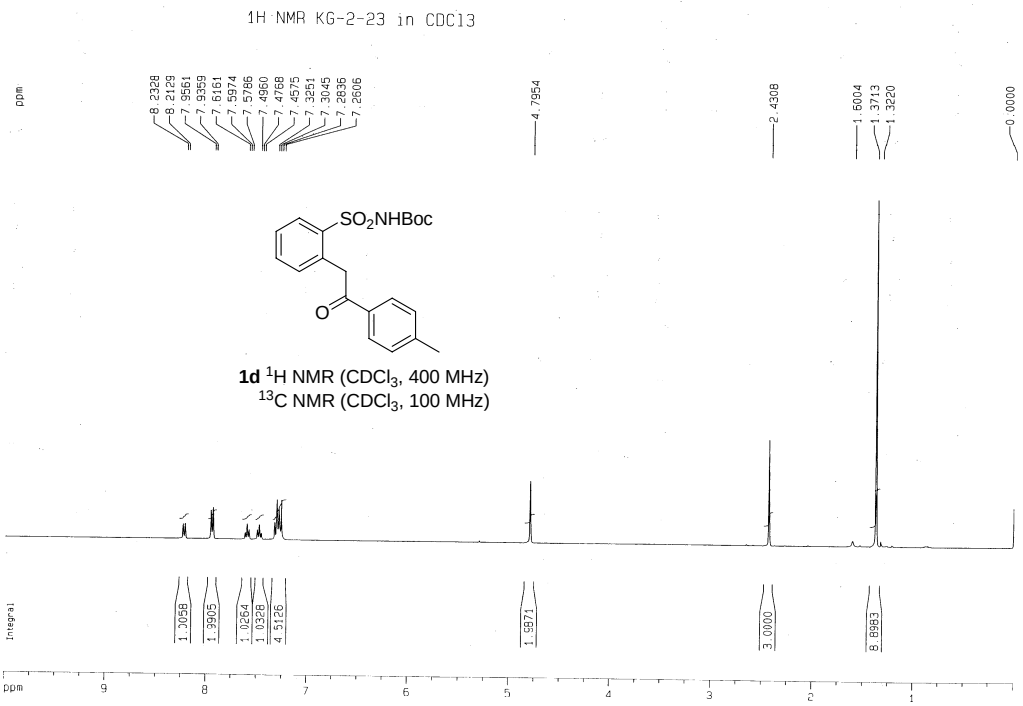
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-4 O: 5-5 Na: 1-1 S: 1-1
CY-8-45
09101902 29 (0.730) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (20:38) 1: TOF MS ES+
4.74e4



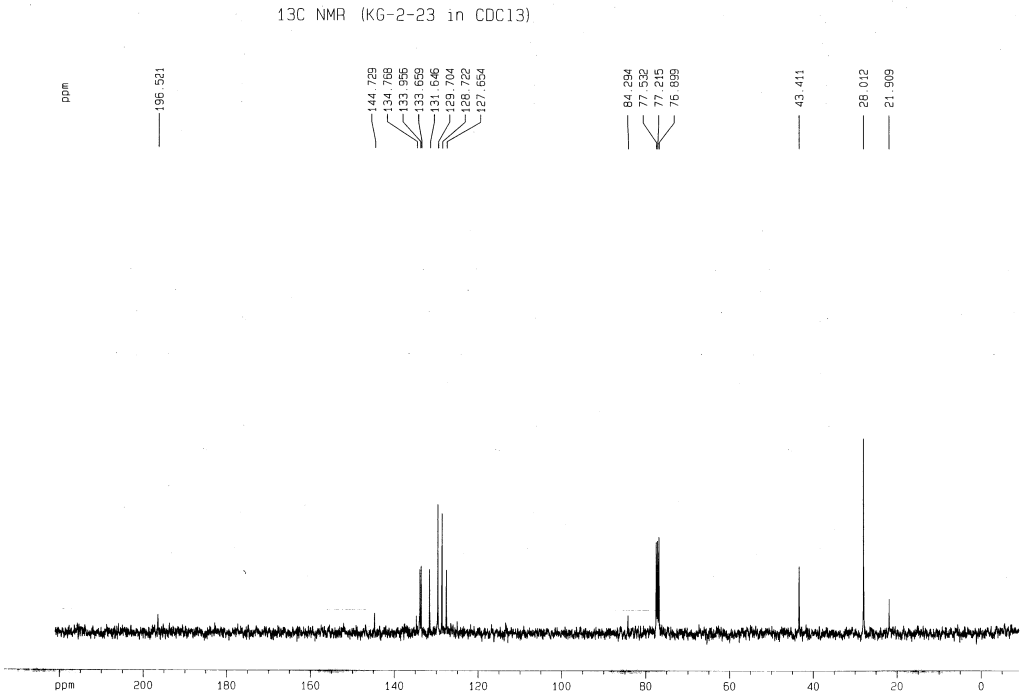
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.1181	412.1195	-1.4	-3.4	9.5	875.0	C20 H23 N O5 Na S



1c HRMS



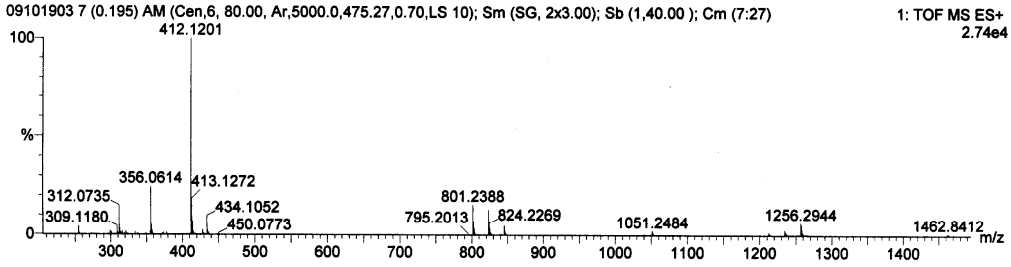
1d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



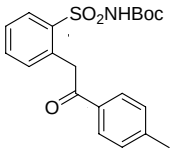
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

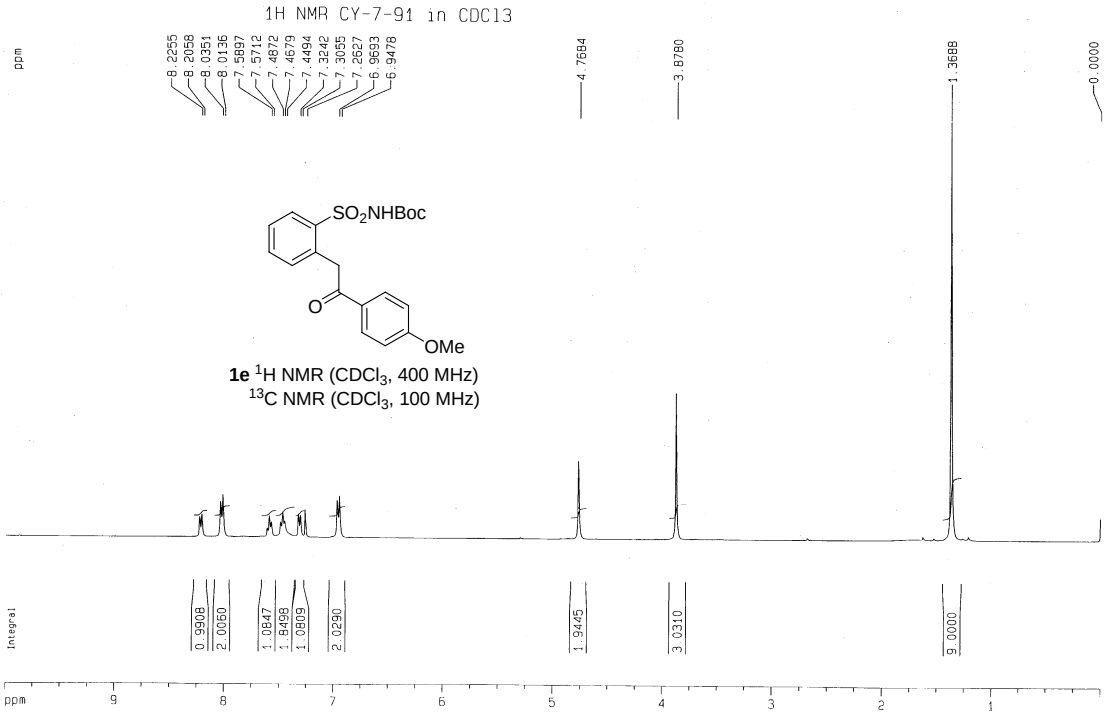
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-4 O: 5-5 Na: 1-1 S: 1-1
KG-2-23
09101903 7 (0.195) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (7:27) 1: TOF MS ES+ 2.74e4



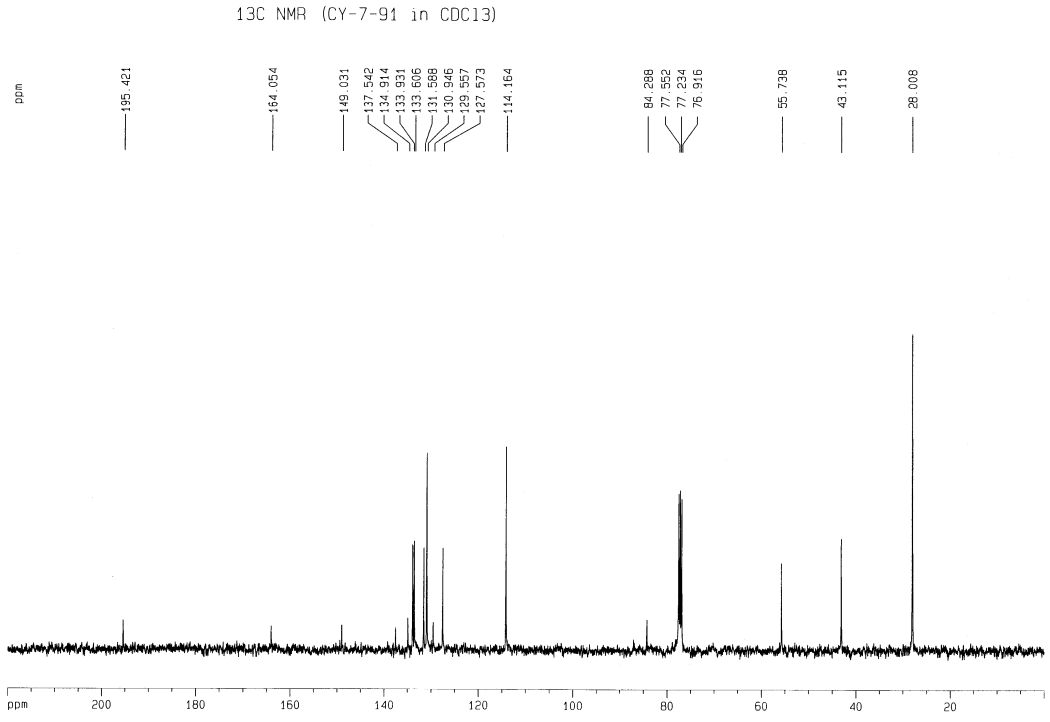
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
412.1201	412.1195	0.6	1.5	9.5	197.5	C20 H23 N O5 Na S



1d HRMS



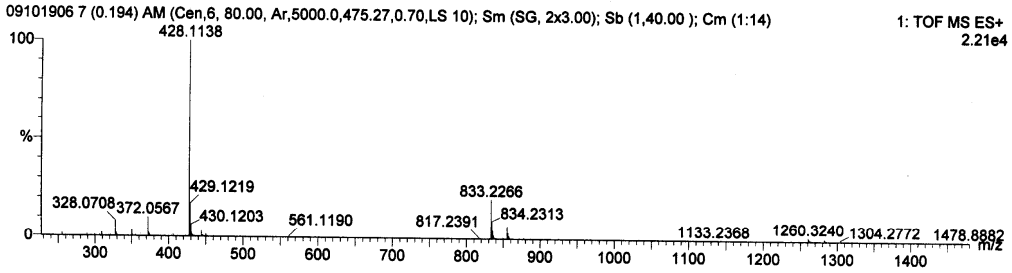
1e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



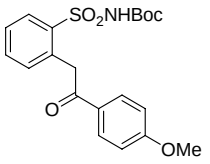
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

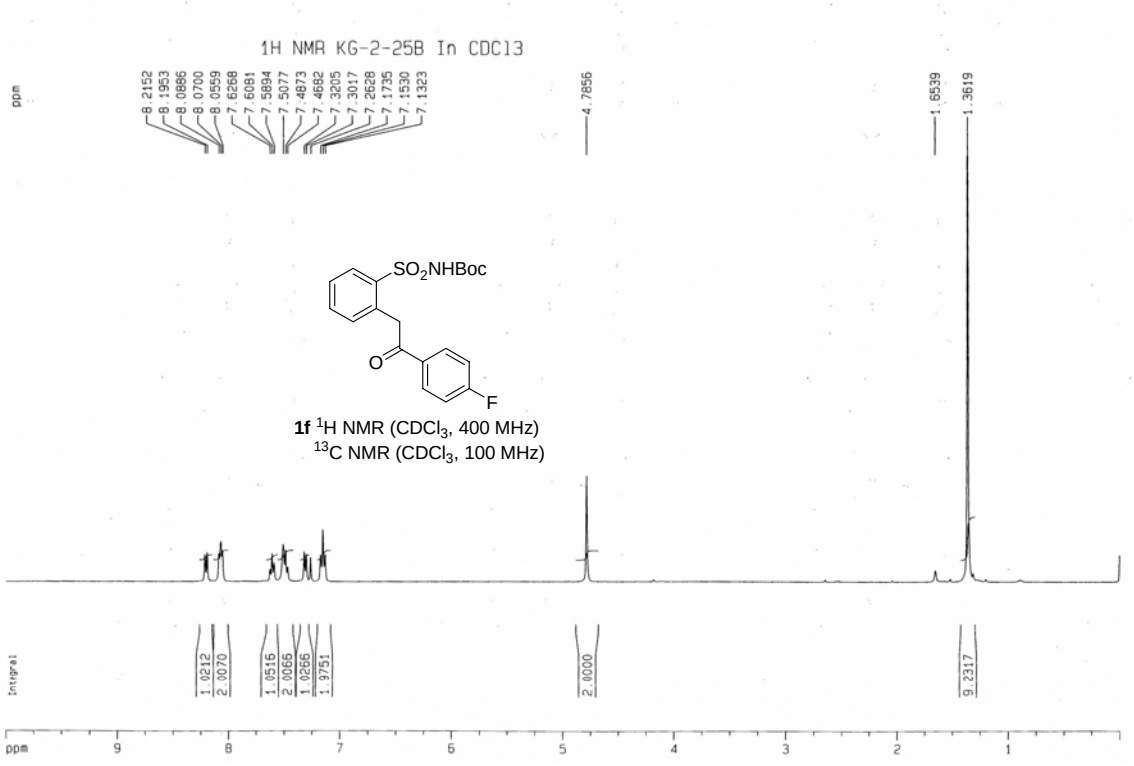
Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-1 O: 5-6 Na: 1-1 S: 1-1
CY-7-91
09101906 7 (0.194) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:14) 1: TOF MS ES+ 2.21e4



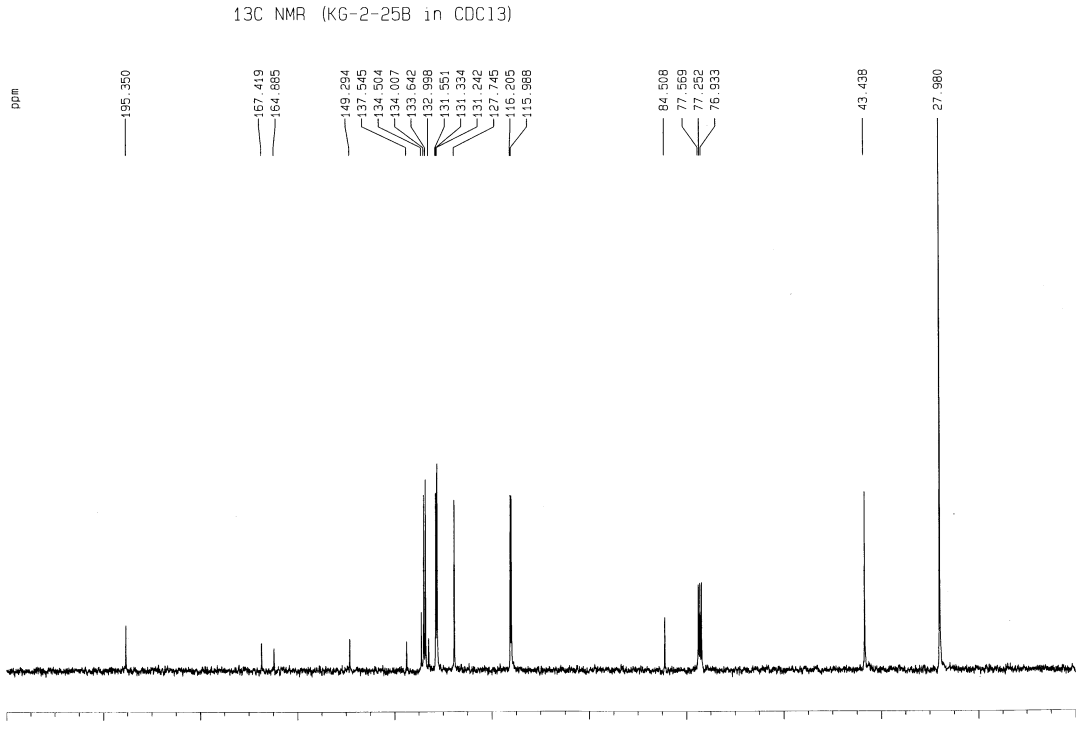
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.1138	428.1144	-0.6	-1.4	9.5	296.2	C20 H23 N O6 Na S



1e HRMS



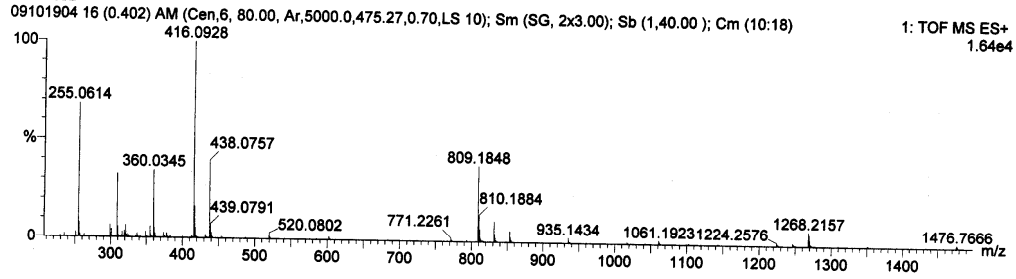
1f ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



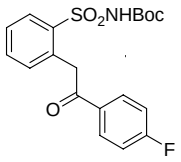
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

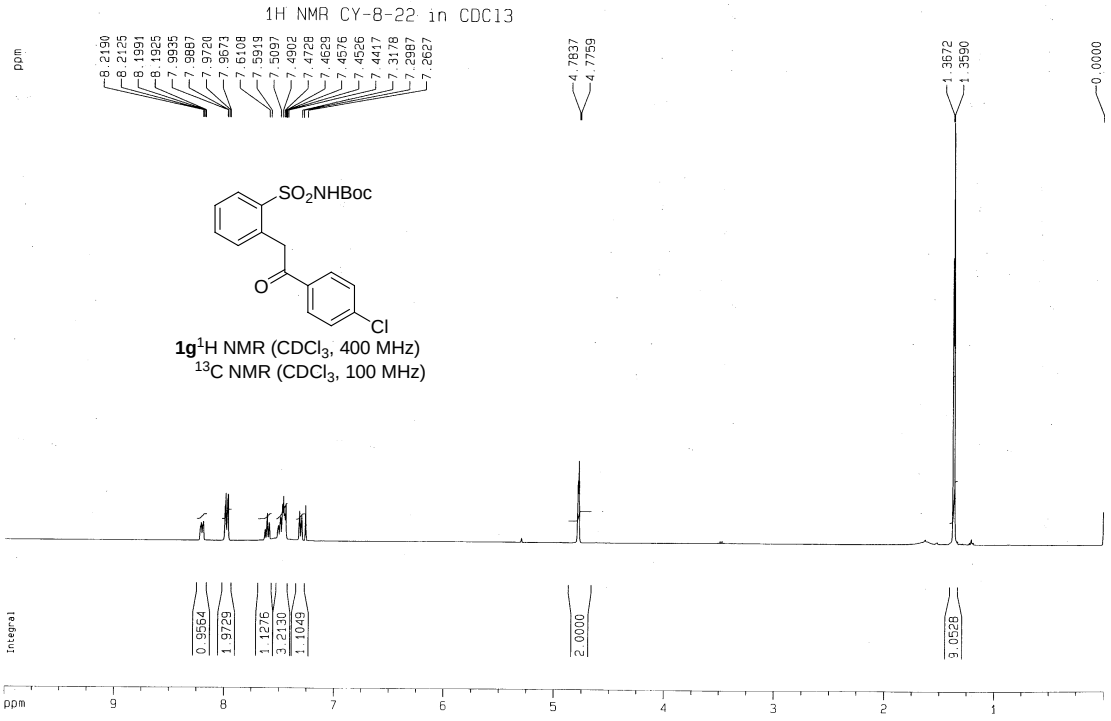
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-1 O: 5-5 F: 1-1 Na: 1-1 S: 1-1
KG-2-25B
09101904 16 (0.402) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (10:18) 1: TOF MS ES+ 1.64e4



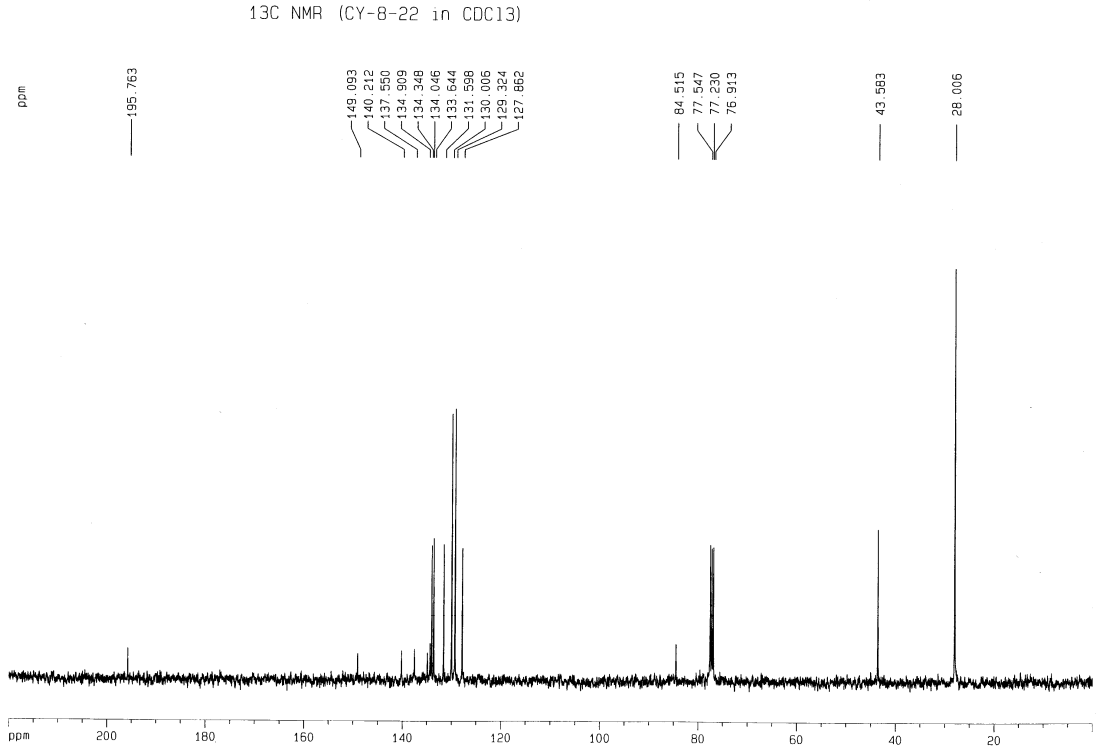
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
416.0928	416.0944	-1.6	-3.8	9.5	208.0	C19 H20 N O5 F Na S



1f HRMS



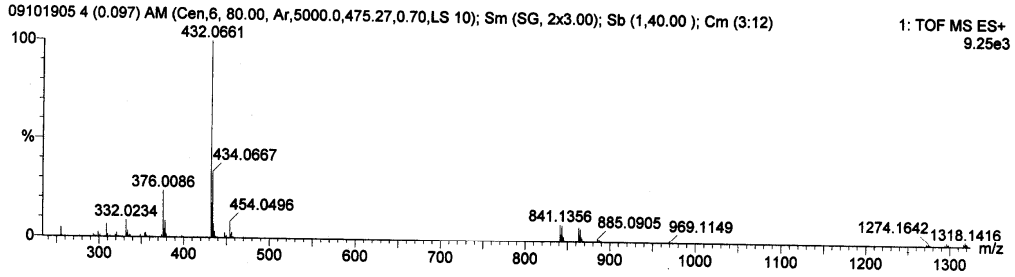
1g ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



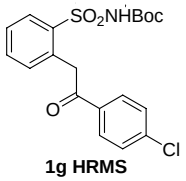
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

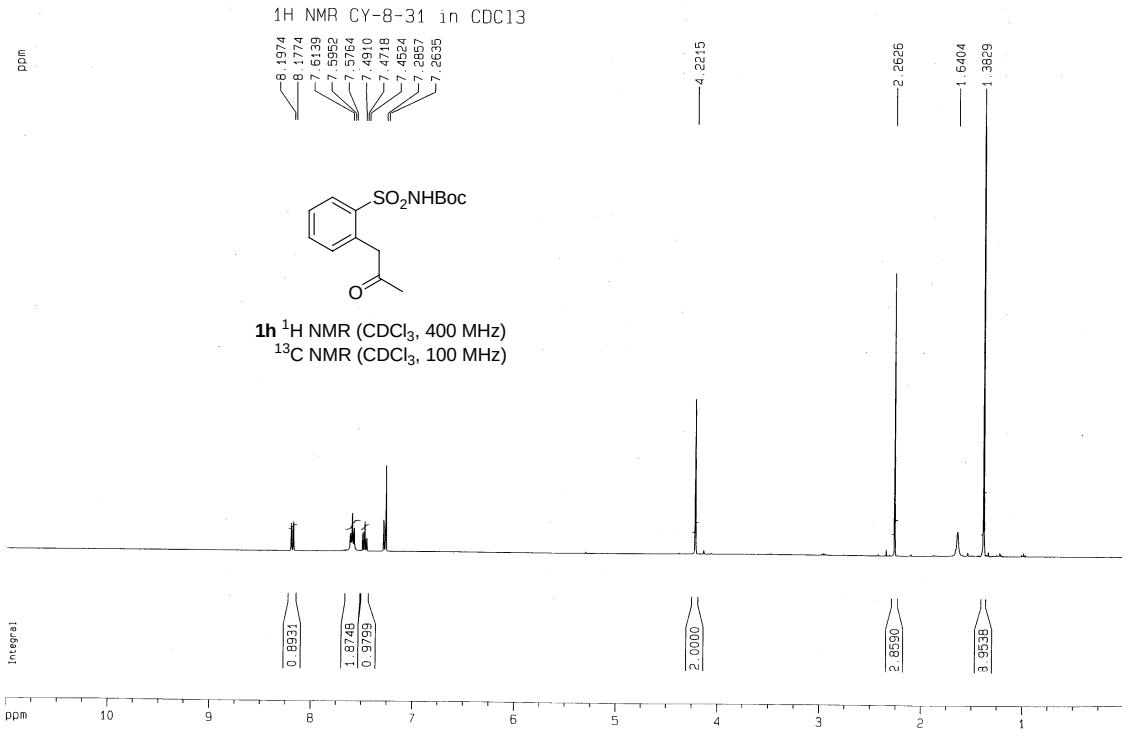
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-1 O: 5-5 Na: 1-1 S: 1-1 Cl: 1-2
KCY-8-22
09101905 4 (0.097) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (3:12) 1: TOF MS ES+ 9.25e3



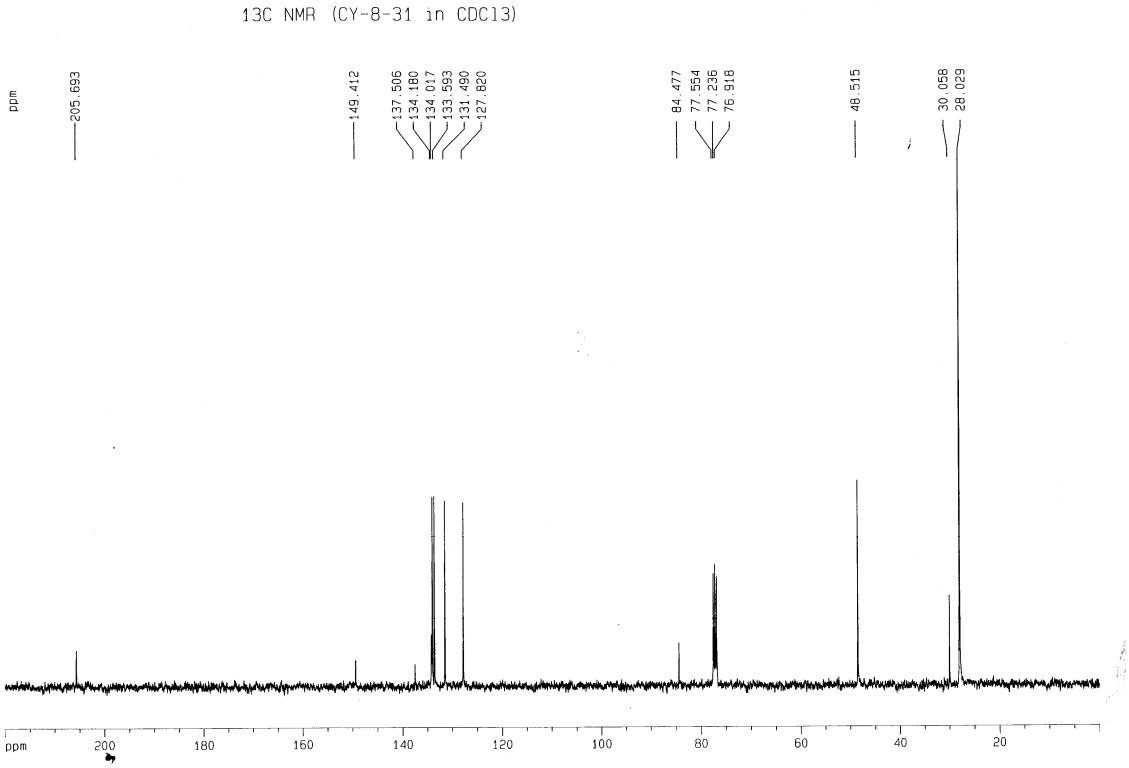
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
432.0661	432.0648	1.3	3.0	9.5	74.9	C19 H20 N O5 Na S Cl



1g HRMS



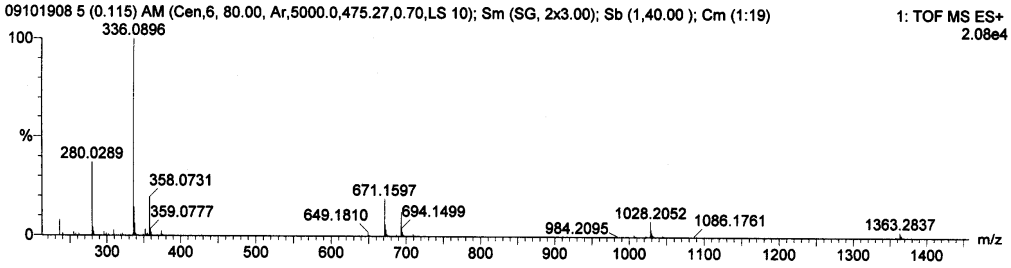
1h ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



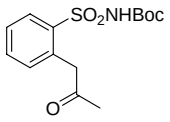
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

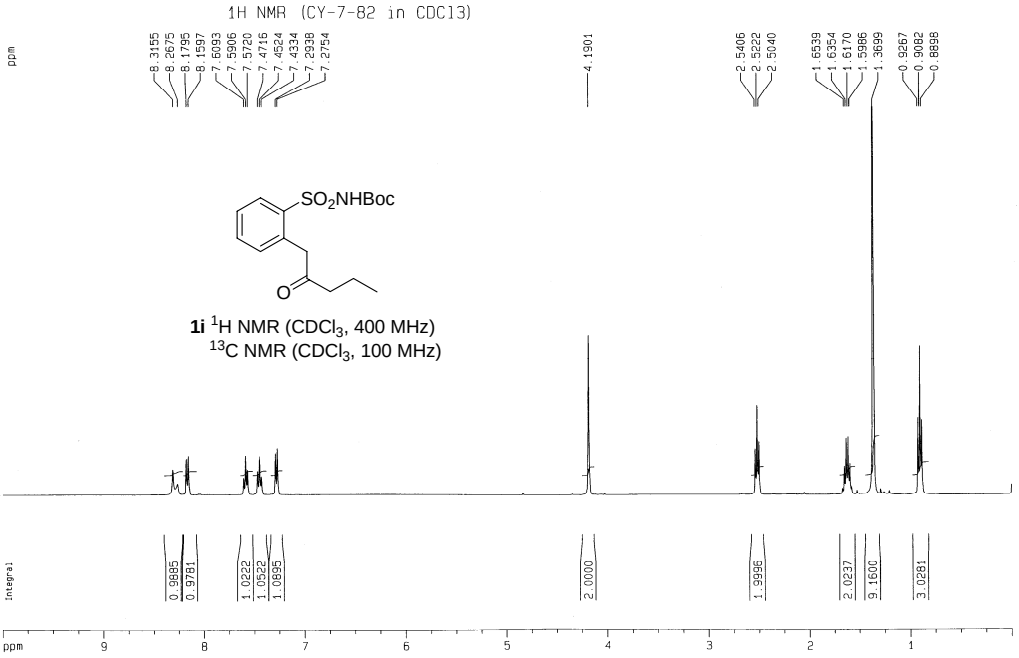
Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-1 O: 1-6 Na: 1-1 S: 1-1
CY-8-31
09101908 5 (0.115) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:19) 1: TOF MS ES+ 2.08e4



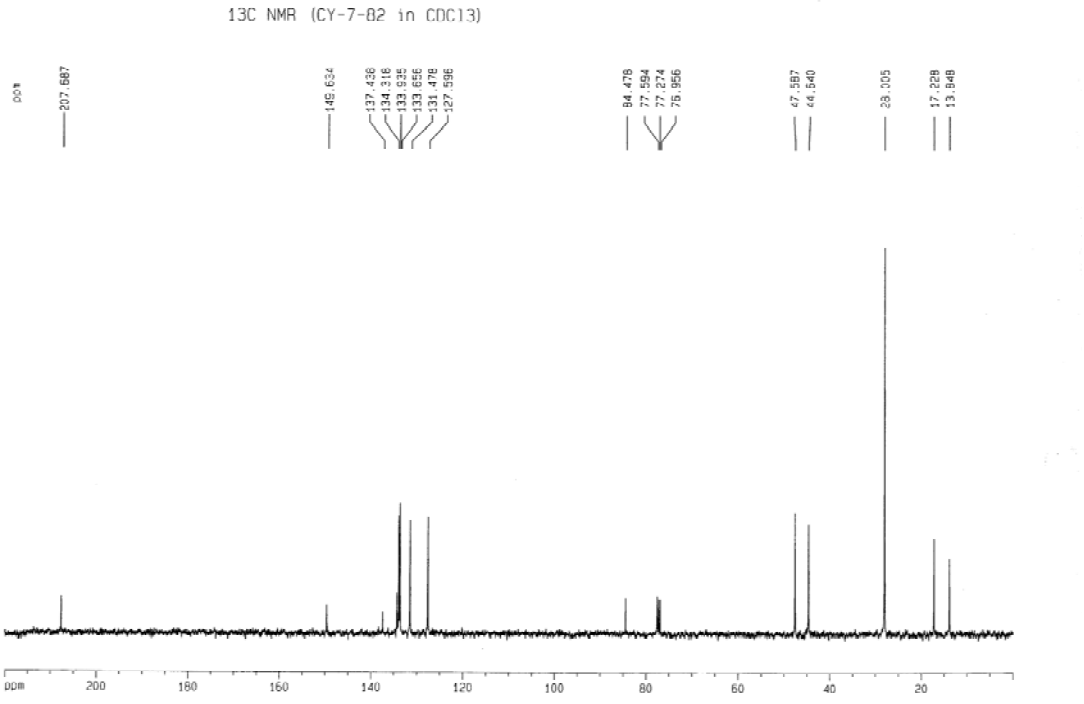
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
336.0896	336.0882	1.4	4.2	5.5	64.2	C14 H19 N O5 Na S



1h HRMS



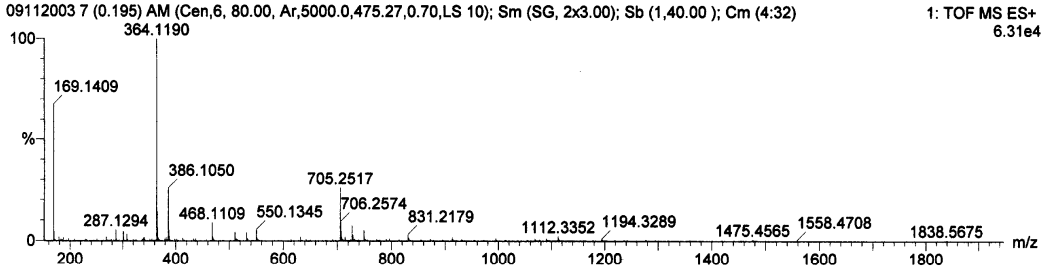
1i ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



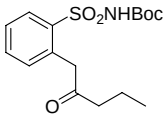
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

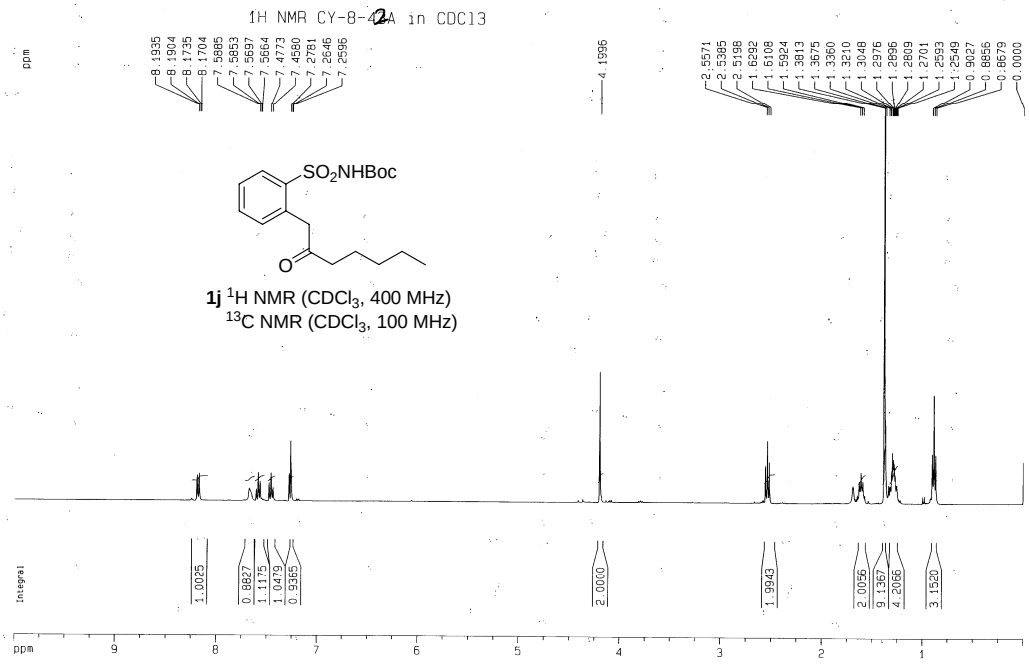
Monoisotopic Mass, Odd and Even Electron Ions
49 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 10-80 N: 1-3 O: 4-6 Na: 1-1 S: 1-2
CY-7-82
09112003 7 (0.195) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (4:32) 1: TOF MS ES+ 6.31e4



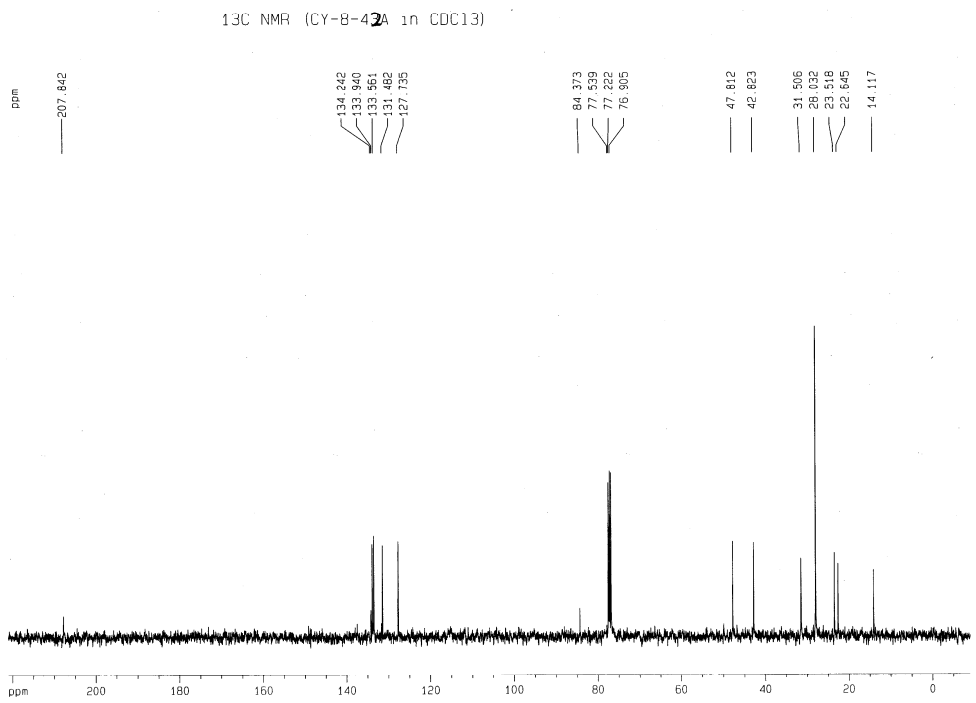
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
364.1190	364.1195	-0.5	-1.4	5.5	536.1	C16 H23 N O5 Na S



