BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis of new tetra- and pentacyclic, methylenedioxy- and ethylenedioxy-substituted derivatives of the dibenzo[*c*,*f*][1,2]thiazepine ring system

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Beilstein J. Org. Chem. **2025,** *21,* 2645–2656. doi:10.3762/bjoc.21.205

Experimental procedures and characterization of compounds 6, 10–19, 20a–e, 21c–p, 23a–e, 24, 26–28, 30–37, 38a–d, 39–44, 45a–c, 46–53, 54a–f. ^{1}H and ^{13}C NMR spectra of all new compounds. 2D NMR spectra of compounds 6–8, 12, 21a, 21b, 25–27, 30, 32, 38b, 42, 50, 51, 54e

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Methyl 2-(1,3-benzodioxol-5-ylsulfamoyl)-4-chlorobenzoate (10). To a vigorously stirred solution of 1,3-benzodioxol-5-amine (14.40 g, 105 mmol) and *N*,*N*-diethylaniline (15.67 g, 105 mmol, 16.7 mL) in MeOH (150 mL), methyl 4-chloro-2-chlorosulfonylbenzoate (**9**, 26.91 g, 100 mmol) was added over a period of 5 min while cooling the reaction mixture with tap water. It was stirred at room temperature for 1 h and at 0–5 °C for 1 h. The crystalline product separated was filtered and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, DCM). After evaporation of the solvents, the solid residue was triturated with MeOH, filtered and air-dried to afford **10** (35.10 g, 95%) as colorless crystals. M. p. 166.5–168.5 °C (CH_3CN). IR (KBr): 3227, 1713, 1292, 1171, 1031, 690 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 10.05 (br s, 1H), 7.86 (d, ^4J = 2.1 Hz, 1H), 7.79 (dd, ^4J = 2.1 Hz, ^3J = 8.3 Hz, 1H), 7.68 (d, ^3J = 8.3 Hz, 1H), 6.82 (d, ^3J = 8.3 Hz, 1H), 6.68 (d, ^4J = 2.2 Hz, 1H), 6.53 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 5.99 (s, 2H), 3.83 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6): 166.72, 147.71, 145.10, 138.78, 135.52, 133.08, 131.35, 131.04, 130.51, 128.25, 115.57, 108.50, 104.13, 101.63, 53.31. MS (EI): M^+=369 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{13}ClNO_6S$ $[M+H]^+$: 370.0146, found: 370.0151.

Methyl 4-chloro-2-(2,3-dihydro-1,4-benzodioxin-6-ylsulfamoyl)benzoate (11). To a vigorously stirred solution of 2,3-dihydro-1,4-benzodioxin-6-amine (29.03 g, 192 mmol) and *N*,*N*-diethylaniline (28.65 g, 192 mmol, 30.6 mL) in MeOH (300 mL), methyl 4-chloro-2-chlorosulfonylbenzoate (**9**, 50.05 g, 186 mmol) was added over a period of 10 min while cooling the reaction mixture with tap water. An exothermic reaction took place, and the product started to crystallize. The brown suspension was stirred at room temperature for 1 h, then at 0–5 °C for 1 h. The crystalline product was filtered and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM). After evaporation of the solvent, the solid residue was triturated with MeOH, filtered and air-dried to afford **11** (66.0 g, 92%) as colorless crystals. M. p. 153–154 °C (MeOH). IR (KBr): 3266, 1715, 1504, 1175 cm^{-1}. ^1H NMR (200 MHz, $CDCl_3$): 7.96 (br s, 1H), 7.83 (d, ^4J = 1.8 Hz, 1H), 7.80 (d, ^3J = 7.7 Hz, 1H), 7.54 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 6.70 (d, ^3J = 8.4 Hz, 1H), 6.70 (d, ^4J = 2.6 Hz, 1H), 6.59 (dd, ^4J = 2.6 Hz, ^3J = 8.8 Hz, 1H), 4.20 (s, 4H), 4.02 (s, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): 167.26, 143.60, 142.25, 140.17, 138.18, 132.42, 132.15, 130.64, 129.27, 128.45, 117.48, 116.99, 113.12, 64.21, 64.11, 53.63. MS (ESI): $[M-H]^-$ = 382 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{15}ClNO_6S$ $[M+H]^+$: 384.0303, found: 384.0309.

Methyl 2-[1,3-benzodioxol-5-yl(methyl)sulfamoyl]-4-chlorobenzoate (12). To a solution of compound **10** (31.08 g, 84 mmol) in DMF (75 mL), anhydrous K_2CO_3 (15.20 g, 110 mmol) was added. To the vigorously stirred suspension iodomethane (15.61 g, 110 mmol, 6.9 mL) was added dropwise and the reaction mixture was stirred at room temperature for 4 h. Water (450 mL) was added and a thick oil separated. The supernatant was decanted, the oil was dissolved in DCM (100 mL), the solution was washed with water (2 × 100 mL), the organic phase was dried over Na_2SO_4 and evaporated in vacuo. The residual dense orange oil was dissolved in a heptane/DCM mixture 2:1 (150 mL), silica gel (20 g, Kieselgel 60 H) was added, and it was stirred at room temperature for 30 min. The filtrate was evaporated in vacuo to afford **12** (31.4 g of dense yellow oil, yield 97%). The TLC pure intermediate was transformed in the next step without further purification. IR (film): 1739, 1484, 1354, 1292, 1253, 1162, 1120, 1057, 1037, 940, 836 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): 7.56 (dd, ^4J = 2.1 Hz, ^3J = 8.2 Hz, 1H), 7.46 (d, ^4J = 2.0 Hz, 1H), 7.44 (d, ^3J = 8.2 Hz, 1H), 6.73 (d, ^3J = 8.3 Hz, 1H), 6.72 (d, ^4J = 2.2 Hz, 1H), 6.60 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 6.00 (s, 2H), 3.89 (s, 3H), 3.26 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): 167.44, 147.94, 147.29, 136.96, 135.97, 134.40, 132.44, 131.66, 129.92, 129.51, 121.11, 109.04, 108.07, 101.74, 53.27, 39.43. COSY: 7.46–7.56–7.44, 6.73–6.60–6.72. HSQC (140 Hz): 7.56–132.44, 7.46–129.92, 7.44–129.51, 6.73–108.07, 6.72–109.04, 6.60–121.11, 6.00–101.72, 3.89–53.27, 3.26–39.43. HMBC (8 Hz, 140 Hz): 7.56–131.66, 7.46–(135.97, 132.44, 131.66), 7.44–(167.44, 136.96, 135.97), 6.73–(147.94, 134.40), 6.72–(147.29, 121.11), 6.60–(147.29, 109.04), 6.00–(147.94, 147.29), 3.89–167.44, 3.26–134.40. HRMS (ESI): m/z calcd. for $C_{16}H_{15}ClNO_6S$ $[M+H]^+$: 384.0304, found: 384.0307.

Methyl 4-chloro-2-[2,3-dihydro-1,4-benzodioxin-6-yl(methyl)sulfamoyl]benzoate (13). To a solution of compound **11** (46.06 g, 120 mmol) in DMF (100 mL), anhydrous K_2CO_3 (21.56 g, 156 mmol) was added, and the suspension was stirred at room temperature for 15 min. To the vigorously stirred suspension iodomethane (22.14 g, 156 mmol, 9.7 mL) was added dropwise while cooling the reaction mixture with tap water. The reaction mixture was stirred at room temperature for 1 h. Water (700 mL) was added and the suspension obtained was stirred at room temperature for 2 h. The product separated was filtered, washed with water (2 × 100 mL), and air-dried to give **13** (47.05 g, 98%) as colorless crystals, suitable to transform in the next step without further purification. A small sample was subjected to dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 2:1, 1:1, DCM). After evaporation of solvents, the oily residue was triturated with cold DIPE to afford pure **13** as colorless crystals. M. p. 97–99 °C (MeOH). IR (KBr): 1733, 1498, 1345, 1294, 1059 cm^{-1}. ^1H NMR (200 MHz, $CDCl_3$): 7.54 (dd, ^4J = 1.8 Hz, ^3J = 8.1 Hz, 1H), 7.43 (d, ^3J = 8.1 Hz,

1H), 7.43 (d, ^4J = 2.2 Hz, 1H), 6.80 (d, ^3J = 8.8 Hz, 1H), 6.72 (d, ^4J = 2.6 Hz, 1H), 6.65 (dd, ^4J = 2.6 Hz, ^3J = 8.8 Hz, 1H), 4.25 (s, 4H), 3.87 (s, 3H), 3.24 (s, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): 167.39, 143.48, 143.33, 136.98, 135.85, 133.80, 132.32, 131.64, 129.83, 129.45, 120.53, 117.31, 116.71, 64.26, 64.16, 53.16, 39.13. MS (GC-EI): M^+ = 397 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{17}ClNO_6S$ $[M+H]^+$: 398.0459, found: 398.0467.

2-[1,3-Benzodioxol-5-yl(methyl)sulfamoyl]-4-chlorobenzoic acid (14). A solution of NaOH (8.00 g, 200 mmol) in water (150 mL) was added to the solution of compound **12** (30.70 g, 80 mmol) in MeOH (150 mL) and it was refluxed for 1 h. Water (750 mL) was added, the solution was cooled with ice-water, and an aqueous HCl solution (5%, 150 mL, 205 mmol HCl) was added in 20 min (pH 1). The colorless suspension obtained was stirred for 30 min while cooling with ice-water, it was filtered, washed with water, and dried over P_2O_5 to afford **14** (28.6 g, 97%) as off-white crystals. M. p. 153–155 °C (CH_3CN, colorless crystals). IR (KBr): 2700, 1706, 1337, 844 cm^{-1}. ^{1}H NMR (500 MHz, DMSO-d_6): 13.7 (br s, 1H), 7.81 (dd, ^4J = 2.0 Hz, ^3J = 8.2 Hz, 1H), 7.66 (d, ^3J = 8.2 Hz, 1H), 7.32 (d, ^4J = 1.8 Hz, 1H), 6.88 (d, ^3J = 8.2 Hz, 1H), 6.82 (d, ^4J = 1.9 Hz, 1H), 6.64 (dd, ^4J = 2.2 Hz, ^3J = 8.2 Hz, 1H), 6.06 (s, 2H), 3.19 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6): 168.03, 147.63, 146.92, 135.70, 134.34, 134.08, 133.88, 133.26, 130.22, 128.85, 121.00, 108.70, 108.20, 101.93, 39.14. MS (EI): M^+ = 369 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{13}ClNO_6S$ $[M+H]^+$: 370.0146, found: 370.0146.

4-Chloro-2-[2,3-dihydro-1,4-benzodioxin-6-yl(methyl)sulfamoyl]benzoic acid (15). A solution of NaOH (11.80 g, 295 mmol) in water (200 mL) was added to the suspension of compound **13** (46.94 g, 118 mmol) in MeOH (200 mL) and the mixture was refluxed for 1 h. The solution obtained was diluted with water (750 mL), cooled with ice-water, and an aqueous HCl solution (5%, 225 mL, 308 mmol HCl) was added in 20 min (pH 1). The partly oily product separated was stirred at room temperature for 3 h. The suspension obtained was filtered, washed thoroughly with water (3 × 100 mL), and dried over P_2O_5 to afford **15** (44.8 g, 99%) as off-white crystals. M. p. 156–158 °C (CH_3CN, colorless crystals). IR (KBr): 3251, 1740, 1504, 1337, 1232, 1065 cm^{-1}. ^{1}H NMR (200 MHz, DMSO-d_6): 13.68 (br s, 1H), 7.81 (dd, ^4J = 1.8 Hz, ^3J = 8.2 Hz, 1H), 7.67 (d, ^3J = 8.2 Hz, 1H), 7.29 (d, ^4J = 1.8 Hz, 1H), 6.85 (d, ^3J = 8.5 Hz, 1H), 6.73 (d, ^4J = 2.1 Hz, 1H), 6.65 (dd, ^4J = 2.4 Hz, ^3J = 8.6 Hz, 1H), 4.24 (s, 4H), 3.19 (s, 3H). ^{13}C NMR (50 MHz, DMSO-d_6): 168.05, 143.40, 143.23, 135.82, 134.16, 133.69, 133.63, 133.24, 130.22, 128.83, 120.15, 117.31, 116.39, 64.23, 38.97. MS (EI): M^+ = 383 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{15}ClNO_6S$ $[M+H]^+$: 384.0303, found: 384.0310.

8-Chloro-5-methyl[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11(5*H*)-one 6,6-dioxide (6). To the suspension of **14** (24.04 g, 65 mmol) in DCM (200 mL), PCl_5 (16.24 g, 78 mmol) was added in portions, and the solution obtained was refluxed for 8.5 h. It was cooled to 0–5 °C, and $SnCl_4$ (37.25 g, 143 mmol, 16.7 mL) was added dropwise over a period of 10 min. The thick suspension obtained was stirred at 0–5 °C for 2 h, then it was allowed to warm to room temperature. The orange suspension was poured onto a mixture of crushed ice (600 g) and conc hydrochloric acid (50 mL) and DCM (100 mL). The mixture was stirred until warming to room temperature (1 h), the product separated was filtered, washed with diluted hydrochloric acid (5%, 2 × 50 mL) and water (2 × 50 mL), and air-dried to give crude **6** (17.17 g of yellow solid). The two-phase filtrate was separated, the strongly acidic aqueous phase was washed with DCM (2 × 50 mL), the combined organic phases were washed with water (100 mL), dried over Na_2SO_4, evaporated, and the oily residue was triturated with ether (50 mL) to afford a second crop of **6** (1.94 g of brown solid). The two crops were purified by dry-column flash chromatography on a short silica gel column (thickness of the stationary phase: 30 mm, eluent: DCM). After evaporation of the solvent, the residue was triturated with Et_2O (50 mL) to give **6** (17.34 g, 76%) as pale yellow crystals. M. p. 268–271 °C (CH_3CN, decomp.). IR (KBr): 1639, 1623, 1482, 1353, 1245, 1033 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): 8.01 (d, ^3J = 8.4 Hz, 1H), 7.95 (d, ^4J = 2.2 Hz, 1H), 7.74 (s, 1H), 7.67 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 6.79 (s, 1H), 6.11 (s, 2H), 3.24 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): 186.97, 153.31, 147.00, 138.76, 137.99, 137.95, 133.99, 133.81, 133.18, 126.34, 125.87, 109.94, 105.60, 102.88, 39.38. COSY: 8.01–7.67–7.95. HSQC (140 Hz): 8.01–133.99, 7.95–125.878, 7.74–109.94, 7.67–133.18, 6.79–105.60, 6.11–102.88, 3.24–39.38. HMBC (8 Hz, 140 Hz): 8.01–(186.97, 138.76, 137.99), 7.95–(133.81, 133.18), 7.74–(186.97, 153.31, 137.95), 7.67–(133.81, 125.87), 6.79–(153.31, 147.00, 137.95, 126.34), 6.11–(153.31, 147.00), 3.24–137.95. MS (EI): M^+ = 351 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{11}ClNO_5S$ $[M+H]^+$: 352.0041, found: 352.0043.