1i HRMS



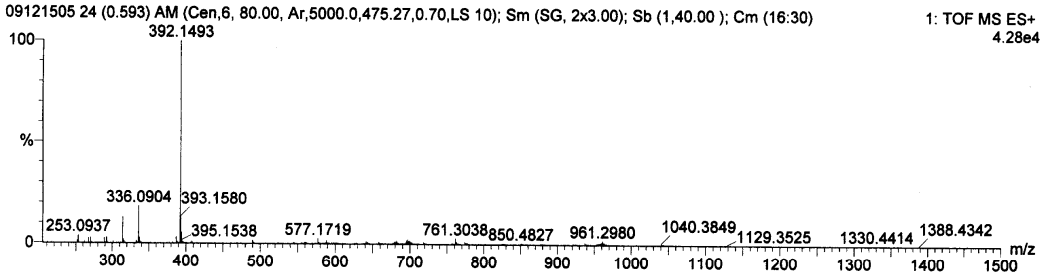
1j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



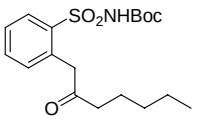
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

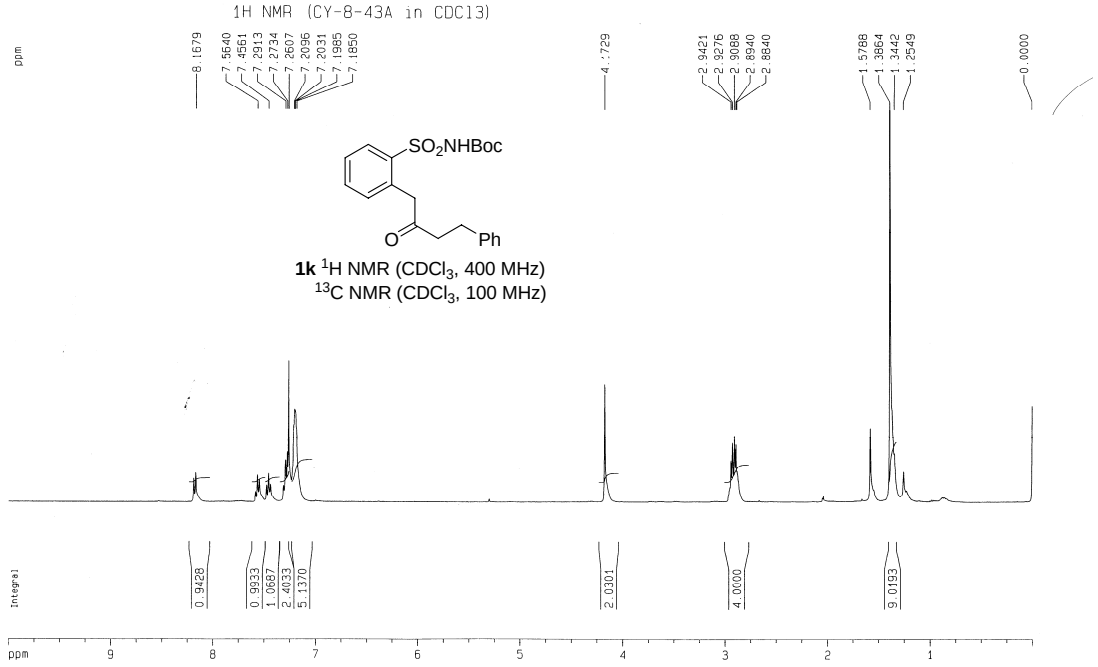
Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-60 H: 8-80 N: 1-1 O: 5-5 Na: 1-1
CY-8-42A
09121505 24 (0.593) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (16:30) 1: TOF MS ES+ 4.28e4



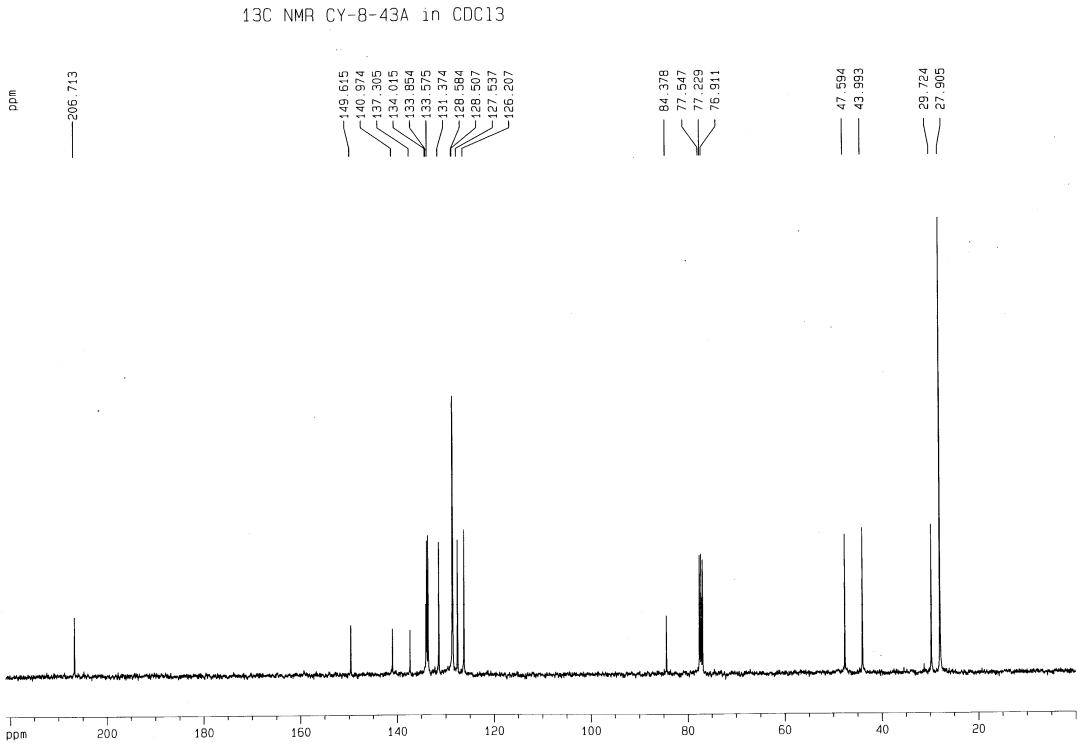
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
392.1493	392.1474	1.9	4.8	10.5	1568.5	C21 H23 N O5 Na



1j HRMS



1k ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

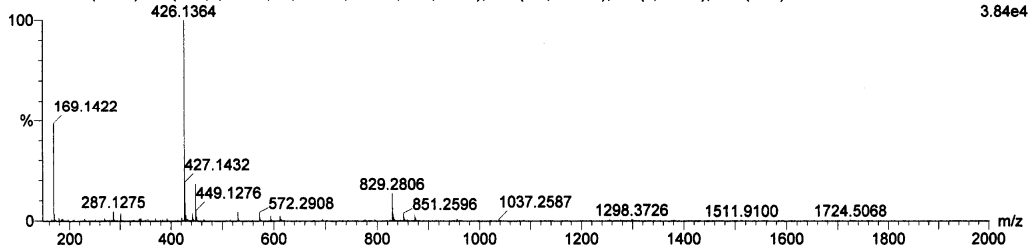


Elemental Composition Report **Page 1**

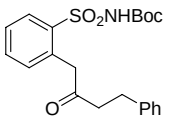
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
32 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 10-80 N: 1-3 O: 4-6 Na: 1-1 S: 1-1

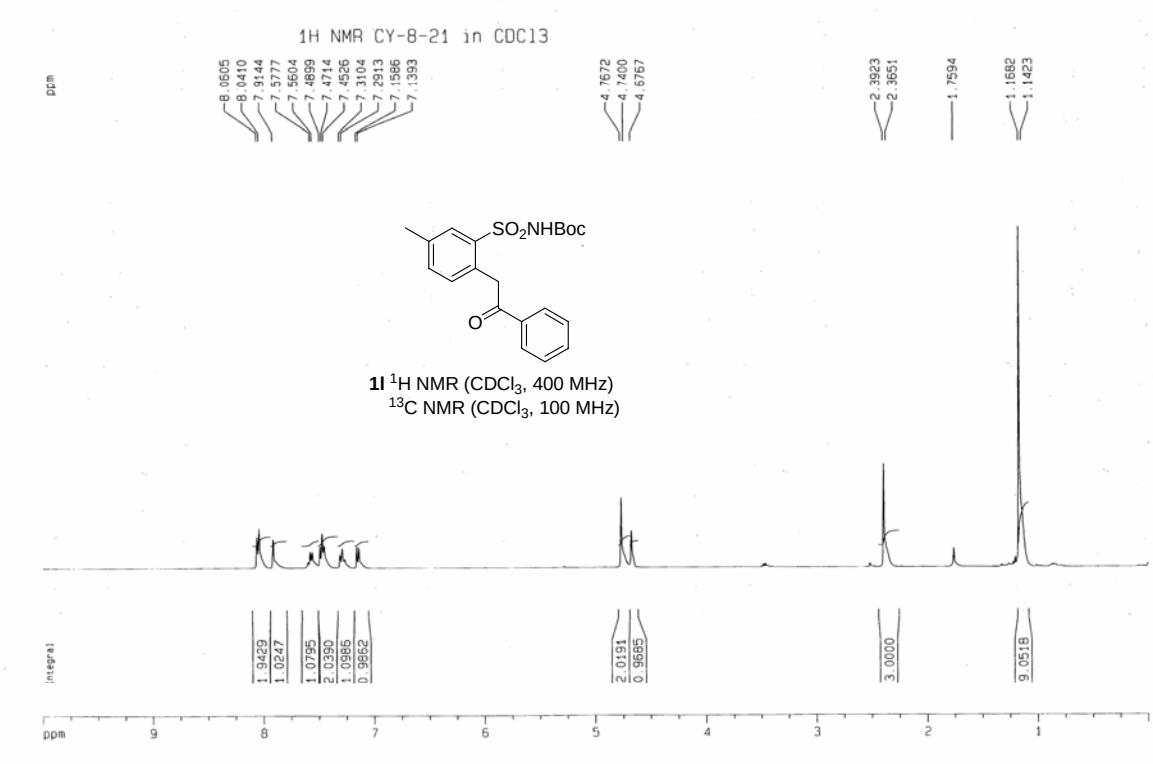
CY-8-43A
09112004 6 (0.134) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:18) 1: TOF MS ES+ 3.84e4



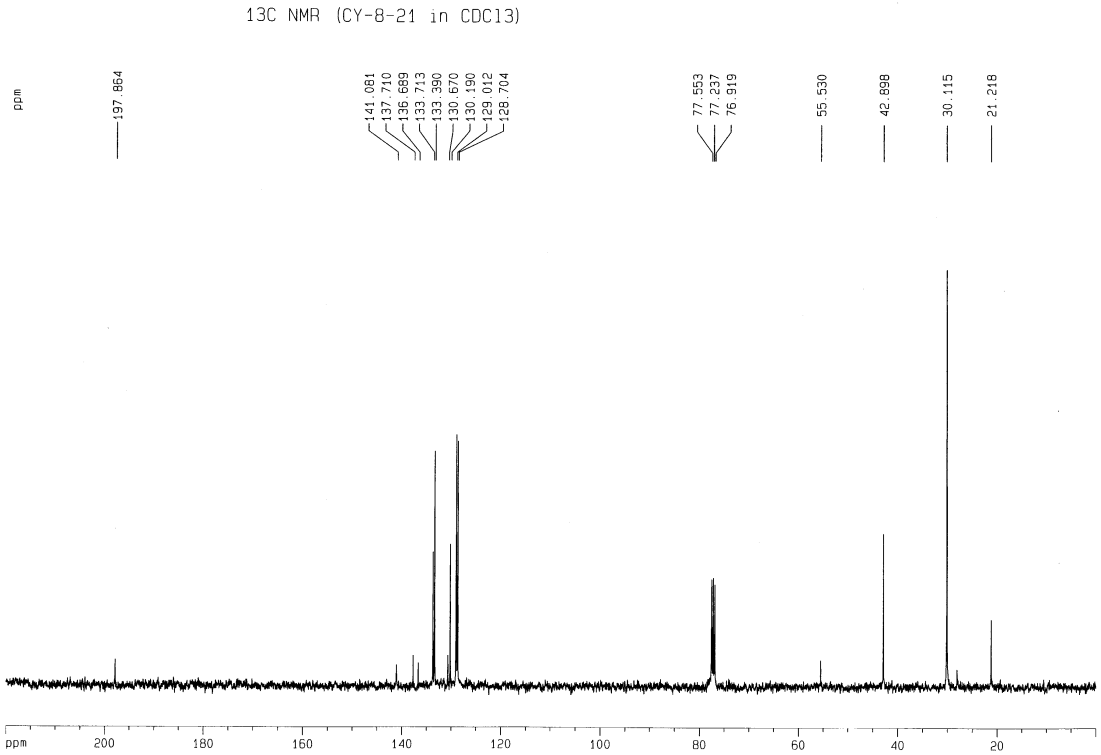
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
426.1364	426.1351	1.3	3.1	9.5	308.8	C21 H25 N O5 Na S



1k HRMS



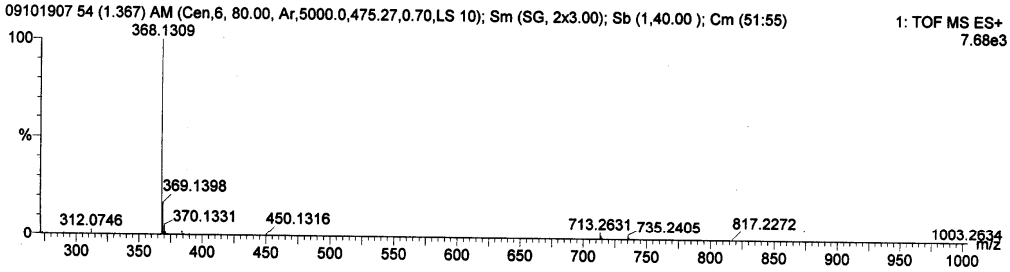
1l ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



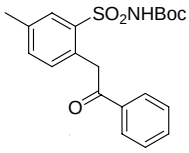
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

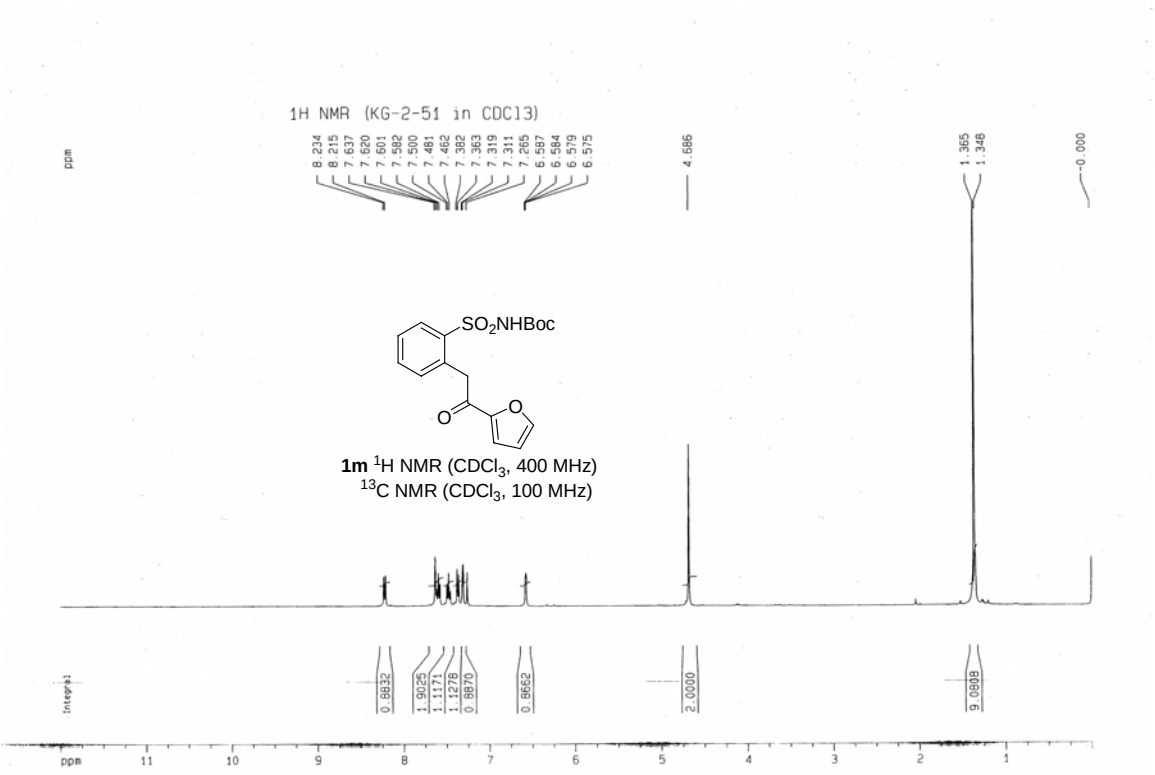
Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-40 H: 10-30 N: 1-1 O: 1-6 Na: 1-1 S: 1-1
CY-8-21
09101907 54 (1.367) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (51:55) 1: TOF MS ES+ 7.68e3



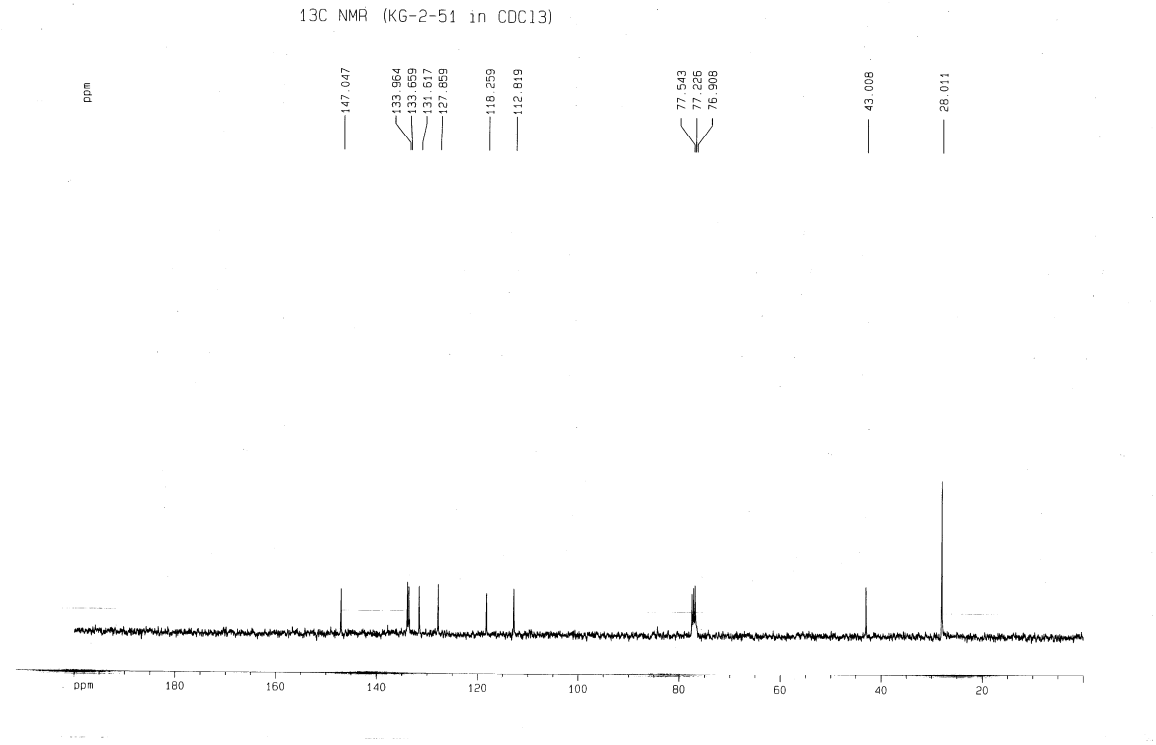
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.1309	368.1296	1.3	3.5	8.5	90.5	C19 H23 N O3 Na S



1l HRMS



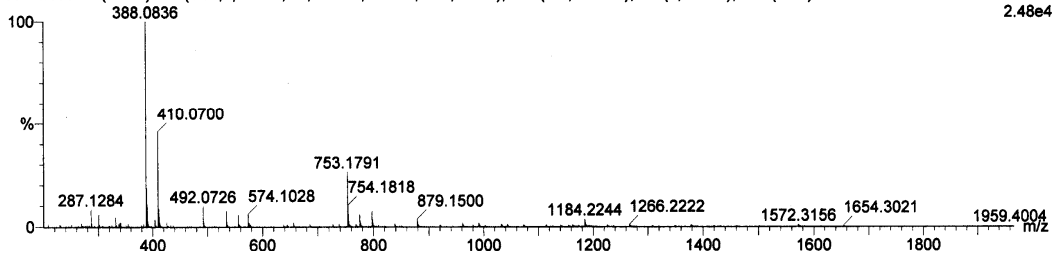
1m ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



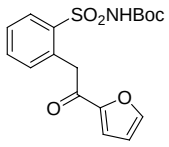
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

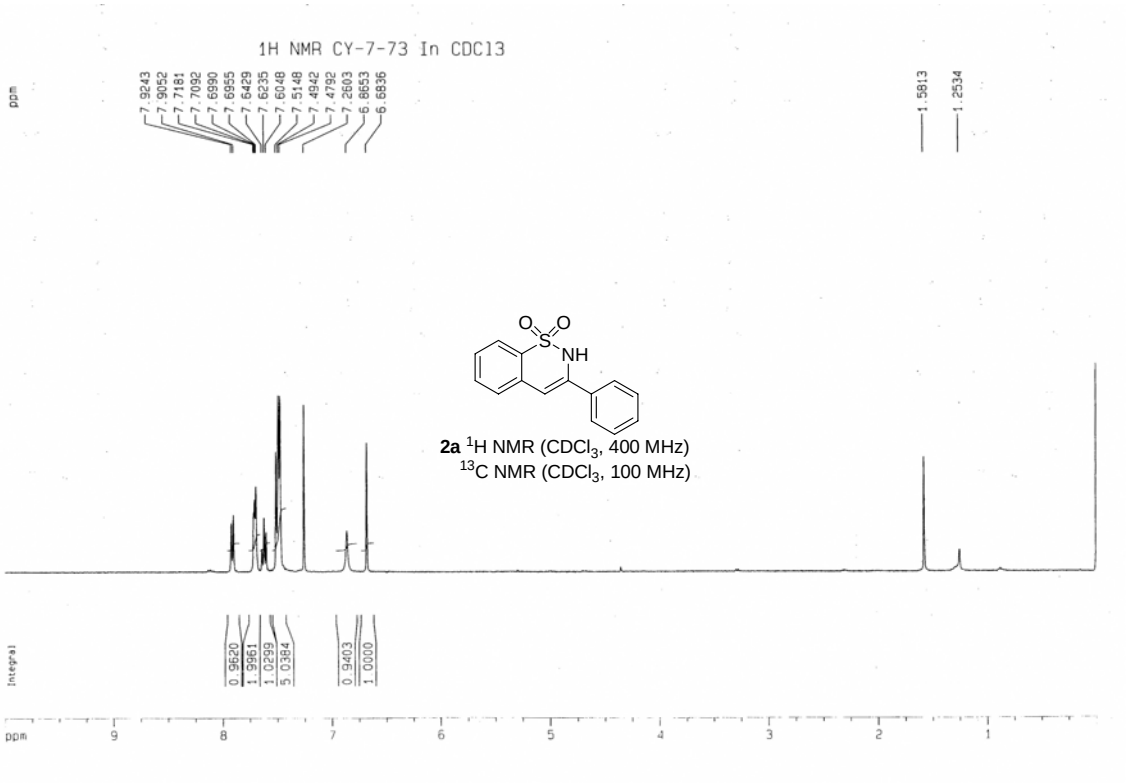
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 10-80 N: 1-3 O: 4-6 Na: 1-1 S: 1-1
KG-2-51
09112005 17 (0.421) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:22) 1: TOF MS ES+ 2.48e4



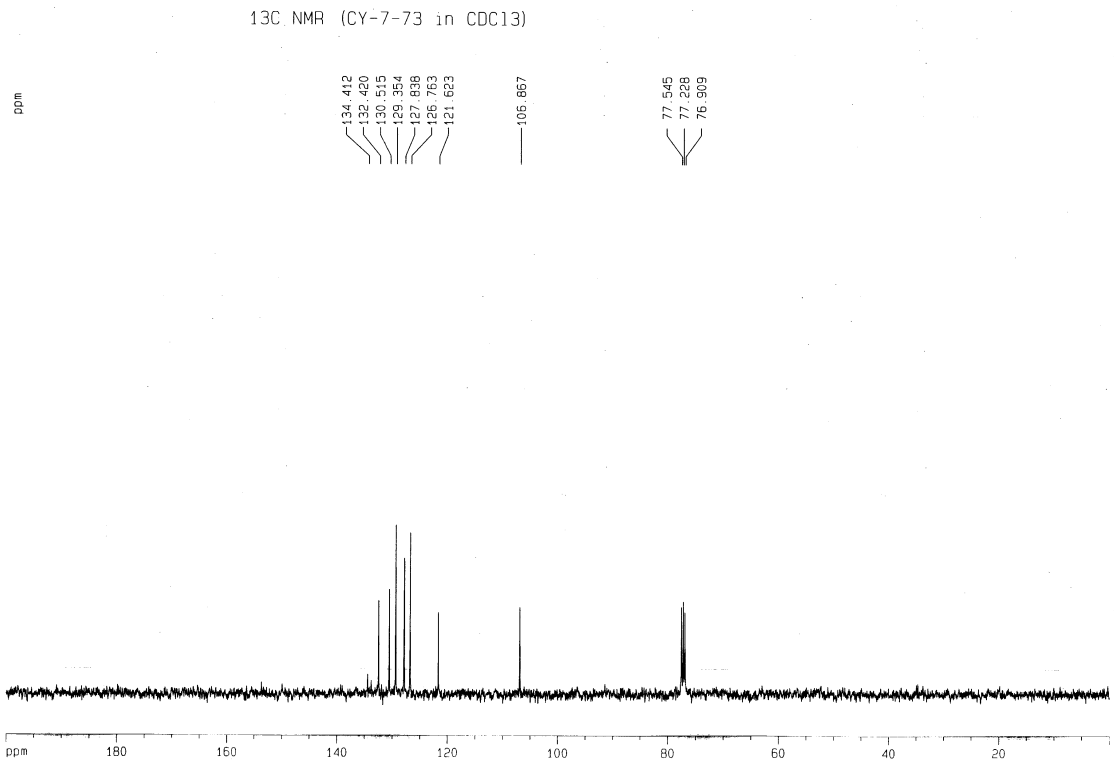
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.0836	388.0831	0.5	1.3	8.5	143.7	C17 H19 N O6 Na S

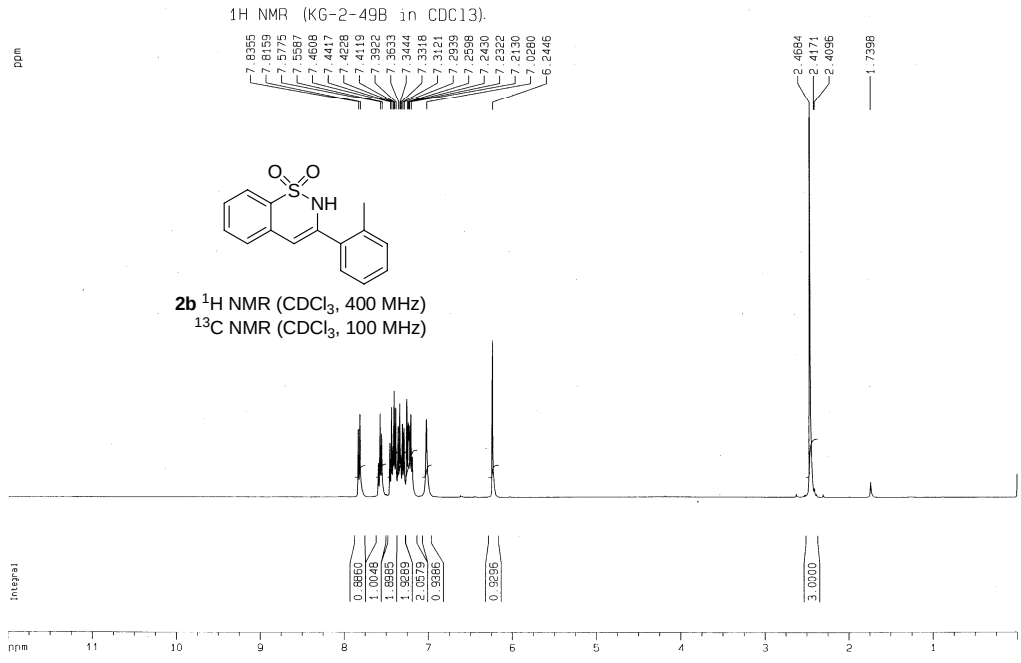


1m HRMS

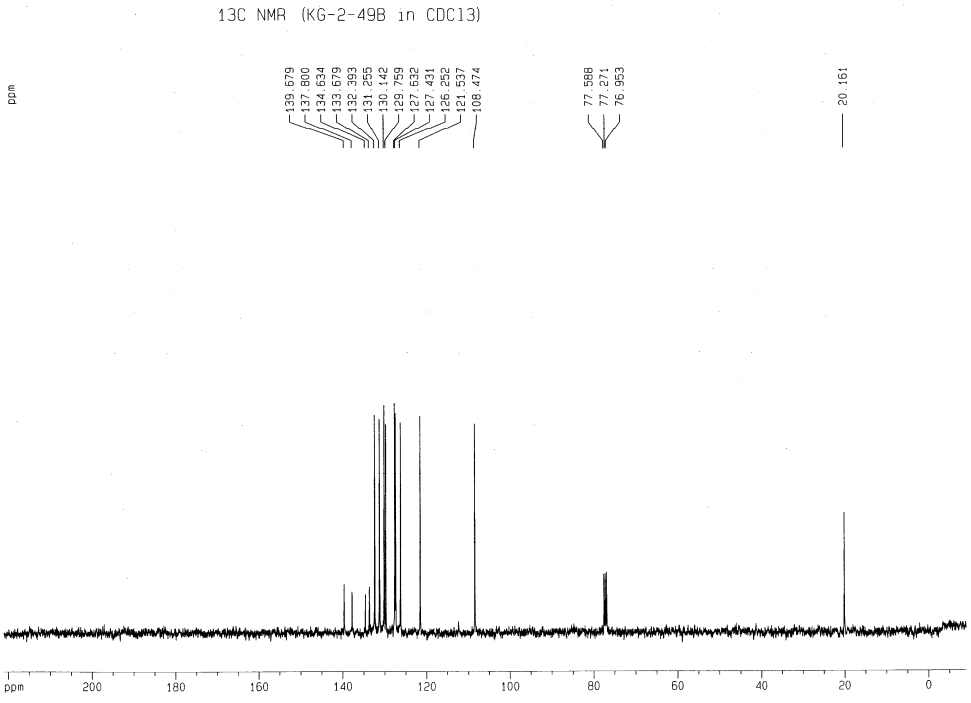


2a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





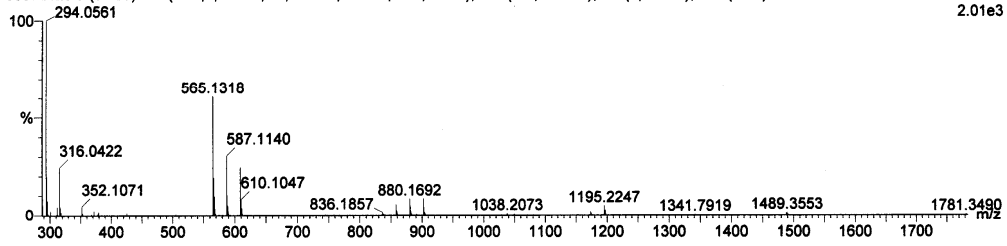
2b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



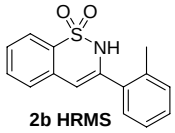
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

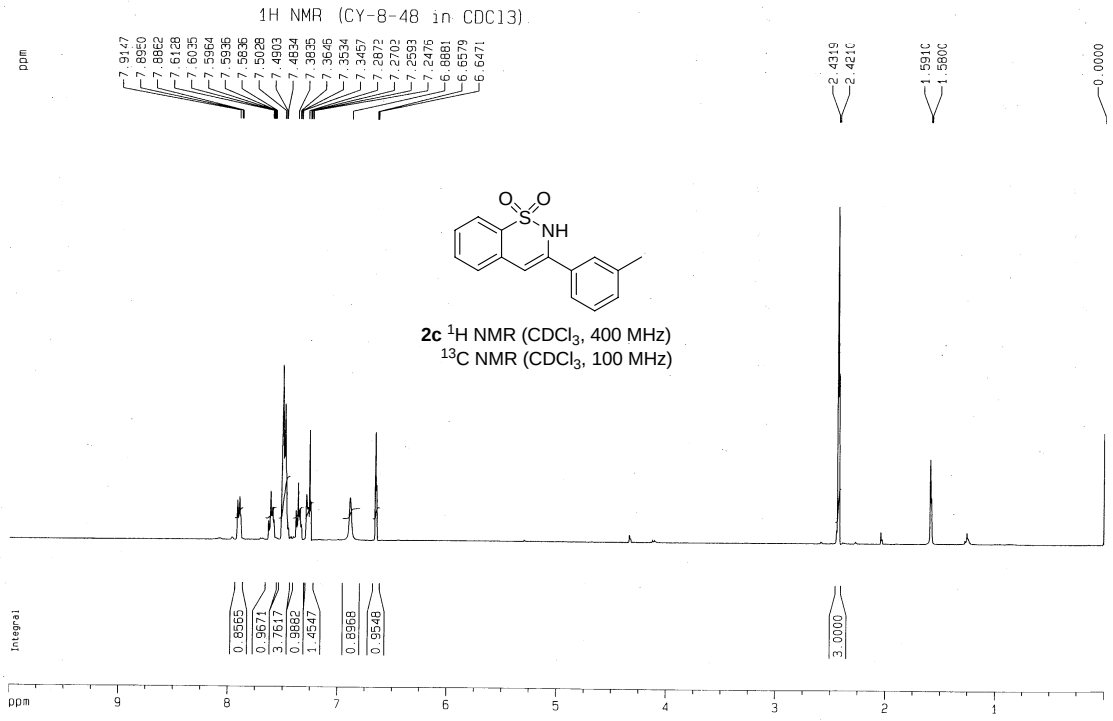
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-2 Na: 1-1 S: 1-1
KG-2-49B
09072125 9 (0.233) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:12) 1: TOF MS ES+ 2.01e3



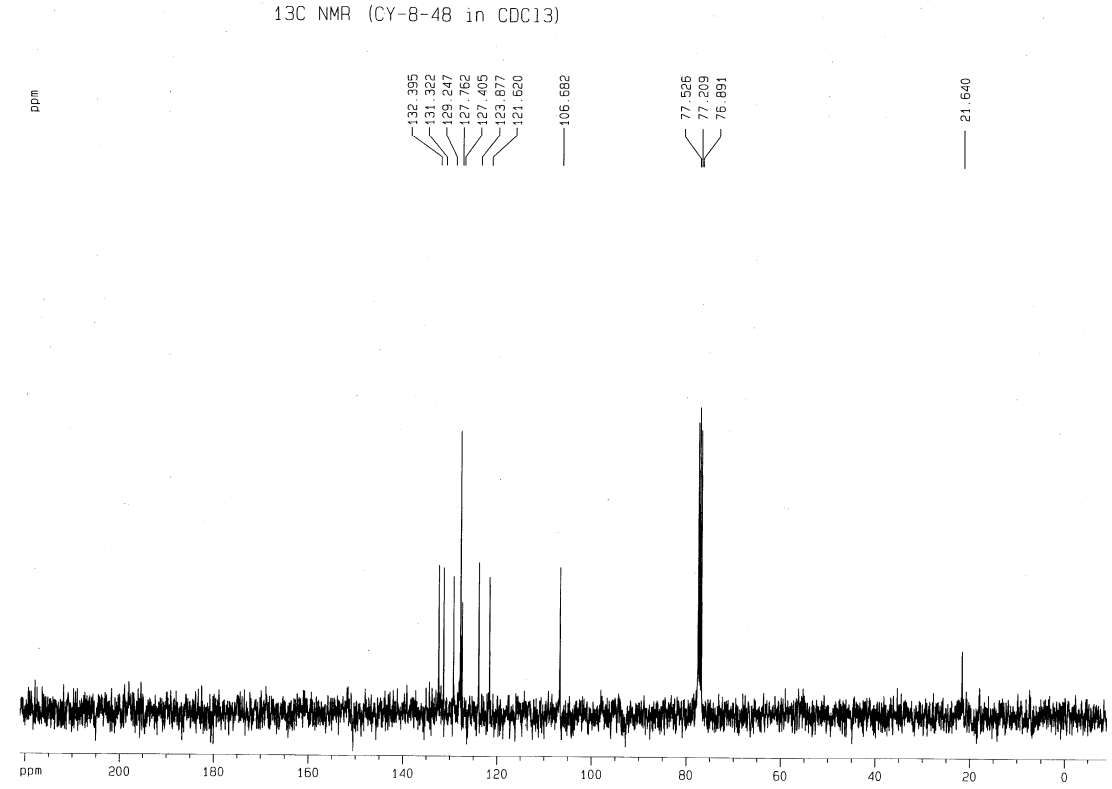
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.0561	294.0565	-0.4	-1.4	9.5	1.9	C15 H13 N O2 Na S



2b HRMS



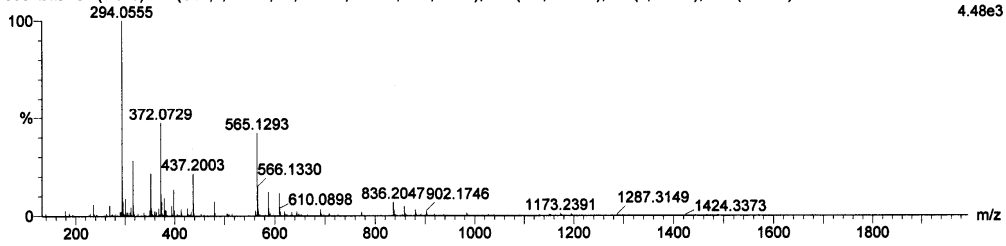
2c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



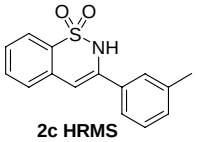
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

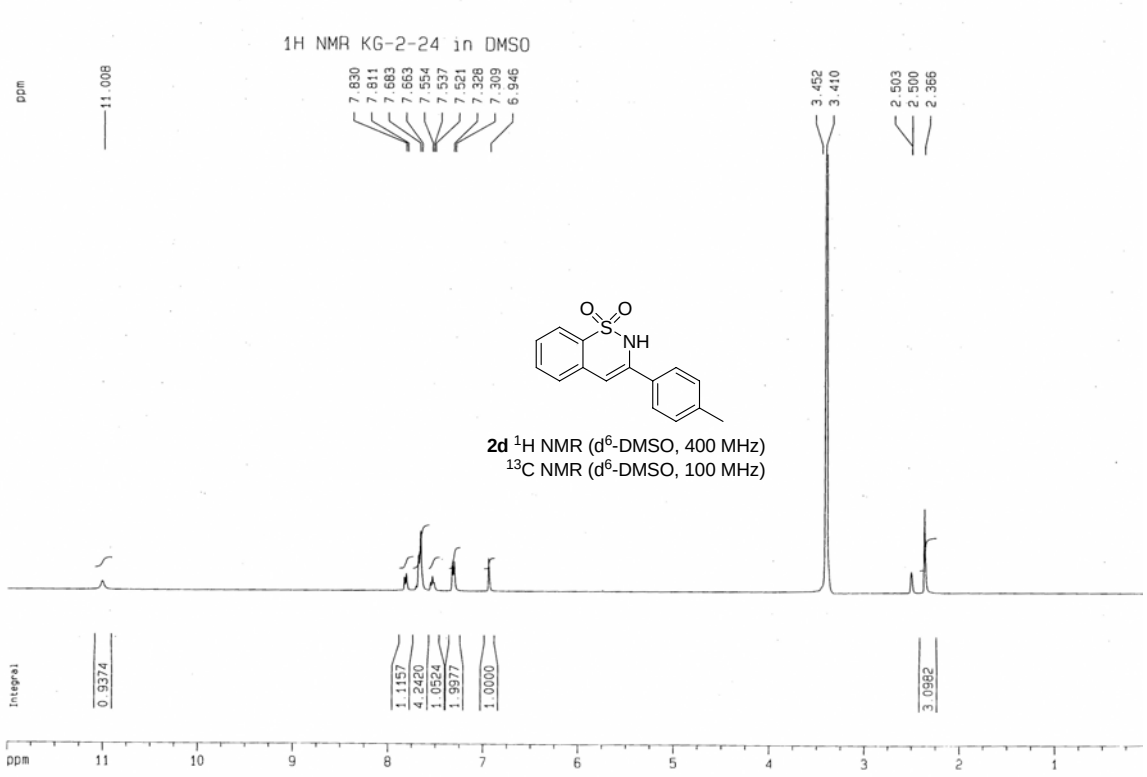
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-3 Na: 1-1 S: 1-1
CY-8-48
09072127 92 (2.319) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (91:117) 1: TOF MS ES+ 4.48e3



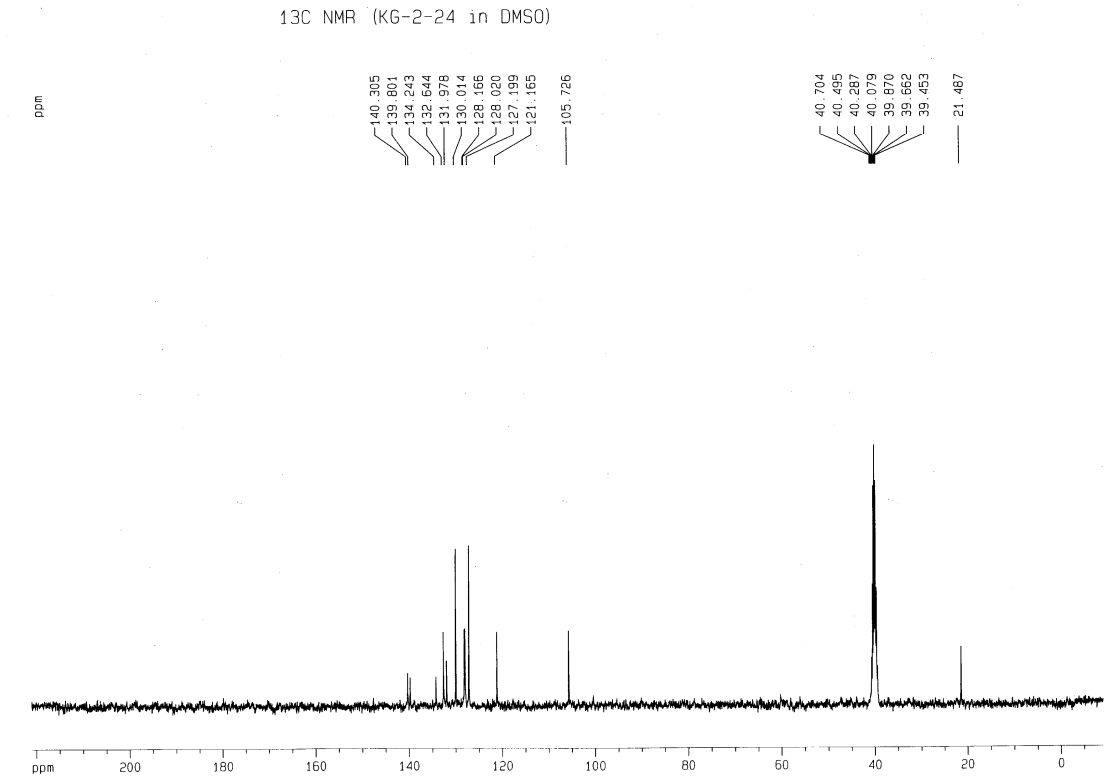
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.0555	294.0565	-1.0	-3.4	9.5	1.6	C15 H13 N O2 Na S



2c HRMS



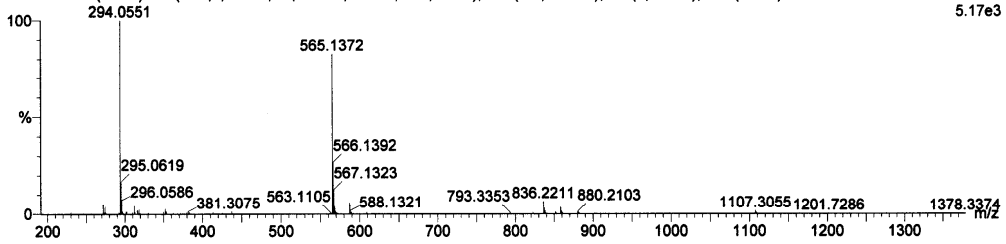
2d ^{1}H NMR (d^{6}-DMSO, 400 MHz)
^{13}C NMR (d^{6}-DMSO, 100 MHz)



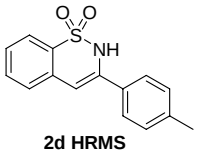
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

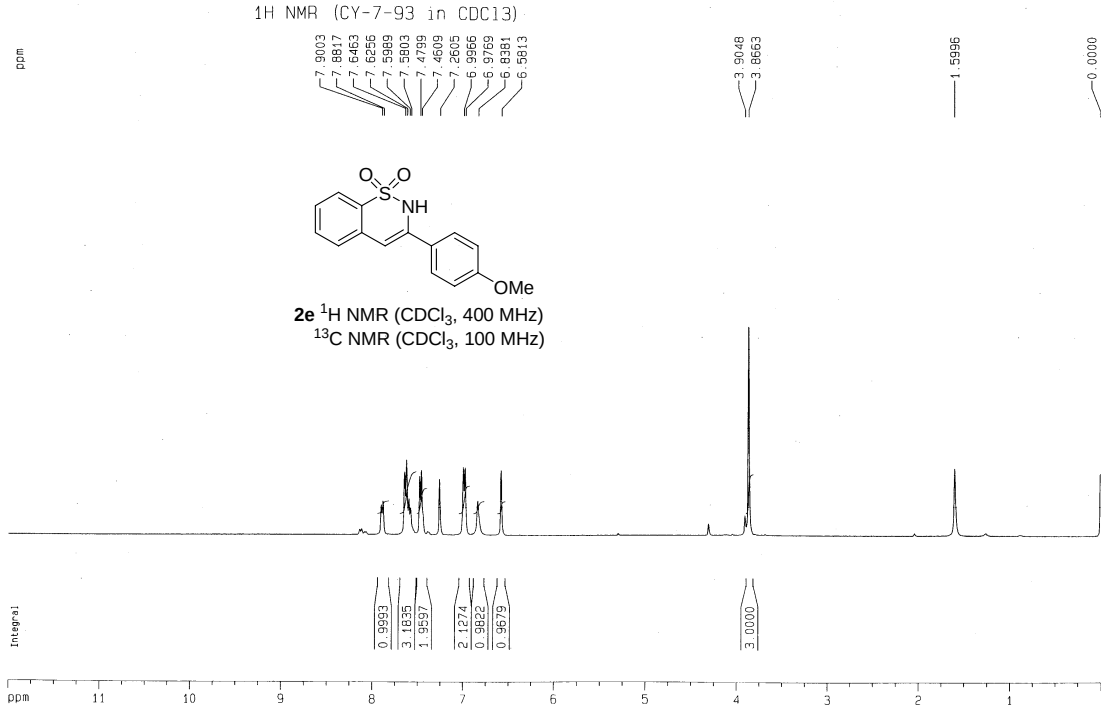
Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-2 Na: 1-1 S: 1-1
KG-2-24
09072108 18 (0.441) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (15:22) 1: TOF MS ES+ 5.17e3



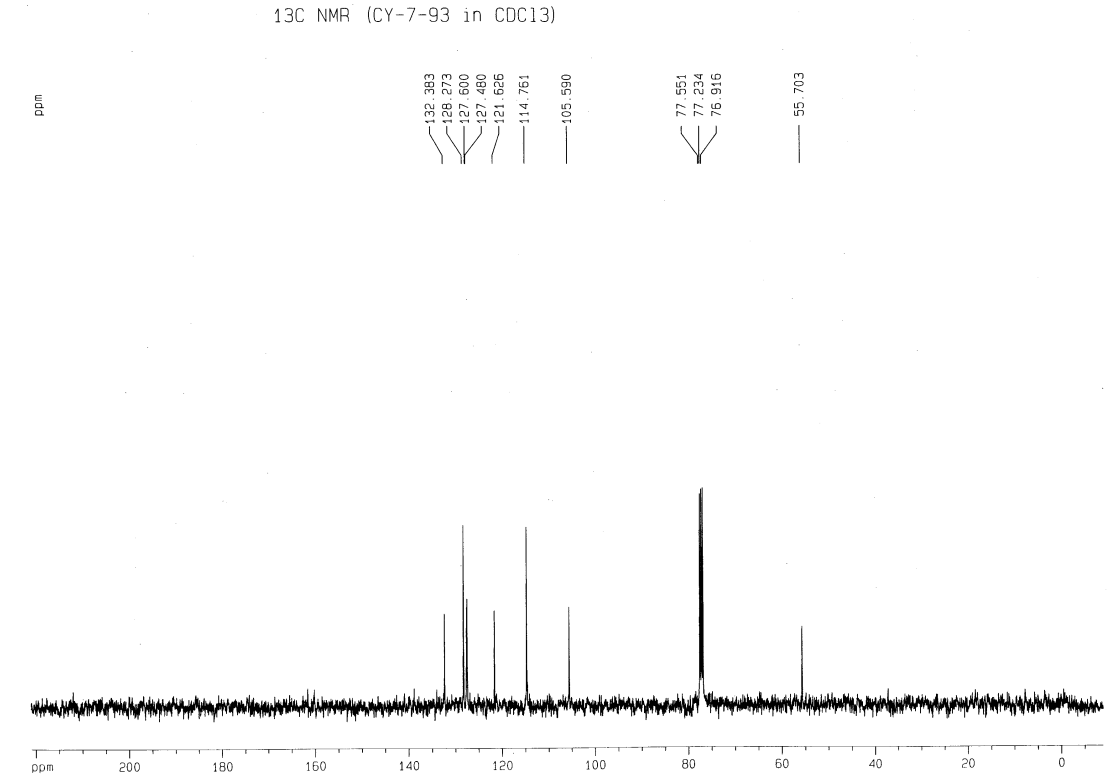
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.0551	294.0565	-1.4	-4.8	9.5	5.9	C15 H13 N O2 Na S



2d HRMS



2e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

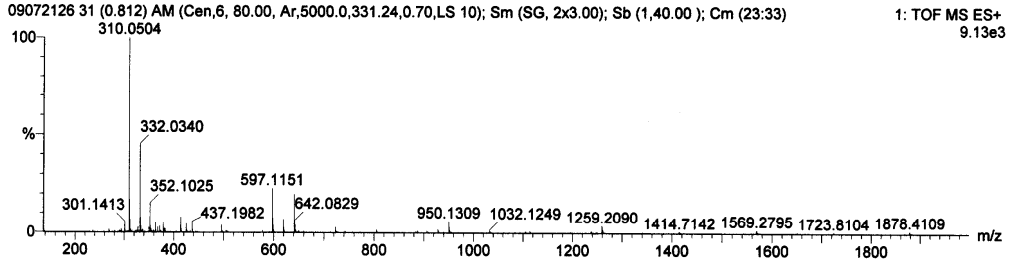


Elemental Composition Report **Page 1**

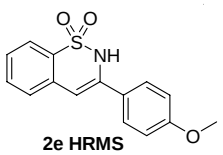
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-3 Na: 1-1 S: 1-1

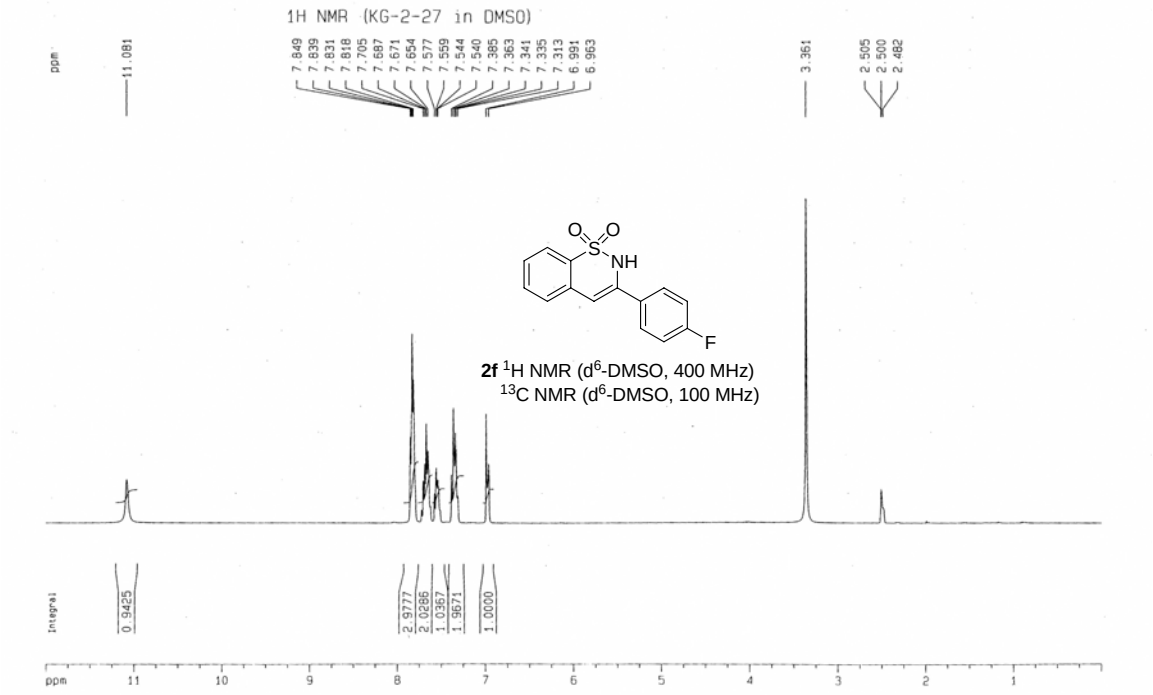
CY-7-93
09072126 31 (0.812) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (23:33) 1: TOF MS ES+ 9.13e3



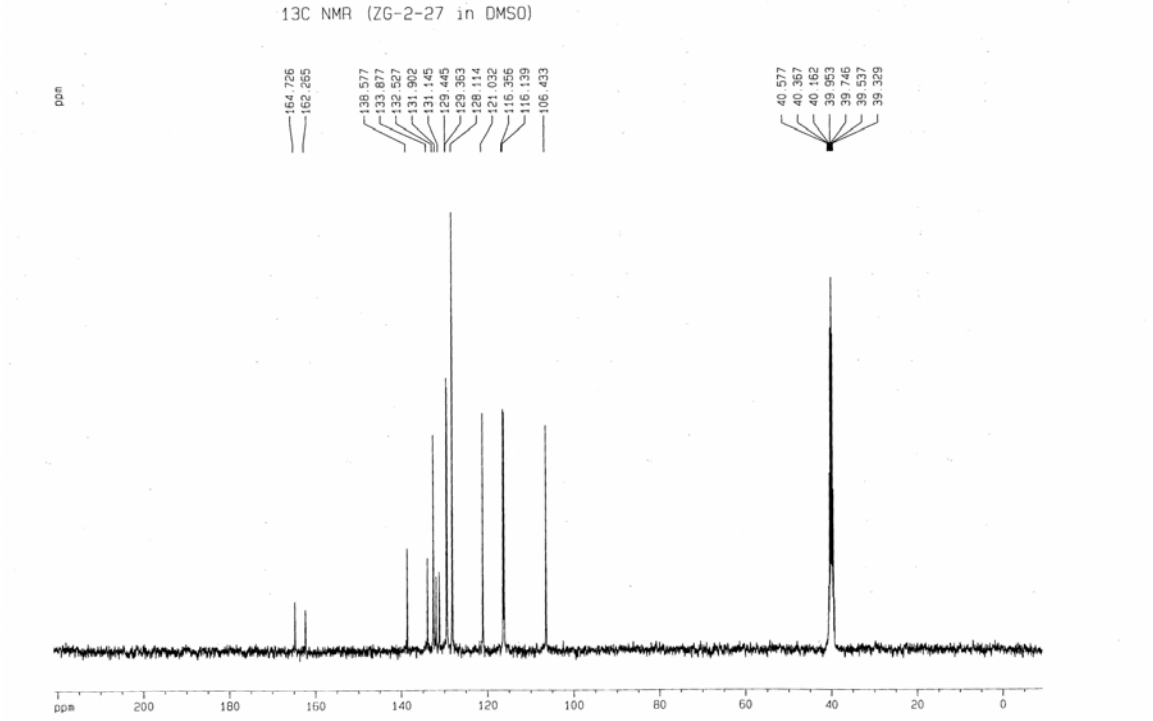
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
310.0504	310.0514	-1.0	-3.2	9.5	4.6	C15 H13 N O3 Na S



2e HRMS



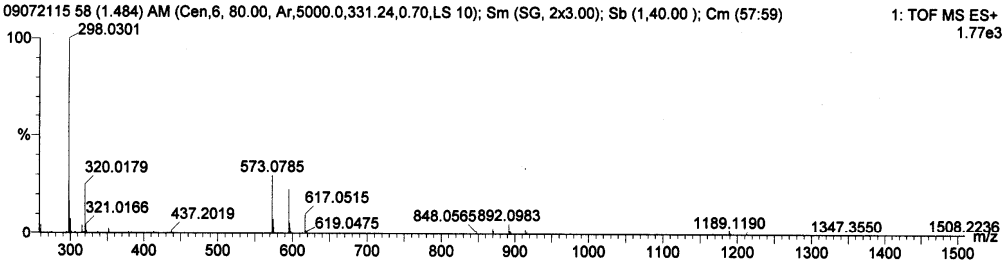
2f ^{1}H NMR (d^{6}-DMSO, 400 MHz)
^{13}C NMR (d^{6}-DMSO, 100 MHz)



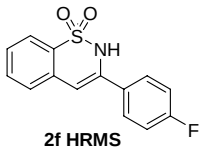
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

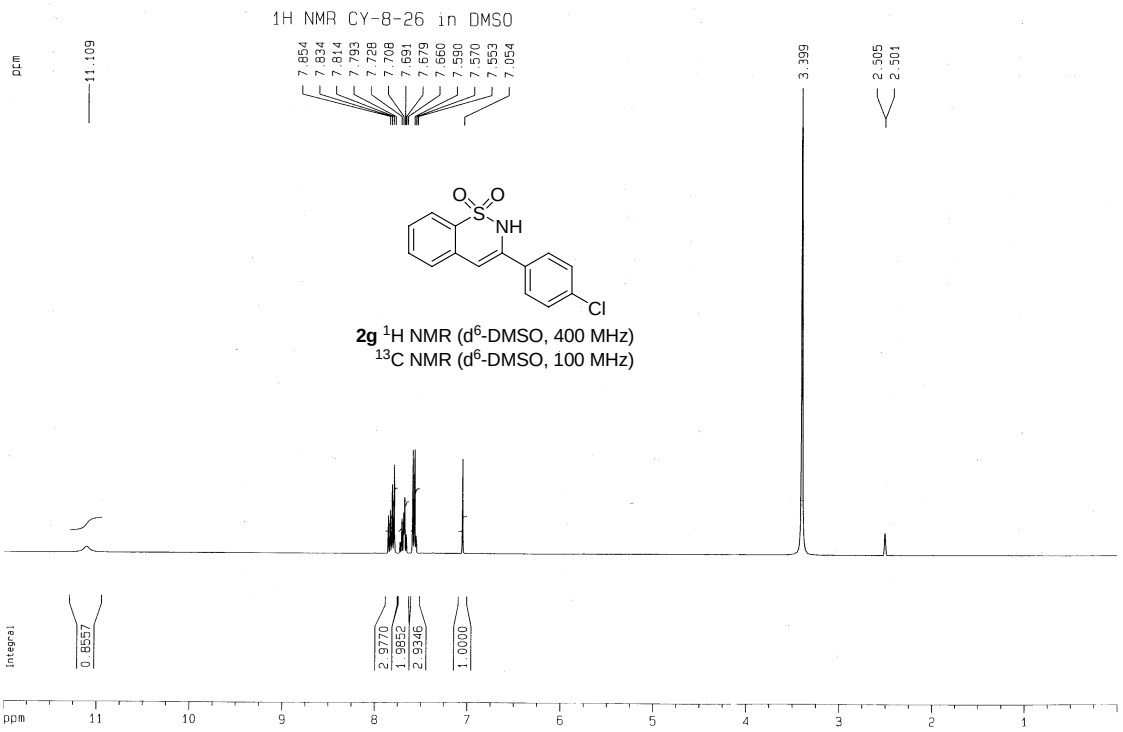
Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-2 F: 1-1 Na: 1-1 S: 1-1
KG-2-27
09072115 58 (1.484) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (57:59) 1: TOF MS ES+ 1.77e3



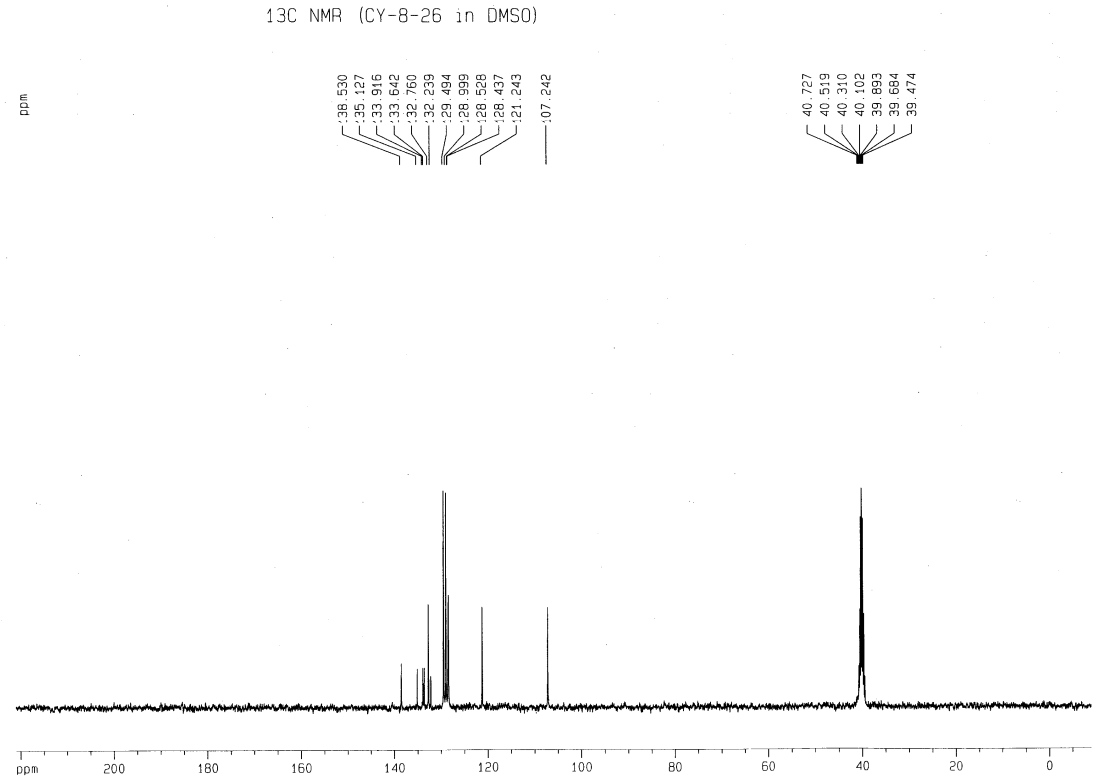
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.0301	298.0314	-1.3	-4.4	9.5	2.4	C14 H10 N O2 F Na S



2f HRMS



2g ^{1}H NMR (d^{6}-DMSO, 400 MHz)
^{13}C NMR (d^{6}-DMSO, 100 MHz)

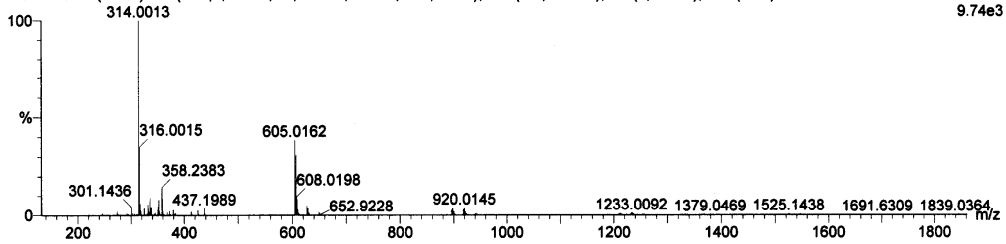


Elemental Composition Report **Page 1**

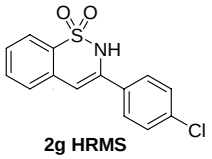
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 1-1 O: 2-2 Na: 1-1 S: 1-1 Cl: 1-1

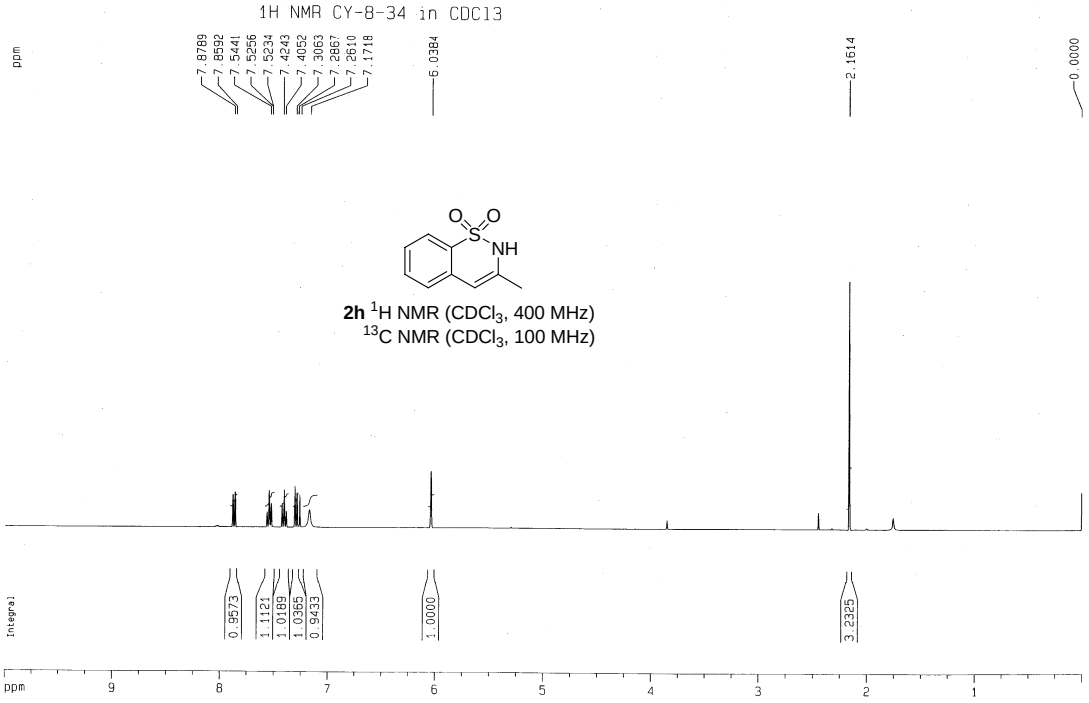
CY-8-26
09072113 12 (0.288) AM (Cen,6, 80.00, Ar,5000.0,331.24,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:12) 1: TOF MS ES+ 9.74e3



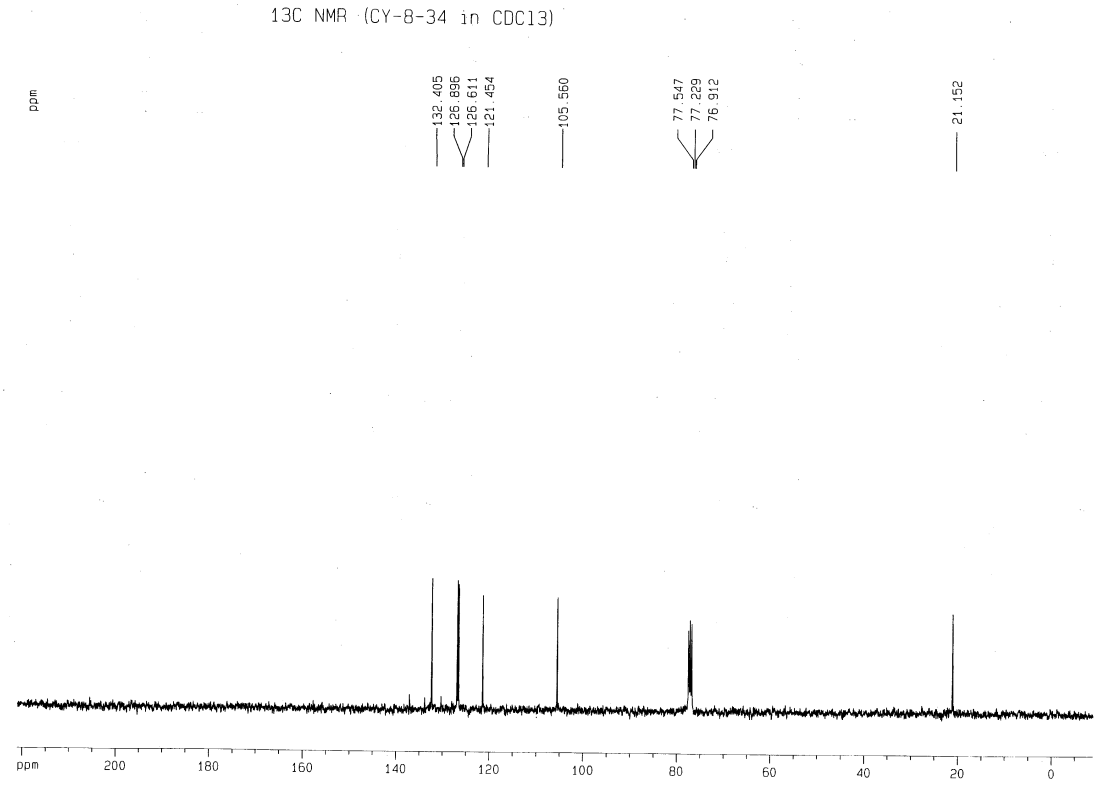
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0013	314.0018	-0.5	-1.6	9.5	24.1	C14 H10 N O2 Na S Cl

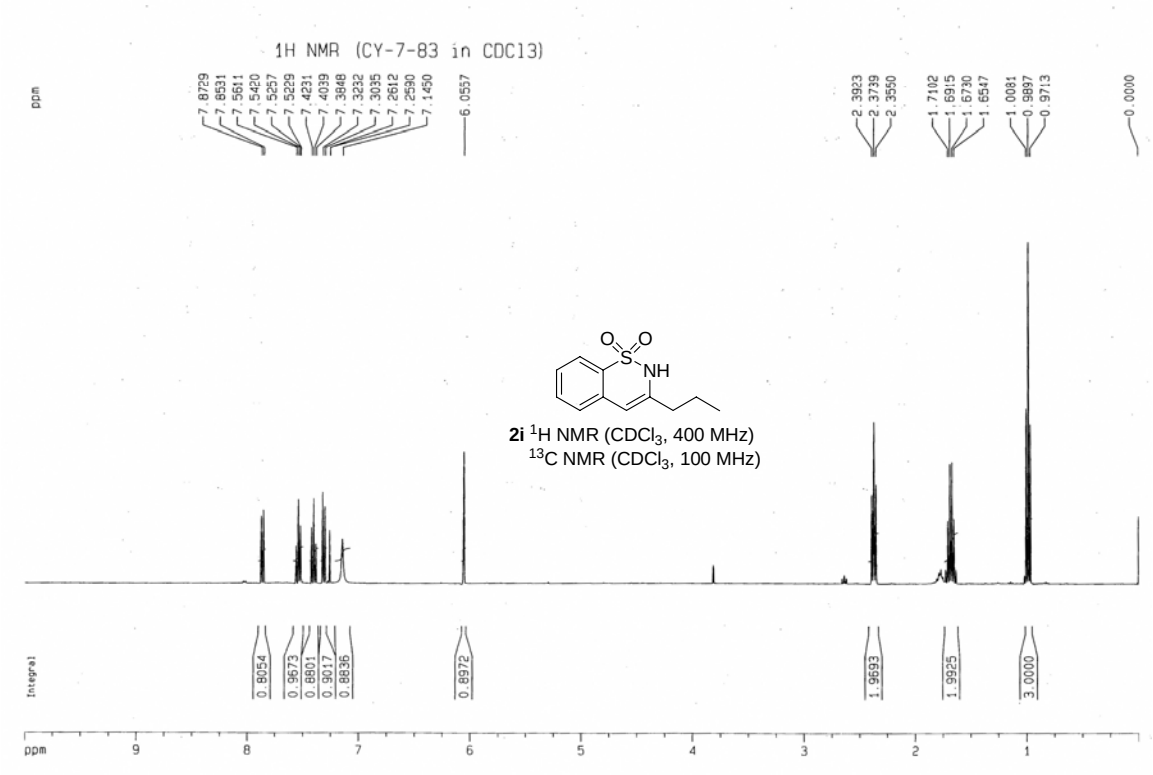


2g HRMS

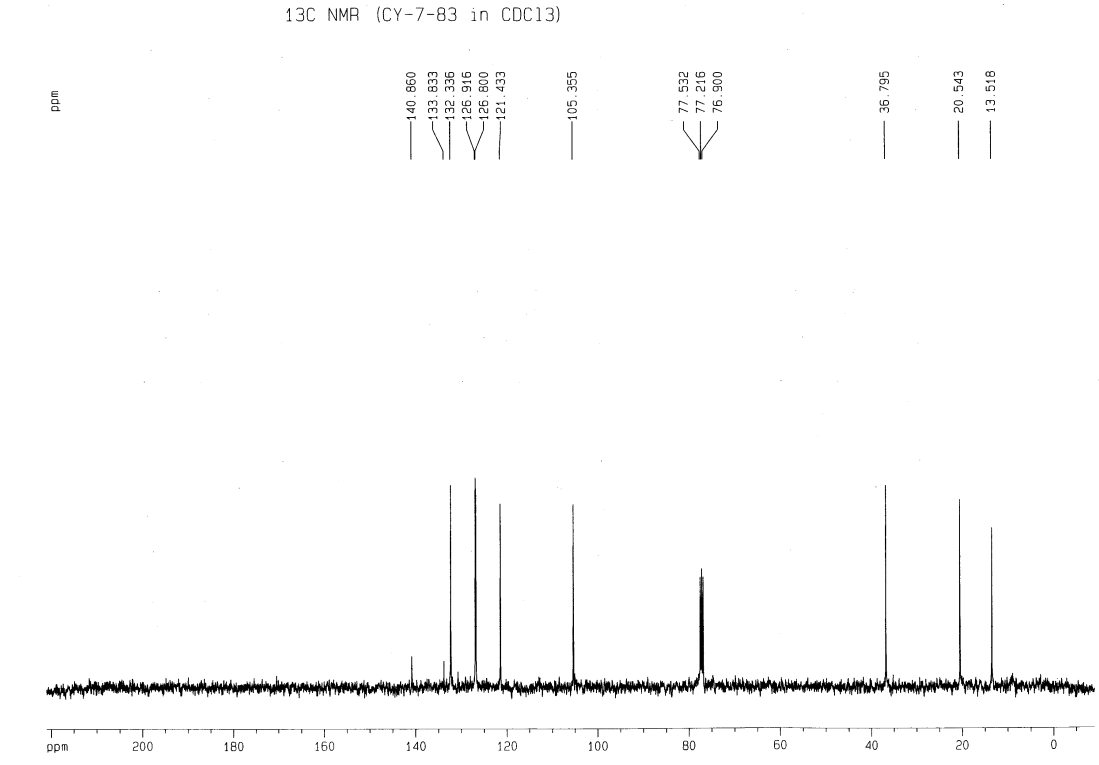


2h ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





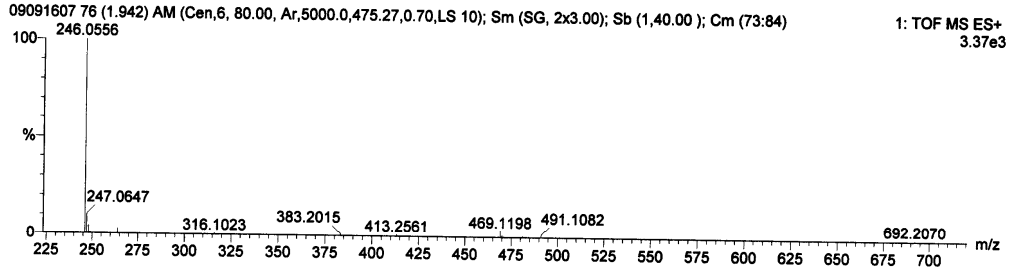
2i ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



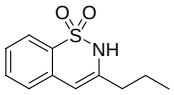
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

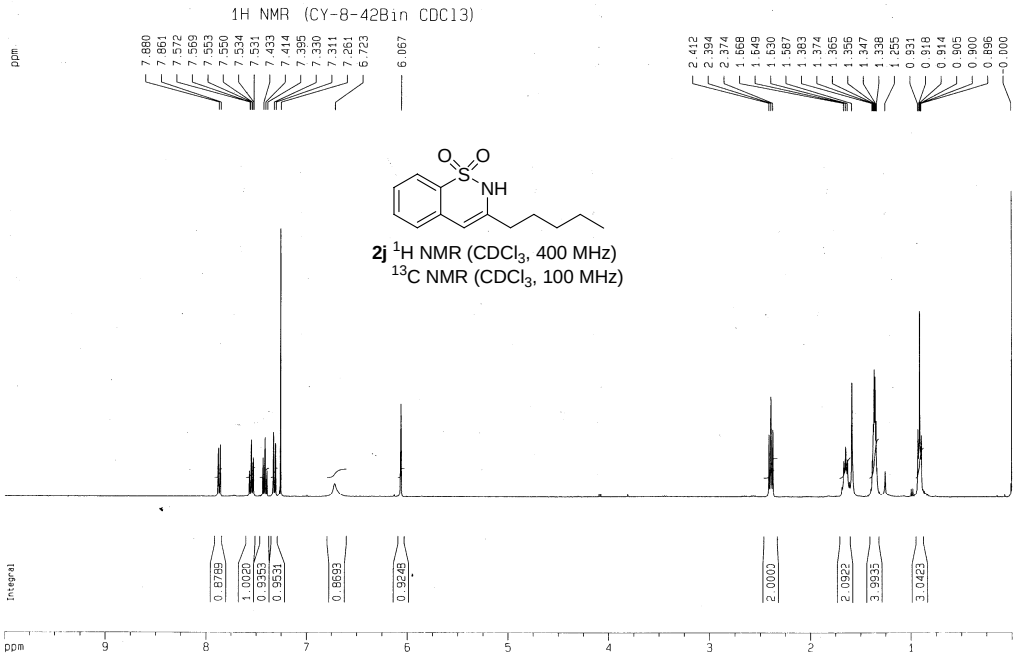
Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1
CY-7-83
09091607 76 (1.942) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (73:84) 1: TOF MS ES+ 3.37e3



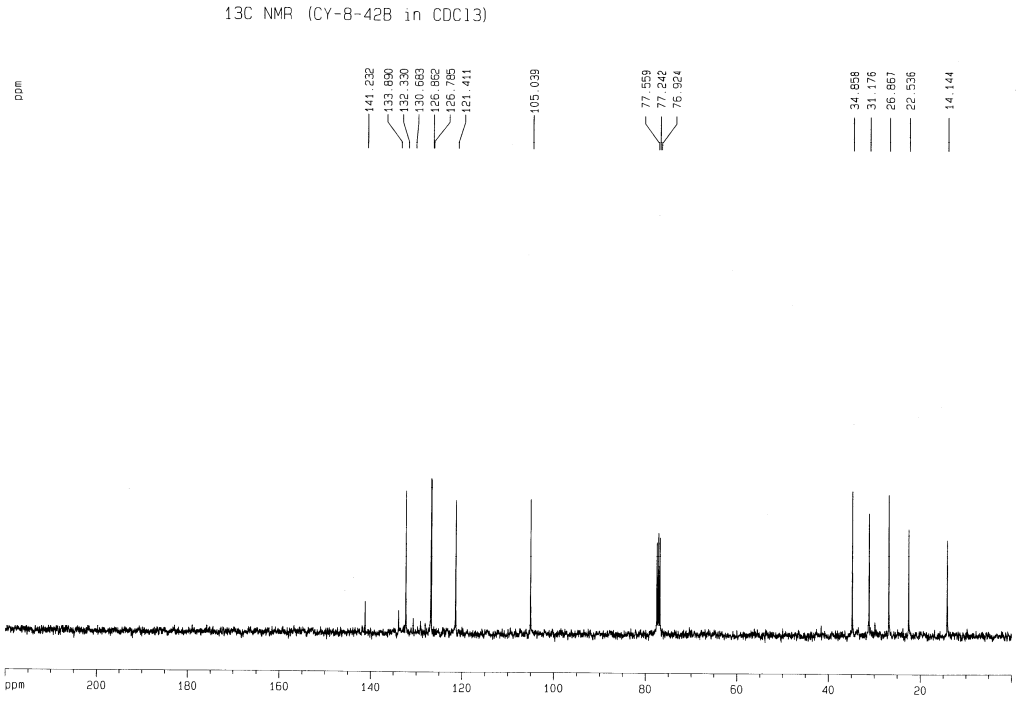
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0556	246.0565	-0.9	-3.7	5.5	24.2	C11 H13 N O2 Na S



2i HRMS



2j ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

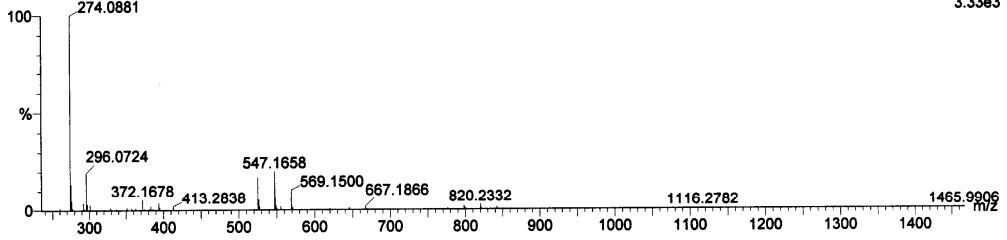


Elemental Composition Report **Page 1**

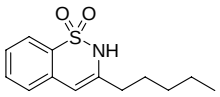
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