8-Chloro-5-methyl-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11-ol 6,6-dioxide (16). To a suspension of **6** (7.04 g, 20 mmol) in DMF (100 mL) and EtOH (100 mL), $NaBH_4$ (1.51 g, 40 mmol) was added, and the reaction mixture was stirred at room temperature for 4.5 h. Water (800 mL) was added dropwise in 30 min. The separated product was filtered, washed with water, and dried in vacuo over P_2O_5 to give **16** (6.72 g, 95%) as colorless crystals. M. p. decomp. from 200 °C (CH_3CN). IR (KBr): 3452, 1503, 1481, 1308, 1141, 1036 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.86 (dd, ^4J = 0.6 Hz, ^3J = 8.7 Hz, 1H), 7.76 (d, ^4J = 2.2 Hz, 1H), 7.70 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 7.18 (s, 1H), 7.04 (s, 1H), 6.60 (d, ^3J = 5.0 Hz, 1H), 6.16 (d, ^3J = 4.9 Hz, 1H), 6.09 (d, ^4J = 1.0 Hz, 1H), 6.04 (d, ^4J = 1.0 Hz, 1H), 3.37 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6): 147.58, 147.33, 140.39, 139.82, 138.34, 132.83, 132.12, 129.01, 128.07, 126.66, 108.70, 105.10, 102.15, 67.51, 37.20. MS (EI): M^+ = 353 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{12}ClNNaO_5S$ $[M+Na]^+$: 376.0017, found: 376.0022.

9-Chloro-6-methyl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-ol 7,7-dioxide (17). To a suspension of **7** (15.00 g, 41 mmol) in DMF (100 mL) and EtOH (100 mL), $NaBH_4$ (3.10 g, 82 mmol) was added, and the reaction mixture was stirred at room temperature for 23 h. Water (800 mL) was added dropwise in 30 min. The product separated was filtered, washed with water, and dried in vacuo over P_2O_5 to give **17** (14.75 g, 98%) as colorless crystals. M. p. decomp. from 180 °C (CH_3CN). IR (KBr): 3531, 1500, 1303, 1134, 1064 cm^{-1}. ^{1}H NMR (200 MHz, DMSO-d_6): 7.85 (d, ^3J = 8.4 Hz, 1H), 7.75 (d, ^4J = 1.8 Hz, 1H), 7.70 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 7.05 (s, 1H), 7.02 (d, ^4J = 0.7 Hz, 1H), 6.53 (d, ^3J = 3.3 Hz, 1H), 6.10 (bd, ^4J = 2.6 Hz, 1H), 4.24 (s, 4H), 3.33 (s, 3H). ^{13}C NMR (50 MHz, DMSO-d_6): 143.53, 143.23, 140.34, 139.44, 136.21, 132.76, 132.23, 128.95, 128.65, 126.67, 117.01, 114.25, 67.95, 64.33, 64.24, 37.88. MS (EI): M^+ = 367 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{14}ClNNaO_5S$ $[M+Na]^+$: 390.0173, found: 390.0176.

8,11-Dichloro-5-methyl-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepine 6,6-dioxide (18). To a vigorously stirred suspension of **16** (6.19 g, 17.5 mmol) in DCM (40 mL), $SOCl_2$ (1.52 mL, 2.50 g, 21 mmol) was added dropwise at room temperature. The solution obtained was stirred at room temperature for 1.5 h, then evaporated in vacuo. The residue was triturated with DIPE (20 mL), filtered and dried in vacuo to give crude **18** (6.51 g, 100%) as colorless crystals. M. p. decomp. from 164 °C. The product is of suitable quality for use in the next step. IR (KBr): 1503, 1490, 1340, 1229, 1031 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.96 (d, ^4J = 2.1 Hz, 1H), 7.48 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.42 (d, ^3J = 8.3 Hz, 1H), 6.94 (s, 1H), 6.82 (s, 1H), 6.06 (d, ^4J = 1.4 Hz, 1H), 6.02 (d, ^4J = 1.3 Hz, 1H), 5.98 (s, 1H), 3.52 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 149.78, 147.65, 141.50, 136.17, 133.54, 133.11, 132.49, 132.33, 131.19, 127.89, 109.51, 108.97, 102.53, 63.30, 38.98. MS (EI): M^+ = 371 (2 Cl). HRMS (TOF MS EI): m/z calcd. for $[C_{15}H_{11}Cl_2NO_4S]^+$: 370.9786, found: 370.9796.

9,12-Dichloro-6-methyl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (19). To a vigorously stirred suspension of **17** (14.71 g, 40 mmol) in DCM (80 mL), $SOCl_2$ (3.5 mL, 5.71 g, 48 mmol) was added dropwise at room temperature. The solution obtained was stirred at room temperature for 3.5 h. Hexane (240 mL) was added to the suspension formed, the product was filtered, washed with hexane (2 × 30 mL) and dried in vacuo to give crude **19** (14.50 g, 94%) as colorless crystals. M. p. decomp. from 160 °C. The product is of suitable quality for use in the next step. IR (KBr): 1512, 1327, 1142,

1065 cm^{-1}. ^1H NMR (200 MHz, $CDCl_3$): 7.97 (d, ^4J = 1.8 Hz, 1H), 7.48 (dd, ^4J = 2.0 Hz, ^3J = 8.4 Hz, 1H), 7.43 (d, ^3J = 8.4 Hz, 1H), 7.02 (s, 1H), 6.90 (s, 1H), 5.99 (s, 1H), 4.26 (s, 4H), 3.52 (s, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): 145.42, 143.38, 141.71, 136.08, 133.52, 132.69, 132.32, 132.11, 130.27, 127.98, 118.30, 118.25, 64.32, 64.25, 63.39, 39.26. MS (EI): M^+ = 385 (2 Cl). HRMS (TOF MS EI): m/z calcd. for $[C_{16}H_{13}Cl_2NO_4S]^+$: 384.9942, found: 384.9945.

Ethyl 7-[(8-chloro-5-methyl-6,6-dioxido-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11-yl)amino]heptanoate (20a). To a solution of ethyl 7-aminoheptanoate (2.77 g, 16 mmol) in CH_3CN (15 mL) crude **18** (2.60 g, 7 mmol) was added, the solution obtained in 5 min was stirred at room temperature for 1 h. It was evaporated in vacuo, the residue was dissolved in DCM (40 mL), washed with water (2 × 20 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue (4.3 g) was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, DCM, DCM/MeOH 100:1, 100:2, 100:4). After evaporation of solvents in vacuo **20a** (2.97 g, 83%) was obtained as a pale yellow oil. IR (film): 2932, 1731, 1487, 1328, 1153, 1037 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (d, ^4J = 1.7 Hz, 1H), 7.42 (m, 2H), 6.87 (s, 1H), 6.80 (s, 1H), 4.93 (s, 1H), 4.11 (q, ^3J = 7.2 Hz, 2H), 3.38 (s, 3H), 2.50 (t, ^3J = 7.1 Hz, 2H), 2.28 (t, ^3J = 7.5 Hz, 2H), 1.76 (br s, 1H), 1.61 (~qn, ^3J = 7.2 Hz, 2H), 1.50 (m, 2H), 1.32 (m, 4H), 1.24 (t, ^3J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 173.63, 147.88, 147.62, 140.73, 137.39, 134.44, 134.13, 131.87, 131.19, 129.90, 128.26, 108.54, 107.98, 101.96, 64.55, 60.11, 48.18, 38.13, 34.15, 29.85, 28.90, 26.88, 24.75, 14.18. MS (ESI): $[M+H]^+$: 509 (1 Cl). HRMS (ESI): m/z calcd. for $C_{24}H_{30}ClN_2O_6S$ $[M+H]^+$: 509.1508, found: 509.1505.

7-[(8-Chloro-5-methyl-6,6-dioxido-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11-yl)amino]heptanoic acid (20b). To a solution of ester **20a** (2.55 g, 5 mmol) in EtOH (30 mL), a solution of NaOH (0.240 g, 6 mmol) in water (7.5 mL) was added at room temperature and it was stirred at room temperature for 25 h. Water (15 mL) was added and the ethanol was removed by evaporation in vacuo. Water (8 mL) was added, and the solution was neutralized with an aqueous HCl solution (0.50 mL of cc. HCl dissolved in 10 mL of water, containing 6 mmol of HCl). The milky reaction mixture was stirred at room temperature for 3 days, the solid product obtained was filtered, washed with water (2 × 3 mL), air-dried and subjected to dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents the solid residue was triturated with CH_3CN (5 mL) to afford **20b** (1.92 g, 80%) as colorless crystals. M. p. 126–128 °C (CH_3CN). IR (KBr): 3081, 1712, 1493, 1326, 1224, 1034 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.75 (d, ^4J = 1.8 Hz, 1H), 7.68 (dd, ^4J = 2.2 Hz, ^3J =

8.5 Hz, 1H), 7.65 (d, ^{3}J = 8.6 Hz, 1H), 7.15 (s, 1H), 7.04 (s, 1H), 6.08 (d, ^{4}J = 0.7 Hz, 1H), 6.06 (d, ^{4}J = 0.6 Hz, 1H), 5.11 (s, 1H), 3.37 (s, 3H), 2.44 (m, 2H), 2.18 (t, ^{3}J = 7.3 Hz, 2H), 1.47 (m, 4H), 1.26 (m, 4H). ^{13}C NMR (125 MHz, DMSO-d_6): 174.68, 147.41, 147.38, 141.30, 138.55, 135.93, 132.77, 131.96, 130.82, 126.86, 109.08, 107.38, 102.18, 61.99, 47.74, 37.83, 33.81, 29.47, 28.69, 26.73, 24.66. MS (ESI): $[M+H]^+$: 481 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{26}ClN_2O_6S$ $[M+H]^+$: 481.1195, found: 481.1201.

8-Chloro-*N*,5-dimethyl-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11-amine 6,6-dioxide (20c). To the solution of methylamine (1.40 g, 45 mmol) in dioxane (45 mL) crude **18** (3.35 g, 9 mmol) was added, and the suspension obtained was stirred at room temperature for 1 h. Water (150 mL) was added dropwise, the product precipitated was filtered, washed with water (2 × 10 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2, 100:4). After evaporation of solvents, the solid residue was triturated with CH_3CN (15 mL) to afford **20c** (1.86 g, 56%) as colorless crystals. M. p. decomp. from 218 °C (CH_3CN). IR (KBr): 1501, 1485, 1325, 1154, 1036 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.93 (d, ^{4}J = 2.1 Hz, 1H), 7.43 (dd, ^{4}J = 2.0 Hz, ^{3}J = 8.4 Hz, 1H), 6.87 (s, 1H), 6.81 (s, 1H), 5.98 (d, ^{4}J = 1.1 Hz, 1H), 5.97 (d, ^{4}J = 1.1 Hz, 1H), 4.82 (s, 1H), 3.37 (s, 3H), 2.38 (s, 3H), 1.86 (br s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 147.96, 147.64, 140.69, 136.96, 134.24, 133.82, 131.90, 131.34, 130.11, 128.35, 108.51, 108.23, 101.99, 66.52, 38.21, 34.98. MS (ESI): $[M+H]^+$: 367 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{16}ClN_2O_4S$ $[M+H]^+$: 367.0514, found: 367.0516.

8-Chloro-5-methyl-*N*-(2-morpholin-4-ylethyl)-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepin-11-amine 6,6-dioxide (20d). To the solution of 4-(2-aminoethyl)morpholine (1.15 g, 8.8 mmol) in CH_3CN (15 mL) crude **18** (1.49 g, 4 mmol) was added, and the suspension obtained was stirred at room temperature for 1 h. Water (50 mL) was added dropwise, the product separated was filtered, washed with water (3 × 3 mL) air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2). After evaporation of solvents, the solid residue was triturated with CH_3CN to afford **20d** (1.58 g, 84%) as colorless crystals. M. p. 207–209 °C (CH_3CN, decomp.). IR (KBr): 3331, 1488, 1326, 1116, 1029 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.93 (m, 1H), 7.42 (m, 2H), 6.89 (s, 1H), 6.81 (s, 1H), 5.98 (d, ^{4}J = 1.3 Hz, 1H), 5.97 (d, ^{4}J = 1.4 Hz, 1H), 4.93 (s, 1H), 3.67 (m, 4H), 3.42 (s, 3H), 2.63 (m, 2H), 2.50 (m, 2H), 2.37 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 147.96, 147.70, 140.84, 137.43, 134.77, 134.24, 131.82, 131.17, 129.80, 128.31, 108.51, 107.75, 102.00, 66.88 (2C), 64.38, 58.05, 53.68 (2C), 44.27,

37.97. MS (ESI): $[M+H]^+$: 466 (1 Cl). HRMS (ESI): m/z calcd. for $C_{21}H_{25}ClN_3O_5S$ $[M+H]^+$: 466.1198, found: 466.1202.

8-Chloro-5-methyl-11-pyrrolidin-1-yl-5,11-dihydro[1,3]benzodioxolo[5,6-*c*]benzo[*f*][1,2]thiazepine 6,6-dioxide (20e). To the cooled solution of pyrrolidine (0.71 g, 10 mmol, 0.83 mL) in CH_3CN (10 mL) crude **18** (1.49 g, 4 mmol) was added. The suspension formed was stirred at room temperature for 1 h. Water (40 mL) was added dropwise, the product separated was filtered, washed with water (3 × 3 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 2:1, 1:1, DCM, DCM/MeOH 100:1). After evaporation of solvents, the solid residue was triturated with CH_3CN (5 mL) to afford TLC pure **20e** (1.11 g, 68%) as colorless crystals. M. p. decomp. from 215 °C (CH_3CN). IR (KBr): 1483, 1316, 1226, 1033 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (d, ^4J = 2.2 Hz, 1H), 7.36 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.30 (d, ^3J = 8.3 Hz, 1H), 6.89 (s, 1H), 6.75 (s, 1H), 6.01 (d, ^4J = 1.3 Hz, 1H), 5.95 (d, ^4J = 1.5 Hz, 1H), 4.05 (br s, 1H), 3.46 (s, 3H), 2.27 (m, 2H), 2.18 (m, 2H), 1.70 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 148.20, 147.64, 142.76, 135.75, 135.52, 134.88, 132.60, 131.18, 131.07, 128.22, 110.64, 109.34, 102.06, 75.99, 53.71 (2C), 39.58, 23.19 (2C). MS (EI): $[M]^+$: 406 (1 Cl). HRMS (ESI): m/z calcd. for $C_{19}H_{20}ClN_2O_4S$ $[M+H]^+$: 407.0827, found: 407.0831.

9-Chloro-*N*,6-dimethyl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21c). To the cold solution of methylamine (0.745 g, 24 mmol) in dioxane (17 mL) crude **19** (1.85 g, 4.8 mmol) was added, and the suspension obtained was stirred at room temperature for 45 min. After evaporation in vacuo the solid residue was triturated with water (15 mL), filtered, air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1). After evaporation of solvents, the solid residue was triturated with DIPE (10 mL) to afford **21c** (1.71 g, 93%) as colorless crystals. M. p. decomp. from 212 °C (CH_3CN). IR (KBr): 1508, 1324, 1064, 594 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.95 (d, ^4J = 2.2 Hz, 1H), 7.44 (dd, ^4J = 2.2 Hz, ^3J = 8.2 Hz, 1H), 7.39 (d, ^3J = 8.3 Hz, 1H), 6.92 (s, 1H), 6.85 (s, 1H), 4.73 (s, 1H), 4.24 (s, 4H), 3.33 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.71, 143.29, 140.74, 136.68, 134.20, 132.02, 131.95, 131.28, 130.99, 128.45, 117.90, 116.92, 67.34, 64.32, 64.27, 38.75, 34.91. MS (EI): $[M]^+$: 380 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{18}ClN_2O_4S$ $[M+H]^+$: 381.0670, found: 381.0677.

9-Chloro-6-methyl-*N*-(2-morpholin-4-ylethyl)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21d). To the solution of 4-(2-aminoethyl)morpholine (1.15 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was

added. The solution obtained was stirred at room temperature for 1 h. Water (50 mL) was added dropwise in 30 min, the product separated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM, DCM/MeOH 100:2). After evaporation of solvents, the solid residue was triturated with CH_3CN (10 mL), filtered and recrystallized from CH_3CN (85 mL) to afford **21d** (1.46 g, 75%) as colorless crystals. M. p. decomp. from 217 °C (CH_3CN). IR (KBr): 1509, 1323, 1147, 1065 cm^{-1}. ^1H NMR (500 MHz, CDCl3): 7.94 (d, ^4J = 2.1 Hz, 1H), 7.43 (dd, ^4J = 2.1 Hz, ^3J = 8.3 Hz, 1H), 7.39 (d, ^3J = 8.3 Hz, 1H), 6.94 (s, 1H), 6.85 (s, 1H), 4.85 (s, 1H), 4.23 (s, 4H), 3.67 (m, 4H), 3.39 (s, 3H), 2.58 (m, 2H), 2.47 (m, 2H), 2.46 (br s, 1H), 2.35 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.65, 143.33, 140.95, 137.18, 134.12, 133.06, 131.82, 130.97, 130.54, 128.30, 117.20, 116.96, 66.85 (2C), 64.96, 64.29, 64.20, 58.04, 53.63 (2C), 44.17, 38.41. MS (EI): $[M]^+$: 479 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{27}ClN_3O_5S$ $[M+H]^+$: 480.1354, found: 480.1353.

9-Chloro-6-methyl-*N*-(3-morpholin-4-ylpropyl)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21e). To the solution of 4-(3-aminopropyl)morpholine (1.27 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1.5 h. Water (100 mL) was added dropwise, the oily product separated was extracted with DCM (2 × 25 mL), the combined organic phases were washed with water (20 mL), dried over Na_2SO_4, and partly evaporated in vacuo (to a volume of 20 mL). The solution obtained was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents, the oily residue was triturated with water (30 mL), filtered and recrystallized from CH_3CN to afford **21e** (1.29 g, 65%) as bright colorless crystals. M. p. 164–166 °C (CH_3CN). IR (KBr): 1500, 1304, 1146, 1116, 1069 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (d, ^4J = 0.7 Hz, 1H), 7.43 (m, 2H), 6.93 (s, 1H), 6.85 (s, 1H), 4.92 (s, 1H), 4.23 (s, 4H), 3.66 (m, 4H), 3.35 (s, 3H), 2.57 (m, 2H), 2.42 (m, 4H), 2.40 (t, ^3J = 7.0 Hz, 2H), 2.35 (br s, 1H), 1.69 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.55, 143.35, 140.68, 137.45, 134.00, 133.13, 131.87, 130.97, 130.04, 128.36, 116.97, 116.93, 66.89 (2C), 64.32, 64.30, 64.21, 57.31, 53.74 (2C), 46.90, 38.39, 26.37. MS (ESI): $[M+H]^+$: 494 (1 Cl). HRMS (ESI): m/z calcd. for $C_{23}H_{29}ClN_3O_5S$ $[M+H]^+$: 494.1511, found: 494.1513.

9-Chloro-6-methyl-*N*-(4-morpholin-4-ylbutyl)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21f). To the solution of 4-(4-aminobutyl)morpholine (1.39 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (60 mL) was added

dropwise in 30 min, the oily product separated was extracted with DCM (3 × 25 mL), the combined organic phases were washed with water (25 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents, the foamy residue was dissolved in CH_3CN (20 mL), the opalescent solution was treated with charcoal, the clear solution obtained was evaporated in vacuo to afford **21f** (1.43 g, 70%) as colorless foam. IR (KBr): 3332, 2936, 1507, 1321, 1116, 1066 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (d, ^4J = 2.0 Hz, 1H), 7.42 (dd, ^4J = 2.1 Hz, ^3J = 8.3 Hz, 1H), 7.39 (d, ^3J = 8.3 Hz, 1H), 6.91 (s, 1H), 6.84 (s, 1H), 4.86 (s, 1H), 4.22 (s, 4H), 3.68 (m, 4H), 3.34 (s, 3H), 2.49 (~q, ^3J = 3.8 Hz, 2H), 2.39 (m, 4H), 2.29 (t, ^3J = 6.8 Hz, 2H), 1.94 (br s, 1H), 1.50 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.56, 143.21, 140.71, 137.06, 133.99, 132.52, 131.84, 131.04, 130.65, 128.27, 117.50, 116.88, 66.83 (2C), 65.14, 64.22, 64.15, 58.65, 53.61 (2C), 47.89, 38.62, 27.84, 24.18. MS (ESI): $[M+H]^+$: 508 (1 Cl). HRMS (ESI): m/z calcd. for $C_{24}H_{31}ClN_3O_5S$ $[M+H]^+$: 508.1667, found: 508.1669.

9-Chloro-6-methyl-12-pyrrolidin-1-yl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (21g). To the cooled suspension of crude **19** (1.74 g, 4.5 mmol) in CH_3CN (15 mL) pyrrolidine (0.80 g, 11.3 mmol, 0.94 mL) was added in one portion. An exothermic reaction took place, a solution was formed, which was followed by rapid precipitation. The suspension obtained was stirred at room temperature for 1 h. Water (60 mL) was added dropwise, the product separated was filtered, washed with water (3 × 3 mL), and air-dried. It was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM). After evaporation of solvent, the solid residue triturated with Et_2O (5 mL) to give **21g** (1.30 g, 69%) as colorless crystals. M. p. decomp. from 216 °C (CH_3CN). IR (KBr): 2933, 1586, 1506, 1320, 1138, 1067 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (d, ^4J = 2.1 Hz, 1H), 7.36 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.29 (d, ^3J = 8.3 Hz, 1H), 6.97 (s, 1H), 6.79 (s, 1H), 4.23 (m, 4H), 4.03 (s, 1H), 3.47 (s, 3H), 2.25 (m, 2H), 2.17 (m, 2H), 1.68 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.84, 143.44, 143.09, 135.79, 134.80, 134.64, 132.72, 131.02, 130.65, 128.33, 119.37, 118.26, 75.64, 64.32, 64.17, 53.68 (2C), 39.93, 23.19 (2C). MS (EI): $[M]^+$: 420 (1 Cl). HRMS (ESI): m/z calcd. for $C_{20}H_{22}ClN_2O_4S$ $[M+H]^+$: 421.0983, found: 421.0985.

9-Chloro-6-methyl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21h). To a cold, 1 m/m % ammonia solution in dioxane (204 g, containing 2.04 g, 120 mmol NH_3) crude **19** (4.63 g, 12 mmol) was added, the thin suspension was stirred at room temperature for 2 h, then evaporated in vacuo. The solid residue (7.1 g) was triturated

with water (20 mL), filtered, washed with water (2 × 10 mL), dried in vacuo and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1). After evaporation of solvents, the foamy residue was triturated with DIPE (20 mL), filtered, washed with DIPE (5 mL) to afford **21h** (2.10 g, 48%) as colorless crystals. M. p. decomp. from 200 °C (EtOH/CH_3CN). IR (KBr): 3368, 1503, 1322, 1143, 1062 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.79 (d, ^3J = 8.5 Hz, 1H), 7.73 (d, ^4J = 2.3 Hz, 1H), 7.69 (dd, ^4J = 2.3 Hz, ^3J = 8.6 Hz, 1H), 7.05 (s, 1H), 7.03 (s, 1H), 5.47 (s, 1H), 4.23 (s, 4H), 3.32 (s, 3H), 2.57 (br s, 2H). ^{13}C NMR (125 MHz, DMSO-d_6): 143.41, 142.90, 140.85, 140.61, 137.22, 132.27, 132.11, 129.57, 129.34, 126.73, 116.56, 115.04, 64.32, 64.22, 53.17, 37.59. MS (EI): $[M]^+$: 366 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{16}ClN_2O_4S$ $[M+H]^+$: 367.0514, found: 367.0519.

7-[(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)amino]-*N*,*N*-dimethylheptanamide (21i). To a solution of 7-amino-*N*,*N*-dimethylheptanamide (1.45 g, 8.4 mmol) in CH_3CN (20 mL) crude **19** (1.545 g, 4 mmol) was added and the solution obtained was stirred at room temperature for 3.5 h. It was evaporated in vacuo, the residue was dissolved in DCM (50 mL), washed with water (3 × 20 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 40 mm, eluent: DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents in vacuo **21i** (1.47 g, 70%) was obtained as a colorless foam. IR (KBr): 3446, 2929, 1641, 1507, 1320, 1143, 1066 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (d, ^4J = 2.0 Hz, 1H), 7.43 (dd, ^4J = 2.0 Hz, ^3J = 8.2 Hz, 1H), 7.40 (d, ^3J = 8.4 Hz, 1H), 6.91 (s, 1H), 6.83 (s, 1H), 4.85 (s, 1H), 4.23 (s, 4H), 3.35 (s, 3H), 2.98 (s, 3H), 2.93 (s, 3H), 2.47 (m, 2H), 2.28 (t, ^3J = 7.5 Hz, 2H), 1.87 (br s, 1H), 1.61 (m, 2H), 1.48 (m, 2H), 1.32 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 172.92, 143.59, 143.27, 140.85, 137.20, 134.01, 132.77, 131.87, 131.08, 130.71, 128.27, 117.51, 116.98, 65.25, 64.26, 64.19, 48.06, 38.63, 37.16, 35.25, 33.13, 29.85, 29.23, 27.04, 24.94. MS (ESI): $[M+H]^+$: 522 (1 Cl). HRMS (ESI): m/z calcd. for $C_{25}H_{33}ClN_3O_5S$ $[M+H]^+$: 522.1824, found: 522.1829.

9-Chloro-6-methyl-*N*-(2-pyrrolidin-1-ylethyl)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21j). To the solution of 4-(2-aminoethyl)pyrrolidine (1.01 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (60 mL) was added, the oily product separated was extracted with DCM (30 + 15 mL), the combined organic phases were washed with water (15 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short silica gel column (thickness of

stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1, 100:2, 100:4). After evaporation of solvents, the solid residue was recrystallized from CH_3CN (50 mL) to afford **21j** (1.35 g, 72%) as colorless crystals. M. p. decomp. from 190 °C (CH_3CN). IR (KBr): 3281, 2788, 1509, 1325, 1159, 1061 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (br s, 1H), 7.41 (m, 2H), 6.94 (s, 1H), 6.85 (s, 1H), 4.86 (s, 1H), 4.22 (s, 4H), 3.40 (s, 3H), 2.59 (m, 4H), 2.41 (m, 4H), 2.35 (br s, 1H), 1.73 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.59, 143.31, 141.14, 137.29, 134.04, 133.32, 131.80, 130.89, 130.69, 128.14, 117.31, 117.03, 65.12, 64.27, 64.18, 55.56, 54.08 (2C), 46.73, 38.32, 23.39 (2C). MS (ESI): $[M+H]^+$: 464 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{27}ClN_3O_4S$ $[M+H]^+$: 464.1405, found: 464.1407.

9-Chloro-6-methyl-*N*-(2-piperidin-1-ylethyl)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-amine 7,7-dioxide (21k). To the solution of 4-(2-aminoethyl)piperidine (1.13 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The thin suspension obtained was stirred at room temperature for 1 h. Water (60 mL) was added dropwise in 30 min, the oily product separated was extracted with DCM (30 + 15 mL), the combined organic phases were washed with water (15 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents, the foamy residue was dissolved in CH_3CN (5 mL), crystallization occurred when cooling it at 5 °C for 3 days to afford **21k** (1.455 g, 76%) as colorless crystals. M. p. decomp. from 141 °C (CH_3CN). IR (KBr): 3302, 2937, 1508, 1323, 1148, 1065 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (m, 1H), 7.41 (m, 2H), 6.94 (s, 1H), 6.84 (s, 1H), 4.86 (d, ^3J = 3.8 Hz, 1H), 4.22 (s, 4H), 3.42 (s, 3H), 2.58 (~q, ^3J = 5.0 Hz, 2H), 2.41 (t, ^3J = 6.0 Hz, 2H), 2.37 (~bq, ^3J = 5.5 Hz, 1H), 2.28 (br s, 4H), 1.52 (~qn, ^3J = 5.6 Hz, 4H), 1.40 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.58, 143.37, 141.14, 137.38, 134.04, 133.54, 131.76, 130.88, 130.48, 128.20, 117.13, 117.08, 64.85, 64.28, 64.19, 58.34, 54.70 (2C), 44.86, 38.41, 25.95 (2C), 24.35. MS (ESI): $[M+H]^+$: 478 (1 Cl). HRMS (ESI): m/z calcd. for $C_{23}H_{29}ClN_3O_4S$ $[M+H]^+$: 478.1562, found: 478.1564.