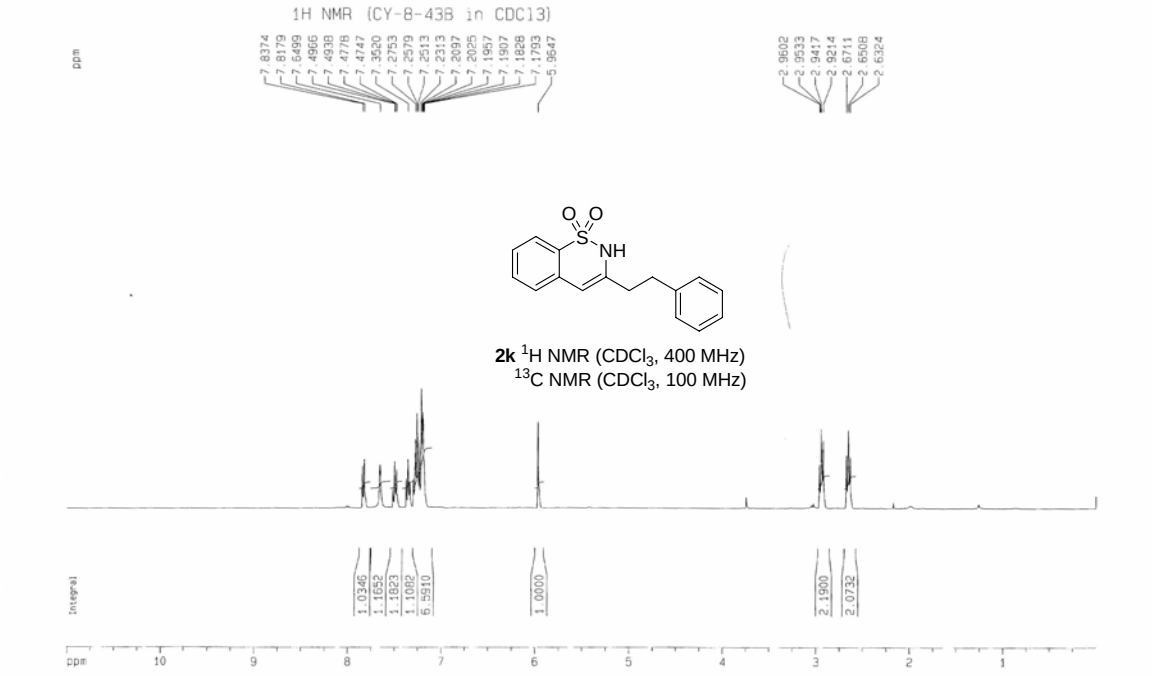
CY-8-42B
09091600 6 (0.135) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:6) 1: TOF MS ES+ 3.33e3



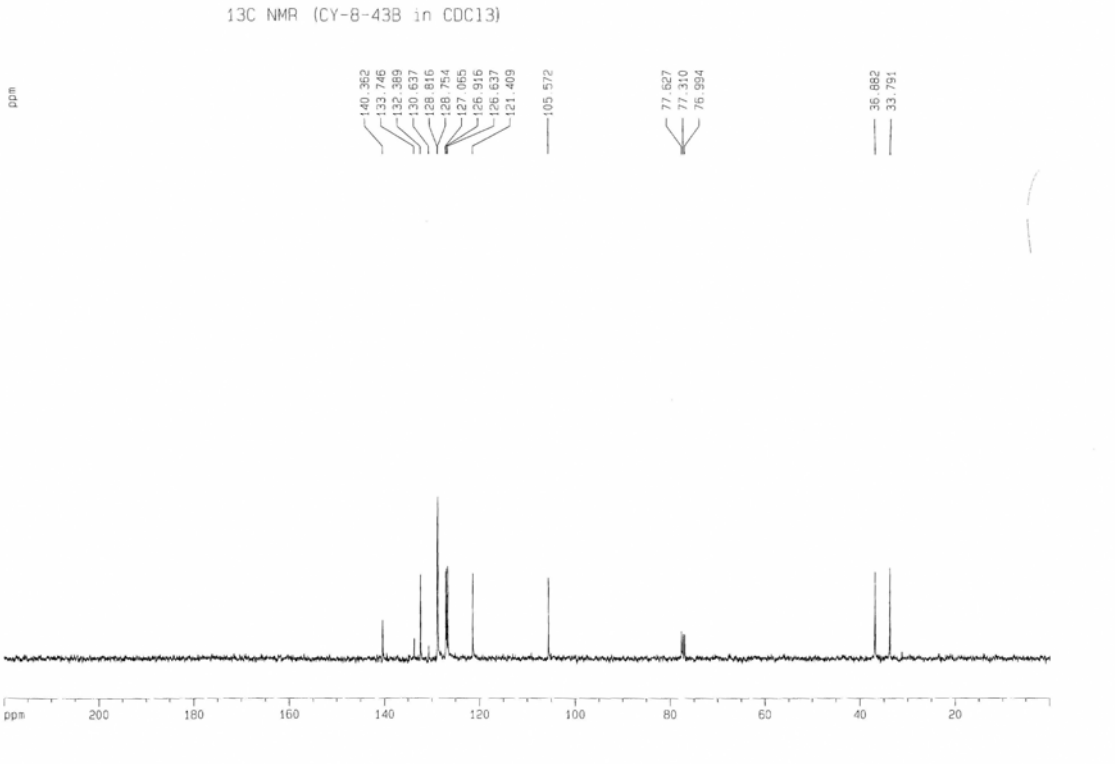
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.0881	274.0878	0.3	1.1	5.5	10.8	C13 H17 N O2 Na S



2j HRMS



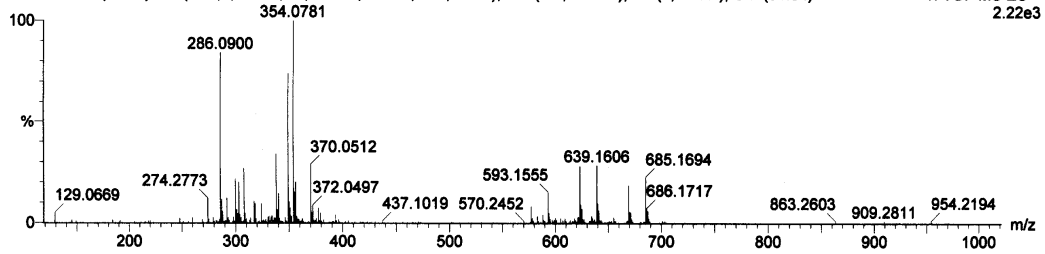
2k ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



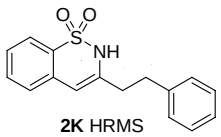
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

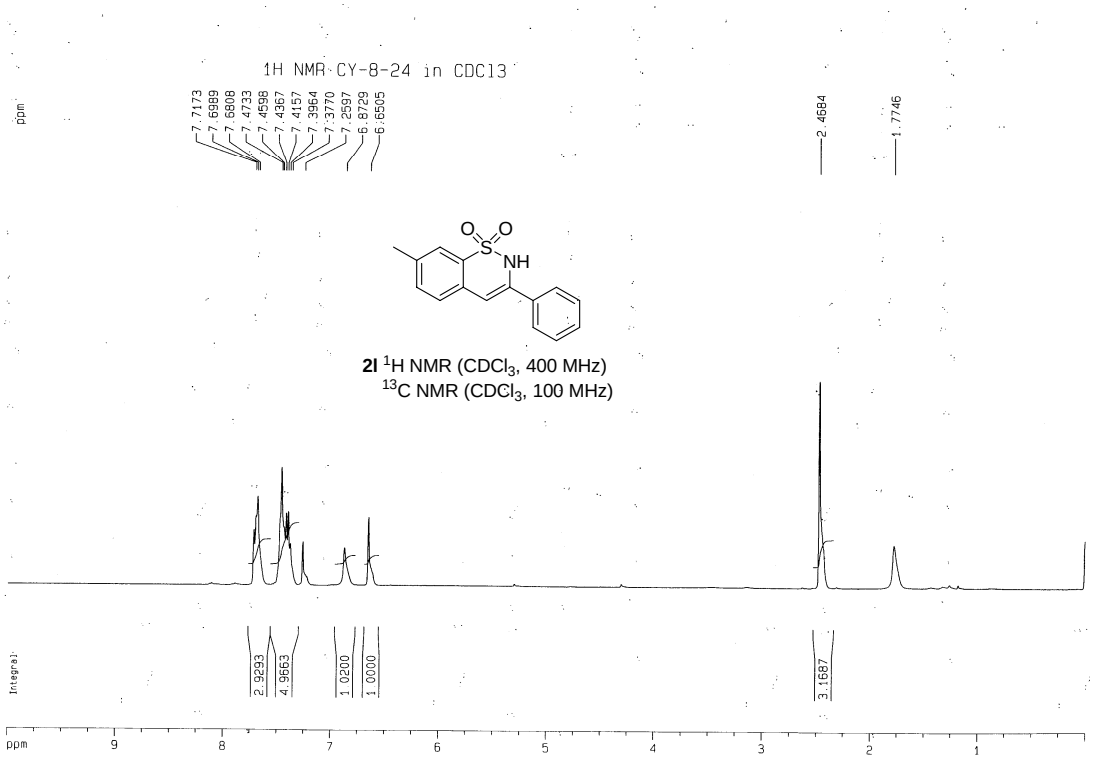
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 2-2 S: 1-1
CY-8-43B
10071805 31 (0.811) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (31:34) 1: TOF MS ES+ 2.22e3



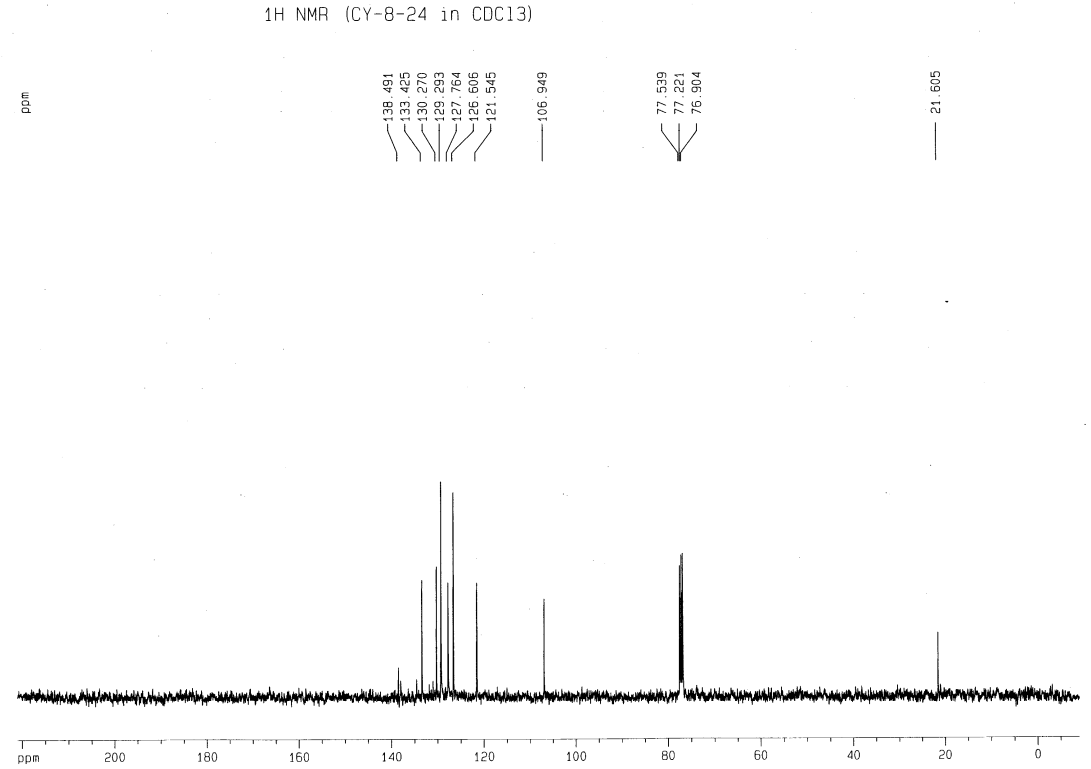
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
286.0900	286.0902	-0.2	-0.7	9.5	17.5	C16 H16 N O2 S



2K HRMS



2l ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

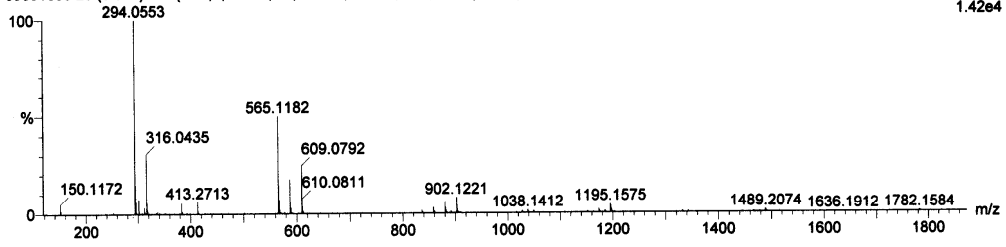


Elemental Composition Report **Page 1**

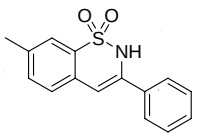
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

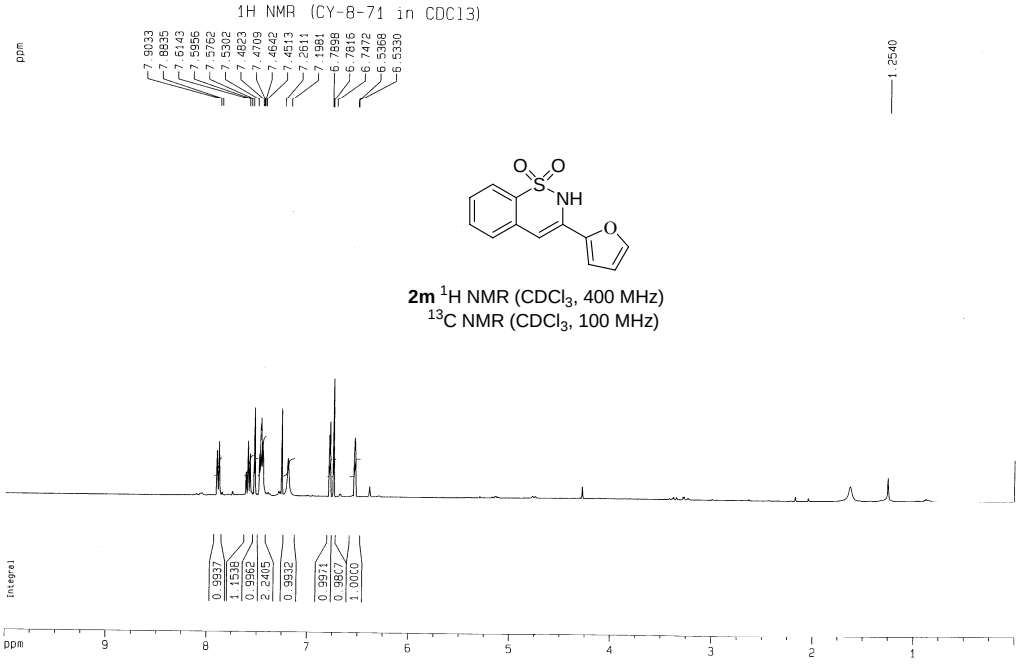
CY-8-24
09091605 20 (0.521) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:20) 1: TOF MS ES+ 1.42e4



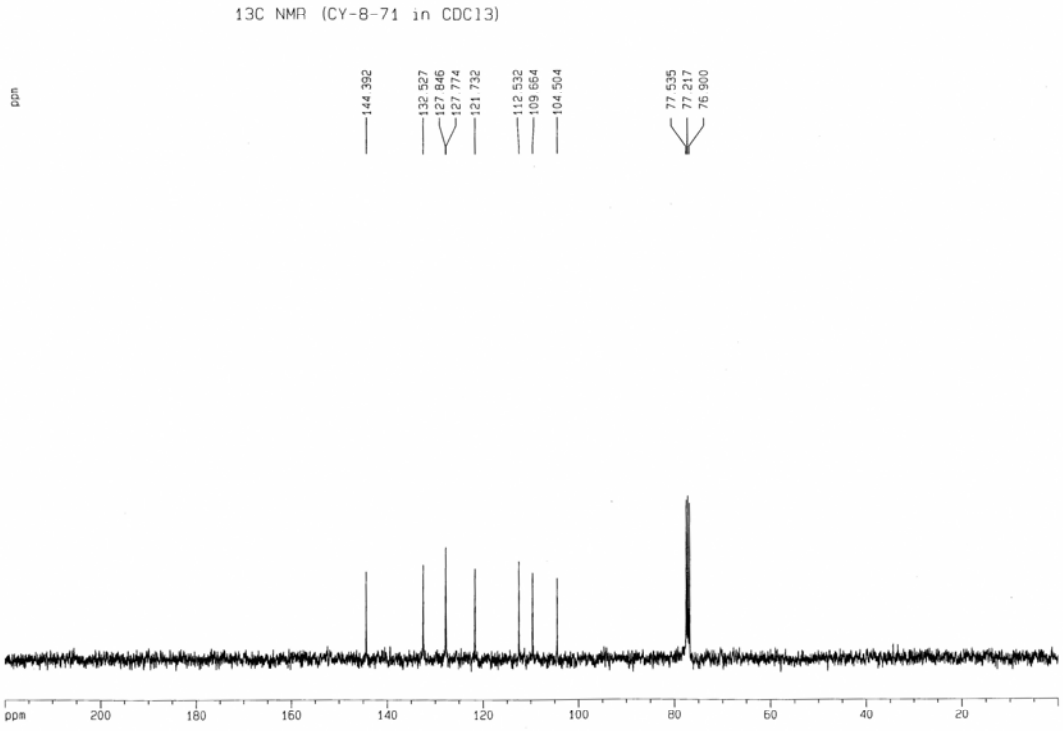
Minimum:				-1.5		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.0553	294.0565	-1.2	-4.1	9.5	43.0	C15 H13 N O2 Na S



2l HRMS



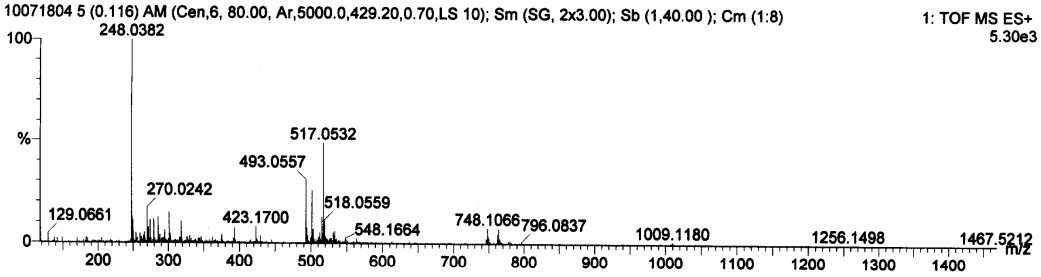
2m ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



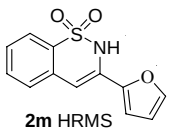
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -10.0, max = 100.0
Selected filters: None

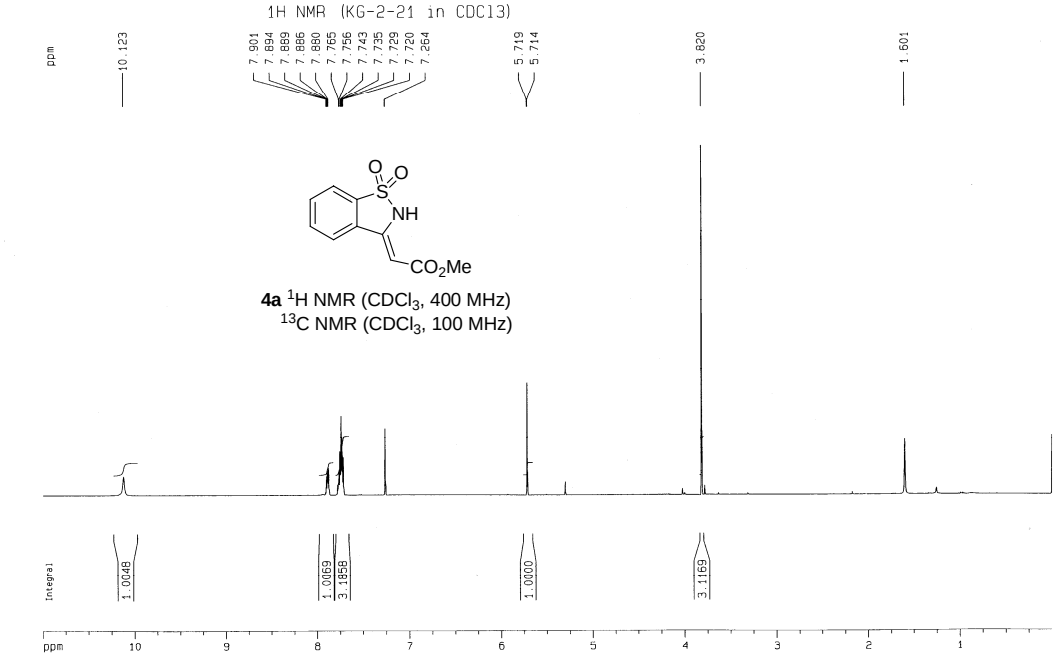
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-90 H: 0-120 N: 1-1 O: 3-3 S: 1-1
CY-8-71
10071804 5 (0.116) AM (Cen,6, 80.00, Ar,5000.0,429.20,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:8) 1: TOF MS ES+ 5.30e3



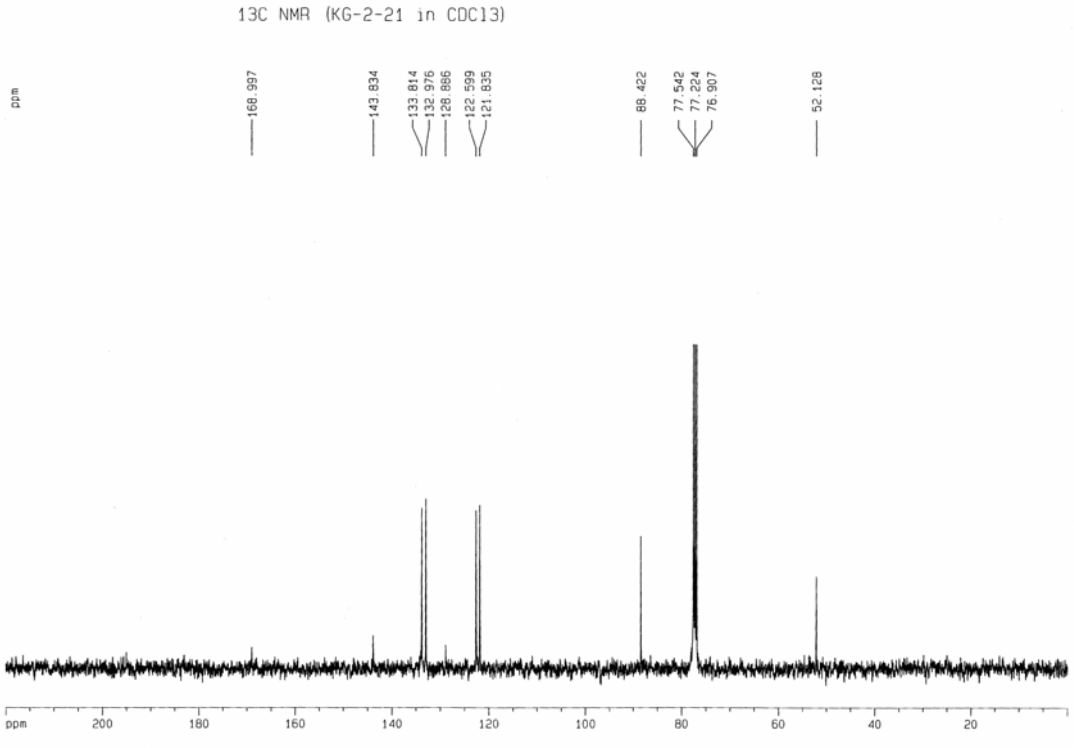
Minimum:				-10.0		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
248.0382	248.0381	0.1	0.4	8.5	67.9	C12 H10 N O3 S



2m HRMS



4a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

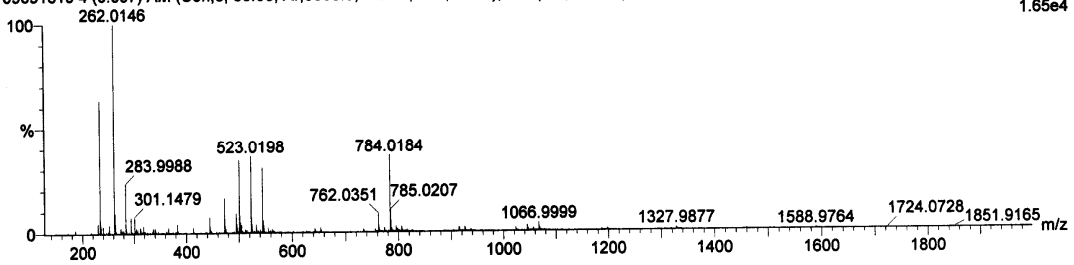


Elemental Composition Report **Page 1**

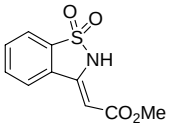
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
6 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 5-20 N: 1-2 O: 2-4 Na: 1-1 S: 1-1

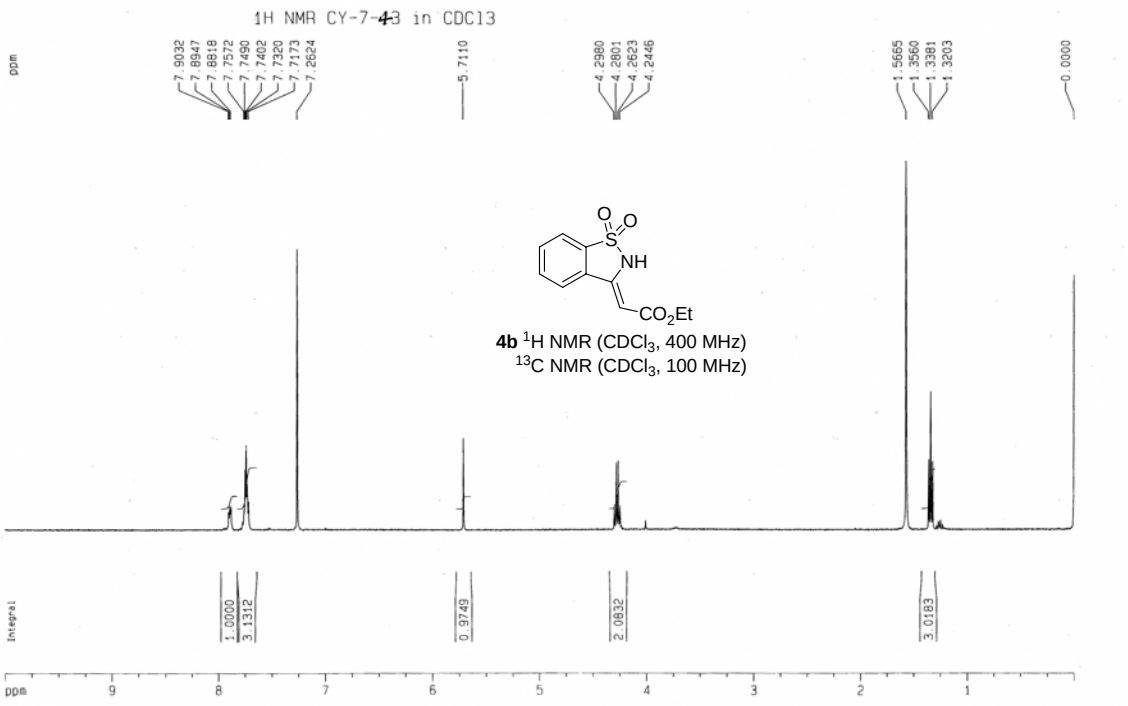
KG-2-21
09091619 4 (0.097) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:10) 1: TOF MS ES+ 1.65e4



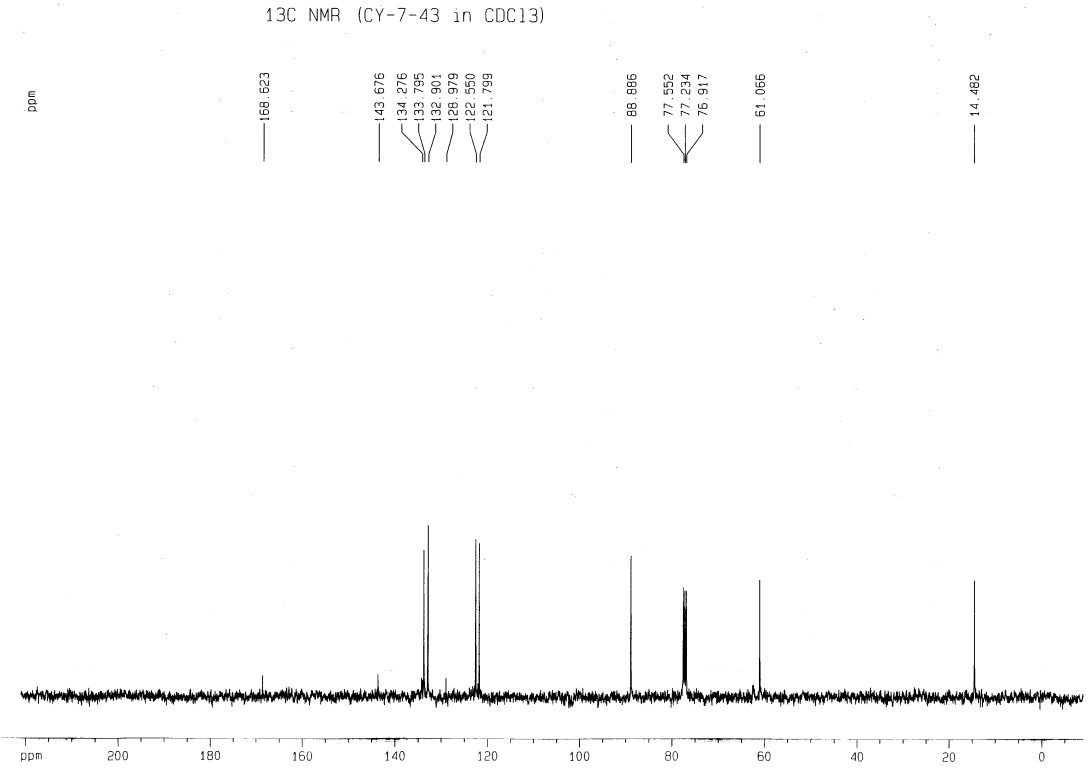
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
262.0146	262.0150	-0.4	-1.5	6.5	118.2	C10 H9 N O4 Na S

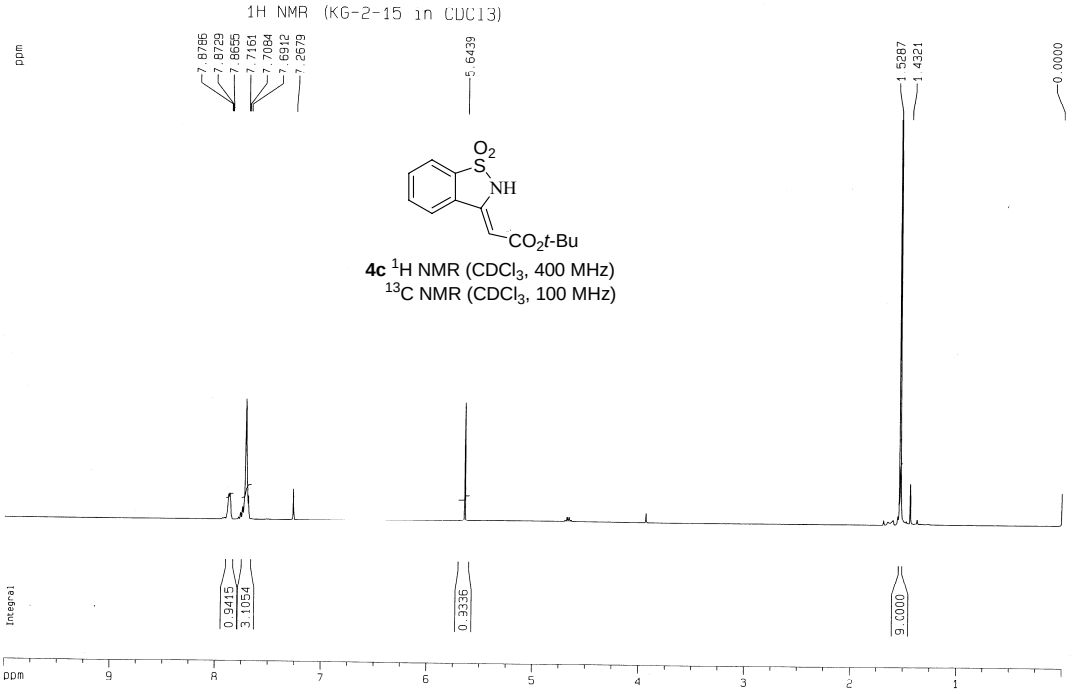


4a HRMS

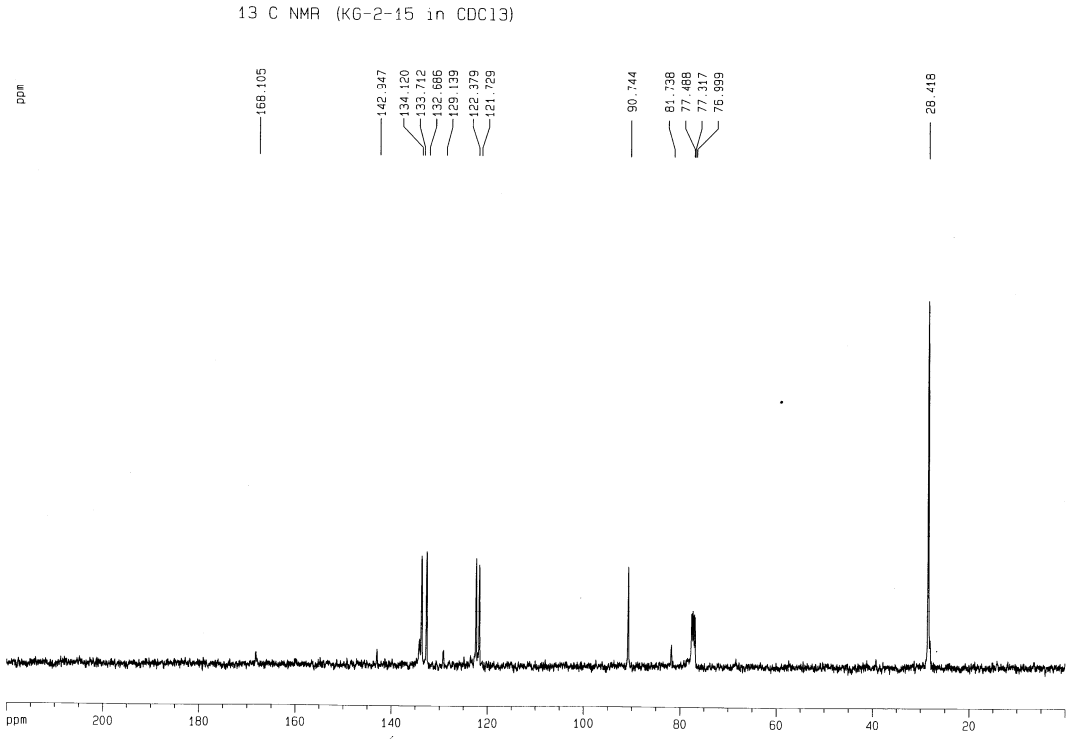


4b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





4c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

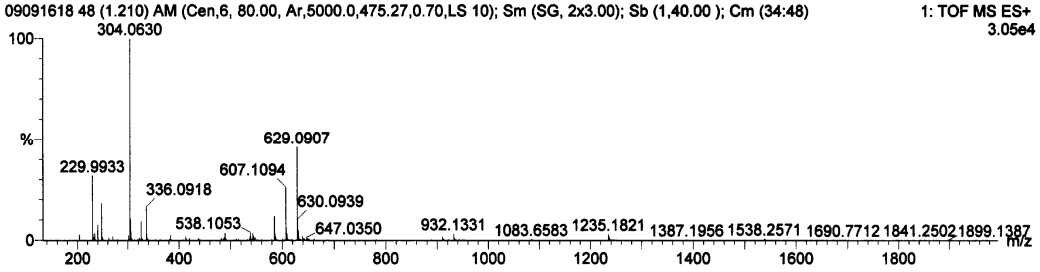


Elemental Composition Report **Page 1**

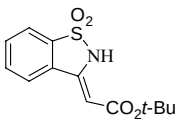
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-4 Na: 1-1 S: 1-1

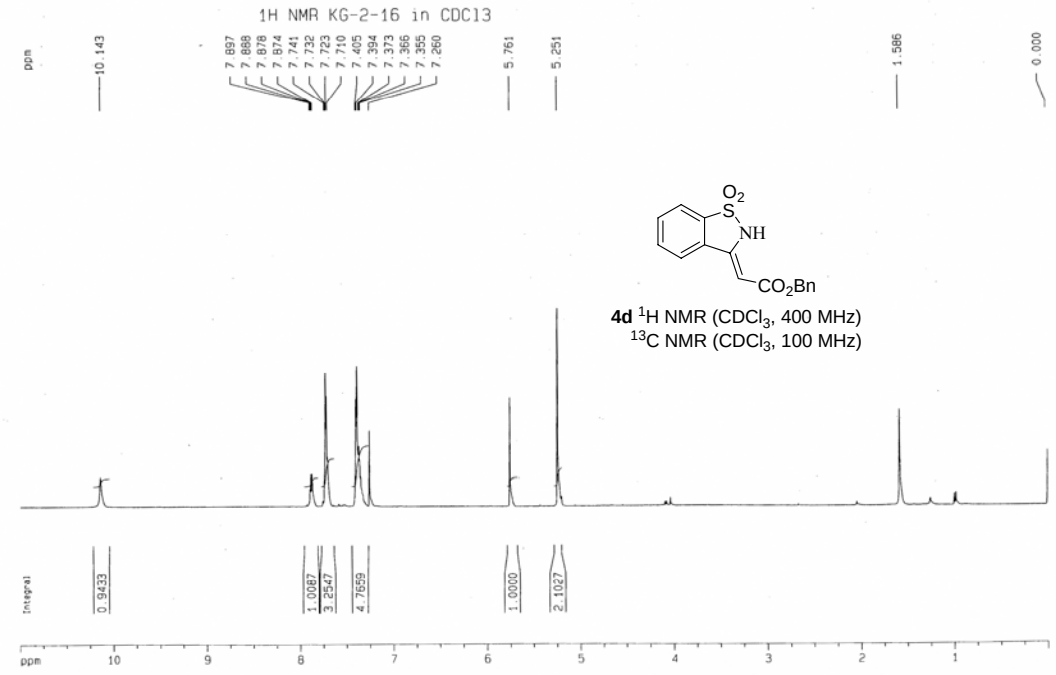
KG-2-15
09091618 48 (1.210) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (34:48) 1: TOF MS ES+ 3.05e4



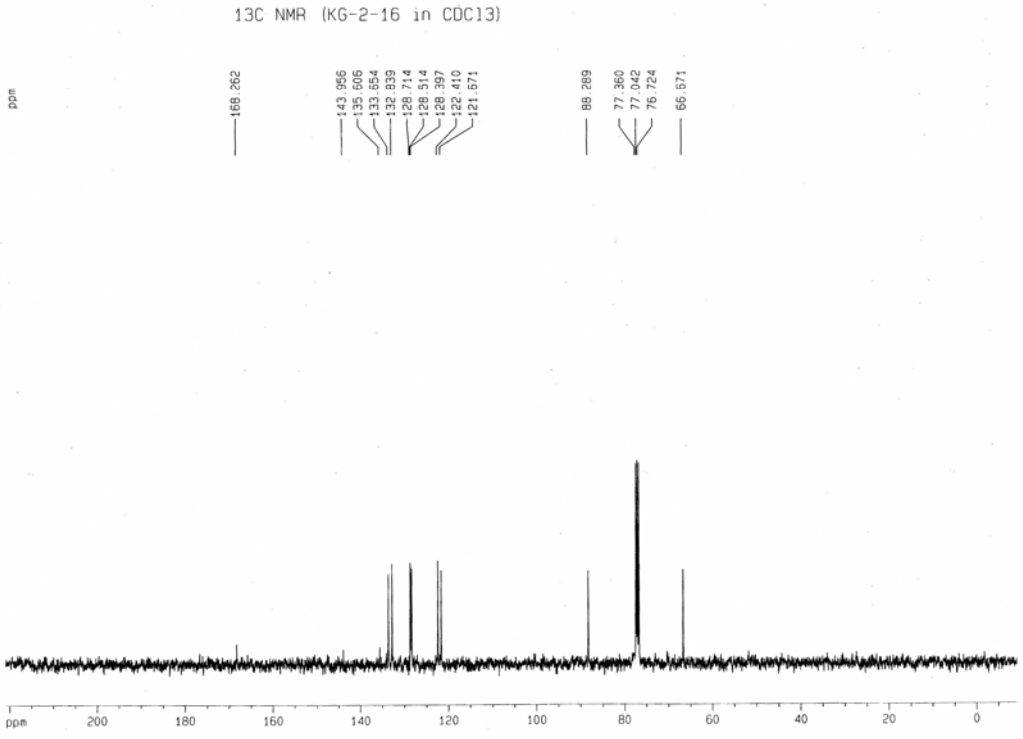
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
304.0630	304.0619	1.1	3.6	6.5	415.9	C13 H15 N O4 Na S