***N*'-(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)-*N*,*N*-dimethylethane-1,2-diamine (21l).** To the solution of 2-(dimethylamino)ethylamine (0.88 g, 10 mmol) in CH_3CN (15 mL) crude **19** (1.70 g, 4.4 mmol) was added. The thick suspension obtained was stirred at room temperature for 1 h. Water (60 mL) was added dropwise, the separated product was filtered, washed with water (2 × 5 mL). The wet crude product was dissolved in DCM (35 mL), water was separated, the organic phase was dried over Na_2SO_4 and evaporated in vacuo. The residue was purified by dry-column

chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents, the solid residue was crystallized from CH_3CN (30 mL) to afford **21l** (1.54 g, 80%) as colorless crystals. M. p. decomp. from 190 °C (CH_3CN). IR (KBr): 2944, 1509, 1325, 1147, 1060 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (br s, 1H), 7.42 (m, 2H), 6.94 (s, 1H), 6.85 (s, 1H), 4.88 (s, 1H), 4.22 (s, 4H), 3.41 (s, 3H), 2.56 (t, ^3J = 5.7 Hz, 2H), 2.39 (t, ^3J = 5.6 Hz, 2H), 2.31 (br s, 1H), 2.15 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.57, 143.32, 141.14, 137.34, 134.02, 133.46, 131.81, 130.84, 130.49, 128.12, 117.14, 117.08, 64.86, 64.26, 64.17, 58.80, 45.52, 45.41 (2C), 38.28. MS (ESI): $[M+H]^+$: 438 (1 Cl). HRMS (ESI): m/z calcd. for $C_{20}H_{25}ClN_3O_4S$ $[M+H]^+$: 438.1249, found: 438.1253.

***N*'-(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)-*N*,*N*-dimethylpropane-1,3-diamine (21m).** To the solution of 3-(dimethylamino)-1-propylamine (0.90 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (60 mL) was added dropwise, the oily product separated was extracted with DCM (30 + 15 mL), the combined organic phases were washed with water (15 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents, the foamy residue was dissolved in CH_3CN (5 mL), crystallization occurred when cooling it at 5 °C overnight to afford **21m** (1.355 g, 75%) as colorless crystals. M. p. 154–156 °C (CH_3CN). IR (KBr): 3199, 1508, 1319, 1066 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (br s, 1H), 7.42 (m, 2H), 6.92 (s, 1H), 6.84 (s, 1H), 4.90 (s, 1H), 4.22 (s, 4H), 3.36 (s, 3H), 2.56 (m, 2H), 2.30 (t, ^3J = 7.0 Hz, 2H), 2.22 (br s, 1H), 2.20 (s, 6H), 1.66 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.52, 143.33, 140.76, 137.41, 133.94, 133.18, 131.86, 130.90, 130.22, 128.26, 117.08, 116.92, 64.53, 64.26, 64.17, 58.04, 46.86, 45.49 (2C), 38.36, 27.81. MS (ESI): $[M+H]^+$: 452 (1 Cl). HRMS (ESI): m/z calcd. for $C_{21}H_{27}ClN_3O_4S$ $[M+H]^+$: 452.1405, found: 452.1406.

Ethyl 1-(9-chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)piperidine-4-carboxylate (21n). To the solution of ethyl piperidine-4-carboxylate (1.04 g, 6.6 mmol) in CH_3CN (10 mL) crude **19** (1.16 g, 3 mmol) was added. The thick suspension obtained was diluted with CH_3CN (5 mL) and stirred at room temperature for 1 h. Water (70 mL) was added dropwise, the product separated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1,

100:2). After evaporation of solvents, the solid residue was recrystallized from CH_3CN to afford **21n** (1.175 g, 77%) as colorless crystals. M. p. 229–231 °C (CH_3CN). IR (KBr): 2949, 1730, 1508, 1318, 1141, 1068 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.94 (d, ^4J = 2.2 Hz, 1H), 7.35 (dd, ^4J = 2.3 Hz, ^3J = 8.3 Hz, 1H), 7.22 (d, ^3J = 8.3 Hz, 1H), 6.98 (s, 1H), 6.74 (s, 1H), 4.24 (m, 2H), 4.21 (m, 2H), 4.11 (q, ^3J = 7.1 Hz, 2H), 3.95 (s, 1H), 3.49 (s, 3H), 2.64 (m, 1H), 2.47 (m, 1H), 2.26 (m, 1H), 1.88 (m, 2H), 1.81 (m, 2H), 1.64 (m, 2H), 1.23 (t, ^3J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 174.79, 144.00, 143.47, 143.16, 135.09, 134.41, 133.61, 133.47, 131.02, 130.29, 128.73, 119.65, 119.00, 76.70, 64.29, 64.15, 60.35, 52.23, 52.01, 40.73, 40.41, 28.35, 27.94, 14.15. MS (ESI): $[M+H]^+$: 507 (1 Cl). HRMS (ESI): m/z calcd. for $C_{24}H_{28}ClN_2O_6S$ $[M+H]^+$: 507.1351, found: 507.1350.

1-(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)piperidine-4-carboxamide (21o). To the solution of piperidine-4-carboxamide (isonipecotamide, 1.41 g, 11 mmol) in CH_3CN (175 mL) crude **19** (1.93 g, 5 mmol) was added and the suspension obtained was stirred at room temperature for 1.5 h. Water (350 mL) was added dropwise in 30 min, the product separated was filtered, washed with water (2 × 15 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:3). After evaporation of solvents, the TLC pure solid residue was triturated with CH_3CN (15 mL) to afford **21o** (2.02 g, 84%) as colorless crystals. M. p. 272–275 °C (CH_3CN, decomp.) IR (KBr): 3437, 3159, 2944, 1685, 1506, 1319, 1065 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.77 (d, ^4J = 2.3 Hz, 1H), 7.64 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.53 (d, ^3J = 8.6 Hz, 1H), 7.21 (br s, 1H), 7.03 (s, 1H), 6.96 (s, 1H), 6.73 (br s, 1H), 4.25 (m, 4H), 4.24 (s, 1H), 3.43 (s, 3H), 2.54 (m, 1H), 2.31 (m, 1H), 2.04 (m, 1H), 1.83 (m, 2H), 1.61 (m, 2H), 1.44 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6): 176.54, 143.76, 143.39, 143.37, 135.12, 134.99, 133.86, 133.66, 131.43, 129.97, 127.42, 119.42, 119.16, 74.61, 64.29, 64.23, 52.08, 51.78, 41.58, 40.28, 28.80, 28.33. MS (ESI): $[M+H]^+$: 478 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{25}ClN_3O_5S$ $[M+H]^+$: 478.1198, found: 478.1199.

1-(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)piperidine-4-carbonitrile (21p). To the solution of piperidine-4-carbonitrile (4-cyanopiperidine) (0.99 g, 9.0 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added. The suspension obtained was stirred at room temperature for 2.5 h. Water (70 mL) was added dropwise, the product separated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM, DCM/MeOH 100:1, 100:2). After

evaporation of solvents, the residue was triturated with CH_3CN, filtered and dried in vacuo (0.1 mm Hg, at 90 °C for 24 h) to afford **21p** (1.60 g, 87%) as colorless crystals. M. p. 229–232 °C (CH_3CN, decomp.). IR (KBr): 2928, 2240, 1508, 1320, 1143, 1067 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.94 (d, ^4J = 2.2 Hz, 1H), 7.37 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.24 (d, ^3J = 8.3 Hz, 1H), 6.98 (s, 1H), 6.75 (s, 1H), 4.22 (m, 4H), 4.01 (s, 1H), 3.46 (s, 3H), 2.65 (m, 1H), 2.47 (m, 1H), 2.37 (m, 1H), 2.24 (m, 1H), 2.13 (m, 1H), 1.80 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 144.15, 143.54, 143.08, 135.29, 133.81, 133.51, 132.87, 131.17, 130.13, 128.73, 121.29, 119.51, 119.06, 76.34, 64.25, 64.12, 50.30 (br), 40.10, 28.61, 25.81. MS (ESI): $[M+H]^+$: 460 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{23}ClN_3O_4S$ $[M+H]^+$: 460.1092, found: 460.1096.

9-Chloro-12-methoxy-6-methyl-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (23a). The suspension of crude **19** (1.74 g, 4.5 mmol) in MeOH (15 mL) was stirred at room temperature for 2 h, while it was transformed to the suspension of the product. It was filtered, washed with MeOH (2 × 2 mL) and subjected to dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 1:1, DCM). After evaporation of solvents, the solid residue was triturated with MeOH to afford **23a** (1.45 g, 84%) as colorless crystals. M. p. 218–220 °C (CH_3CN). IR (KBr): 1507, 1322, 1068, 596 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.91 (d, ^4J = 2.1 Hz, 1H), 7.58 (d, ^3J = 8.4 Hz, 1H), 7.44 (dd, ^4J = 2.2 Hz, ^3J = 8.5 Hz, 1H), 6.99 (s, 1H), 6.91 (s, 1H), 5.49 (s, 1H), 4.23 (m, 4H), 3.46 (s, 3H), 3.40 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.93, 143.73, 140.42, 135.84, 134.57, 132.88, 131.87, 129.87, 128.53, 128.00, 117.53, 115.36, 80.51, 64.31, 64.19, 57.85, 38.00. MS (EI): M^+ = 381 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{16}ClNNaO_5S$ $[M+Na]^+$: 404.0330, found: 404.0331.

2-[(9-Chloro-6-methyl-7,7-dioxido-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-yl)oxy]-*N*,*N*-dimethylethanamine (23b). To the solution of 2-(dimethylamino)ethanol (0.89 g, 10 mmol) in CH_3CN (15 mL) crude **19** (1.70 g, 4.4 mmol) was added, and the solution obtained was stirred at room temperature for 3 h. Water (60 mL) was added dropwise, the precipitate was collected by filtration, washed with water (2 × 3 mL), air-dried and purified by dry-column chromatography on a short aluminum oxide column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents, the solid residue was recrystallized from CH_3CN (14 mL) to afford **23b** (1.14 g, 59%) as colorless crystals. M. p. 175–178 °C (decomp.). IR (KBr): 1508, 1323, 1147, 1060 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.2 Hz, 1H), 7.63 (d, ^3J = 8.4 Hz, 1H), 7.43 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 6.98 (s, 1H), 6.94 (s, 1H), 4.23 (m, 4H), 3.68 (m, 1H), 3.62 (m, 1H), 3.41 (s, 3H), 2.61 (m, 2H), 2.28 (s, 6H). ^{13}C NMR

(125 MHz, $CDCl_3$): 143.83, 143.73, 140.29, 136.22, 134.41, 133.37, 131.87, 129.69, 128.33, 127.94, 117.33, 115.15, 78.67, 68.60, 64.29, 64.18, 58.93, 46.02 (2 Me), 37.86. MS (ESI): $[M+H]^+$ = 439 (1 Cl). HRMS (ESI): m/z calcd. for $C_{20}H_{24}ClN_2O_5S$ $[M+H]^+$: 439.1089, found: 439.1091.

9-Chloro-6-methyl-12-(2-pyrrolidin-1-ylethoxy)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (23c). To the solution of 1-(2-hydroxyethyl)pyrrolidine (2.30 g, 20 mmol) in CH_3CN (30 mL) crude **19** (3.40 g, 8.8 mmol) was added, and the solution obtained was stirred at room temperature for 2.5 h. Water (120 mL) was added dropwise, the oily product separated was extracted with DCM (2 × 50 mL). The combined organic phases were washed with water (50 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2, 100:4). After evaporation of solvents, the solid residue was triturated with EtOH to afford **23c** (1.56 g, 38%). M. p. 145–146 °C (CH_3CN, colorless crystals). IR (KBr): 2946, 1509, 1325, 1160, 1060 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.2 Hz, 1H), 7.64 (d, ^3J = 8.5 Hz, 1H), 7.43 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 6.97 (s, 1H), 6.95 (s, 1H), 4.22 (s, 4H), 3.71 (m, 1H), 3.65 (m, 1H), 3.40 (s, 3H), 2.79 (t, ^3J = 6.2 Hz, 2H), 2.55 (m, 4H), 1.77 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.81, 143.70, 140.29, 136.23, 134.38, 133.33, 131.84, 129.69, 128.39, 127.91, 117.30, 115.22, 78.70, 69.53, 64.27, 64.17, 55.51, 54.72 (2C), 37.89, 23.47 (2C). MS (ESI): $[M+H]^+$ = 465 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{26}ClN_2O_5S$ $[M+H]^+$: 465.1245, found: 465.1249.

9-Chloro-6-methyl-12-(2-piperidin-1-ylethoxy)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (23d). To the solution of 1-(2-hydroxyethyl)piperidine (1.29 g, 10 mmol) in CH_3CN (15 mL) crude **19** (1.70 g, 4.4 mmol) was added, and the solution obtained was stirred at room temperature for 2 h. Water (60 mL) was added dropwise, the oily product separated was extracted with DCM (2 × 30 mL). The combined organic phases were washed with water (30 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column chromatography on a short aluminum oxide column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 2:1, 1:1, DCM, DCM/MeOH 100:1). After evaporation of solvents the residue was triturated with CH_3CN to afford **23d** (1.40 g, 66%) as colorless crystals. M. p. 133–135 °C (CH_3CN). IR (KBr): 1494, 1319, 1144, 1066 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.2 Hz, 1H), 7.66 (d, ^3J = 8.6 Hz, 1H), 7.43 (dd, ^4J = 2.1 Hz, ^3J = 8.4 Hz, 1H), 6.97 (s, 1H), 6.96 (s, 1H), 5.69 (s, 1H), 4.22 (s, 4H), 3.69 (m, 1H), 3.64 (m, 1H), 3.40 (s, 3H), 2.63 (m, 2H), 2.42 (m, 4H), 1.57 (m,

4H), 1.43 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.79, 143.67, 140.29, 136.25, 134.35, 133.28, 131.82, 129.74, 128.53, 127.86, 117.27, 115.29, 78.70, 68.17, 64.26, 64.16, 58.52, 55.08 (2C), 37.97, 25.95 (2C), 24.16. MS (ESI): $[M+H]^+$ = 479 (1 Cl). HRMS (ESI): m/z calcd. for $C_{23}H_{28}ClN_2O_5S$ $[M+H]^+$: 479.1402, found: 479.1403.

9-Chloro-6-methyl-12-(2-morpholin-4-ylethoxy)-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (23e). To the solution of 4-(2-hydroxyethyl)morpholine (1.15 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added and the solution obtained was stirred at room temperature for 2 h. Water (60 mL) was added dropwise, the product separated was filtered, washed with water (2 × 3 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents the residue was triturated with CH_3CN to afford **23e** (1.61 g, 84%) as colorless crystals. M. p. 191–194 °C (CH_3CN, decomp.). IR (KBr): 1510, 1325, 1146, 1066 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.1 Hz, 1H), 7.65 (d, ^3J = 8.4 Hz, 1H), 7.44 (dd, ^4J = 2.0 Hz, ^3J = 8.4 Hz, 1H), 6.98 (s, 1H), 6.97 (s, 1H), 5.70 (s, 1H), 4.22 (s, 4H), 3.71 (m, 1H), 3.70 (m, 4H), 3.65 (m, 1H), 3.40 (s, 3H), 2.68 (t, ^3J = 5.7 Hz, 2H), 2.50 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.82, 143.66, 140.18, 136.15, 134.39, 133.05, 131.85, 129.73, 128.25, 127.90, 117.19, 115.11, 78.55, 67.74, 66.86 (2C), 64.25, 64.15, 58.18, 54.06 (2C), 37.91. MS (ESI): $[M+H]^+$ = 481 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{26}ClN_2O_6S$ $[M+H]^+$: 481.1195, found: 481.1200.

9-Chloro-6-methyl-12-[(2-morpholin-4-ylethyl)sulfanyl]-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (24). To the solution of 2-(morpholin-4-yl)ethanethiol (1.30 g, 8.8 mmol) in CH_3CN (15 mL) crude **19** (1.55 g, 4 mmol) was added and it was stirred at room temperature for 1 h. Water (60 mL) was added dropwise, the product separated was filtered, washed with water (2 × 3 mL), and air-dried to give crude **24**. It was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM, DCM/MeOH 100:2). After evaporation of solvents, the solid residue was triturated with CH_3CN (10 mL) and filtered to afford crude **24** (1.93 g), which was recrystallized from CH_3CN to give **24** (1.44 g, 72%) as colorless crystals. M. p. decomp. from 240 °C (CH_3CN). IR (KBr): 1511, 1326, 1301, 1114, 1063 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.94 (d, ^3J = 8.2 Hz, 1H), 7.40 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.31 (d, ^3J = 8.3 Hz, 1H), 6.99 (s, 1H), 6.75 (s, 1H), 4.95 (s, 1H), 4.25 (m, 4H), 3.69 (m, 4H), 3.51 (s, 3H), 2.60 (m, 1H), 2.50 (m, 2H), 2.46 (m, 1H), 2.40 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 144.32, 143.05, 142.31, 134.63, 134.55, 132.50, 131.89, 131.72, 131.44, 127.79, 118.10, 117.90, 66.82 (2C), 64.33,

64.26, 58.22, 54.34, 53.54 (2C), 39.35, 30.28. MS (ESI): $[M+H]^+$ = 497 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{26}ClN_2O_5S_2$ $[M+H]^+$: 497.0966, found: 497.0970.

9-Chloro-2,3-dihydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12(6*H*)-one 7,7-dioxide (28). Compound **7** (14.89 g, 40.7 mmol) was mixed with pyridine hydrochloride (47 g, 407 mol) and the mixture was melted. The melt was stirred at 180 °C for 27 h. Water (230 mL) was added to the cooled reaction mixture (dark brown melt), the suspension obtained was stirred for 2 h, the product was filtered and washed thoroughly with water. The wet crude product on the sintered glass filter was treated with aqueous NaOH solution (80 + 30 mL, 116 g of 5 m/m % solution, containing 5.8 g, ca. 145 mmol NaOH). The filtrate was acidified with AcOH (10 mL, 173 mmol), the product precipitated was collected by filtration, washed with water (3 × 30 mL), air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 35 mm, eluent: $CHCl_3$, $CHCl_3$/MeOH 100:3) After evaporation of the solvents the solid residue was triturated with CH_3CN (40 mL) to afford **28** (6.27 g, 51%) as yellow solid. M. p. 276–278 °C (CH_3CN, bright yellow crystals). IR (KBr): 3146, 1600, 1503, 1289 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 11.72 (br s, 1H), 7.90 (dd, ^4J = 2.1 Hz, ^3J = 8.2 Hz, 1H), 7.88 (dd, ^4J = 0.4 Hz, ^4J = 2.1 Hz, 1H), 7.83 (dd, ^4J = 0.5 Hz, ^3J = 8.2 Hz, 1H), 7.51 (s, 1H), 6.70 (s, 1H), 4.36 (m, 2H), 4.29 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6): 189.20, 149.53, 140.53, 139.65, 137.14, 134.46, 133.51, 132.97, 132.40, 122.01, 120.37, 118.36, 108.75, 65.18, 64.07. MS (EI): M^+ = 351 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{11}ClNO_5S$ $[M+H]^+$: 352.0041, found: 352.0046.

6-(2-Bromoethyl)-9-chloro-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-ol 7,7-dioxide (30). To the suspension of **29** (9.175 g, 20 mmol) in a mixture of THF (20 mL) and EtOH (20 mL), $NaBH_4$ (0.91 g, 24 mmol) was added in portions and the stirring was continued at room temperature for 30 min. Water (200 mL) was added, and the oily product separated was extracted with DCM (2 × 100 mL). The combined organic phases were washed with water (50 mL), dried over Na_2SO_4, and evaporated in vacuo to give crude **30** (9.09 g, 99%) as colorless foam suitable for next reaction step. IR (KBr): 3484, 1499, 1327, 1304, 1141, 1065 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.2 Hz, 1H), 7.65 (d, ^3J = 8.4 Hz, 1H), 7.49 (dd, ^4J = 2.1 Hz, ^3J = 8.4 Hz, 1H), 7.04 (s, 1H), 6.94 (s, 1H), 6.07 (d, ^3J = 6.1 Hz, 1H), 4.25 (s, 4H), 4.03 (m, 2H), 3.54 (m, 1H), 3.47 (m, 1H), 3.38 (d, ^3J = 6.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): 143.99, 143.97, 139.94, 136.91, 134.70, 133.42, 132.65, 129.22, 128.05, 127.92, 117.26, 116.74, 72.29, 64.31, 64.26, 52.83, 29.10. COSY: 7.89–7.49–7.65, 6.07–3.38, 4.03–(3.54, 3.47). HSQC (140 Hz): 7.89–127.92, 7.65–129.22, 7.49–132.65, 7.04–116.74, 6.94–117.26, 6.07–72.29, 4.25–64.31, 4.25–64.26, 4.03–52.83,

3.54–29.10, 3.47–29.10. HMBC (8 Hz, 140 Hz): 7.89–(136.91, 134.70, 132.65), 7.65–(139.94, 134.70, 72.29), 7.49–(136.91, 134.70, 127.92), 7.04–(143.97, 128.05, 72.29), 6.94–(143.99, 133.42), 6.07–(139.94, 136.91, 133.42, 129.22, 128.05, 116.74), 4.25–(143.99, 64.26), 4.25–(143.97, 64.31), 4.03–(128.05, 29.10), (3.54, 3.47)–52.83, 3.38–(136.91, 133.42, 72.29). MS (EI): M^+ = 459 (1 Br, 1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{15}BrClNNaO_5S$ $[M+Na]^+$: 481.9435, found: 481.9438.

6-(2-Bromoethyl)-9,12-dichloro-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (31). To a vigorously stirred yellow solution of **30** (8.75 g, 19 mmol) in DCM (100 mL), $SOCl_2$ (4.52 g, 38 mmol, 2.76 mL) was added dropwise at room temperature and stirring was continued for 2.5 h. To the solution hexane (400 mL) was added dropwise, the product precipitated was filtered, washed with hexane (2 × 20 mL), and dried in vacuo to give **31** (6.02 g, 66%) as beige crystals. M. p. decomp. from 144 °C. The mother liquor of this product was evaporated in vacuo, the solid residue was triturated with a little cold Et_2O to give a second crop of crude **31** (2.21 g, 24%) as beige crystals. Total yield: 8.23 g, 90%. IR (KBr): 1510, 1332, 1303, 1160, 1064 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): 7.96 (d, ^4J = 2.1 Hz, 1H), 7.48 (dd, ^4J = 2.1 Hz, ^3J = 8.4 Hz, 1H), 7.44 (d, ^3J = 8.4 Hz, 1H), 7.10 (s, 1H), 6.92 (s, 1H), 6.04 (s, 1H), 4.33 (m, 1H), 4.26 (m, 4H), 4.01 (m, 1H), 3.73 (t, ^3J = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 145.25, 143.97, 141.40, 136.19, 133.33, 132.89, 132.60, 130.58, 130.34, 128.20, 119.97, 118.87, 64.31, 64.29, 63.08, 54.27, 29.60. HRMS (TOF MS EI): m/z calcd. for $[C_{17}H_{14}BrCl_2NO_4S]^+$: 476.9204, found: 476.9200.

***S*-[2-(9-Chloro-12-hydroxy-7,7-dioxido-2,3-dihydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-6(12*H*)-yl)ethyl] ethanethioate (32).** To a solution of **30** (1.015 g, 2.2 mmol) in CH_3CN (10 mL), potassium thioacetate (0.43 g, 3.75 mmol, 1.7 equiv) and tetrabutylammonium bromide (0.032 g, 0.1 mmol, 4.5 mol%) were added, and the thin suspension was vigorously stirred at room temperature for 4 h. To the thin suspension obtained, water (50 mL) and EtOAc (25 mL) were added with stirring (25 min). The phases were separated, the aqueous phase was washed with EtOAc (10 mL), the combined organic phases were washed with water (15 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was subjected to dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2). After evaporation of the solvents, the residue was dried in vacuo to afford **32** (0.84 g, 84%) as colorless foam. IR (KBr): 3479, 1692, 1500, 1306, 1155, 1139, 1064 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): 7.92 (d, ^4J = 1.9 Hz, 1H), 7.64 (d, ^3J = 8.3 Hz, 1H), 7.51 (dd, ^4J = 1.9 Hz, ^3J = 8.3 Hz, 1H), 7.05 (s, 1H), 6.98 (s, 1H), 5.96 (d, ^3J = 7.3 Hz, 1H), 4.26 (s, 4H), 3.77 (t, ^3J = 7.3 Hz, 2H),

3.54 (d, ^3J = 7.3 Hz, 1H), 3.03 (m, 2H), 2.30 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): 195.08, 144.10, 143.67, 140.01, 136.61, 134.70, 132.70, 132.08, 129.76, 128.68, 127.94, 117.39, 116.81, 73.23, 64.32 (2C), 50.75, 30.58, 28.07. COSY: 7.64–7.51, 5.96–3.54, 3.77–3.03. HSQC (140 Hz): 7.92–127.94, 7.64–129.76, 7.51–132.70, 7.05–117.39, 6.98–116.81, 5.96–73.23, 4.26–64.32, 3.77–50.75, 3.03–28.07, 2.30–30.58. HMBC (140 Hz, 8 Hz): 7.92–(136.61, 134.70, 132.70), 7.64–(140.01, 134.70, 73.23), 7.51–(136.61, 127.94), 7.05–(144.10, 128.68, 73.23), 6.98–(143.67, 132.08), 5.96–(140.01, 136.61, 132.08, 129.76, 128.68, 117.39), 4.26–(143.67, 140.01, 64.32), 3.77–(128.68, 28.07), 3.54–(136.61, 132.08, 73.23), 3.03–(195.08, 50.75), 2.30–195.08. HRMS (ESI): m/z calcd. for $C_{19}H_{18}ClNNaO_6S_2$ $[M+Na]^+$: 478.0156, found: 478.0158.

9-Chloro-2,3-dihydro-12*H*-12,6-(epithioethano)[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (26). To the solution of compound **32** (0.64 g, 1.4 mmol) in MeOH (12 mL), K_2CO_3 (0.31 g, 2.24 mmol) was added, and the reaction mixture was stirred under argon atmosphere at room temperature for 30 min. The solution obtained was diluted with water (30 mL), and aqueous HCl solution (5 m/m%, 4.2 mL) was added dropwise. The thiol intermediate separated was dissolved by adding DCM (40 mL), the layers were separated, and the aqueous layer was washed with DCM (10 mL). The combined organic phases were washed with water (15 mL), dried over Na_2SO_4 and evaporated in vacuo to give crude thiol intermediate as a dense colorless oil. It was dissolved in DCM (100 mL), *p*-TsOH·H_2O (0.057 g, 0.3 mmol, 21 mol %) was added and the reaction mixture was stirred under argon atmosphere at room temperature for 1 h. Then it was evaporated to 30 mL of volume and purified by passing it through a short silica gel column (thickness of stationary phase: 30 mm, eluent: DCM). After evaporation of the solvent, the partly crystalline residue was triturated with DIPE (5 mL) to afford **26** (0.504 g, 91%) as colorless crystals. M. p. 258–259.5 °C (CH_3CN). IR (KBr): 3449, 1506, 1338, 1304, 1159, 1062, 595 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): 7.90 (d, ^4J = 2.2 Hz, 1H), 7.46 (dd, ^4J = 2.2 Hz, ^3J = 8.4 Hz, 1H), 7.32 (d, ^3J = 8.4 Hz, 1H), 6.99 (s, 1H), 6.78 (s, 1H), 4.78 (s, 1H), 4.47 (dt, ^3J = 14.6 Hz, ^3J = 3.0 Hz, 1H), 4.24 (m, 4H), 3.50 (~t, ^3J = 14.6 Hz, 1H), 3.29 (~t, ^3J = 15.3 Hz, 1H), 2.59 (dt, ^3J = 15.3 Hz, ^4J = 2.9 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): 143.93, 143.65, 143.57, 137.04, 134.65, 133.07, 132.81, 132.15, 131.20, 127.24, 120.19, 116.13, 64.34, 64.15, 51.70, 51.52, 27.79. COSY: 7.46–7.32, (4.47, 3.50)–(3.29, 2.59). HSQC (140 Hz): 7.90–127.24, 7.46–132.81, 7.32–132.15, 6.99–120.19, 6.78–116.13, 4.78–51.52, (4.47, 3.50)–51.70, 4.24–64.34/64.15, (3.29, 2.59)–27.79. HMBC (140 Hz, 8 Hz): 7.90–(134.65, 132.81), 7.46–(134.65, 127.24), 7.32–(143.65, 133.07, 51.52), 6.99–(143.93, 137.04, 132.10), 6.78–(143.57, 131.20, 51.52), 4.78–(143.65, 137.04, 131.20,

116.13, 27.79), (4.47, 3.50)–(131.20, 27.79), 4.24–(143.93, 143.57), (3.29, 2.59)–(51.70, 51.52). HRMS (ESI): m/z calcd. for $C_{17}H_{15}ClNO_4S_2$ $[M+H]^+$: 396.0126, found: 396.0128.

9-Chloro-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepin-12-ol 7,7-dioxide (33). To a solution of **28** (9.74 g, 27.7 mmol) in an aqueous NaOH solution (5.54 g, 138.5 mmol NaOH dissolved in 250 mL of water), $NaBH_4$ (5.24 g, 138.5 mmol) was added in several portions while cooling the reaction mixture with tap water. After stirring at room temperature for 69 h (weekend), the yellow solution was cooled with ice-water, and an aqueous HCl solution (6 M, 60 mL) was added dropwise over a period of 30 min. The oily product separated was dissolved by adding DCM (300 mL), the phases were separated, the organic phase was dried over Na_2SO_4 and purified by passing through a short silica gel column (thickness of stationary phase: 35 mm, eluent: DCM, DCM/MeOH 100:1). After evaporation of the solvents, the residue (10.9 g of greyish foam) was triturated with CH_3CN to afford **33** (8.18 g, 83%) as pale pink crystals. M. p. decomp. from 180 °C. IR (KBr): 3488, 3238, 1509, 1322, 1138, 1066 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 10.37 (br s, 1H), 7.87 (m, 1H), 7.71 (m, 2H), 7.10 (s, 1H), 6.70 (s, 1H), 6.66 (br s, 1H), 6.49 (s, 1H), 4.21 (m, 4H). ^{13}C NMR (125 MHz, DMSO-d_6): 142.72, 142.26, 139.71, 139.41, 132.61, 132.42, 132.07, 127.44, 125.58, 125.27, 115.06, 113.64, 65.80, 64.32, 64.31. MS (ESI): $[M-H]^-$ = 352 (1 Cl). HRMS (ESI): m/z calcd. for $C_{15}H_{12}ClNNaO_5S$ $[M+Na]^+$: 376.0017, found: 376.0020.