4c HRMS



4d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

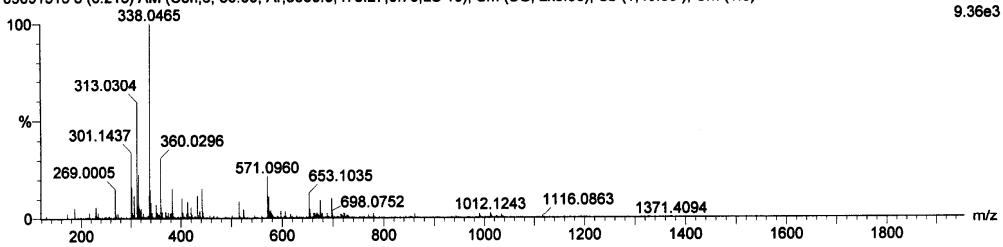


Elemental Composition Report **Page 1**

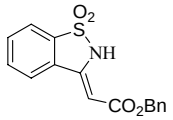
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 4-4 Na: 1-1 S: 1-1

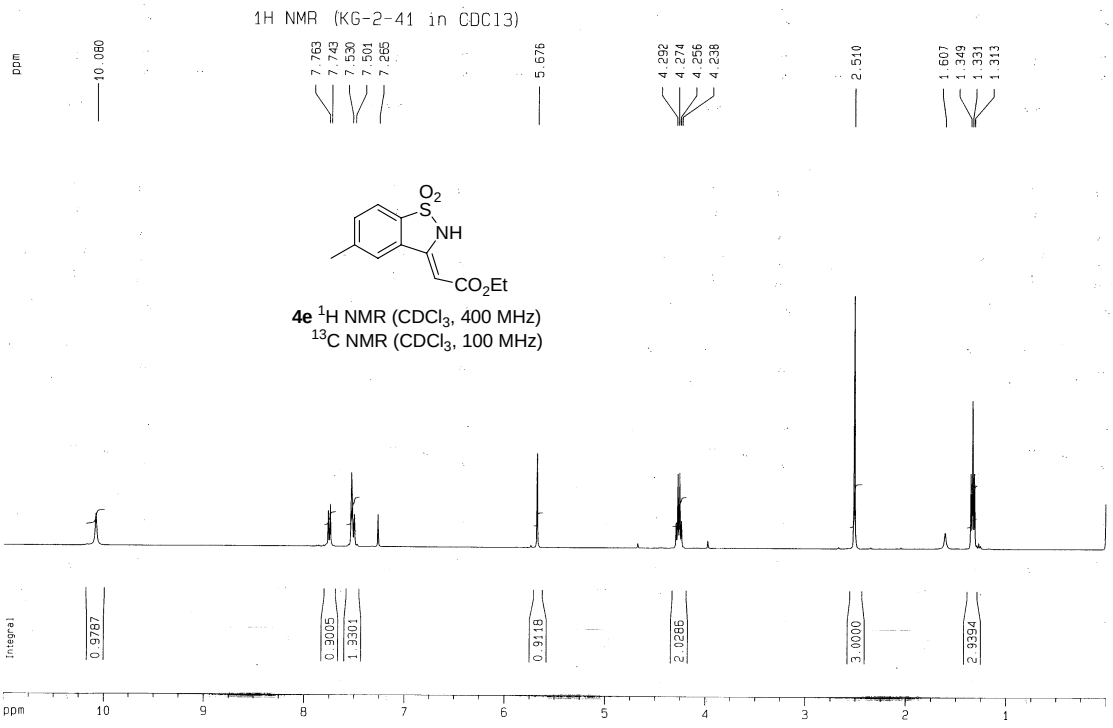
KG-2-16
09091515 8 (0.213) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:8) 1: TOF MS ES+ 9.36e3



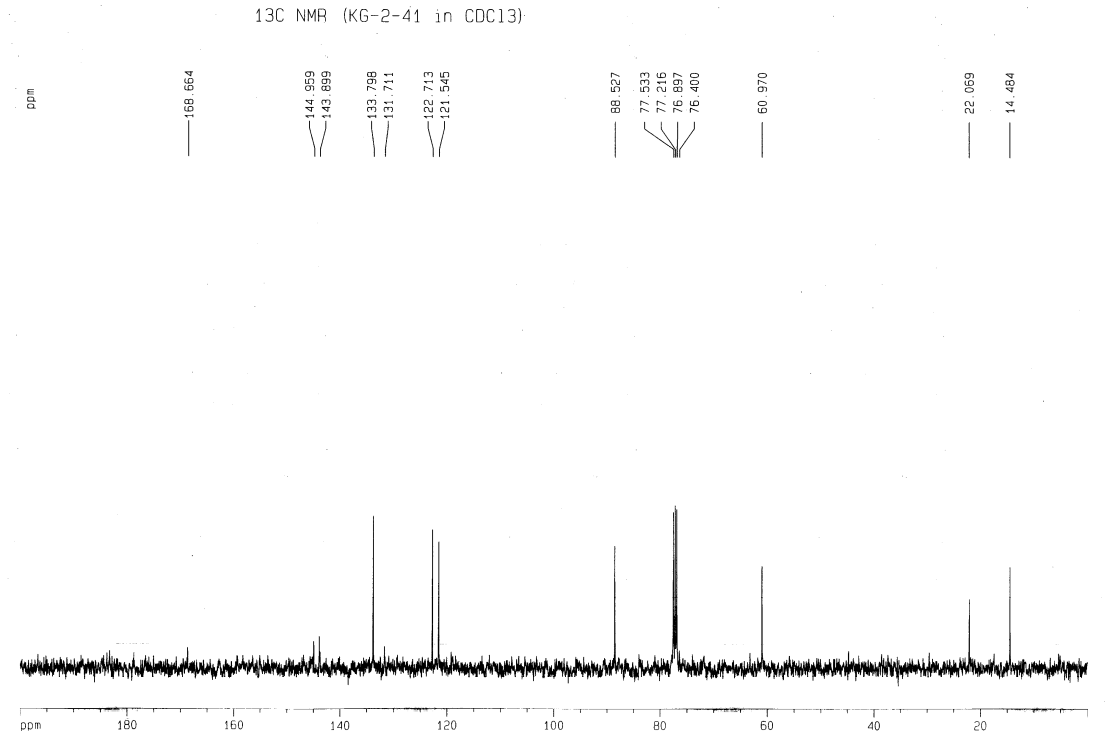
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
338.0465	338.0463	0.2	0.6	10.5	46.2	C16 H13 N O4 Na S



4d HRMS



4e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

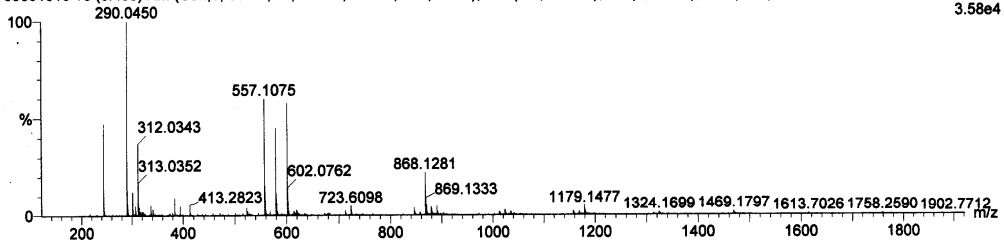


Elemental Composition Report **Page 1**

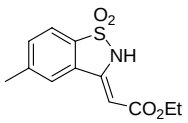
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 4-4 Na: 1-1 S: 1-1

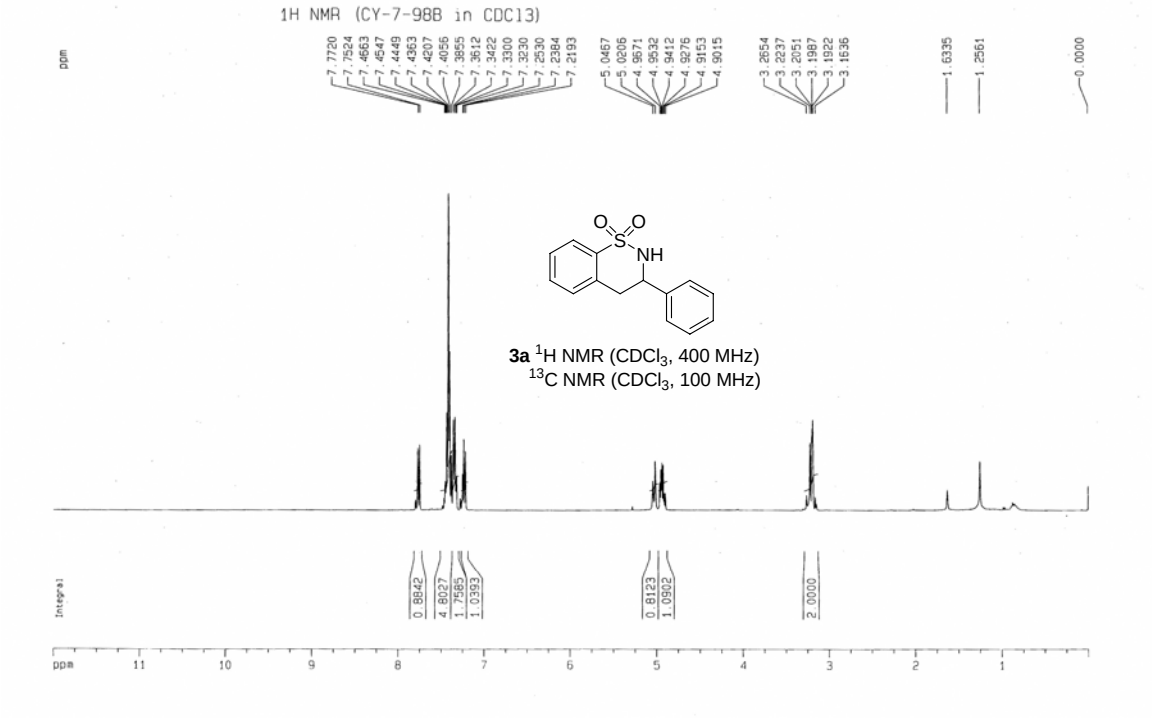
KG-2-42
09091516 16 (0.405) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:29) 1: TOF MS ES+ 3.58e4



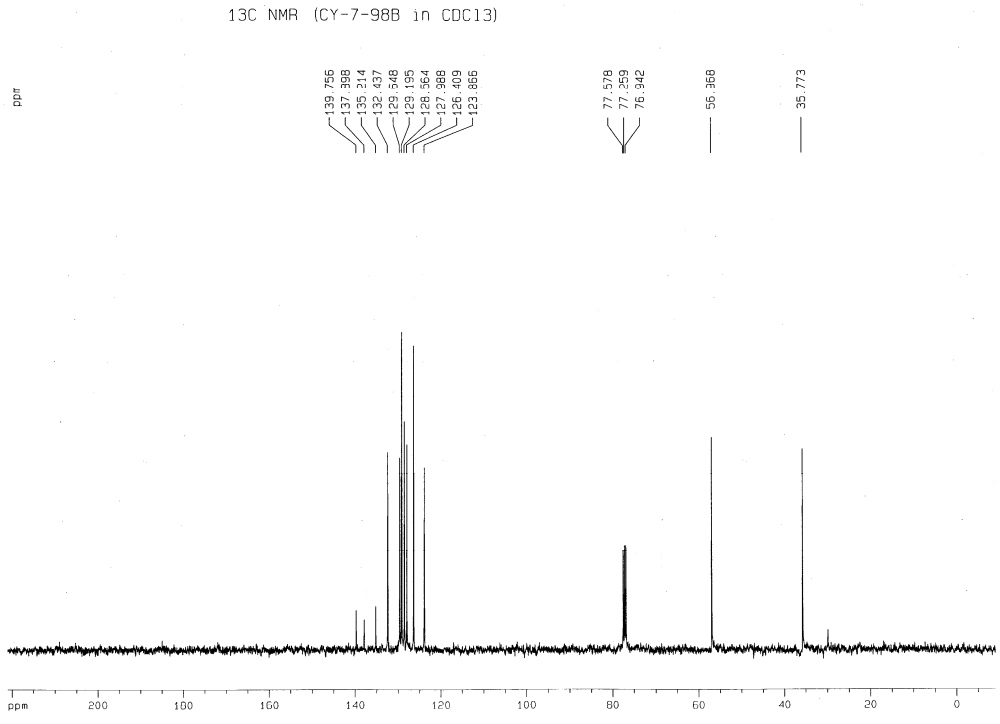
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0450	290.0463	-1.3	-4.5	6.5	45.9	C12 H13 N O4 Na S

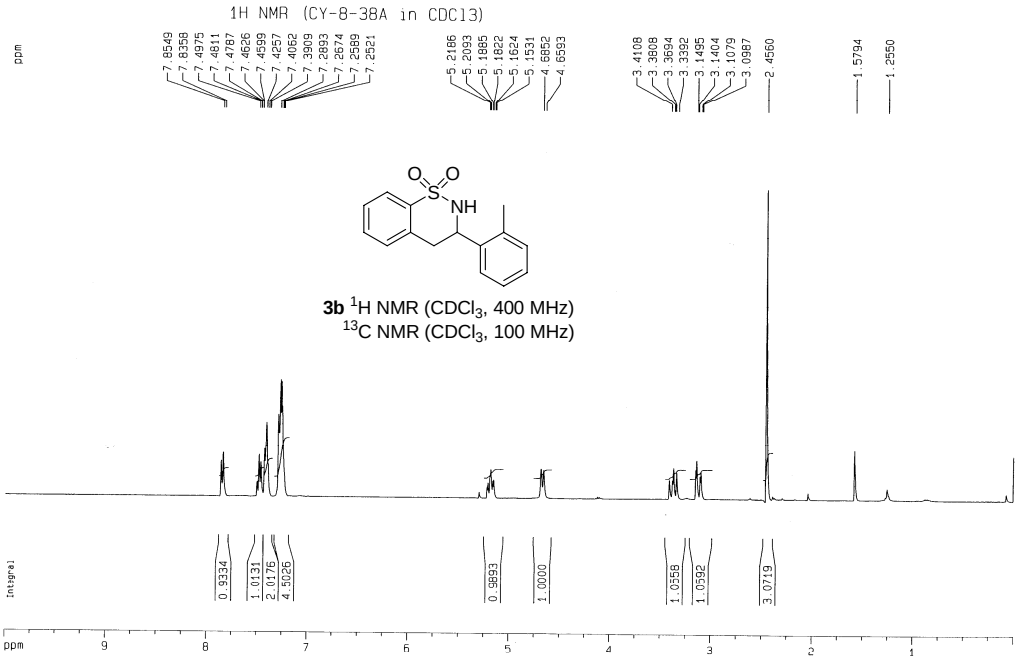


4e HRMS

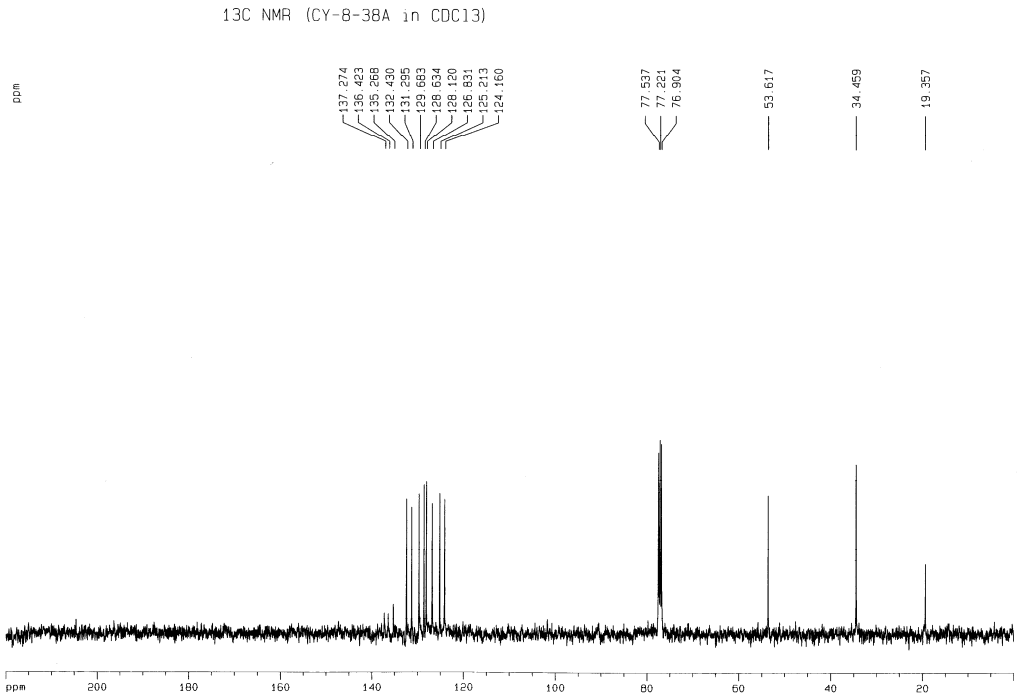


3a ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)





3b ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

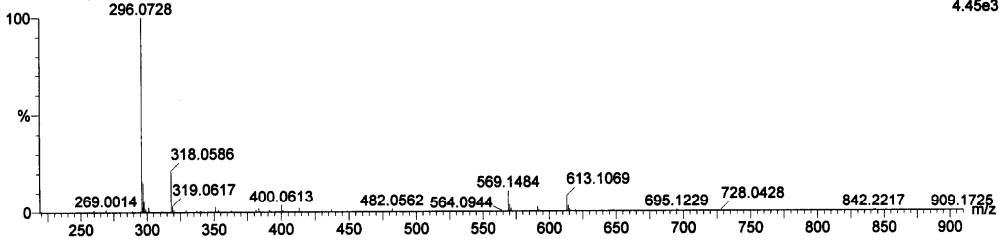


Elemental Composition Report **Page 1**

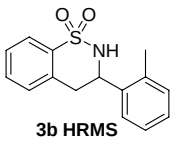
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

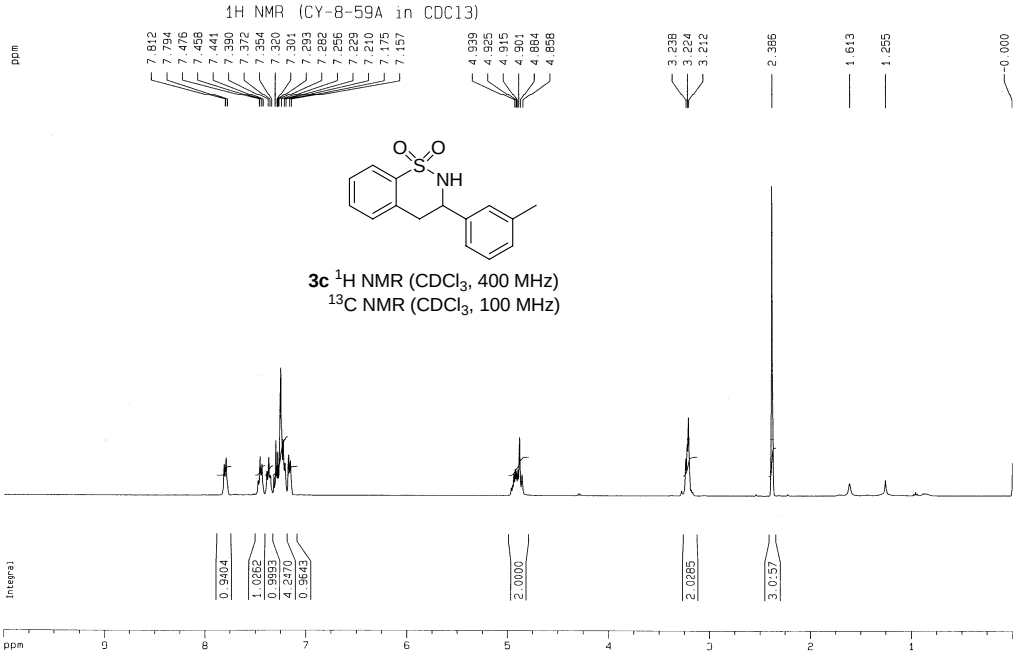
CY-8-38A
09091602 3 (0.079) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:11) 1: TOF MS ES+ 4.45e3



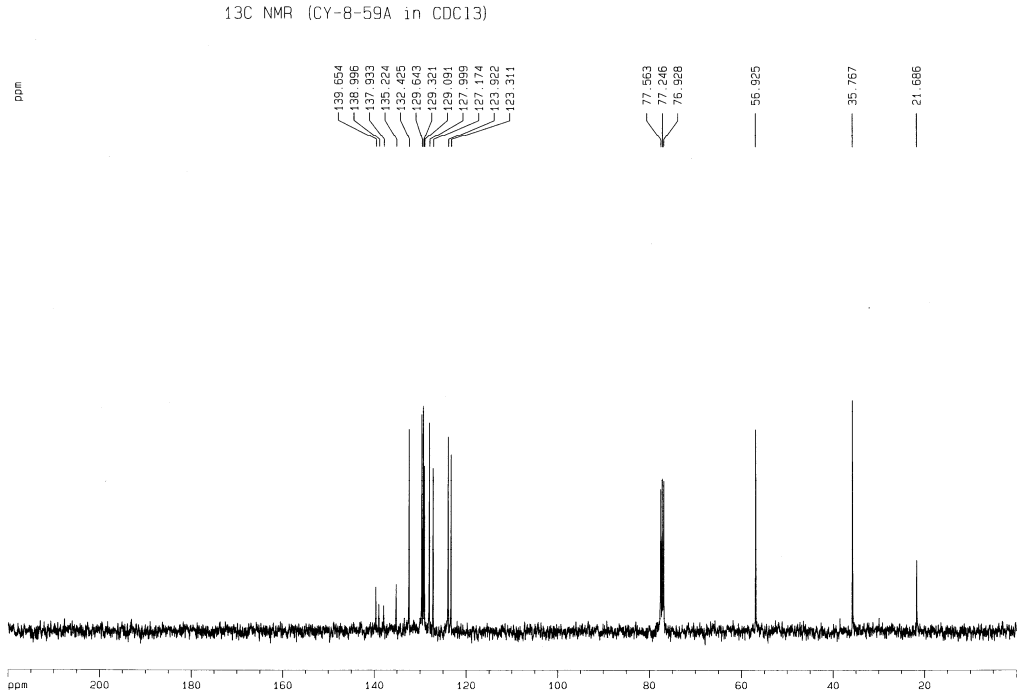
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0728	296.0721	0.7	2.4	8.5	13.3	C15 H15 N O2 Na S



3b HRMS



3c ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

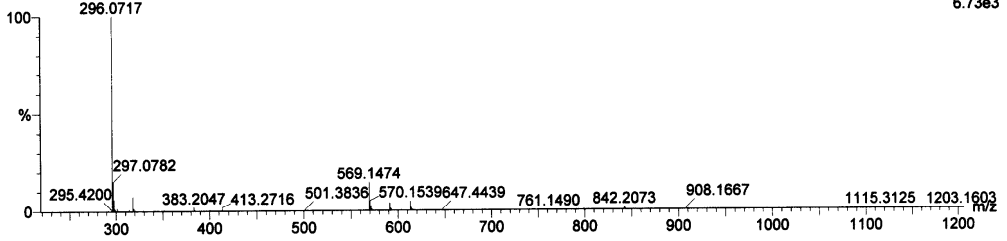


Elemental Composition Report **Page 1**

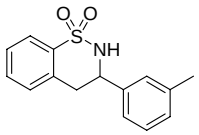
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

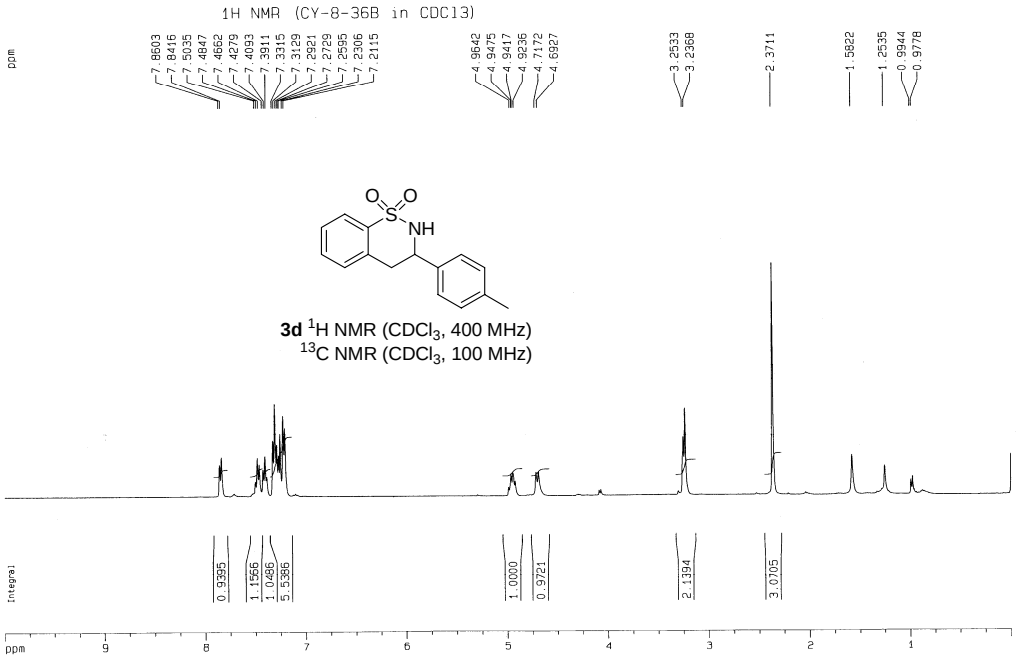
CY-8-59A
09091603 20 (0.521) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:20) 1: TOF MS ES+ 6.73e3



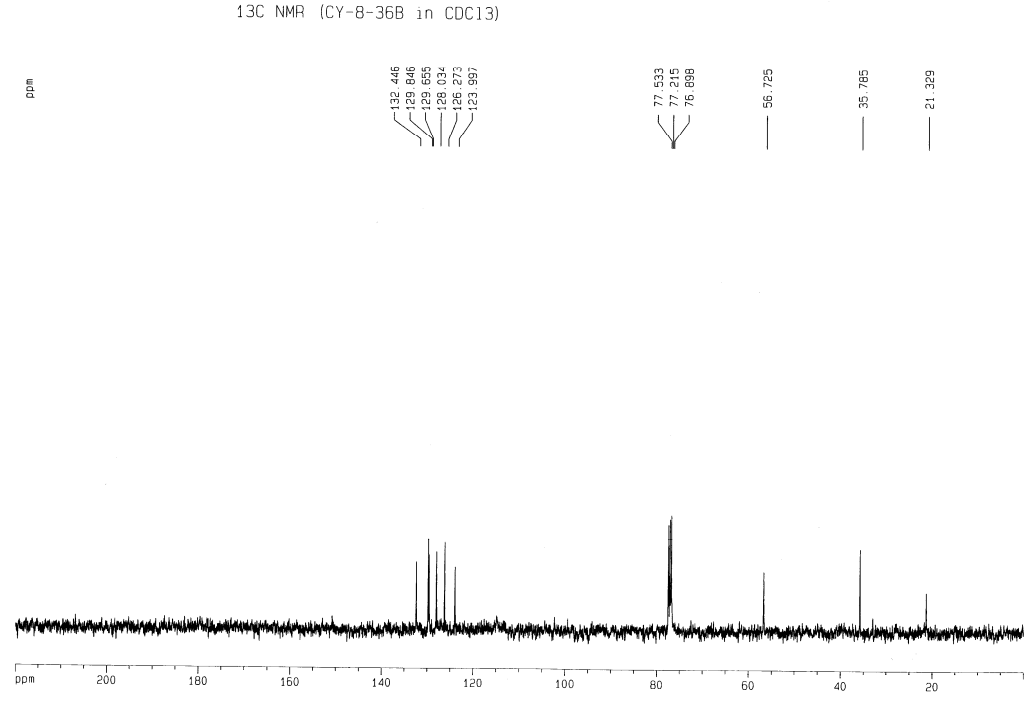
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0717	296.0721	-0.4	-1.4	8.5	20.0	C15 H15 N O2 Na S



3c HRMS



3d ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

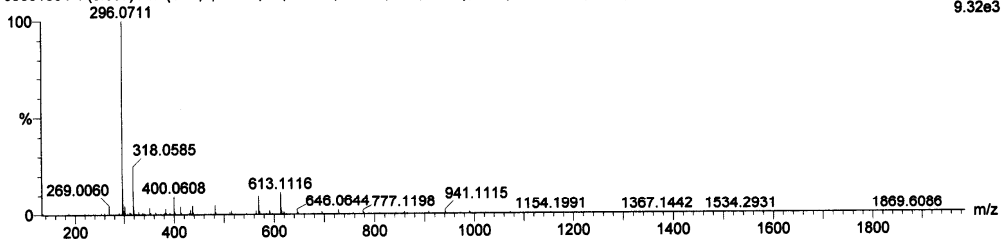


Elemental Composition Report **Page 1**

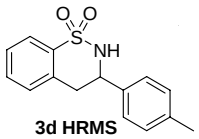
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

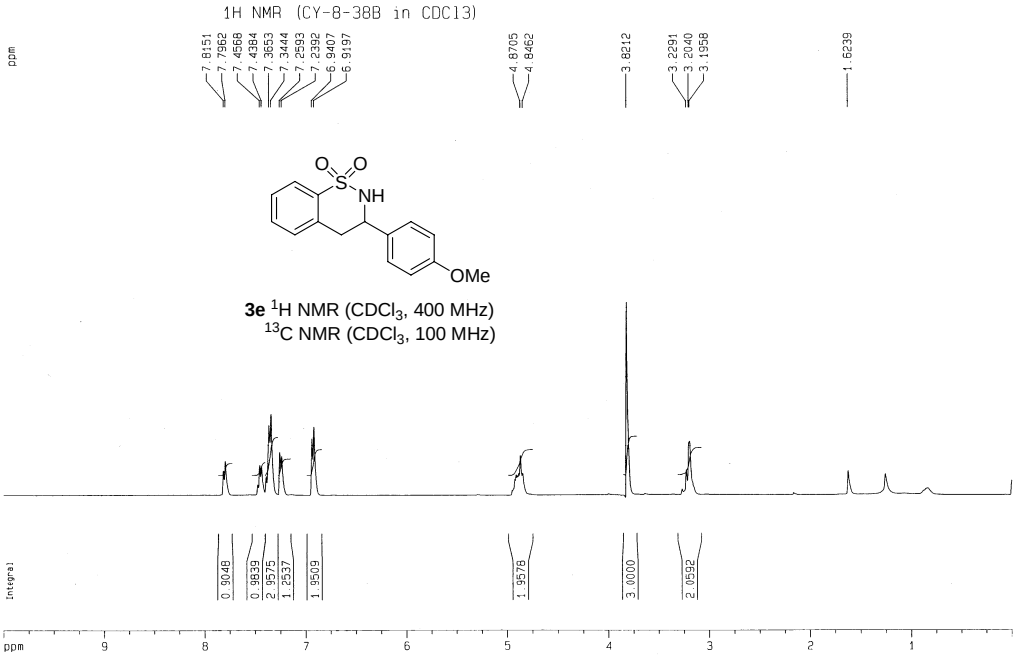
CY-8-37A
09091604 4 (0.097) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:12) 1: TOF MS ES+ 9.32e3



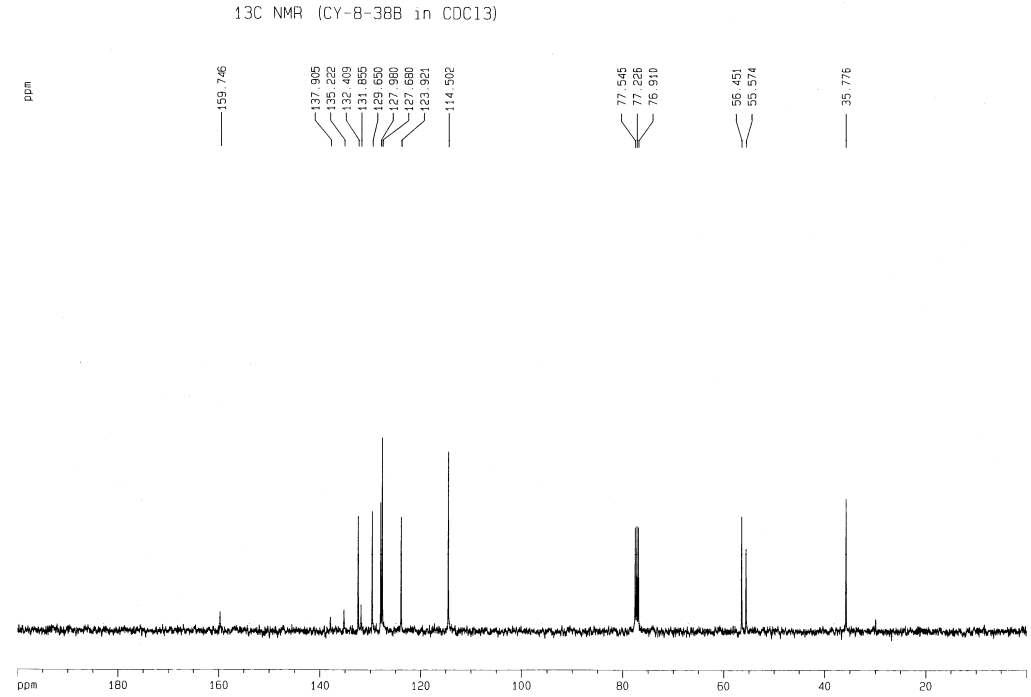
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0711	296.0721	-1.0	-3.4	8.5	63.6	C15 H15 N O2 Na S

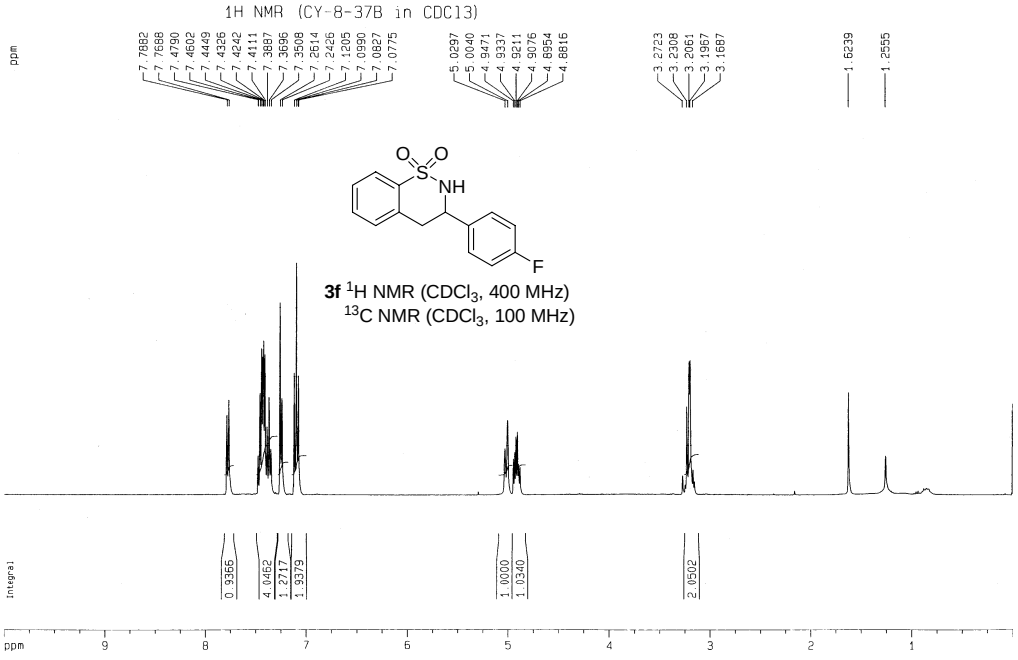


3d HRMS

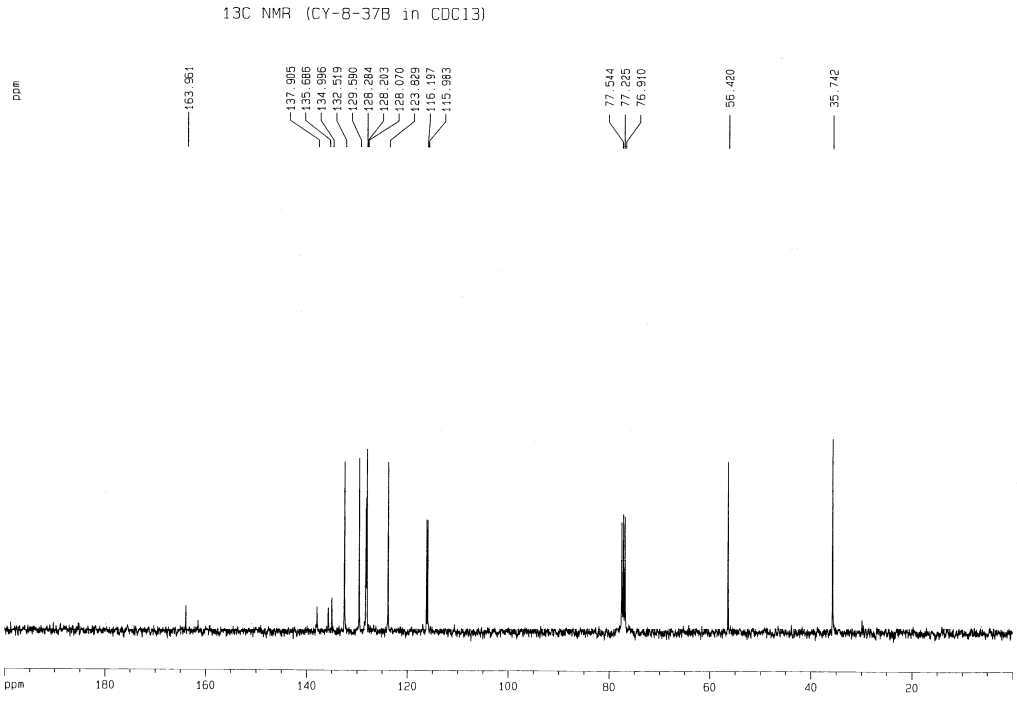


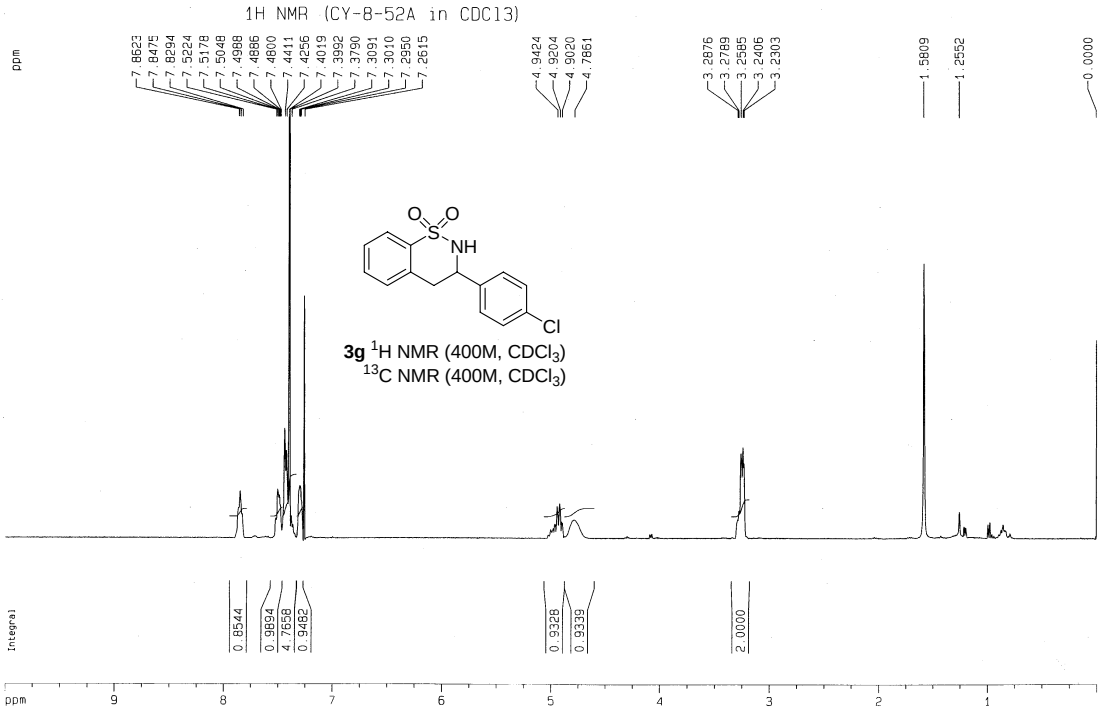
3e ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)