9,12-Dichloro-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (34). To a vigorously stirred suspension of **33** (2.12 g, 6 mmol) in DCM (15 mL), $SOCl_2$ (0.95 g, 8 mmol, 0.58 mL) was added at room temperature. After 5 min of stirring the starting material was completely dissolved, and the product began to crystallize. Stirring was continued for 2 h, hexane (80 mL) was added dropwise to the suspension. The product was filtered, washed with hexane, and dried in vacuo to give crude **34** (2.23 g, 100%) as beige crystals. M. p. decomp. from 105 °C. IR (KBr): 3263, 1512, 1328, 1161, 1061 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.91 (d, ^4J = 2.2 Hz, 1H), 7.46 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.36 (d, ^3J = 8.4 Hz, 1H), 7.23 (br s, 1H), 7.08 (s, 1H), 6.88 (s, 1H), 5.86 (s, 1H), 4.25 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 145.13, 143.80, 141.92, 136.82, 133.38, 132.49, 131.79, 130.76, 129.06, 126.21, 121.30, 117.65, 64.30, 64.24, 63.27. MS (ESI): $[M-Cl+OH-H]^-$ = 352 (1 Cl) (after a rapid hydrolysis of **34** the compound **33** was detected).

12-(2-Bromoethoxy)-9-chloro-2,3,6,12-tetrahydro[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (35). To a stirred solution of 2-bromoethanol (4.50 g, 36 mmol, 2.56 mL) in CH_3CN (15 mL), **34** (2.23 g, 6 mmol) was added in portions at 20 °C. The thin suspension obtained was stirred at room temperature for 6 h, then it was evaporated in

vacuo. The oily residue was purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, 1:2, DCM). After evaporation of the solvents the residue was triturated with Et_2O (5 mL), filtered and dried in vacuo to give **35** (1.69 g, 61%) as off-white crystals. M. p. decomp. from 180 °C. IR (KBr): 3210, 1498, 1320, 1158, 1064 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.2 Hz, 1H), 7.67 (br s, 1H), 7.43 (dd, J_1 =2.2 Hz, ^3J = 8.3 Hz, 1H), 7.37 (d, ^3J = 8.3 Hz, 1H), 7.01 (s, 1H), 6.83 (s, 1H), 5.29 (br s, 1H), 4.22 (m, 4H), 3.84 (m, 1H), 3.79 (m, 1H), 3.50 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 144.24, 143.55, 142.13, 136.24, 133.77, 132.02, 131.12, 130.59, 129.03, 125.84, 120.05, 116.90, 83.67, 69.27, 64.31, 64.19, 30.51. MS (ESI): $[M-H]^-$ = 458 (1 Br, 1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{15}BrClNNaO_5S$ $[M+Na]^+$: 481.9435, found: 481.9431.

9-Chloro-2,3-dihydro-12*H*-12,6-(epoxyethano)[1,4]benzodioxino[6,7-*c*]benzo[*f*][1,2]thiazepine 7,7-dioxide (27). To a solution of **35** (1.475 g, 3.2 mmol) in CH_3CN (40 mL), K_2CO_3 (1.38 g, 10 mmol) was added, and the suspension obtained was stirred at room temperature for 5 h. Water (200 mL) was added dropwise. The product precipitated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column flash chromatography on a short aluminum oxide column (thickness of stationary phase: 30 mm, eluent: hexane/DCM 1:1, 1:2, DCM). After evaporation of the solvents the residue was recrystallized from CH_3CN (12 mL) to afford **27** (0.86 g, 71%) as colorless crystals. M. p. 228–229 °C (CH_3CN). IR (KBr): 1506, 1338, 1164, 1061, 612 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.89 (d, ^4J = 2.1 Hz, 1H), 7.47 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.33 (d, ^3J = 8.2 Hz, 1H), 7.03 (s, 1H), 6.81 (s, 1H), 5.48 (s, 1H), 4.23 (m, 2H), 4.21 (m, 2H), 4.18 (m, 1H), 4.10 (m, 1H), 3.74 (m, 1H), 3.56 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 144.71, 144.18, 144.03, 136.35, 134.31, 133.07, 132.47, 131.44, 130.43, 127.94, 119.70, 117.28, 83.18, 64.29, 64.17, 61.88, 52.62. NOE: 3.74–(7.03, 6.81, 5.48, 4.10, 3.56), 3.56–(7.03, 6.81, 5.48, 4.18, 3.74). COSY: 7.89–7.47–7.33, 4.23–4.21, (4.18, 3.56)–(4.10, 3.74). HSQC (140 Hz): 7.89–127.94, 7.47–132.47, 7.33–133.09, 7.03–119.70, 6.81–117.28, 5.48–83.18, 4.23–64.17, 4.21–64.29, 4.18–52.62, 4.10–61.88, 3.74–61.88, 3.56–52.62. HMQC (140 Hz, 8 Hz): 7.89–(136.35, 132.47, 131.44), 7.47–(136.35, 131.44, 127.94), 7.33–(144.71, 136.35, 83.18), 7.03–(144.03, 134.31, 130.43), 6.81–(144.18, 130.43, 119.70, 83.18), 5.48–(144.71, 134.31, 130.43, 117.28, 61.88), 4.23–(144.18, 64.29), 4.21–(144.03, 64.17), 4.18–(130.43, 83.18), 4.10–83.18, 3.74–83.18, 3.56–61.88. MS (ESI): $[M+H]^+$ = 380 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{15}ClNO_5S$ $[M+H]^+$: 380.0354, found: 380.0354.

10-Chloro-7-methyl-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepin-13-ol 8,8-dioxide (36). To a suspension of **8** (2.23 g, 6.1 mmol) in DMF (15 mL) and EtOH (15 mL), $NaBH_4$ (0.46 g, 12.2 mmol) was added, and the reaction mixture was stirred at room

temperature for 3 h. To the solution obtained water (150 mL) was added dropwise. The separated product was filtered, washed with water, and dried in vacuo to give **36** (2.00 g, 89%) as colorless crystals. The quality of the rigorously dried compound was suitable for the next reaction step. A sample of **36** (0.65 g) was purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 20 mm, eluent: DCM, DCM/MeOH 100:1). After evaporation of solvents, the oily residue was triturated with DIPE, filtered and dried in vacuo to afford **36** (0.585 g, 84%) as colorless crystals. M. p. decomp. from 155 °C. IR (KBr): 3544, 1490, 1346, 847, 589 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.77 (d, ^4J = 2.2 Hz, 1H), 7.68 (dd, ^4J = 2.3 Hz, ^3J = 8.3 Hz, 1H), 7.61 (d, ^3J = 8.3 Hz, 1H), 6.99 (d, ^3J = 8.5 Hz, 1H), 6.92 (d, ^3J = 8.5 Hz, 1H), 6.22 (d, ^3J = 4.3 Hz, 1H), 6.14 (d, ^3J = 4.2 Hz, 1H), 4.33 (m, 2H), 4.26 (m, 2H), 3.41 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6): 143.50, 142.88, 140.77, 136.68, 134.35, 133.90, 132.16, 131.50, 130.18, 126.93, 122.62, 117.62, 66.79, 64.51, 63.89, 40.72. MS (EI): $[M]^+$ = 367 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{14}ClNNaO_5S$ $[M+Na]^+$: 390.0173, found: 390.0179.

10,13-Dichloro-7-methyl-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepine 8,8-dioxide (37). To a vigorously stirred suspension of **36** (2.39 g, 6.5 mmol) in DCM (25 mL), $SOCl_2$ (0.93 g, 7.8 mmol, 0.57 mL) was added dropwise at room temperature. The solution obtained was stirred at room temperature for 1.5 h. To the suspension obtained hexane (75 mL) was added, the product was filtered, washed with hexane (2 × 8 mL) and dried in vacuo to give crude **37** (2.36 g, 94%) as colorless crystals. M. p. decomp. from 90 °C. The product was used without purification for the next reaction step. IR (KBr): 1497, 1337, 1161, 1061, 854, 577 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.97 (m, 1H), 7.47 (m, 2H), 7.00 (d, ^3J = 8.7 Hz, 1H), 6.96 (d, ^3J = 8.7 Hz, 1H), 6.72 (s, 1H), 4.20–4.40 (m, 4H), 3.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.45, 142.21, 140.50, 136.13, 133.43, 133.20, 132.73, 132.25, 127.87, 126.13, 121.52, 119.34, 64.64, 63.79, 53.59, 39.44. MS (EI): $[M]^+$ = 385 (2 Cl). HRMS (TOF MS EI): m/z calcd. for $[C_{16}H_{13}Cl_2NO_4S]^+$: 384.9942, found: 384.9940.

10-Chloro-7-methyl-13-pyrrolidin-1-yl-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepine 8,8-dioxide (38a). To the cooled solution of pyrrolidine (0.106 g, 1.5 mmol) in CH_3CN (2 mL) **37** (0.1785 g, 0.46 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (10 mL) was added dropwise, the product separated was filtered, washed with water (2 × 1 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 20 mm, eluent: DCM, DCM/MeOH 100:2). After evaporation of solvents, the residue (0.19 g of colorless oil) was triturated with DIPE (2 mL) to afford **38a** (0.153 g, 79%) as colorless crystals. M. p.

decomp. from 213 °C (CH_3CN, bright colorless crystals). IR (KBr): 1491, 1324, 1154, 1109, 1067 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.92 (m, 1H), 7.36 (m, 2H), 6.95 (d, ^3J = 8.6 Hz, 1H), 6.84 (d, ^3J = 8.7 Hz, 1H), 4.87 (s, 1H), 4.26 (m, 2H), 4.25 (m, 1H), 4.20 (m, 1H), 3.49 (s, 3H), 2.27 (m, 2H), 2.20 (m, 2H), 1.67 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 143.80, 143.56, 141.29, 135.17, 134.87, 133.62, 131.40, 130.91, 129.94, 128.12, 122.94, 117.69, 64.74, 64.20, 63.91, 53.24 (2C), 40.07, 23.17 (2C). MS (ESI): $[M+H]^+$ = 421 (1 Cl). HRMS (ESI): m/z calcd. for $C_{20}H_{22}ClN_2O_4S$ $[M+H]^+$: 421.0983, found: 421.0985.

10-Chloro-7-methyl-*N*-(2-morpholin-4-ylethyl)-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepin-13-amine 8,8-dioxide (38b). To the solution of 4-(2-aminoethyl)morpholine (0.664 g, 5.1 mmol) in CH_3CN (10 mL) **37** (0.608 g, 1.57 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (50 mL) was added dropwise in 30 min, the product separated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2). After evaporation of solvents, the residue was triturated with CH_3CN to afford **38b** (0.588 g, 78%) as colorless crystals. M. p. 203–205 °C (CH_3CN). IR (KBr): 3350, 1493, 1313, 1119, 1062 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): 7.95 (d, ^4J = 2.2 Hz, 1H), 7.42 (dd, ^4J = 2.2 Hz, ^3J = 8.2 Hz, 1H), 6.96 (d, ^3J = 8.8 Hz, 1H), 6.87 (d, ^3J = 8.7 Hz, 1H), 5.25 (s, 1H), 4.28 (m, 2H), 4.25 (m, 1H), 4.22 (m, 1H), 3.63 (m, 4H), 3.49 (s, 3H), 2.80 (br s, 1H), 2.60 (m, 2H), 2.50 (m, 1H), 2.35 (m, 1H), 2.24 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$): 143.32, 142.17, 140.80, 136.04, 134.53, 133.22, 131.56, 131.48, 128.69, 128.20, 120.32, 117.77, 66.81 (2C), 64.37, 63.83, 57.90 (2C), 53.44 (2C), 43.54, 38.51. COSY: 7.95–7.42–7.33, 6.96–6.87, 4.28–(4.25, 4.22), 3.63–2.24, 2.60–(2.50, 2.35). HSQC (140 Hz): 7.95–128.20, 7.42–131.48, 7.33–133.22, 6.96–120.32, 6.87–117.77, 5.25–57.90, 4.28–64.37, 4.25–63.83, 4.22–63.83, 3.63–66.81, 3.49–38.51, 2.60–43.54, 2.50–57.90, 2.35–57.90, 2.24–53.44. HMBC (8 Hz, 140 Hz): 7.95–(136.04, 134.53, 131.48), 7.42–(136.04, 134.53, 128.20), 7.33–(142.17, 134.53, 57.90), 6.96–(143.32, 128.69), 6.87–(140.83, 131.56), 5.25–(142.17, 140.83, 136.04, 133.22, 131.56, 128.69, 43.54), 4.28–(140.83, 63.83), (4.25, 4.22)–(143.32, 64.37), 3.63–66.81, 3.49–131.56, 2.60–57.90, (2.50, 2.35)–(53.44, 43.54), 2.24–53.44. MS (EI): $[M]^+$ = 479 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{27}ClN_3O_5S$ $[M+H]^+$: 480.1354, found: 480.1357.

Ethyl 7-[(10-chloro-7-methyl-8,8-dioxido-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepin-13-yl)amino]heptanoate (38c). To a solution of ethyl 7-aminoheptanoate (1.73 g, 10 mmol) in CH_3CN (15 mL) **37** (1.425 g, 3.7 mmol) was added, the solution obtained was stirred at room temperature for 1 h. The solution was evaporated in vacuo,

the oily residue was dissolved in DCM (40 mL), washed with water (2 × 20 mL), dried over Na_2SO_4, and evaporated in vacuo. The oily residue was purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 2:1, 1:1, DCM, DCM/MeOH 100:1). After evaporation of solvents in vacuo **38c** was obtained (1.63 g, 84%) as dense colorless oil which slowly solidified when stored at 5 °C. A small sample (0.20 g) was triturated with a little EtOH to afford **38c** (0.13 g) as colorless crystals. M. p. 81–83 °C. IR (KBr): 3326, 2928, 1726, 1493, 1322, 1146 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.94 (d, ^4J = 2.2 Hz, 1H), 7.43 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.36 (d, ^3J = 8.3 Hz, 1H), 6.93 (d, ^3J = 8.7 Hz, 1H), 6.86 (d, ^3J = 8.7 Hz, 1H), 5.30 (s, 1H), 4.19-4.33 (m, 4H), 4.11 (q, ^3J = 7.2 Hz, 2H), 3.40 (s, 3H), 2.46 (t, ^3J = 7.1 Hz, 2H), 2.25 (t, ^3J = 7.5 Hz, 2H), 2.02 (br s, 1H), 1.58 (m, 2H), 1.44 (m, 2H), 1.27 (m, 4H), 1.24 (t, ^3J = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 173.65, 143.18, 141.91, 141.24, 136.13, 134.41, 133.17, 131.78, 131.67, 128.22, 128.13, 120.44, 117.67, 64.32, 63.83, 60.11, 58.21, 47.79, 38.72, 34.17, 29.75, 28.89, 26.88, 24.77, 14.19. MS (ESI): $[M+H]^+$ = 523 (1 Cl). HRMS (ESI): m/z calcd. for $C_{25}H_{32}ClN_2O_6S$ $[M+H]^+$: 523.1664, found: 523.1671.

7-[(10-Chloro-7-methyl-8,8-dioxido-2,3,7,13-tetrahydro[1,4]benzodioxino[6,5-*c*]benzo[*f*][1,2]thiazepin-13-yl)amino]heptanoic acid (38d). To a solution of ester **38c** (1.41 g, 2.7 mmol) in EtOH (20 mL), NaOH (0.130 g, 3.25 mmol) dissolved in water (5 mL) was added at room temperature and the reaction mixture (gradually diluting suspension, later solution) was stirred at room temperature for 19 h (overnight stirring). Water (15 mL) was added, and the reaction mixture was partly evaporated in vacuo to remove ethanol. The solution obtained was neutralized with aqueous HCl solution (0.27 mL of cc. HCl dissolved in 2.7 mL of water, containing 3.25 mmol of HCl). It was stirred at room temperature for 4 h, the crystalline product obtained was filtered, washed with water (2 × 3 mL), and dried in vacuo to give **38d** (0.804, 60%) as an off-white amorphous solid. Melting range (glass-transition range): 76–85 °C. The aqueous mother liquor was extracted with EtOAc (2 × 20 mL), the combined organic phases were dried over Na_2SO_4, evaporated in vacuo, the residue was triturated with water (2 mL), the wet product was dried in vacuo to give a second crop of **38d** (0.30 g, 22%) as an off-white amorphous solid. Melting range (glass-transition range): 76–85 °C. Total yield: 1.10 g, 82%. IR (KBr): 2932, 1713, 1493, 1330, 1109, 1067 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.93 (d, ^4J = 1.5 Hz, 1H), 7.42 (m, 2H), 6.93 (d, ^3J = 8.8 Hz, 1H), 6.88 (d, ^3J = 8.7 Hz, 1H), 6.76 (br s, 2H), 5.43 (s, 1H), 4.28 (m, 3H), 4.23 (m, 1H), 3.38 (s, 3H), 2.50 (m, 2H), 2.18 (t, ^3J = 7.3 Hz, 2H), 1.52 (m, 2H), 1.45 (m, 2H), 1.24 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 177.84, 143.14, 141.78, 141.31, 134.93, 134.62, 133.69, 131.89, 131.84, 128.10, 126.14,

119.69, 118.08, 64.39, 63.85, 57.33, 47.14, 38.08, 34.44, 28.93, 28.84, 26.83, 24.83. MS (ESI): $[M+H]^+$ = 495 (1 Cl). HRMS (ESI): m/z calcd. for $C_{23}H_{28}ClN_2O_6S$ $[M+H]^+$: 495.1351, found: 495.1355.

Methyl 4-chloro-2-(2,3-dihydro-1,4-benzodioxin-5-ylsulfamoyl)benzoate (39). To a vigorously stirred solution of 2,3-dihydro-1,4-benzodioxin-5-amine (11.50 g, 76 mmol) and *N*,*N*-diethylaniline (11.34 g, 76 mmol, 12.1 mL) in MeOH (100 mL), methyl 4-chloro-2-chlorosulfonylbenzoate (**9**, 19.38 g, 72 mmol) was added over a period of 10 min while cooling the reaction mixture with tap water. The suspension formed was stirred at room temperature for 1 h, then at 0–5 °C for 1 h. The crystalline product was filtered and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, DCM). After evaporation of solvents, the solid residue was triturated with MeOH, filtered and air-dried to afford **39** (22.76 g, 82%) as colorless crystals. M. p. 134–136 °C (MeOH, bright colorless crystals). IR (KBr): 3288, 1727, 1300, 1169, 1087 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 8.30 (br s, 1H), 7.91 (d, ^4J = 2.2 Hz, 1H), 7.81 (d, ^3J = 8.3 Hz, 1H), 7.54 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.15 (dd, ^4J = 1.5 Hz, ^3J = 8.2 Hz, 1H), 6.79 (~t, ^3J = 8.2 Hz, 1H), 6.66 (dd, ^4J = 1.5 Hz, ^3J = 8.3 Hz, 1H), 4.10 (m, 2H), 4.01 (s, 3H), 4.00 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 166.37, 143.50, 140.97, 137.88, 135.52, 132.28, 132.10, 129.89, 128.53, 125.26, 120.82, 115.60, 114.30, 64.28, 63.90, 53.39. MS (ESI): $[M-H]^-$ = 382 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{15}ClNO_6S$ $[M+H]^+$: 384.0303, found: 384.0299.

Methyl 4-chloro-2-[2,3-dihydro-1,4-benzodioxin-5-yl(methyl)sulfamoyl]benzoate (40). To a solution of compound **39** (22.26 g, 58 mmol) in DMF (100 mL), anhydrous K_2CO_3 (10.42 g, 75.4 mmol) was added, and the suspension was stirred at room temperature for 15 min. To the vigorously stirred suspension iodomethane (10.70 g, 75.4 mmol, 4.7 mL) was added dropwise while cooling the reaction mixture with tap water. It was stirred at room temperature for 2 h, then water (500 mL) was added. The oily product separated, the supernatant was decanted, the oil was dissolved in DCM (100 mL), the solution was washed with water (2 × 80 mL), dried over Na_2SO_4 and diluted with heptane (125 mL). Kieselgel 60 H (for TLC, 5–40 μm, 7 g) was added and the mixture was stirred for half an hour. The adsorbent was removed by filtration, and the filtrate was evaporated in vacuo. The residue was triturated with MeOH (50 mL), the product was filtered, washed with MeOH and air-dried to afford **40** (20.00 g, 87%) as bright colorless crystals. M. p. 103–105 °C (MeOH). IR (KBr): 1745, 1477, 1350, 1283, 1117, 1079 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.73 (d, ^4J = 2.0 Hz, 1H), 7.53 (dd, ^4J = 2.1 Hz, ^3J = 8.2 Hz, 1H), 7.41 (d, ^3J = 8.2 Hz, 1H), 6.90 (dd, ^4J = 1.7 Hz, ^3J = 7.7 Hz, 1H), 6.88 (dd, ^4J = 1.7 Hz, ^3J = 8.2 Hz, 1H), 6.82 (~t, ^3J = 8.0 Hz, 1H), 4.14 (m, 2H), 3.92 (m, 2H), 3.77 (s, 3H), 3.29 (s,

3H). ^{13}C NMR (125 MHz, $CDCl_3$): 167.48, 144.37, 141.08, 139.11, 135.63, 131.80, 131.51, 129.34, 129.15, 128.32, 123.71, 120.44, 117.65, 64.05, 63.81, 53.06, 38.21. MS (EI): $[M]^+$ = 397 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{17}ClNO_6S$ $[M+H]^+$: 398.0460, found: 398.0461.

4-Chloro-2-[2,3-dihydro-1,4-benzodioxin-5-yl(methyl)sulfamoyl]benzoic acid (41). A solution of NaOH (5.48 g, 137 mmol) in water (100 mL) was added to the suspension of compound **40** (21.80 g, 54.8 mmol) in MeOH (100 mL) and the mixture was refluxed for 1 h. The solution thus obtained was diluted with water (600 mL), aqueous HCl solution (5 m/m %, 100 mL, 105 g, 144 mmol HCl) was added while cooling the reaction mixture with tap water. The sticky oily product separated from the reaction mixture (pH 1) slowly crystallized while stirring at room temperature for 1 h. It was filtered, washed with water (3 × 60 mL), and dried over P_2O_5 to afford crude **41** (20.45 g, 97%) as off-white crystals of suitable quality for next reaction step. M. p. 188–191 °C (CH_3CN, decomp.). IR (KBr): 2883, 1707, 1353, 1303, 1169, 1080, 1060, 979 cm^{-1}. ^{1}H NMR (500 MHz, DMSO-*d*$_6$): 13.57 (br s, 1H), 7.80 (dd, ^4J = 2.2 Hz, ^3J = 8.2 Hz, 1H), 7.64 (d, ^3J = 8.2 Hz, 1H), 7.52 (d, ^4J = 2.0 Hz, 1H), 6.90 (dd, ^4J = 1.8 Hz, ^3J = 8.1 Hz, 1H), 6.83 (~t, ^3J = 8.0 Hz, 1H), 6.79 (dd, ^4J = 2.0 Hz, ^3J = 8.1 Hz, 1H), 4.15 (m, 2H), 3.93 (m, 2H), 3.20 (s, 3H). ^{13}C NMR (125 MHz, DMSO-*d6*): 168.21, 144.50, 141.21, 137.75, 133.97, 133.44, 132.77, 129.92, 128.49, 128.35, 123.24, 120.39, 117.60, 64.23, 63.83, 38.17. MS (ESI): $[M-H]^-$ = 382 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{15}ClNO_6S$ $[M+H]^+$: 384.0303, found: 384.0302.

10-Chloro-13-methyl-2,3-dihydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepin-7(13*H*)-one 12,12-dioxide (42). To the thin suspension of **41** (19.80 g, 51.6 mmol) in DCM (165 mL), PCl_5 (12.91 g, 62 mmol, 1.2 equiv) was added in two portions (effervescence!), and the solution obtained was refluxed for 9 h. The solution was cooled to 0–5 °C, and $SnCl_4$ (29.60 g, 113.5 mmol, 13.3 mL, 2.2 equiv) was added. The suspension obtained was stirred at 0–5 °C for 1.5 h, then it was allowed to warm to room temperature (approx. 1 h). It was diluted with DCM (165 mL), poured onto a mixture of crushed ice (600 g) and conc. hydrochloric acid (85 mL, 100 g, 1 mol of HCl). The crystalline product separated was filtered, washed with diluted hydrochloric acid (5%, 2 × 50 mL) and water (2 × 50 mL), and air-dried to give crude **42** (10.93 g of off-white solid). The two-phase filtrate was separated, the strongly acidic aqueous phase was washed with DCM (100 mL), the combined organic phases were washed with aqueous HCl solution (5 m/m %, 100 mL), dried over Na_2SO_4, evaporated in vacuo, and the residue was triturated with DIPE to afford a second crop of crude **42** (6.88 g of pale pink solid). The two crops combined were purified by dry-column flash chromatography on a short silica gel column (thickness of the stationary phase: 30 mm, eluent: DCM). After evaporation of the

solvent, the residue was triturated with CH_3CN (50 mL) to give pure **42** (16.28 g, 86%) as colorless crystals. M. p. 265–267 °C (CH_3CN/EtOH 1:1). IR (KBr): 1643, 1601, 1578, 1354, 1278, 1170, 1078, 996 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$+CD_3OD): 8.01 (d, ^3J = 8.4 Hz, 1H), 7.98 (d, ^4J = 2.1 Hz, 1H), 7.89 (d, ^3J = 9.0 Hz, 1H), 7.70 (dd, ^4J = 2.1 Hz, ^3J = 8.3 Hz, 1H), 6.98 (d, ^3J = 9.0 Hz, 1H), 4.41 (m, 2H), 4.39 (m, 2H), 3.10 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$+CD_3OD): 187.60, 149.34, 138.61, 138.50, 137.56, 134.08, 133.85, 133.11, 130.50, 126.43, 125.94, 124.37, 116.27, 64.33, 64.10, 37.74. HSQC (140 Hz): 8.01–133.85, 7.98–126.43, 7.89–124.37, 7.70–133.11, 6.98–116.27, 4.41–64.10, 4.39–64.33, 3.10–37.74. HMQC (140 Hz, 8 Hz): 8.01–(187.60, 138.50, 137.56), 7.98–(138.50, 133.11), 7.89–(187.60, 149.34, 130.50), 7.70–(138.50, 134.08, 126.43), 6.98–(149.34, 138.61, 125.94), 4.41–(138.61, 64.33), 4.39–(149.34, 64.10), 3.10–130.50. MS (EI): $[M]^+$ = 365 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{13}ClNO_5S$ $[M+H]^+$: 366.0197, found: 366.0200.

10-Chloro-13-methyl-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepin-7-ol 12,12-dioxide (43). To a suspension of **42** (5.49 g, 15 mmol) in DMF (30 mL) and EtOH (30 mL), $NaBH_4$ (1.135 g, 30 mmol) was added, and the reaction mixture was stirred at room temperature for 4.5 h. Water (300 mL) was added dropwise over 30 min. The separated product was filtered, washed with water and Et_2O, and air-dried to give TLC pure crude **43** (5.32 g, 96%) as colorless crystals. M. p. decomp. from 208 °C (CH_3CN/EtOH 1:1). IR (KBr): 3484, 1493, 1304, 1070, 984 cm^{-1}. This compound is a 6:4 mixture of two conformers in DMSO-d_6 solution at 25 °C. ^1H NMR (500 MHz, DMSO-d_6): 7.92 (m, 0.6H), 7.80–7.65 (m, 2.2H), 7.05–6.98 (d, 1H), 6.96–6.86 (m, 1H), 6.57 (br s, 0.6H), 6.24 (br s, 0.4H), 6.18 (br s, 0.6H), 5.73 (br s, 0.4H), 4.40–4.20 (m, 4H), 3.40–3.20 (m, 3H, overlapped with water signal of DMSO-d_6). ^{13}C NMR (125 MHz, DMSO-d_6): 144.49, 143.49, 141.62, 140.83, 140.00, 138.14, 137.42, 134.06, 133.83, 133.45, 132.53, 132.29, 131.98, 127.06, 126.65 (126.60, shoulder), 122.57, 121.16, 117.54, 116.68, 115.94, 75.41, 65.97, 64.58, 64.08, 40.30, 40.13, 39.96, 39.79, 38.90, 36.02. MS (EI): $[M]^+$: 367 (1 Cl). HRMS (ESI): m/z calcd. for $C_{16}H_{14}ClNNaO_5S$ $[M+Na]^+$: 390.0173, found: 390.0170.