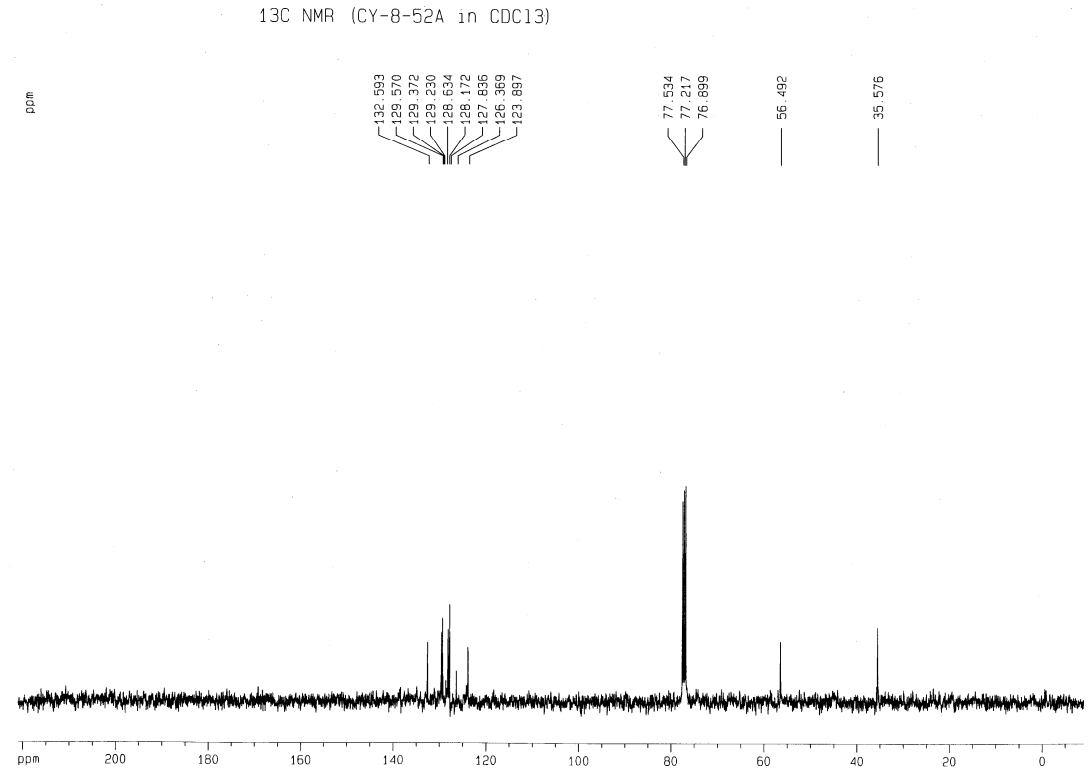


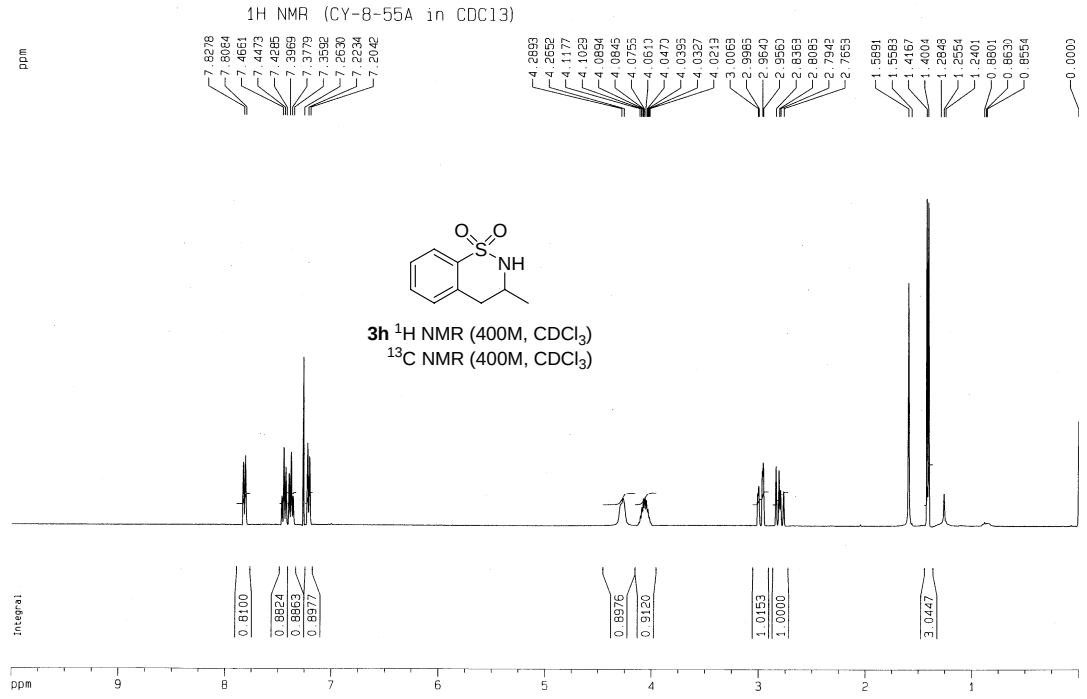
3f ^{1}H NMR ($CDCl_3$, 400 MHz)
^{13}C NMR ($CDCl_3$, 100 MHz)

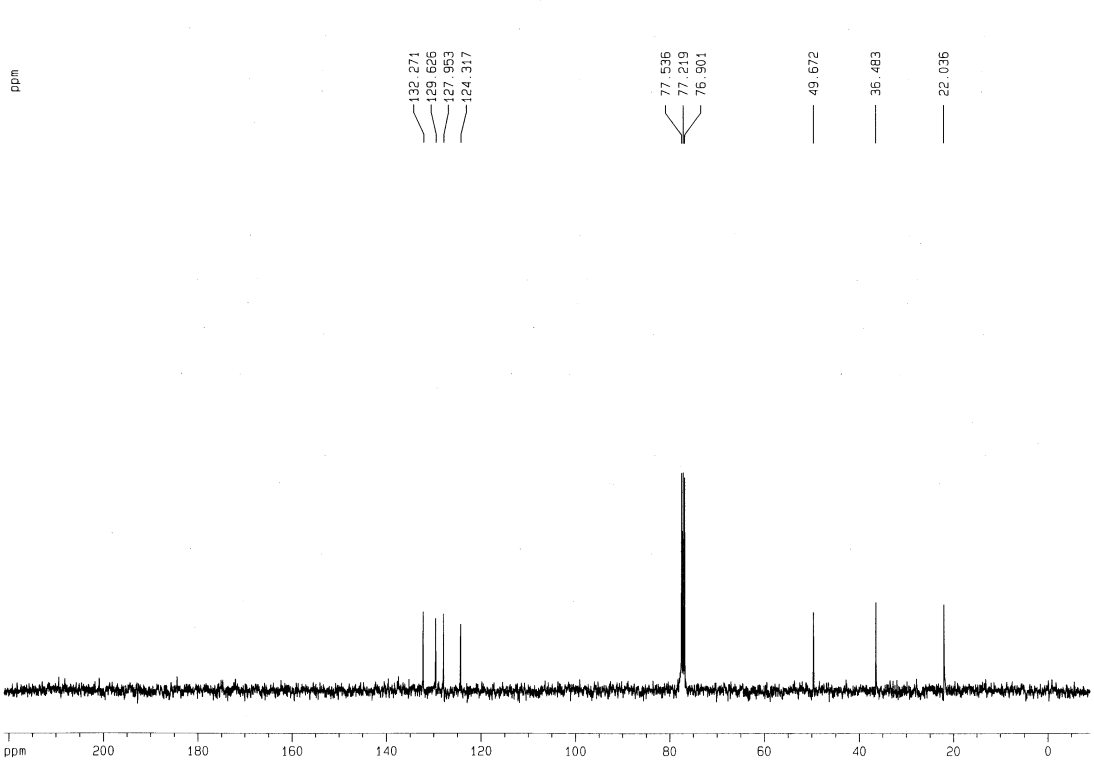


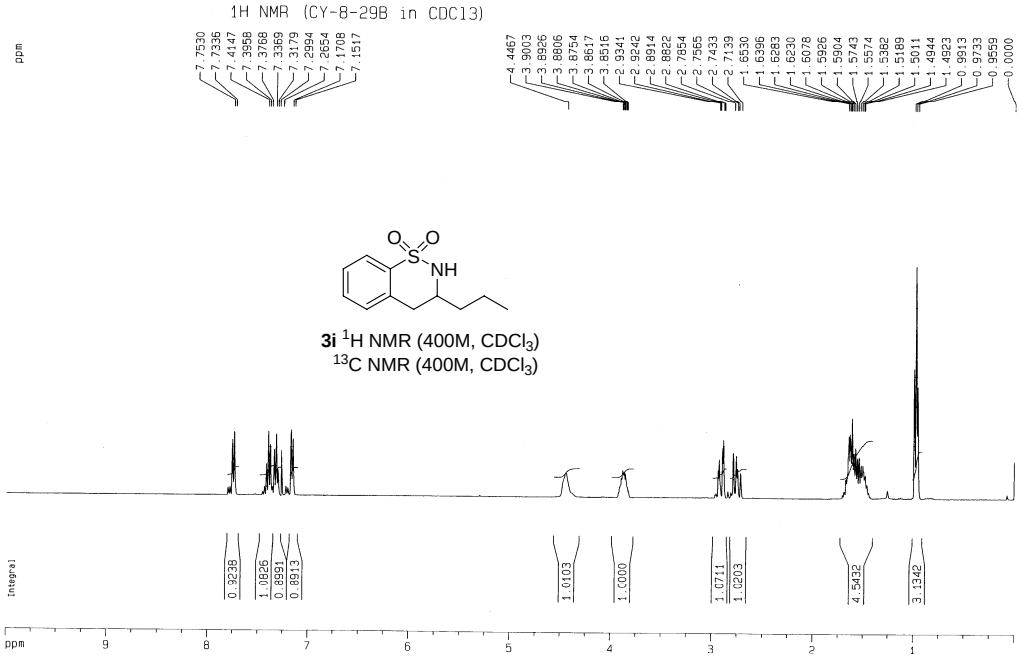


3g ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (400M, $CDCl_3$)

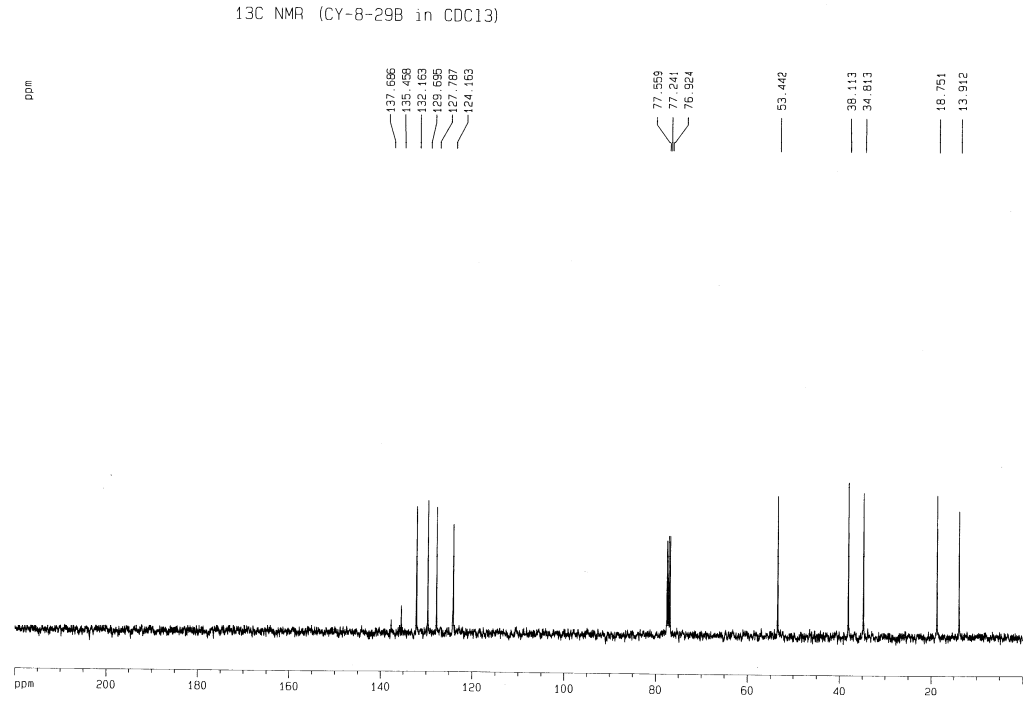



1H NMR (CY-8-55A in CDCl3)
ppm
7.8278
7.8064
7.4661
7.4473
7.4285
7.3969
7.3779
7.3592
7.2630
7.2234
7.2042
4.2893
4.2652
4.1177
4.1029
4.0894
4.0845
4.0755
4.0610
4.0473
4.0395
4.0327
4.0219
3.0069
2.9965
2.9640
2.9561
2.8363
2.8085
2.7942
2.7653
1.5891
1.5583
1.4167
1.4004
1.2848
1.2554
1.2401
0.8801
0.8639
0.8554
0.0000
O
O
S
NH
3h 1H NMR (400M, CDCl3)
13C NMR (400M, CDCl3)
Integral
0.8100
0.8824
0.8863
0.8977
0.8976
0.9120
1.0153
1.0000
3.0447
ppm
9
8
7
6
5
4
3
2
1


13C NMR (CY-8-55A in CDCl3)
ppm
132.271
129.626
127.953
124.317
77.536
77.219
76.901
49.672
36.483
22.036
ppm
200
180
160
140
120
100
80
60
40
20
0



3i ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (400M, $CDCl_3$)

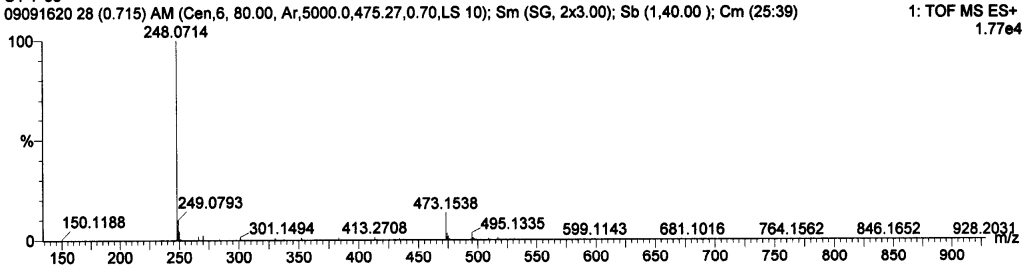


Elemental Composition Report **Page 1**

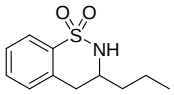
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 5-20 N: 1-2 O: 2-4 Na: 1-1 S: 1-1

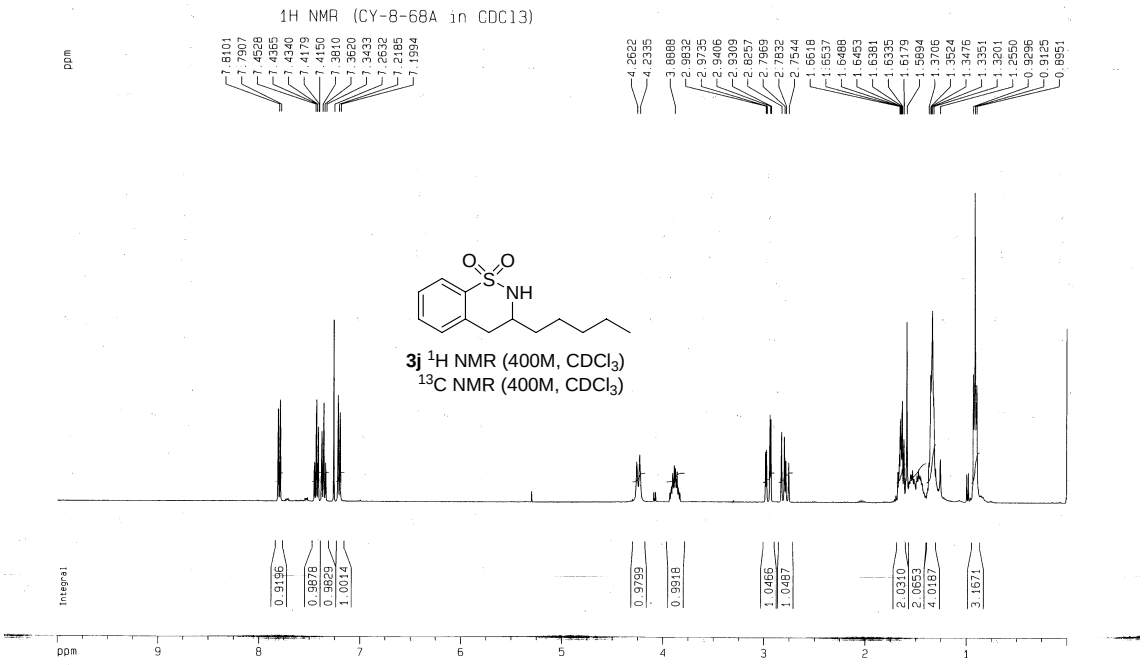
CY-7-88
09091620 28 (0.715) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (25:39) 1: TOF MS ES+ 1.77e4



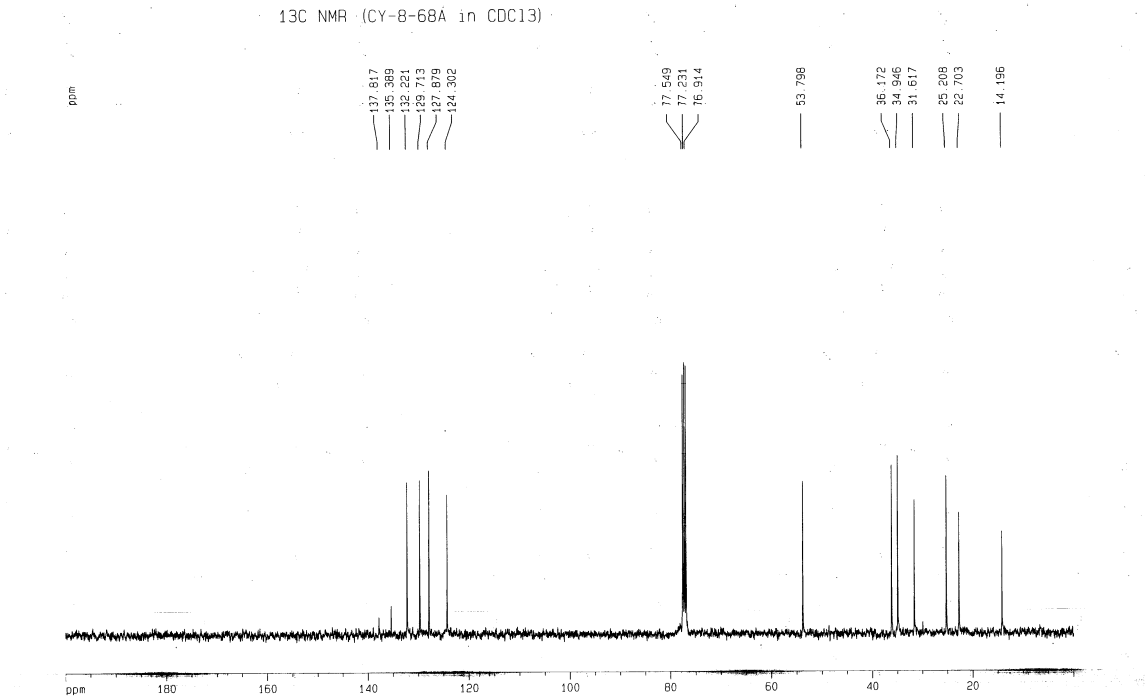
Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
248.0714	248.0721	-0.7	-2.8	4.5	141.8	C11 H15 N O2 Na S



3i HRMS



3j ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (400M, $CDCl_3$)

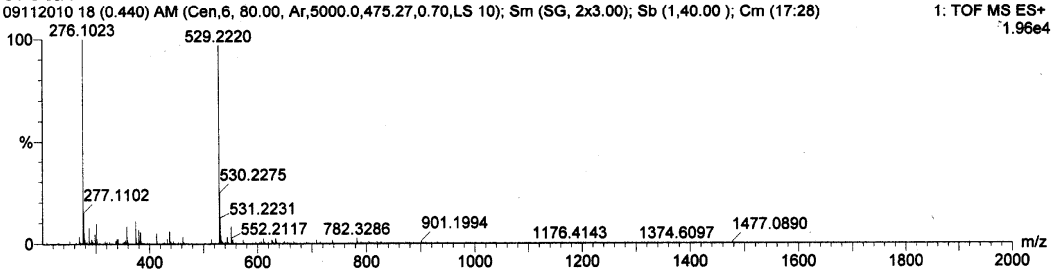


Elemental Composition Report **Page 1**

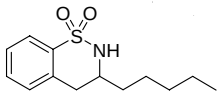
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
19 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 8-80 N: 1-3 O: 2-6 Na: 1-1 S: 1-1

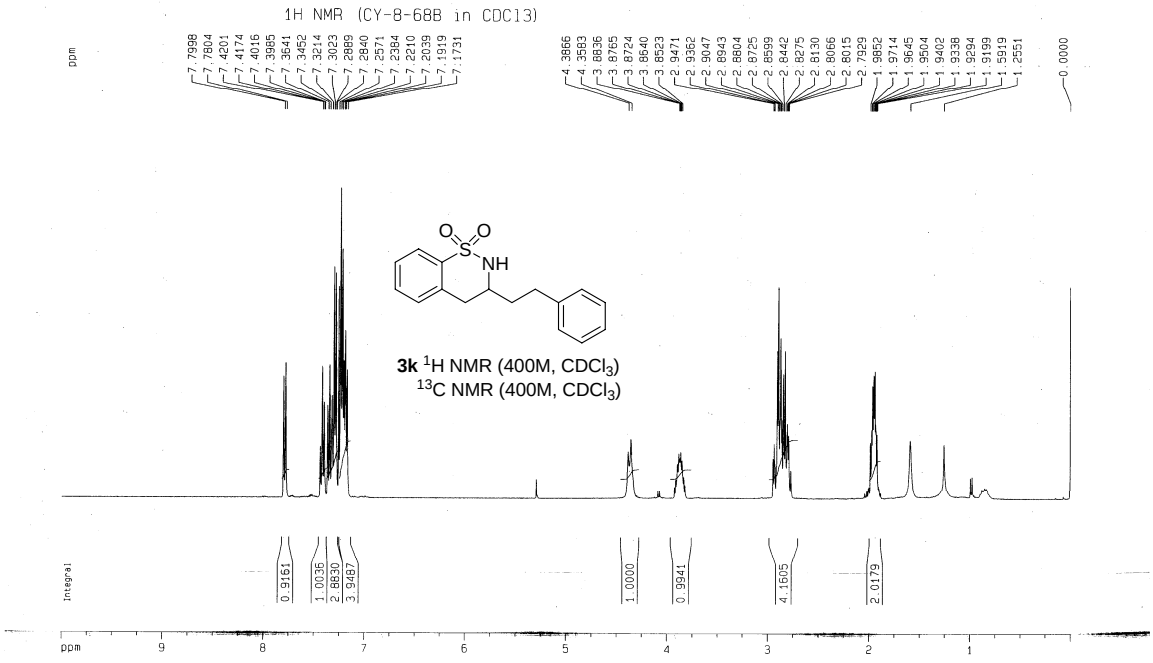
CY-8-68A
09112010 18 (0.440) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (17:28) 1: TOF MS ES+
1.96e4



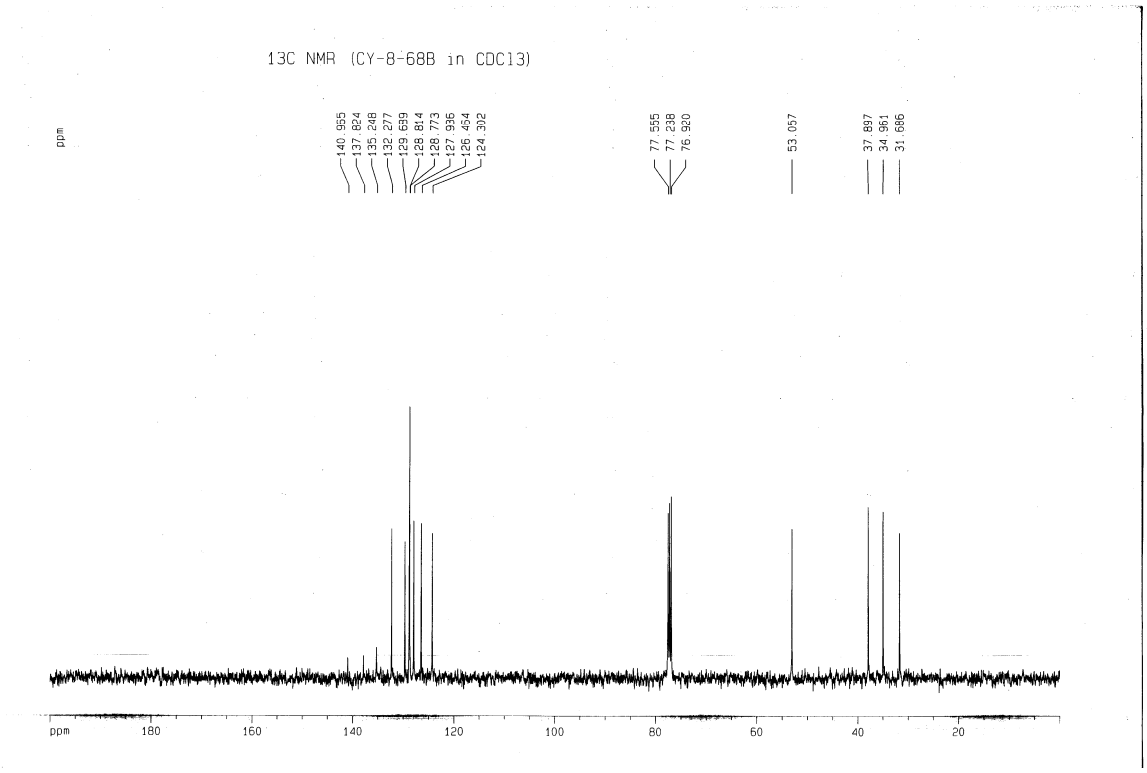
Minimum:		5.0	5.0	-1.5		
Maximum:				100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
276.1023	276.1034	-1.1	-4.0	4.5	21.8	C13 H19 N O2 Na S



3J HRMS



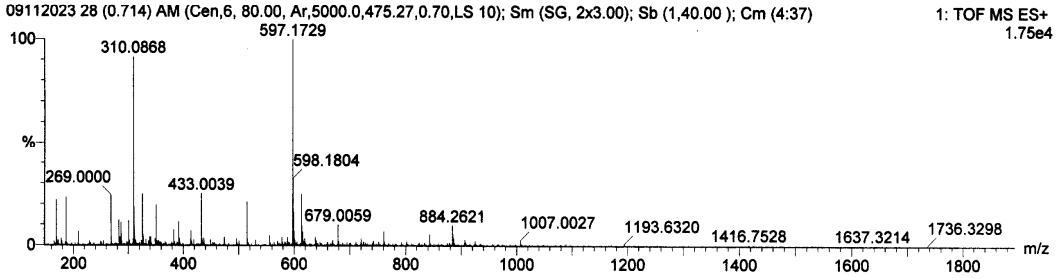
3k ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (400M, $CDCl_3$)



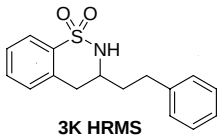
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

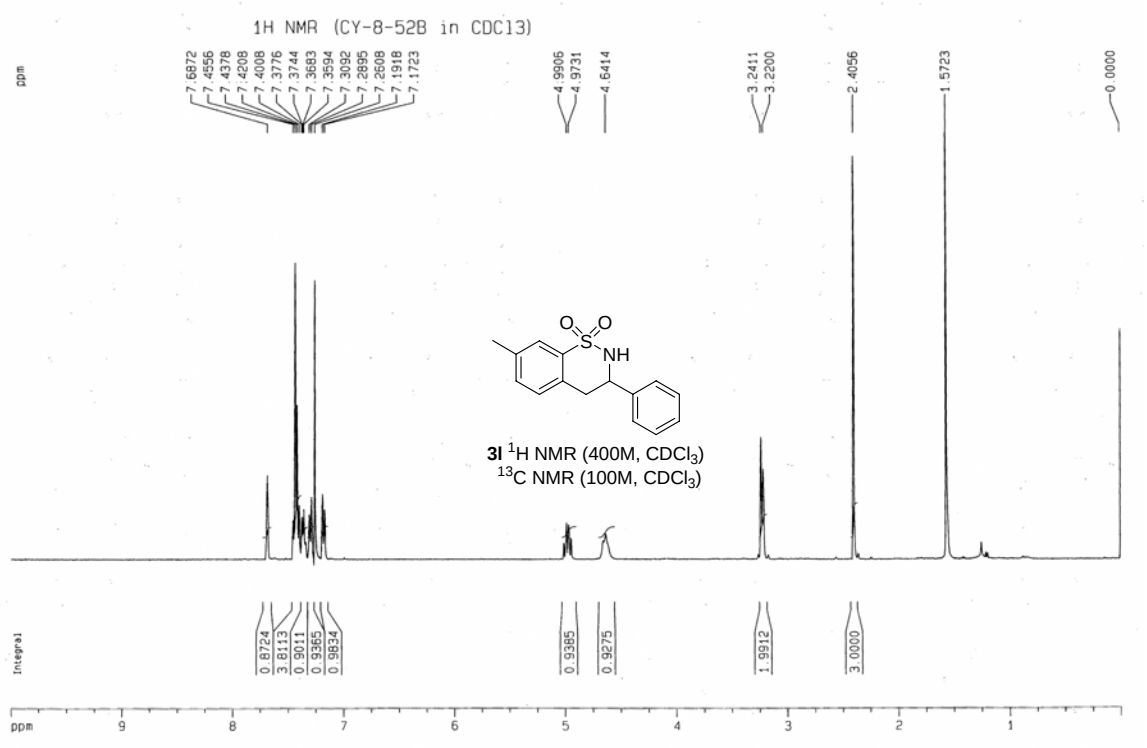
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 8-80 N: 1-1 O: 2-2 Na: 1-1 S: 1-1
QC-8-68B
09112023 28 (0.714) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (4:37) 1: TOF MS ES+ 1.75e4



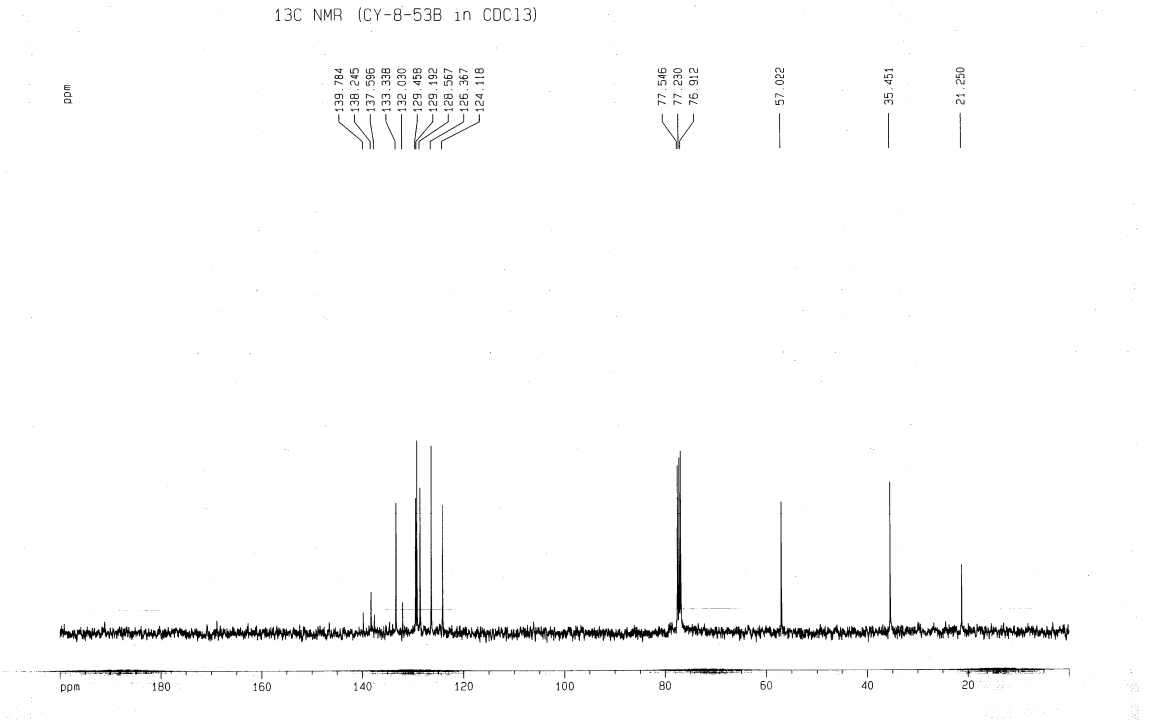
Minimum:				-1.5		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
310.0868	310.0878	-1.0	-3.2	8.5	16.9	C16 H17 N O2 Na S



3K HRMS



3l ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)

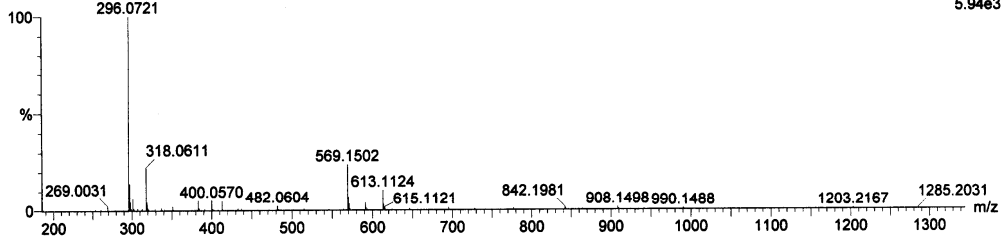


Elemental Composition Report **Page 1**

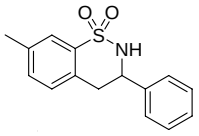
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-20 H: 10-20 N: 1-2 O: 2-2 Na: 1-1 S: 1-1

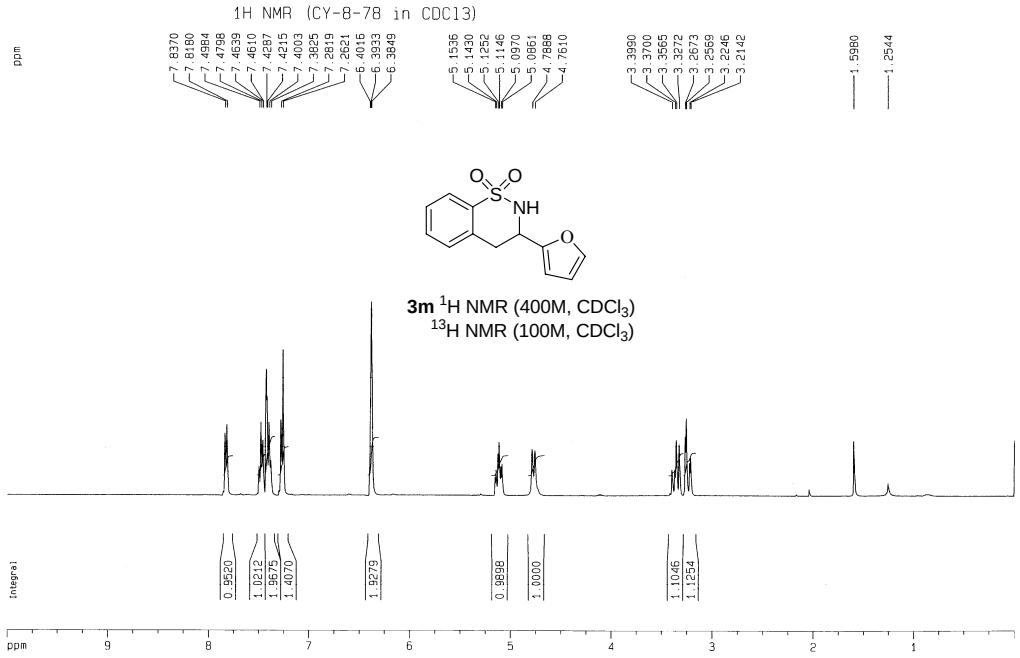
CY-8-53B
09091601 29 (0.728) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (28:35) 1: TOF MS ES+ 5.94e3

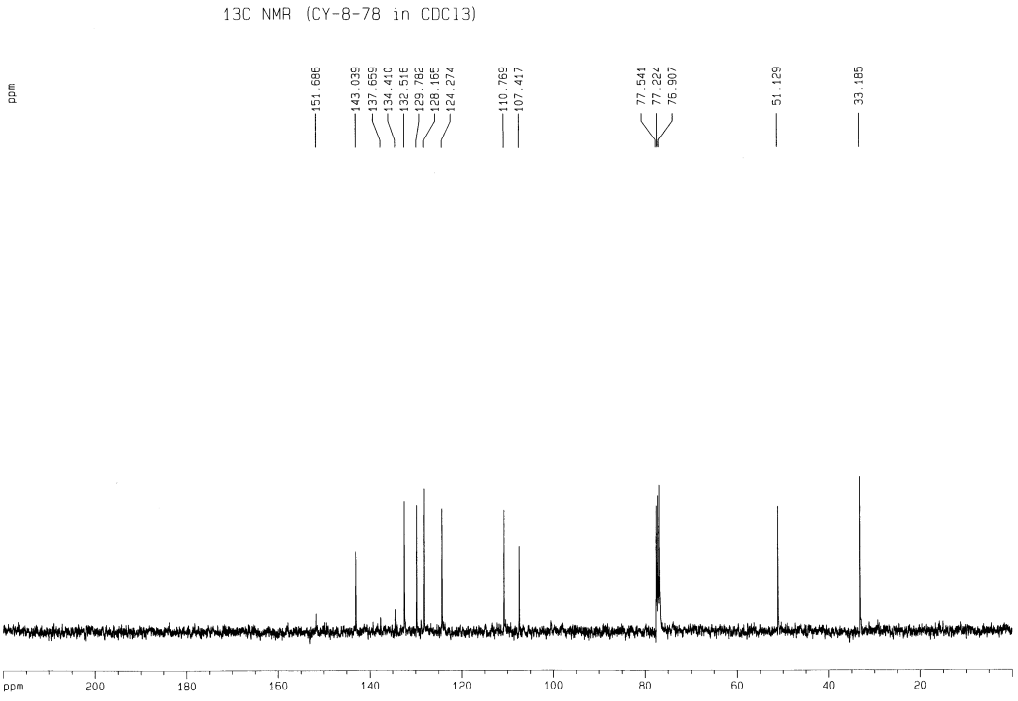


Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0721	296.0721	0.0	0.0	8.5	42.9	C15 H15 N O2 Na S



3l HRMS

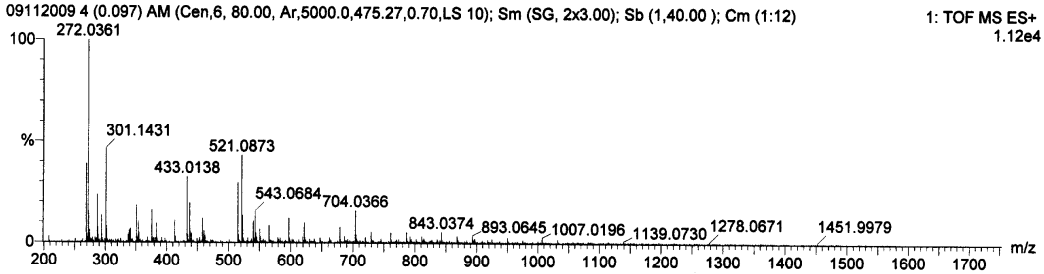

1H NMR (CY-8-78 in CDCl3)
ppm
7.8370
7.8180
7.4984
7.4798
7.4639
7.4610
7.4287
7.4215
7.4003
7.3825
7.2819
7.2621
6.4016
6.3933
6.3849
5.1536
5.1430
5.1252
5.1146
5.0970
5.0861
4.7888
4.7610
3.3990
3.3700
3.3565
3.3272
3.2673
3.2569
3.2246
3.2142
1.5980
1.2544
O
O
S
NH
O
3m 1H NMR (400M, CDCl3)
13H NMR (100M, CDCl3)
Integral
0.9520
1.0212
1.9675
1.4070
1.9279
0.9898
1.0000
1.1046
1.1254
ppm
9
8
7
6
5
4
3
2
1


13C NMR (CY-8-78 in CDCl3)
ppm
151.686
143.035
137.655
134.410
132.516
129.782
128.165
124.274
110.765
107.417
77.541
77.224
76.907
51.129
33.185
ppm
200
180
160
140
120
100
80
60
40
20

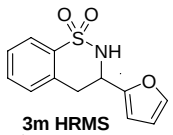
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

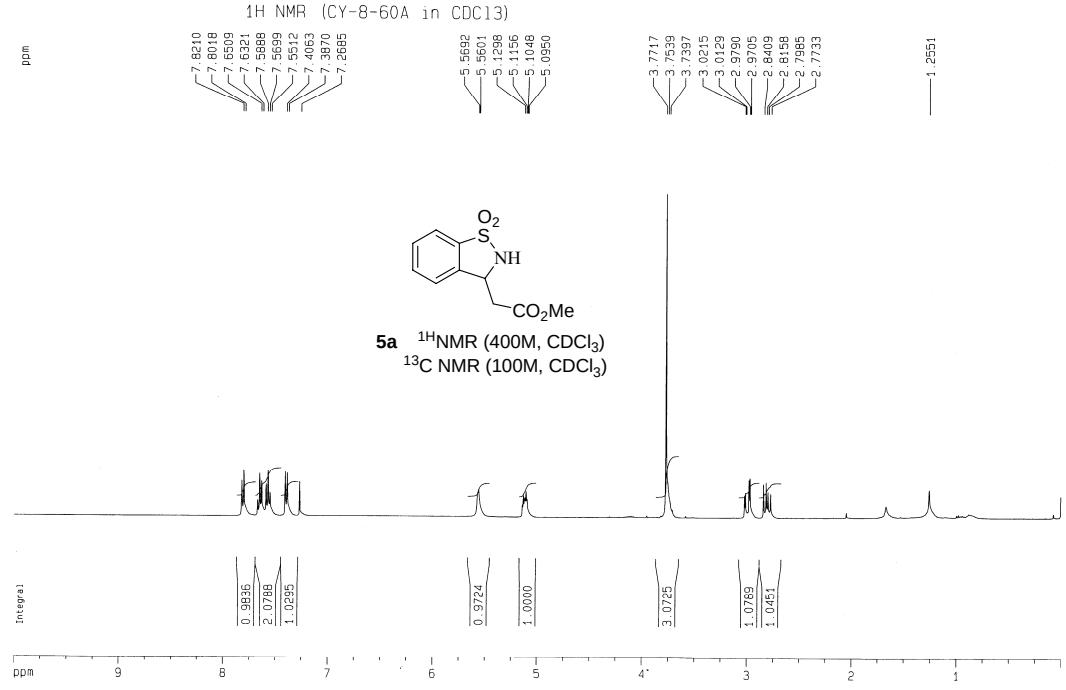
Monoisotopic Mass, Odd and Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 8-80 N: 1-3 O: 3-6 Na: 1-1 S: 1-1
CY-8-78
09112009 4 (0.097) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (1:12) 1: TOF MS ES+ 1.12e4



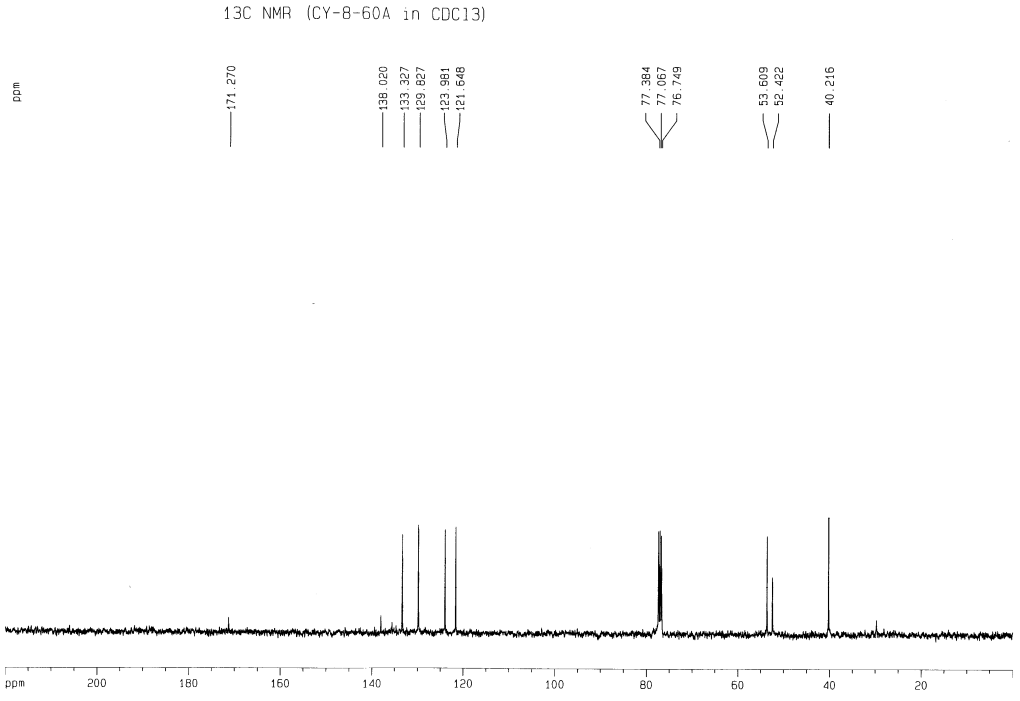
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
272.0361	272.0357	0.4	1.5	7.5	3.0	C12 H11 N O3 Na S

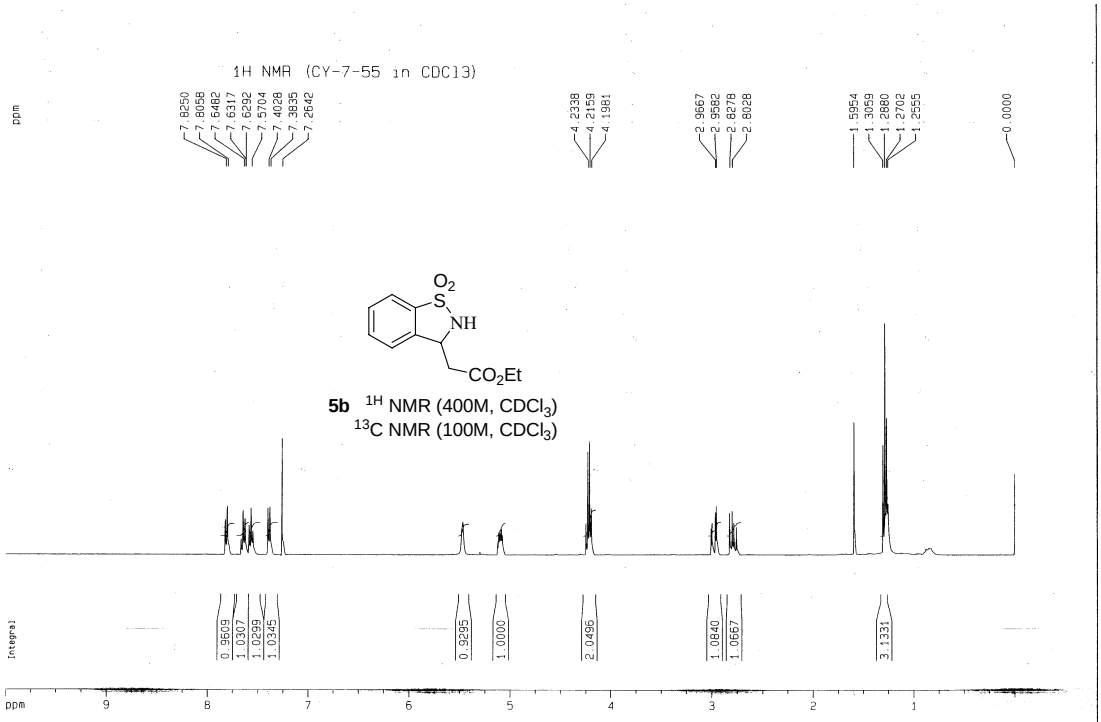


3m HRMS

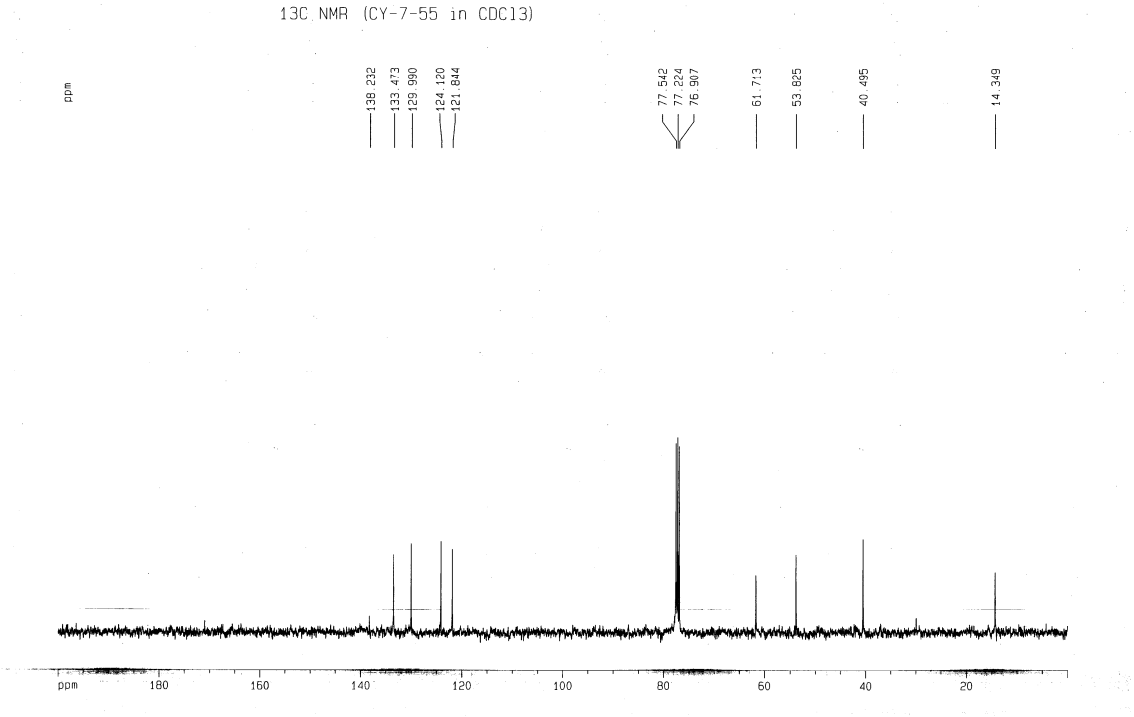


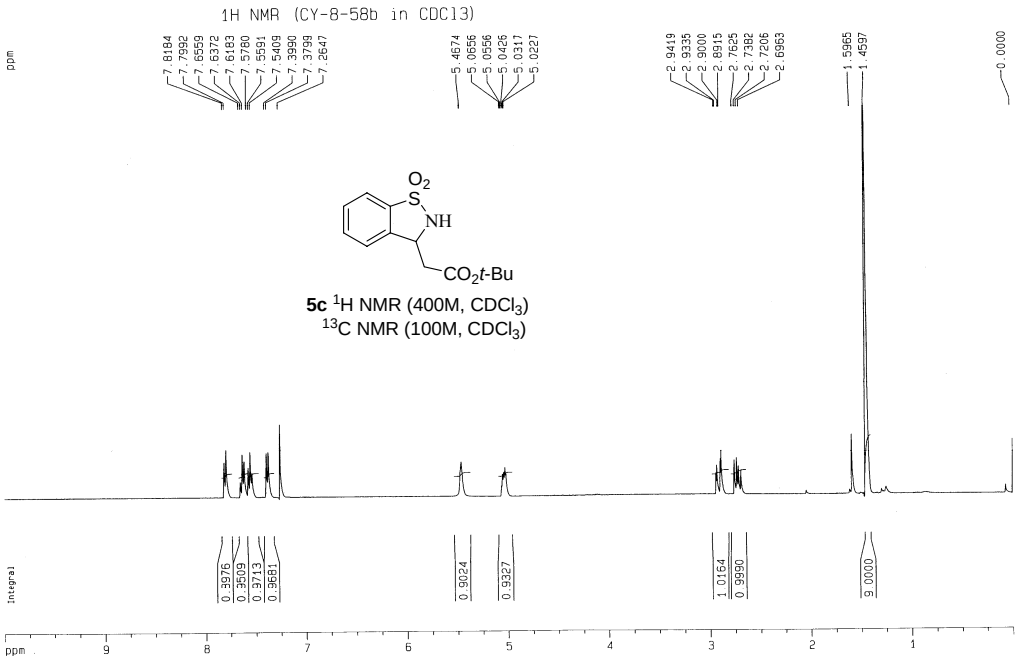
5a ^{1H}NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)



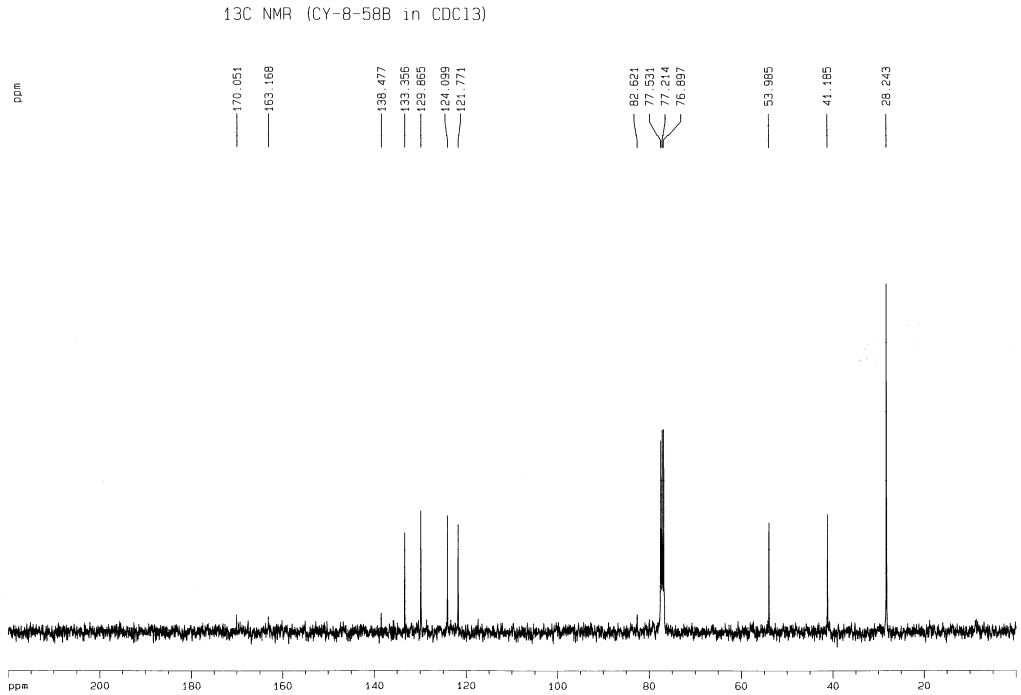


5b ^{1H} NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)





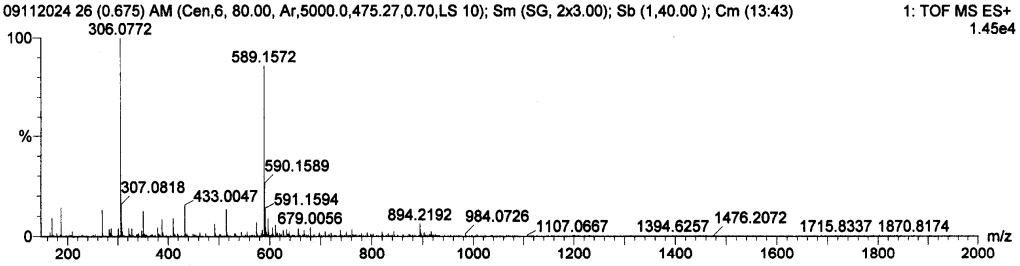
5c ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)



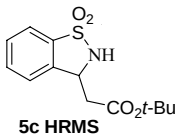
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

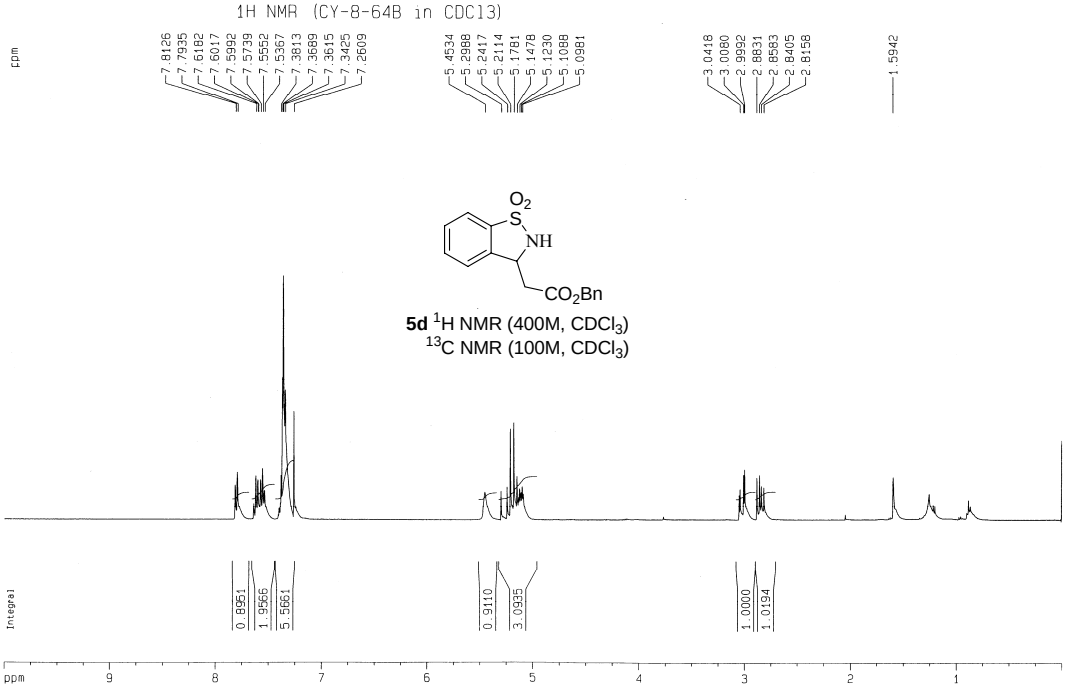
Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 8-80 N: 1-1 O: 4-4 Na: 1-1 S: 1-1
QC-8-58B
09112024 26 (0.675) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (13:43) 1: TOF MS ES+ 1.45e4



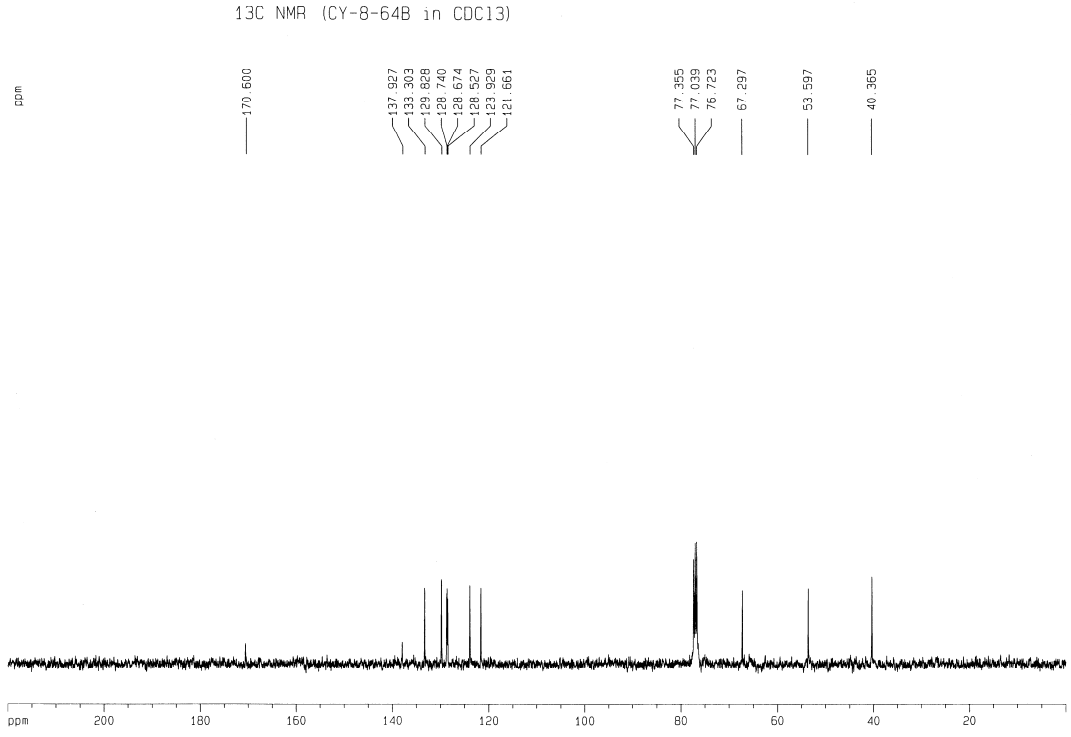
Minimum:				-1.5		
Maximum:		5.0	50.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
306.0772	306.0776	-0.4	-1.3	5.5	4.2	C13 H17 N O4 Na S



5c HRMS



5d ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)

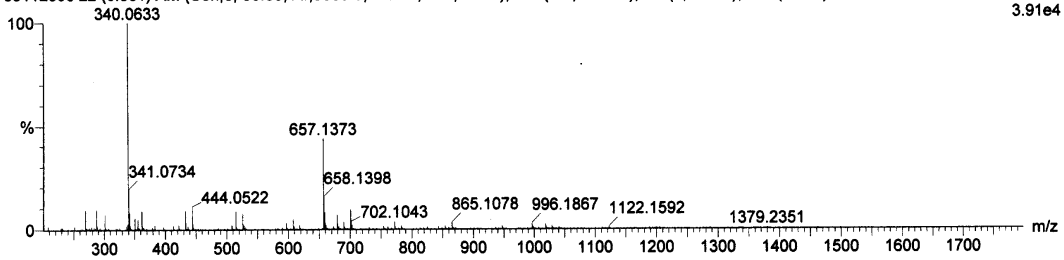


Elemental Composition Report **Page 1**

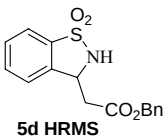
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 10-80 N: 1-3 O: 4-6 Na: 1-1 S: 1-1

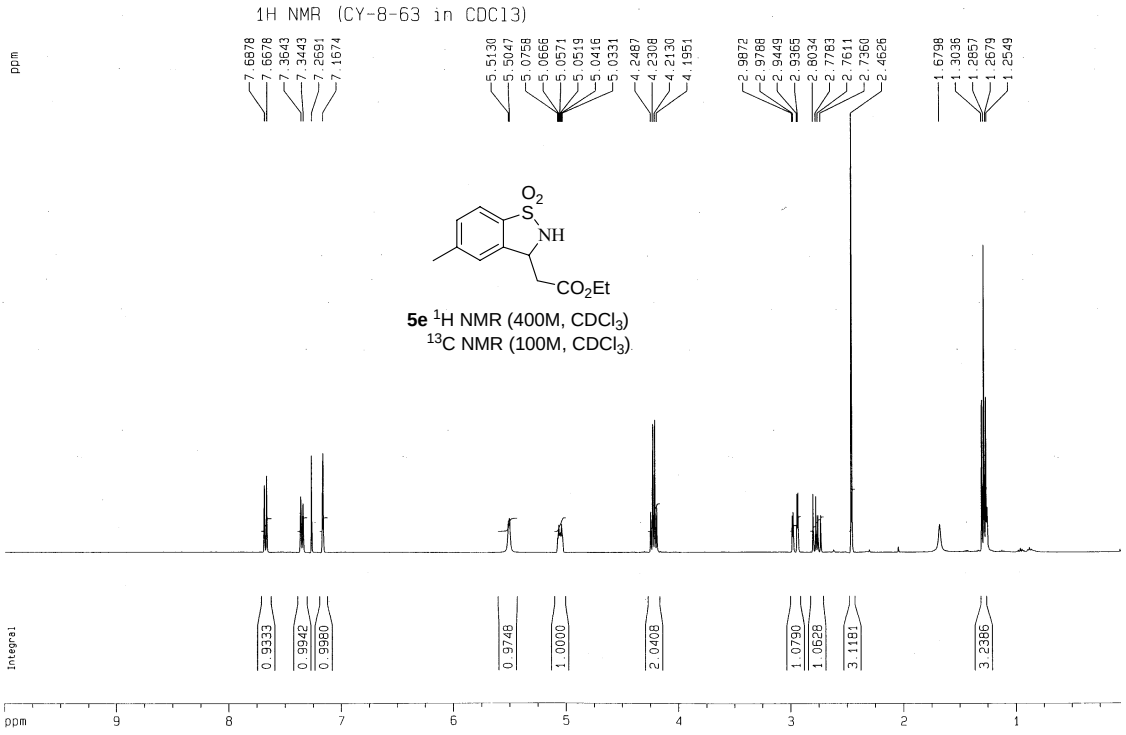
CY-8-64B
09112006 22 (0.561) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (14:43) 1: TOF MS ES+ 3.91e4



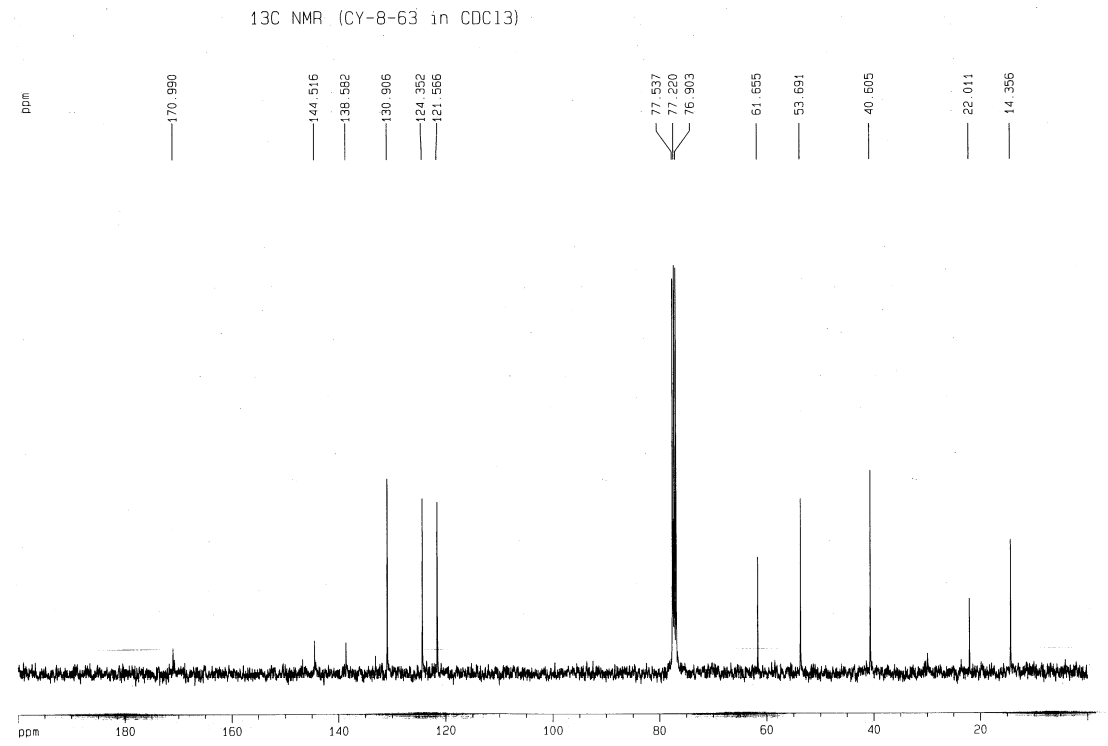
Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
340.0633	340.0619	1.4	4.1	9.5	38.8	C16 H15 N O4 Na S



5d HRMS



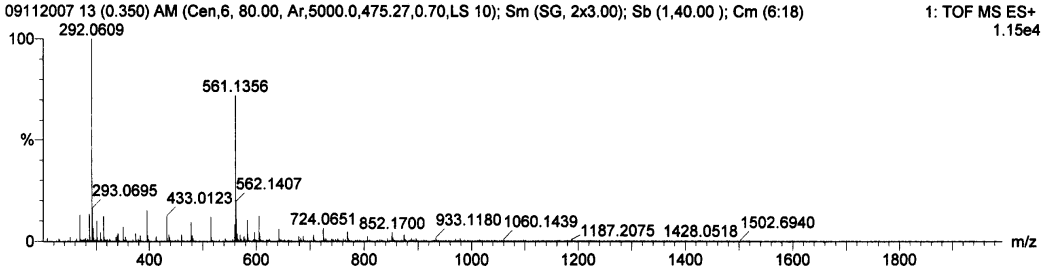
5e ^{1}H NMR (400M, $CDCl_3$)
^{13}C NMR (100M, $CDCl_3$)



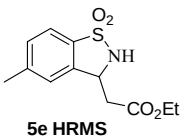
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
9 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-76 H: 10-80 N: 1-3 O: 4-6 Na: 1-1 S: 1-1
CY-8-72
09112007 13 (0.350) AM (Cen,6, 80.00, Ar,5000.0,475.27,0.70,LS 10); Sm (SG, 2x3.00); Sb (1,40.00); Cm (6:18) 1: TOF MS ES+ 1.15e4



Minimum:				-1.5		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.0609	292.0619	-1.0	-3.4	5.5	6.8	C12 H15 N O4 Na S



5e HRMS

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006325.D Sample Name: CY-7-81 (+/-)

OD-H, H/i-PrOH = 70/30, 0.8 mL/min

```
==========================================================================
Injection Date  : 4/21/2009 4:18:00 PM
Sample Name     : CY-7-81 (+/-)                  Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 4/21/2009 4:16:30 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:19:04 AM
                  (modified after loading)
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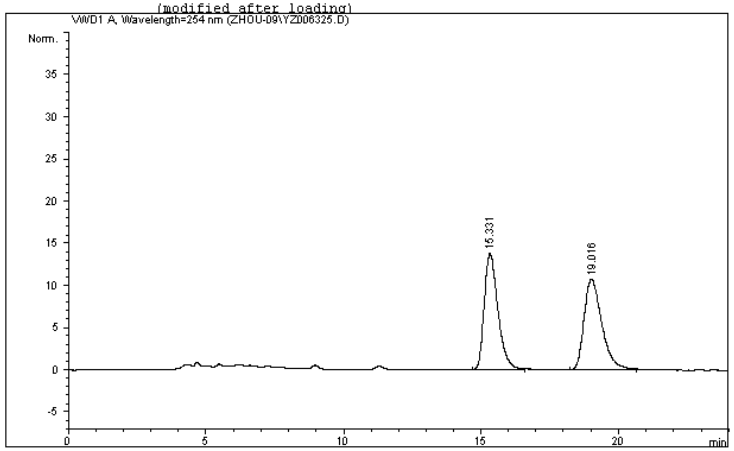



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  15.331 PB    0.5215  473.68723   13.74377  49.9676
   2  19.016 BB    0.6858  474.30237   10.70506  50.0324

Totals :                  947.98959   24.44883

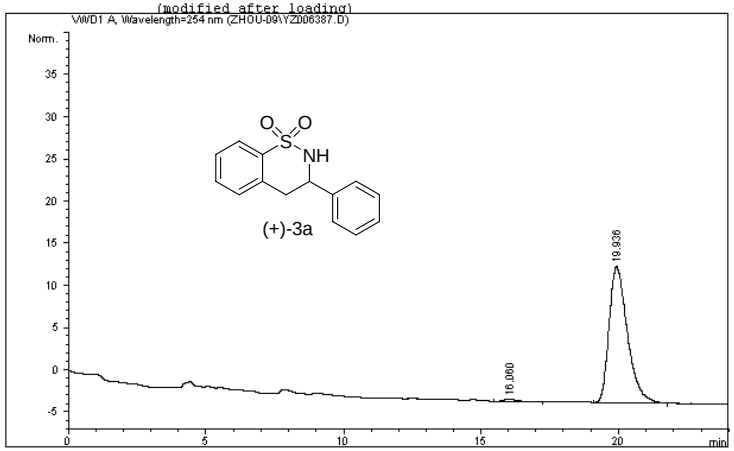
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:20:25 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006387.D Sample Name: CY-8-13

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 6/2/2009 11:03:57 AM
Sample Name     : CY-8-13                        Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/2/2009 10:52:53 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:18:57 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  16.060 PB    0.3775    7.06317 2.23437e-1   0.9309
   2  19.936 PP    0.7129  751.70172   16.12078  99.0691

Totals :                  758.76489   16.34421

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:19:01 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006542.D Sample Name: CY-8-41A(+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/13/2009 4:27:06 PM
Sample Name     : CY-8-41A(+/-)                  Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/13/2009 4:25:13 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:41:40 AM
                  (modified after loading)
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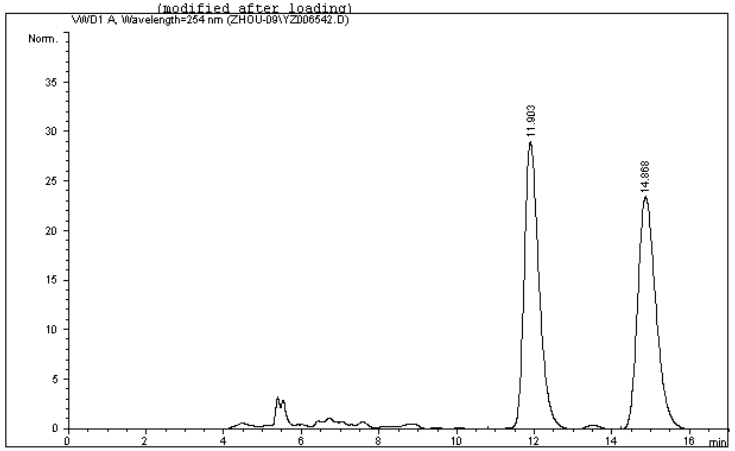


```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  11.903 BB    0.4079  787.06458   29.17456  50.2003
   2  14.868 BB    0.5078  780.78528   23.62893  49.7997

Totals :                  1567.84985   52.80349

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:41:45 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006543.D Sample Name: CY-8-38A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/13/2009 4:49:53 PM
Sample Name     : CY-8-38A                       Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/13/2009 4:45:01 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:46:24 AM
                  (modified after loading)
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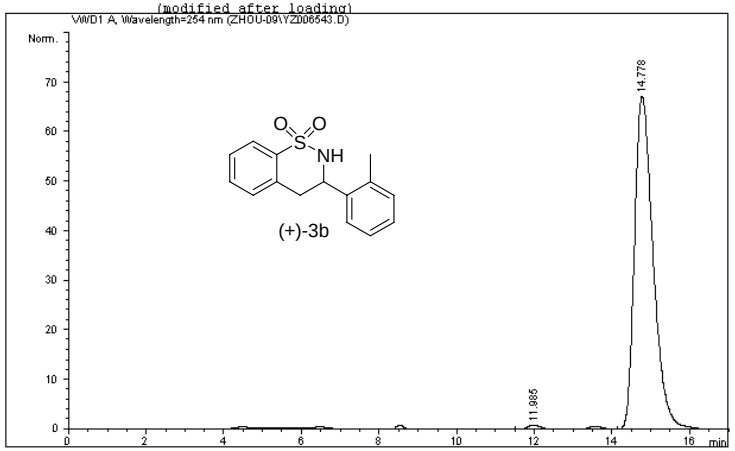


```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  11.985 BB    0.3724   21.83636 7.96275e-1   0.9651
   2  14.778 VB    0.5105 2240.75415   67.33521  99.0349

Totals :                  2262.59051   68.13148

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:47:39 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006529.D Sample Name: CY-8-60C

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 7/11/2009 11:33:30 AM
Sample Name     : CY-8-60C                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/11/2009 11:30:58 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:52:24 AM
                  (modified after loading)
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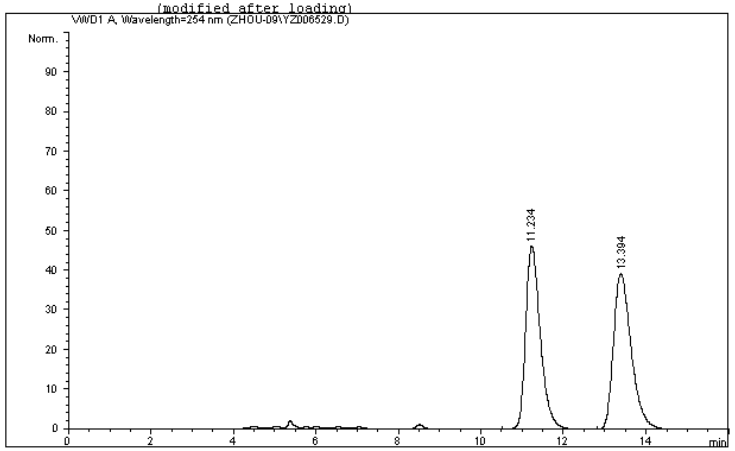


```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  11.234 BB    0.3806 1150.45117   46.23342  49.1333
   2  13.394 BB    0.4643 1191.03967   39.29092  50.8667

Totals :                  2341.49084   85.52434

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 10/19/2009 10:52:28 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006528.D Sample Name: CY-8-59A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 7/11/2009 11:14:59 AM
Sample Name     : CY-8-59A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/11/2009 11:13:58 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:53:53 AM
                  (modified after loading)
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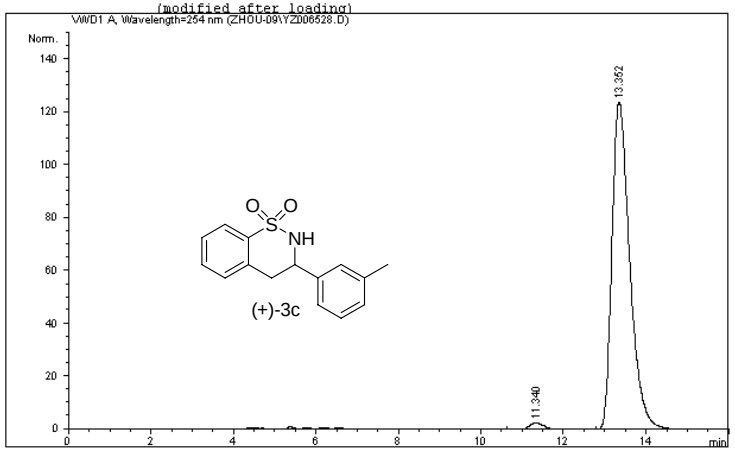



```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  11.340 BB    0.3963   67.84648    2.58672   1.7795
   2  13.352 PB    0.4603 3744.81104  123.91671  98.2205

Totals :                  3812.65752  126.50343

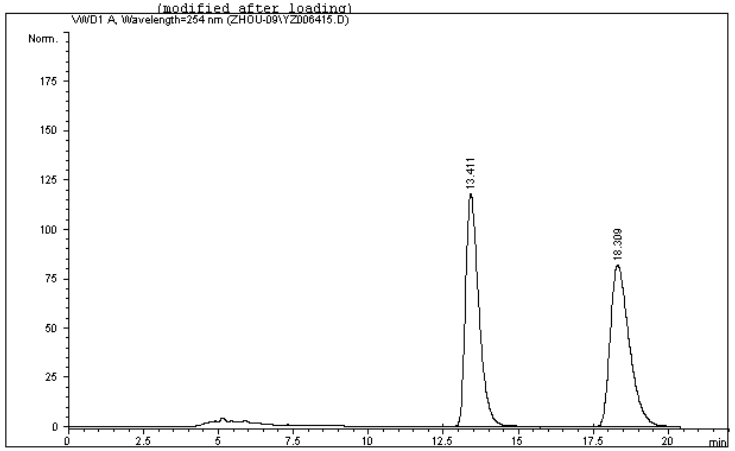
 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 10/19/2009 10:53:59 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006415.D Sample Name: CY-8-36B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 6/18/2009 9:56:23 AM
Sample Name     : CY-8-36B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/18/2009 9:54:53 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:13:32 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|---------|----------|--------|
   1  13.411 VB    0.4700 3658.53223  117.82305  50.0305
   2  18.309 BBA   0.6795 3654.07251   82.08787  49.9695

Totals :                  7312.60474  199.91092

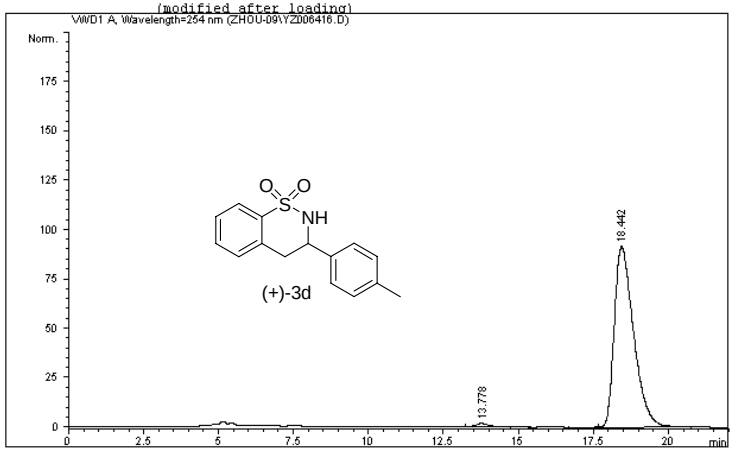
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:13:35 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006416.D Sample Name: CY-8-37A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 6/18/2009 10:18:28 AM
Sample Name     : CY-8-37A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/18/2009 10:16:59 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:14:50 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|---------|----------|--------|
   1  13.778 BB    0.4825   58.99335    1.82257   1.4172
   2  18.442 BB    0.6834 4103.72070   91.50468  98.5828

Totals :                  4162.71405   93.32725

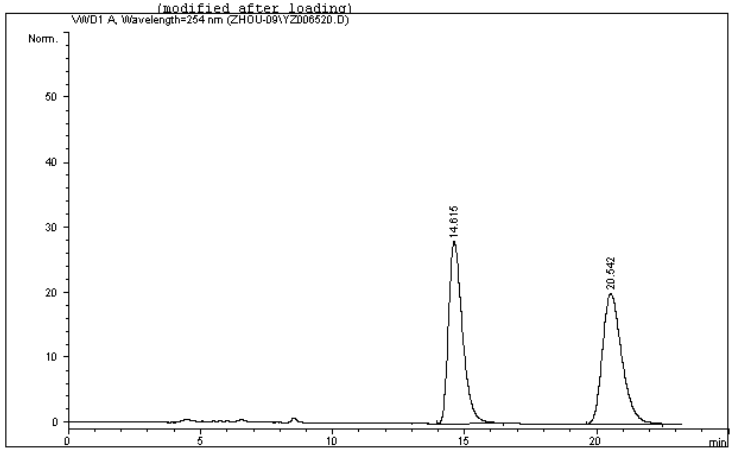
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:14:53 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006520.D Sample Name: CY-8-41B(+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 7/10/2009 3:02:55 PM
Sample Name     : CY-8-41B(+/-)                 Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/10/2009 3:00:20 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:59:40 AM
                  (modified after loading)
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  14.615 PB    0.5572 1022.07184   27.98180  49.9524
   2  20.542 BB    0.7763 1024.01990   20.05411  50.0476

Totals :                  2046.09174   48.03591

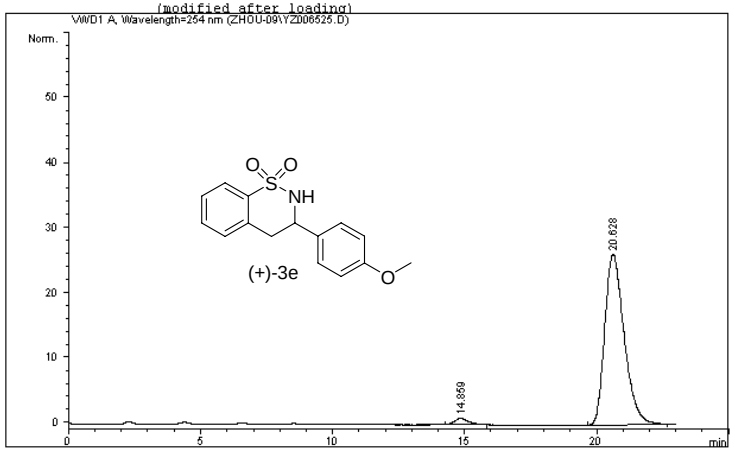
 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 10/19/2009 10:59:47 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006525.D Sample Name: CY-8-38B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 7/10/2009 4:51:37 PM
Sample Name     : CY-8-38B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/10/2009 4:45:28 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:59:48 AM
                  (modified after loading)
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  14.859 BB    0.4755   34.42447 9.23731e-1   2.4949
   2  20.628 BB    0.7852 1345.37183   26.20942  97.5051

Totals :                  1379.79630   27.13315

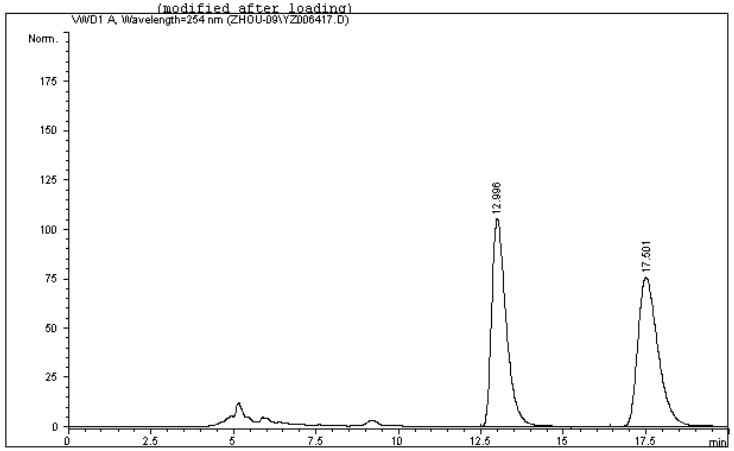
 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 10/19/2009 11:01:16 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006417.D Sample Name: CY-8-36C

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 6/18/2009 10:50:01 AM
Sample Name     : CY-8-36C                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/18/2009 10:48:28 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:10:58 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  12.996 PP    0.4617 3198.27148  105.41691  49.9076
   2  17.501 BB    0.6494 3210.11914   75.64262  50.0924

Totals :                  6408.39063  181.05953

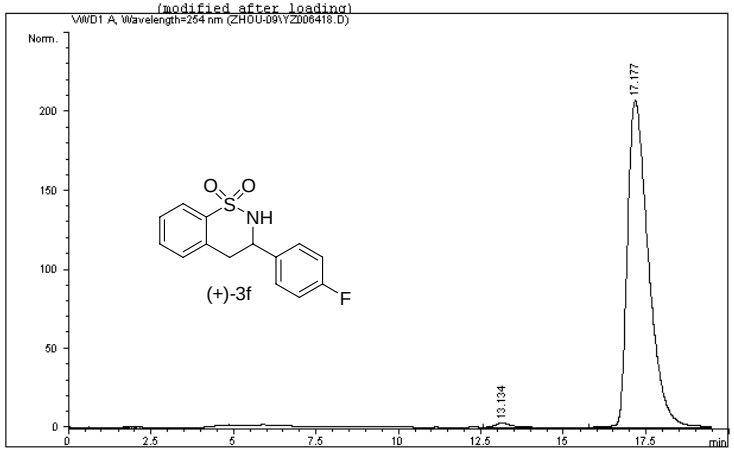
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:11:02 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006418.D Sample Name: CY-8-37B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 6/18/2009 11:12:28 AM
Sample Name     : CY-8-37B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/18/2009 11:10:57 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:12:14 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  13.134 VB    0.4631   83.23767    2.66705   0.9085
   2  17.177 BBA   0.6721 9078.99414  206.89391  99.0915

Totals :                  9162.23181  209.56096

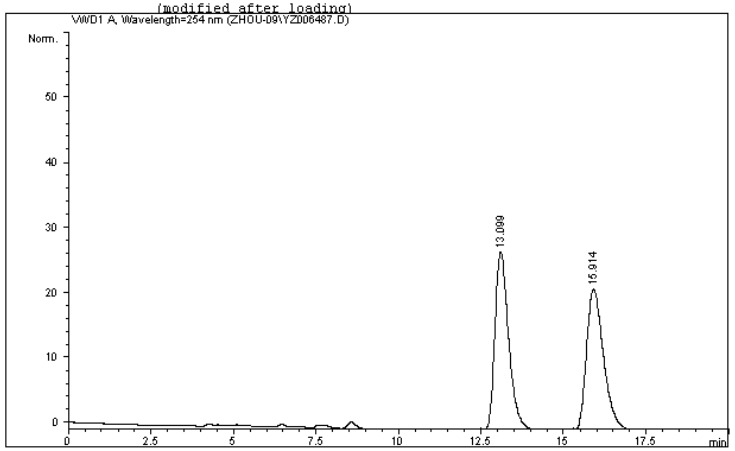
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:12:16 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006487.D Sample Name: CY-8-52A (+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
Injection Date  : 7/4/2009 10:52:44 AM
Sample Name     : CY-8-52A (+/-)                Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/4/2009 10:46:43 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:08:13 AM
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  13.099 VB    0.4416  793.50446   27.49201  50.2153
   2  15.914 VBA   0.5517  786.70056   21.81926  49.7847

Totals :                  1580.20502   49.31127

 Results obtained with enhanced integrator!

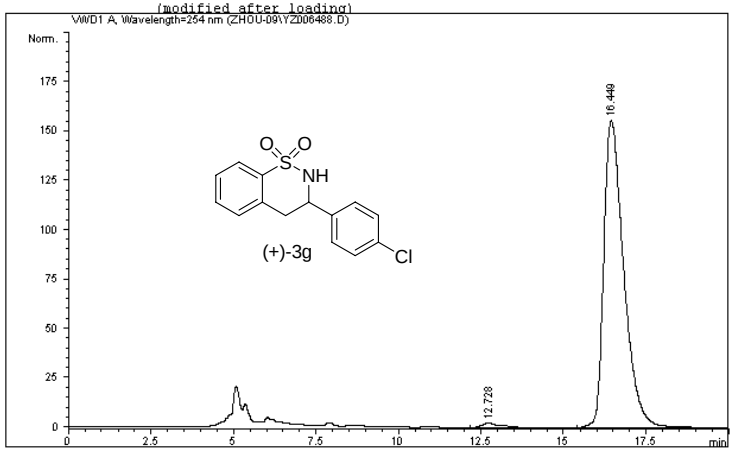
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:08:15 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006488.D Sample Name: CY-8-53A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
Injection Date  : 7/4/2009 11:15:12 AM
Sample Name     : CY-8-53A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/4/2009 11:10:25 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:09:34 AM
                  (modified after loading)
```




```
                        Area Percent Report

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  12.728 BB    0.5302   80.08139    2.09599   1.2097
   2  16.449 BB    0.6386 6539.97900  155.68066  98.7903

Totals :                  6620.06039  157.77665

 Results obtained with enhanced integrator!

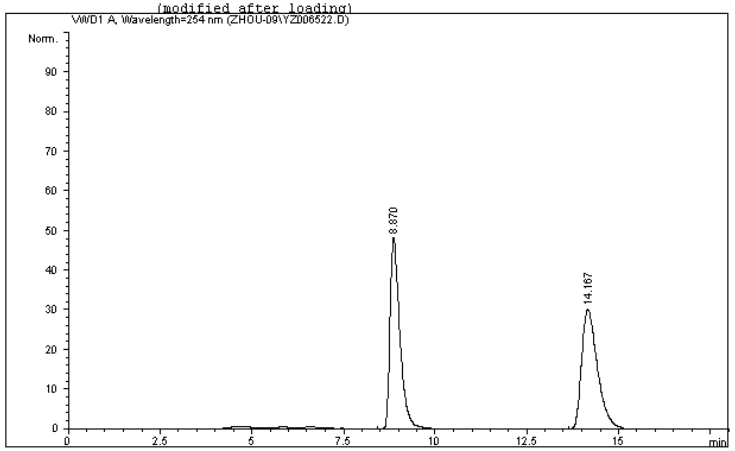
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:09:38 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006522.D Sample Name: CY-8-55A(+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/10/2009 3:58:28 PM
Sample Name     : CY-8-55A(+/-)                  Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/10/2009 3:54:14 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:56:13 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|---------|----------|--------|
   1   8.870 PB    0.2866  906.81799   48.16644  48.7649
   2  14.167 BP    0.4740  952.75482   30.59462  51.2351

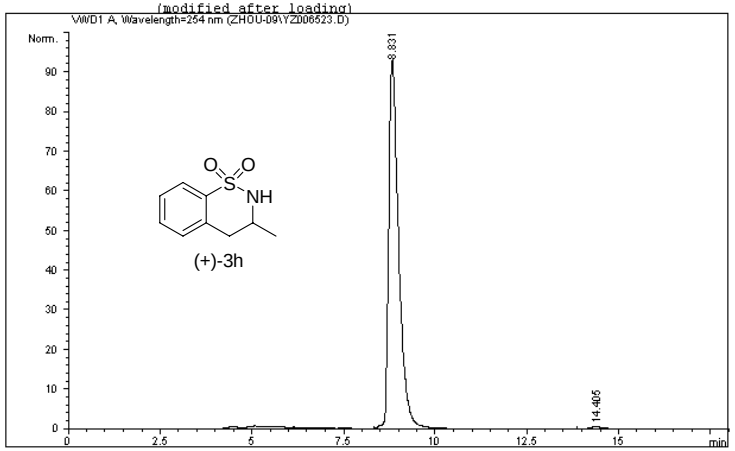
Totals :                  1859.57281   78.76106

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```


Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006523.D Sample Name: CY-8-57A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/10/2009 4:24:26 PM
Sample Name     : CY-8-57A                       Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/10/2009 4:18:40 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:56:17 AM
                  (modified after loading)
```



(+)-3h

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|---------|----------|--------|
   1   8.831 BB    0.2905 1780.38965   92.94349  99.0163
   2  14.405 PB    0.3906   17.68837 5.44513e-1   0.9837

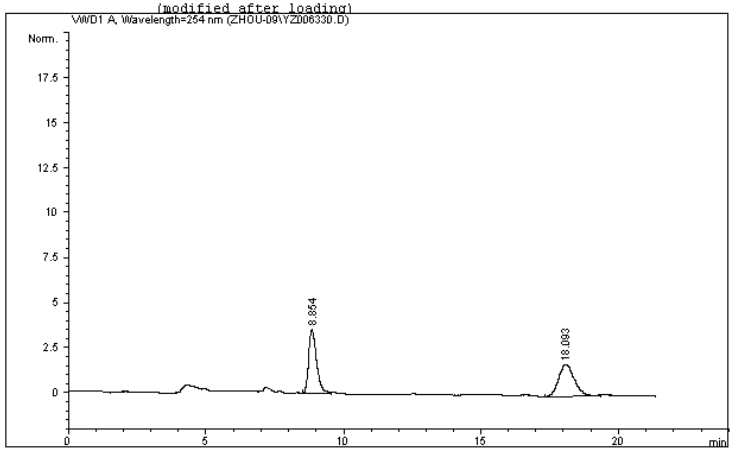
Totals :                  1798.07802   93.48800

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006330.D Sample Name: CY-7-87 (+/-)

OD-H, H/i-PrOH = 70/30, 0.8 mL/min

```
==================================================================
Injection Date  : 4/24/2009 2:38:06 PM
Sample Name     : CY-7-87 (+/-)                 Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 4/24/2009 2:36:02 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:24:20 AM
                  (modified after loading)
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1   8.854 BB    0.3028   69.04240    3.50286  49.7358
   2  18.093 PB    0.5171   69.77578    1.76304  50.2642

Totals :                   138.81818    5.26591

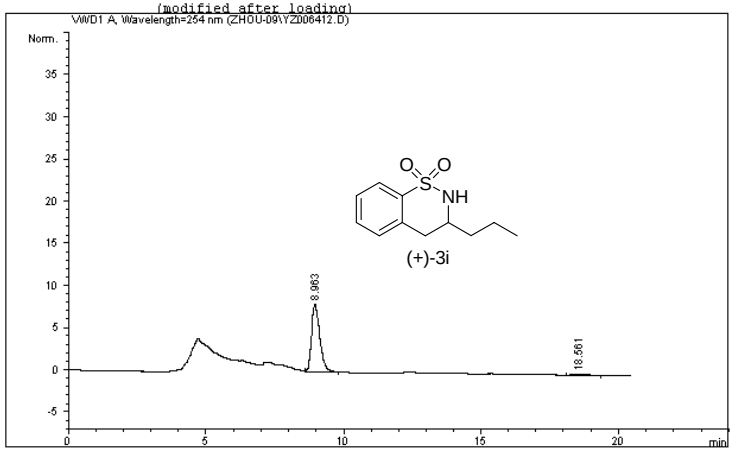
 Results obtained with enhanced integrator!
==================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:24:25 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006412.D Sample Name: CY-8-33A

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 6/18/2009 8:54:13 AM
Sample Name     : CY-8-33A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 6/18/2009 8:53:37 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:20:28 AM
                  (modified after loading)
```



(+)-3i

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1   8.963 VB    0.3261  167.51826    7.99169  97.7775
   2  18.561 PB    0.4332    3.80774 1.06119e-1   2.2225

Totals :                   171.32600    8.09781

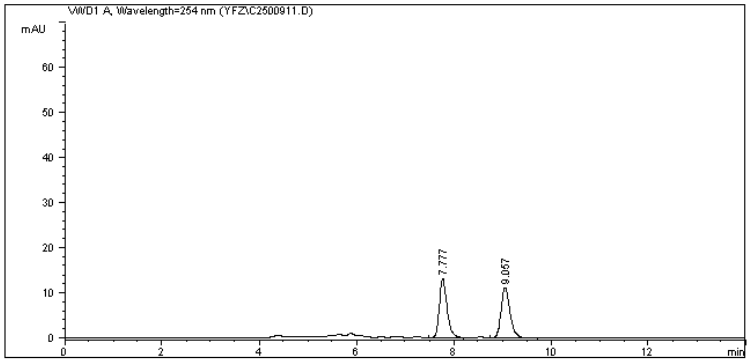
 Results obtained with enhanced integrator!
==================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:22:32 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500911.D Sample Name: CY-8-68A

AD-H, H/i-PrOH = 70/30, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 11/11/2010 2:10:04 PM
Sample Name     : CY-8-68A                    Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/11/2010 1:21:10 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/11/2010 3:11:55 PM by ZX
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.777	VV	0.1663	145.02368	13.17133	50.5582
2	9.057	VB	0.1935	141.82162	11.15575	49.4418
Totals :				286.84531	24.32707	

Results obtained with enhanced integrator!

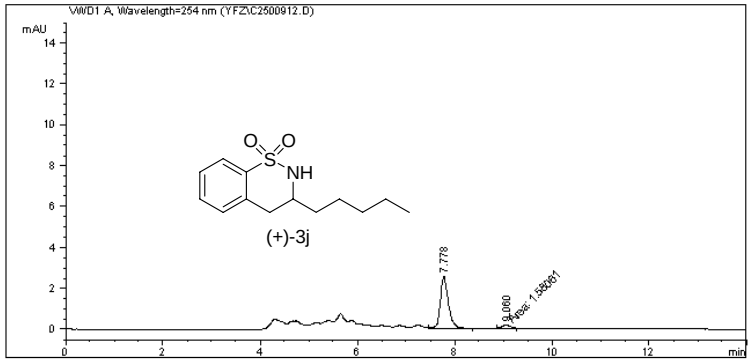
*** End of Report ***

Instrument 1 11/11/2010 3:11:59 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\YFZ\C2500912.D Sample Name: CY-8-65A

AD-H, H/i-PrOH = 70/30, 0.7 mL/min, 30 oC, 254 nm

```
Injection Date  : 11/11/2010 2:47:29 PM
Sample Name     : CY-8-65A                    Location : Vial 1
Acq. Operator   : ZX
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/11/2010 2:45:34 PM by ZX
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/11/2010 3:09:15 PM by ZX
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
```

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	7.778	VB	0.1764	30.26665	2.54800	95.0369
2	9.060	MM	0.2035	1.58061	1.29459e-1	4.9631
Totals :				31.84725	2.67746	

Results obtained with enhanced integrator!

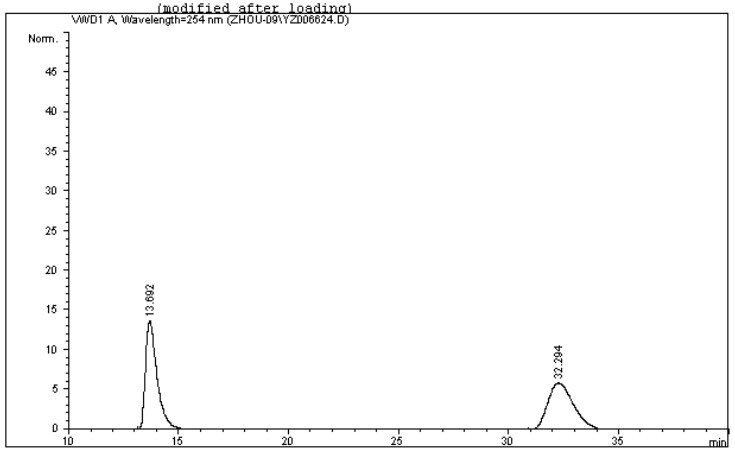
*** End of Report ***

Instrument 1 11/11/2010 3:09:20 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006624.D Sample Name: CY-8-68A(+/-)

OD-H, H/i-PrOH =70/30, 0.7mL/min

```
==================================================================
Injection Date  : 7/27/2009 1:48:28 PM
Sample Name     : CY-8-68A(+/-)                 Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/27/2009 1:42:26 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:25:34 AM
                  (modified after loading)
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.692 PB    0.5350  492.24985   13.62858  49.9011
   2  32.294 PB    1.0024  494.20071    5.97760  50.0989

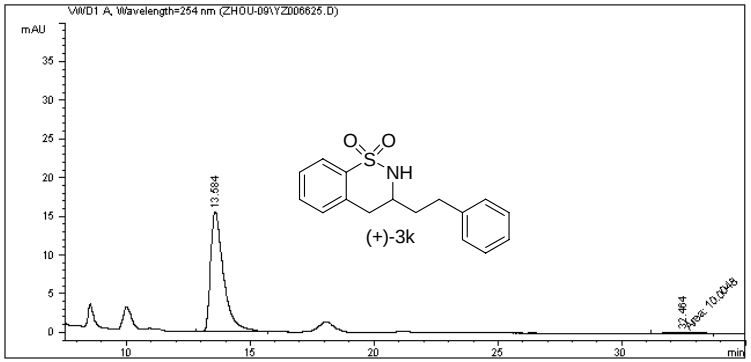
Totals :                  986.45056   19.60618

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```


Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006625.D Sample Name: CY-8-65B

OD-H, H/i-PrOH =70/30, 0.7mL/min

```
==================================================================
Injection Date  : 7/27/2009 2:41:15 PM
Sample Name     : CY-8-65B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/27/2009 2:34:26 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/22/2010 3:59:28 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  13.584 VB    0.5491  566.07373   15.47369  98.2633
   2  32.464 MM    1.1006   10.00484 1.51508e-1   1.7367

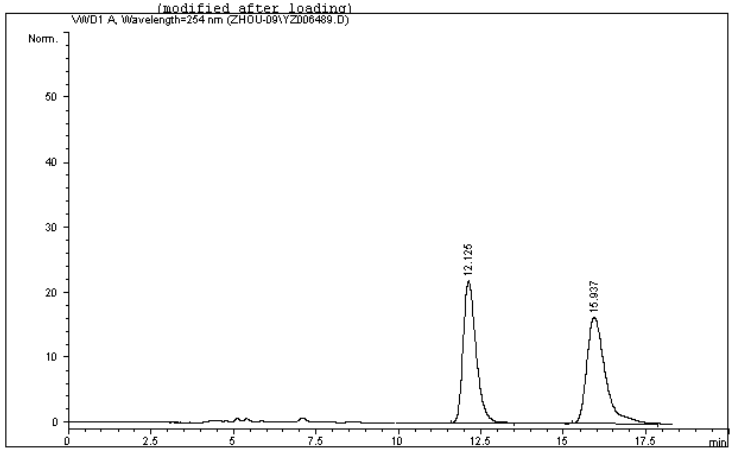
Totals :                  576.07857   15.62520

 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006489.D Sample Name: CY-8-52B (+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/4/2009 11:52:32 AM
Sample Name     : CY-8-52B (+/-)                Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/4/2009 11:48:08 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:02:44 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  12.125 BB    0.4197  595.33978   21.85488  48.4934
   2  15.937 BB    0.5864  632.33093   16.41004  51.5066

Totals :                  1227.67072   38.26493

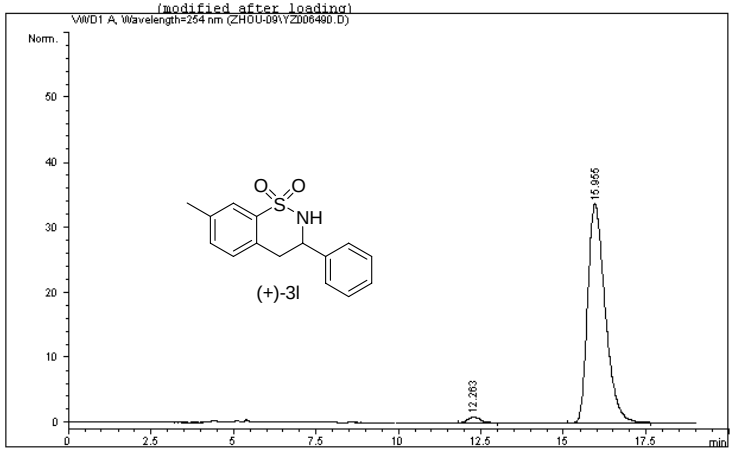
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:02:48 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006490.D Sample Name: CY-8-53B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/4/2009 12:15:49 PM
Sample Name     : CY-8-53B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/4/2009 12:10:36 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 11:02:48 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  12.263 BB    0.3796   25.24533 9.33519e-1   1.9931
   2  15.955 BB    0.5610 1241.42114   33.68610  98.0069

Totals :                  1266.66647   34.61962

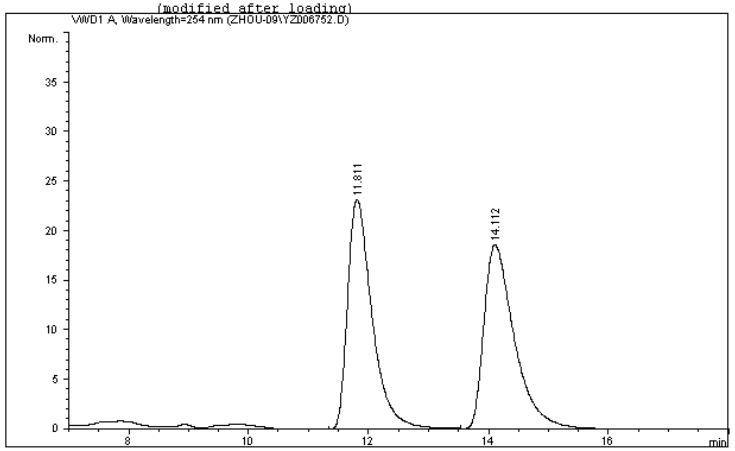
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 11:04:29 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006752.D Sample Name: CY-8-79(+/-)

OD-H, H/i-PrOH =85/15, 0.8 mL/min

```
==================================================================
Injection Date  : 8/29/2009 12:36:46 PM
Sample Name     : CY-8-79(+/-)                  Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 8/29/2009 11:59:10 AM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:04:29 AM
                  (modified after loading)
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.811 PB    0.4310  661.22162   23.23702  50.4067
   2  14.112 BB    0.5341  650.55273   18.56136  49.5933

Totals :                  1311.77435   41.79837

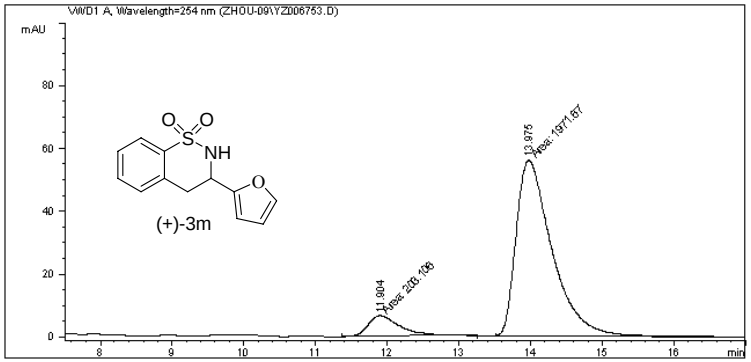
 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 10/19/2009 10:04:36 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006753.D Sample Name: CY-8-78

OD-H, H/i-PrOH =70/30, 0.7 mL/min

```
==================================================================
Injection Date  : 8/29/2009 1:04:10 PM
Sample Name     : CY-8-78                       Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 8/29/2009 12:58:43 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/22/2010 4:02:59 PM by ZX
                  (modified after loading)
==================================================================
```




```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  11.904 MM    0.5196  203.10611    6.51495   9.3392
   2  13.975 MM    0.5869 1971.67285   55.98711  90.6608

Totals :                  2174.77896   62.50207

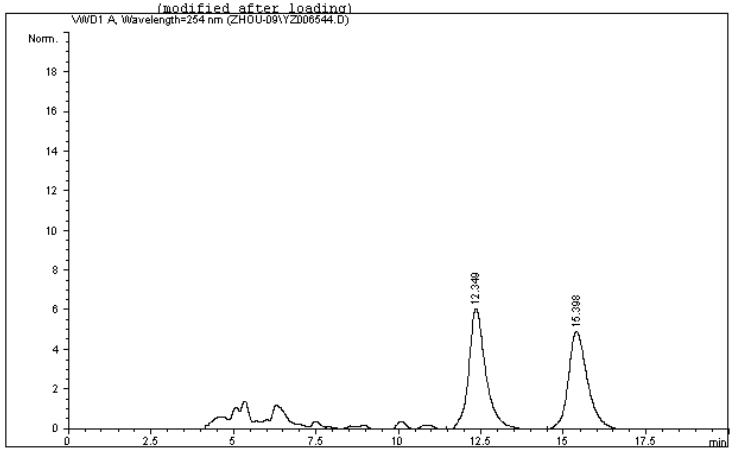
 Results obtained with enhanced integrator!
==================================================================
                      *** End of Report ***
```

Instrument 1 7/22/2010 4:03:48 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006544.D Sample Name: CY-8-60A(+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/13/2009 5:12:48 PM
Sample Name     : CY-8-60A(+/-)                 Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/13/2009 5:07:54 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:33:23 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  12.349 VB    0.5295  221.04391    6.11454  51.9139
   2  15.398 BB    0.6169  204.74542    4.97619  48.0861

Totals :                   425.78934   11.09073

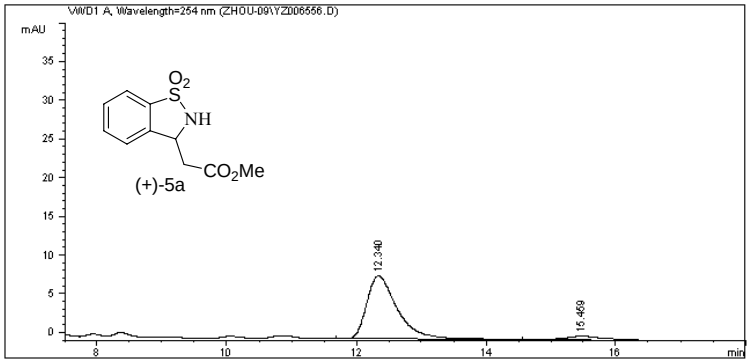
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:33:31 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006556.D Sample Name: CY-8-58A

OD-H, H/i-PrOH =70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/16/2009 8:04:12 PM
Sample Name     : CY-8-58A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/16/2009 7:51:51 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/22/2010 3:56:13 PM by ZX
                  (modified after loading)
==========================================================================
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1  12.340 VB    0.4878  267.50034    8.14986  92.9138
   2  15.459 BV    0.5129   20.40129 4.76220e-1   7.0862

Totals :                   287.90163    8.62608

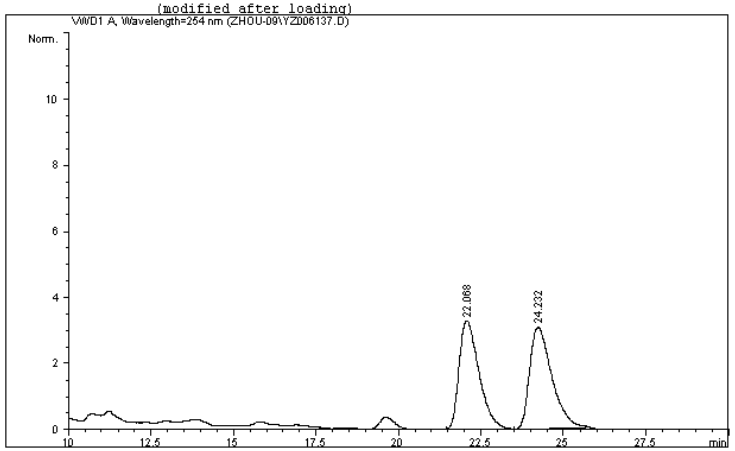
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 7/22/2010 3:56:18 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006137.D Sample Name: CY-7-47A (+/-)

OJ-H, H/i-PrOH = 70/30, 0.8 mL/min

```
Injection Date  : 12/31/2008 4:15:20 PM
Sample Name     : CY-7-47A (+/-)                Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 12/31/2008 4:13:53 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 11/5/2009 7:02:04 PM
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  22.068 PB    0.6046  135.62302    3.28041  48.9226
   2  24.232 PB    0.6542  141.59677    3.05561  51.0774

Totals :                  277.21979    6.33602

 Results obtained with enhanced integrator!
```

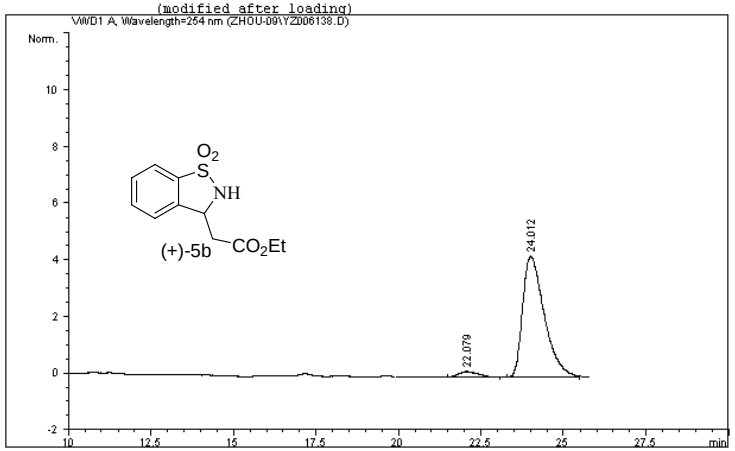
*** End of Report ***

Instrument 1 11/5/2009 7:02:08 PM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006138.D Sample Name: CY-7-47A

OJ-H, H/i-PrOH = 70/30, 0.8 mL/min

```
Injection Date  : 12/31/2008 4:43:18 PM
Sample Name     : CY-7-47A                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 12/31/2008 4:41:11 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 11/5/2009 7:04:04 PM
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]        [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  22.079 BB    0.5207    8.45855 1.98402e-1   4.1944
   2  24.012 PB    0.6579  193.20268    4.25496  95.8056

Totals :                  201.66123    4.45337

 Results obtained with enhanced integrator!
```

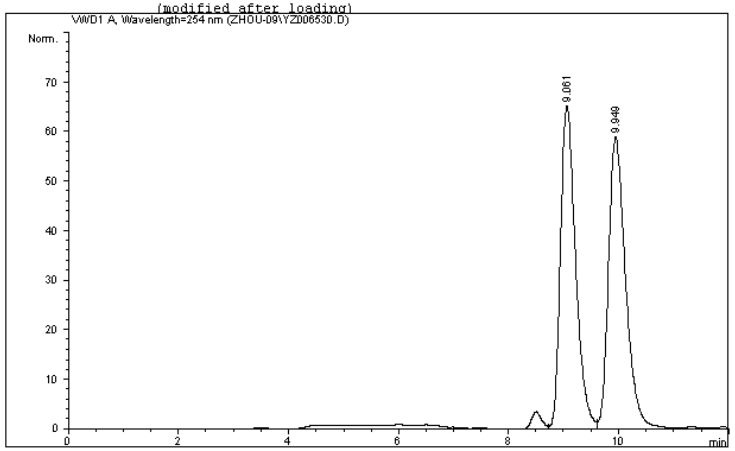
*** End of Report ***

Instrument 1 11/5/2009 7:04:08 PM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006530.D Sample Name: CY-8-60B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/11/2009 11:50:43 AM
Sample Name     : CY-8-60B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/11/2009 11:49:04 AM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:49:21 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.061 VV     0.2944 1253.74219   65.16142  49.4300
   2   9.949 VV     0.3327 1282.65881   58.90273  50.5700

Totals :                  2536.40100  124.06414

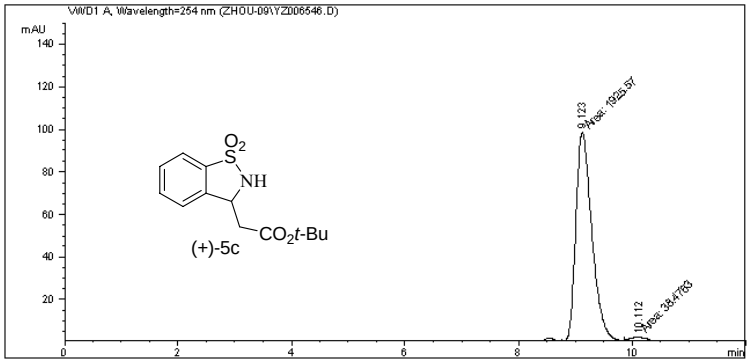
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:49:26 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006546.D Sample Name: CY-8-58B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
==========================================================================
Injection Date  : 7/13/2009 6:09:00 PM
Sample Name     : CY-8-58B                      Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 7/13/2009 6:04:43 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 7/23/2010 3:01:40 PM by ZX
                  (modified after loading)
==========================================================================
```



(+)-5c

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]  mAU   *s   [mAU   ]      %
----|-------|----|-------|----------|----------|--------|
   1   9.123 MM     0.3260 1925.57471   98.43872  98.0410
   2  10.112 MM     0.3251   38.47634    1.97232   1.9590

Totals :                  1964.05105  100.41104

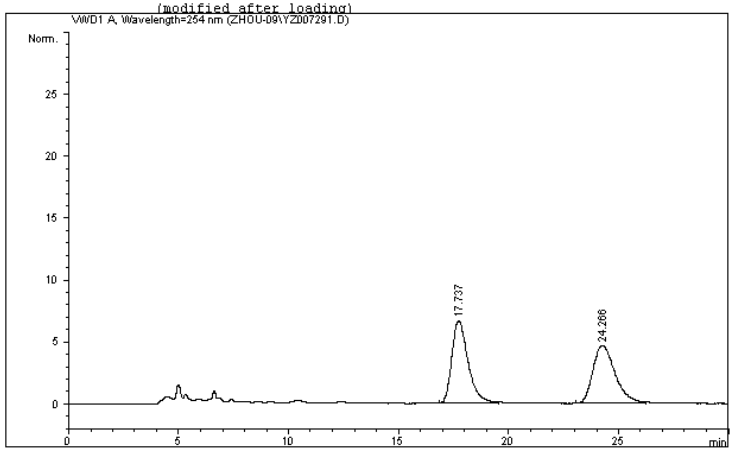
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 7/23/2010 3:02:02 PM ZX Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ007291.D Sample Name: CY-8-64B(+/-)

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
Injection Date  : 11/2/2009 8:35:46 PM
Sample Name     : CY-8-64B(+/-)                 Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/2/2009 7:41:34 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 11/5/2009 7:06:55 PM
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  17.737 BB    0.7721  336.12210    6.62894  51.1150
   2  24.266 BB    1.0424  321.45767    4.66674  48.8850

Totals :                  657.57977   11.29568

 Results obtained with enhanced integrator!
```

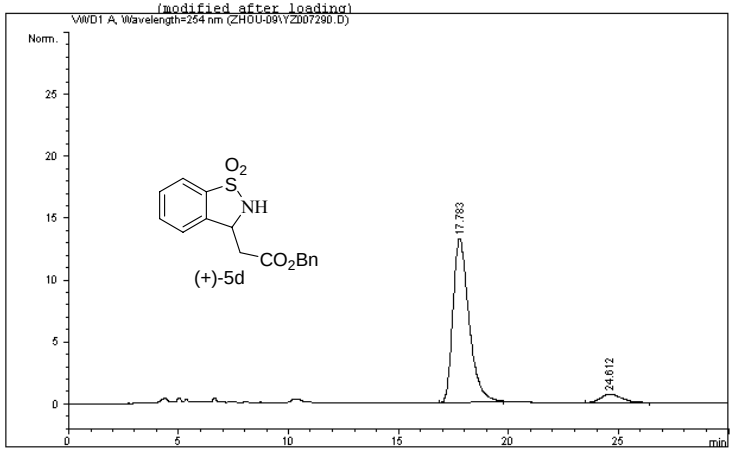
*** End of Report ***

Instrument 1 11/5/2009 7:07:56 PM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ007290.D Sample Name: CY-8-64B

OD-H, H/i-PrOH = 70/30, 0.7 mL/min

```
Injection Date  : 11/2/2009 7:55:20 PM
Sample Name     : CY-8-64B                      Location : Vial 1
Acq. Operator   :
Acq. Method     : C:\HPCHEM\1\METHODS\SW.M
Last changed    : 11/2/2009 7:41:34 PM
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 11/5/2009 7:06:51 PM
                  (modified after loading)
```



Area Percent Report

```
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min] mAU   *s   [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  17.783 PB    0.7782  669.59509   13.19926  93.2223
   2  24.612 PB    0.8280   48.68282 6.93286e-1   6.7777

Totals :                  718.27791   13.89255

 Results obtained with enhanced integrator!
```

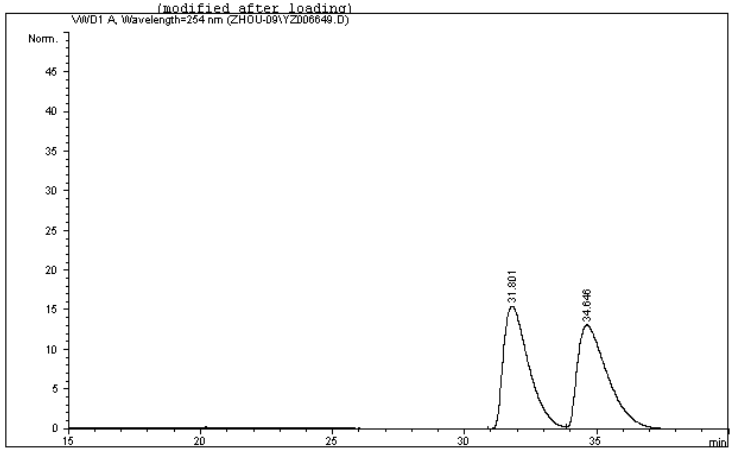
*** End of Report ***

Instrument 1 11/5/2009 7:06:55 PM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006649.D Sample Name: CY-8-63(+/-)

AS-H, H/i-PrOH =80/20, 0.8mL/min

```
==========================================================================
Injection Date  : 8/15/2009 3:56:17 PM
Sample Name     : CY-8-63(+/-)                  Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 8/15/2009 3:53:14 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:10:28 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  31.801 BV    0.9699 1022.71344   15.45791  49.8942
   2  34.646 VB    1.1093 1027.05078   13.06477  50.1058

Totals :                  2049.76422   28.52268

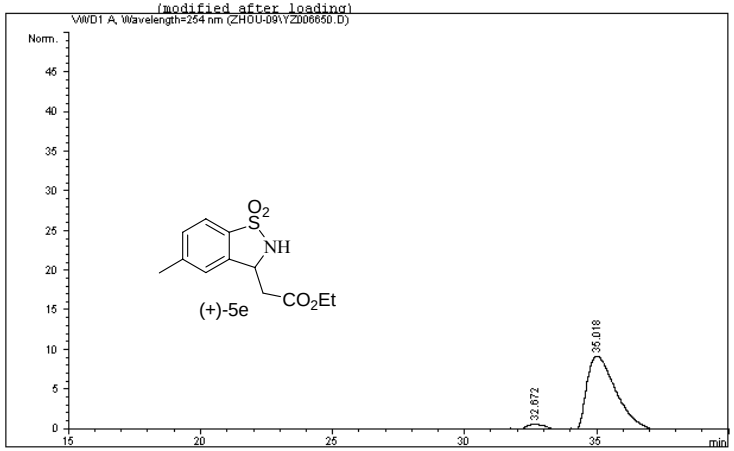
 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:10:40 AM Page 1 of 1

Data File C:\HPCHEM\1\DATA\ZHOU-09\YZ006650.D Sample Name: CY-8-72

OJ-H, H/i-PrOH =80/20, 0.8mL/min

```
==========================================================================
Injection Date  : 8/15/2009 4:40:12 PM
Sample Name     : CY-8-72                       Location : Vial 1
Acq. Operator   : WANG
Acq. Method     : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 8/15/2009 4:36:51 PM by WANG
                  (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\2012.M
Last changed    : 10/19/2009 10:12:16 AM
                  (modified after loading)
```




```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #  [min]       [min]  mAU   *s    [mAU   ]      %
---|-------|----|-------|----------|----------|--------|
   1  32.672 PV    0.6908   49.73135 8.65418e-1   6.3755
   2  35.018 VB    1.1101  730.30341    9.43135  93.6245

Totals :                  780.03476   10.29677

 Results obtained with enhanced integrator!
==========================================================================
                        *** End of Report ***
```

Instrument 1 10/19/2009 10:12:19 AM Page 1 of 1