7,10-Dichloro-13-methyl-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepine 12,12-dioxide (44). To a vigorously stirred suspension of **43** (5.74 g, 15.6 mmol) in DCM (250 mL), $SOCl_2$ (7.43 g, 62.4 mmol, 4.5 mL, 4 equiv) was added dropwise at room temperature. The suspension was stirred at room temperature for 2 h (no solution was obtained). To the suspension hexane (500 mL) was added, the product was filtered, washed with hexane (2 × 30 mL) and dried in vacuo to give crude **44** (5.65 g, 94%). M. p. decomp. from 250 °C. The compound is of suitable quality for the next step. IR (KBr): 1504,

1477, 1336, 1319, 1160, 670 cm^{-1}. No NMR spectra of **44** could be recorded due to the extremely low solubility of this compound in the usual NMR solvents and their mixtures as well.

10-Chloro-*N*,13-dimethyl-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepin-7-amine 12,12-dioxide (45a). To the cold solution of methylamine (0.62 g, 20 mmol) in dioxane (15 mL) crude **44** (1.545 g, 4 mmol) was added, and the suspension obtained was stirred at 5–10 °C for 2 h and at room temperature for 1 h. To the thin suspension water (50 mL) was added dropwise, the product precipitated was filtered, washed with water (2 × 5 mL), air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents, the solid residue was triturated with CH_3CN (5 mL) to afford **45a** (1.30 g, 85%) as colorless crystals. M. p. 187–189 °C (CH_3CN). IR (KBr): 3323, 1498, 1327, 1157, 1070 cm^{-1}. This compound is a 16:9 mixture of two conformers in DMSO-d_6 solution at 25 °C. At elevated temperature (352 K) the signals of the two species coalesced. ^{1}H NMR (500 MHz, $CDCl_3$): 7.77–7.64 (m, 2.2H), 7.58 (d, ^3J = 8.4 Hz, 0.64H), 6.93–6.86 (m, 2H), 5.12 (d, ^3J = 8.4 Hz, 0.35H), 4.67 (s, 0.63H), 4.40–4.20 (m, 4H), 3.37 (s, 1.9H), 3.24 (s, 1.06H), 3.01 (m, 0.4H), 2.33 (d, ^3J = 4.4 Hz, 1.1H), 2.28 (br s, 0.64H), 2.09 (br s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): (33 signals) 144.42, 143.28, 143.20, 142.03, 141.41, 140.39, 138.77, 136.87, 134.65, 133.52, 133.31, 132.27, 132.11, 131.72, 128.81, 127.36, 126.51, 126.13, 125.01, 122.58, 117.81, 117.23, 116.79, 70.22, 64.53, 64.51, 64.07, 64.03, 60.40, 38.41, 36.49, 34.90, 34.59. MS (ESI): $[M+H]^+$ = 381 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{18}ClN_2O_4S$ $[M+H]^+$: 381.0670, found: 381.0668.

10-Chloro-13-methyl-7-pyrrolidin-1-yl-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepine 12,12-dioxide (45b). To the solution of pyrrolidine (0.85 g, 12 mmol, 1.0 mL) in CH_3CN (30 mL) crude **44** (1.55 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1 h. Water (150 mL) was added dropwise, the product separated was filtered, washed with water (3 × 5 mL), air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1). After evaporation of solvents, the residue was triturated with Et_2O (5 mL) to afford **45b** (1.24 g, 74%) as colorless crystals. M. p. 189–191 °C (CH_3CN). IR (KBr): 2937, 1496, 1306, 1153, 1069 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.94 (d, ^4J = 2.2 Hz, 1H), 7.35 (dd, ^4J = 2.2 Hz, ^3J = 8.3 Hz, 1H), 7.29 (d, ^3J = 8.3 Hz, 1H), 6.79 (d, ^3J = 8.4 Hz, 1H), 6.73 (d, ^3J = 8.6 Hz, 1H), 4.37 (m, 1H), 4.35 (m, 1H), 4.28 (m, 2H), 4.04 (s, 1H), 3.42 (s, 3H), 2.21 (m, 2H), 2.14 (m, 2H), 1.67 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 144.58,

143.45, 142.35, 135.64, 134.82, 134.77, 133.05, 130.88, 128.09, 125.66, 121.29, 117.12, 76.53, 64.48, 64.11, 53.65 (2C), 38.11, 23.16 (2C). MS (ESI): $[M+H]^+$ = 421 (1 Cl). HRMS (ESI): m/z calcd. for $C_{20}H_{22}ClN_2O_4S$ $[M+H]^+$: 421.0983, found: 421.0983.

1-(10-Chloro-13-methyl-12,12-dioxido-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepin-7-yl)piperidine-4-carboxamide (45c). To the solution of piperidine-4-carboxamide (isonipecotamide, 1.13 g, 8.8 mmol) in CH_3CN (140 mL) crude **44** (1.545 g, 4 mmol) was added. The suspension obtained was stirred at room temperature for 1 h. Water (300 mL) was added dropwise, the product separated was collected by filtration, washed with water (2 × 10 mL), air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM/MeOH 100:3). After evaporation of solvents, the solid residue was triturated with CH_3CN (15 mL) to afford **45c** (1.60 g, 84%) as colorless crystals. M. p. decomp. from 272 °C (CH_3CN). IR (KBr): 3419, 3198, 1682, 1494, 1307, 1151 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.77 (d, ^4J = 2.2 Hz, 1H), 7.64 (dd, ^4J = 2.2 Hz, J_2 =8.3 Hz, 1H), 7.56 (d, ^3J = 8.4 Hz, 1H), 7.20 (br s, 1H), 6.88 (d, ^3J = 8.4 Hz, 1H), 6.86 (d, ^3J = 8.4 Hz, 1H), 6.72 (br s, 1H), 4.39 (m, 1H), 4.31 (m, 2H), 4.26 (s, 1H), 4.25 (m, 1H), 3.37 (s, 3H), 2.50 (m, 1H), 2.28 (m, 1H), 2.04 (m, 1H), 1.82 (m, 2H), 1.59 (m, 2H), 1.43 (m, 2H). ^{13}C NMR (125 MHz, DMSO-d_6): 176.52, 144.54, 143.44, 142.54, 135.11, 135.04, 133.95, 133.88, 131.42, 127.31, 125.04, 122.28, 117.11, 75.35, 64.52, 64.07, 52.14, 51.82, 41.57, 38.70, 28.85, 28.38. MS (ESI): $[M+H]^+$ = 478 (1 Cl). HRMS (ESI): m/z calcd. for $C_{22}H_{25}ClN_3O_5S$ $[M+H]^+$: 478.1198, found: 478.1201.

10-Chloro-7-methoxy-13-methyl-2,3,7,13-tetrahydro[1,4]benzodioxino[5,6-*c*]benzo[*f*][1,2]thiazepine 12,12-dioxide (46). To a suspension of crude **44** (0.309 g, 0.8 mmol) in DCM (3 mL) MeOH (3 mL) was added and the solution obtained in 5 min was stirred at room temperature for further 40 min. The solution was evaporated in vacuo, the residue was subjected to dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 1:2, DCM). After evaporation of solvents, the solid residue was triturated with Et_2O to afford **46** (0.233 g, 76%) as colorless crystals. M. p. decomp. from 185 °C (MeOH). IR (KBr): 2937, 1493, 1319, 1302, 1074, 982 cm^{-1}. This compound is a 6:4 mixture of two conformers in $CDCl_3$ solution at 25 °C. ^1H NMR (500 MHz, $CDCl_3$): 7.97 (br s, 0.40H), 7.87 (br s, 0.32H), 7.71 (m, 0.43H), 7.48–7.35 (m, 1.5H), 6.85 (m, 2H), 5.75 (br s, 0.43H), 5.00 (br s, 0.55H), 4.42–4.25 (m, 4H), 3.58 (br s, 1.33H), 3.47 (br s, 1.33H), 3.37 (br s, 1.67H), 3.22 (br s, 1.67H). ^{13}C NMR (125 MHz, $CDCl_3$): (31 signals) 145.32, 143.88, 142.60, 142.31, 142.20, 139.96, 137.49, 135.52, 135.30, 133.88, 133.39, 133.26, 131.74, 131.62, 131.13, 128.01, 127.89, 126.21, 125.43, 123.09, 122.14, 118.00,

117.00, 115.42, 87.33, 64.47, 64.11, 58.46, 56.80, 38.31, 35.69. MS (EI): $[M]^+$ = 381 (1 Cl). HRMS (ESI): m/z calcd. for $C_{17}H_{20}ClN_2O_5S$ $[M+NH_4]^+$: 399.0776, found: 399.0775.

Methyl 2-[(2,3-dihydro-1,4-benzodioxin-6-ylsulfonyl)amino]benzoate (48). To the solution of 2,3-dihydro-1,4-benzodioxine-6-sulfonyl chloride (**47**, 23.47 g, 100 mmol) in pyridine (100 mL) methyl anthranilate (13.61 g, 90 mmol, 11.6 mL) was added at 0—5 °C, and the reaction mixture (suspension after 10 min) was stirred at 0–5 °C for 4 h, then at room temperature for 13 h. Water (600 mL) was added dropwise, the product was filtered, washed with water (3 × 80 mL) to give crude **48** (29.78 g, 95%) as colorless crystals. M. p. 158–160 °C (MeOH). IR (KBr): 3151, 1690, 1499, 1286, 1254, 1154, 1085 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 10.62 (br s, 1H), 7.92 (m, 1H), 7.66 (m, 1H), 7.45 (m, 1H), 7.38 (d, ^4J = 2.2 Hz, 1H), 7.34 (dd, ^4J = 2.3 Hz, ^3J = 8.5 Hz, 1H), 7.03 (m, 1H), 6.86 (d, ^3J = 8.5 Hz, 1H), 4.26 (m, 2H), 4.23 (m, 2H), 3.88 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 168.25, 147.63, 143.40, 140.48, 134.45, 131.72, 131.09, 122.65, 120.96, 118.71, 117.60, 116.86, 115.67, 64.43, 64.03, 52.41. MS (EI): $[M]^+$ = 349. HRMS (ESI): m/z calcd. for $C_{16}H_{16}NO_6S$ $[M+H]^+$: 350.0693, found: 350.0698.

Methyl 2-[(2,3-dihydro-1,4-benzodioxin-6-ylsulfonyl)(methyl)amino]benzoate (49).

Method A: To a suspension of compound **48** (29.70 g, 85 mmol) in DMF (85 mL), anhydrous K_2CO_3 (15.27 g, 110.5 mmol, 1.3 equiv) was added, and the suspension was stirred at room temperature for 15 min. Iodomethane (15.68 g, 110.5 mmol, 6.9 mL, 1.3 equiv) was added dropwise while cooling the reaction mixture with tap water. The suspension was stirred at room temperature for 22 h. Water (425 mL) was added, the product precipitated was filtered, washed with water, and air-dried to afford crude **49** (30.73 g, 99%) as off-white crystals. The product was of suitable quality for the next reaction step. Method B: To the ice-cooled solution of 2,3-dihydro-1,4-benzodioxine-6-sulfonyl chloride (**47**, 2.35 g, 10 mmol) in abs. pyridine (10 mL) methyl *N*-methylanthranilate (1.65 g, 10 mmol, 1.47 mL) was added dropwise. The reaction mixture was stirred at 0–5 °C for 2 h, then at room temperature for 17 h (overnight). The suspension obtained was added to an aqueous HCl solution (5 m/m %, 100 mL). The oily product was separated, DCM (50 mL) was added, the phases were separated, the aqueous phase was washed with DCM (40 mL), the combined organic phases were washed with aqueous HCl solution (5 m/m %, 20 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 30 mm, eluent: heptane/DCM 1:1, DCM, DCM/MeOH 100:1). After evaporation of solvents, the oily residue was triturated with MeOH to afford **49** (2.60 g, 71%) as colorless crystals. M. p. 96–98 °C (MeOH). IR (KBr): 1734, 1496, 1338, 1290, 1255, 1064

cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): 7.83 (dd, ^{4}J = 1.8 Hz, ^{3}J = 7.7 Hz, 1H), 7.43 (m, 1H), 7.37 (m, 1H), 7.21 (d, ^{4}J = 2.2 Hz, 1H), 7.11 (dd, ^{4}J = 2.2 Hz, ^{3}J = 8.5 Hz, 1H), 6.98 (dd, ^{4}J = 1.3 Hz, ^{3}J = 7.7 Hz, 1H), 6.90 (d, ^{3}J = 8.6 Hz, 1H), 4.31 (m, 2H), 4.29 (m, 2H), 3.88 (s, 3H), 3.25 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): 166.87, 147.27, 142.32, 140.15, 132.22, 132.12, 130.97, 128.57, 128.02, 121.36, 117.41, 117.16, 64.49, 64.11, 52.36, 38.79. MS (EI): $[M]^+$ = 363. HRMS (ESI): m/z calcd. for $C_{17}H_{18}NO_6S$ $[M+H]^+$: 364.0849, found: 364.0850.

2-[(2,3-Dihydro-1,4-benzodioxin-6-ylsulfonyl)(methyl)amino]benzoic acid (50). A solution of NaOH (8.46 g, 211.5 mmol) in water (140 mL) was added to the suspension of crude **49** (30.71 g, 84.5 mmol) in MeOH (140 mL) and the mixture was refluxed for 1 h. The solution thus obtained was diluted with water (700 mL), aqueous HCl solution (5 m/m %, 200 mL, 210 g, 288 mmol HCl) was added over 20 min while cooling the reaction mixture with ice water. The sticky oily product separated slowly crystallized while stirring at room temperature for 1 h. It was collected by filtration, washed with water (3 × 60 mL) and dried in vacuo over P_2O_5 to afford crude **50** (29.01 g, 95%) as colorless crystals. M. p. 171–173 °C (CH_3CN, decomp.). The quality of the dried product was suitable for the next reaction step. IR (KBr): 1679, 1496, 1346, 1290, 1062 cm^{-1}. ^{1}H NMR (600 MHz, DMSO-d_6): 12.94 (br s, 1H), 7.74 (m, 1H), 7.48 (m, 1H), 7.44 (m, 1H), 7.04 (m, 1H), 7.04 (m, 1H), 7.03 (m, 1H), 6.91 (m, 1H), 4.35 (m, 2H), 4.31 (m, 2H), 3.14 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6): 167.62, 147.54, 143.50, 139.65, 133.66, 132.09, 130.43, 130.35, 128.35, 128.29, 121.13, 117.81, 116.44, 64.64, 64.25, 38.87. COSY: 7.74–7.44–7.48-6.91, 7.04–7.04–7.03, 4.35–4.31. HSQC (140 Hz): 7.74–130.43, 7.48–132.09, 7.44–128.35, 7.04–121.13, 7.04–117.81, 7.03–116.44, 6.91–128.29, 4.35–64.64, 4.31–64.25, 3.14–38.87. HMBC (8 Hz, 140 Hz): 7.74–(167.62, 139.65, 132.09), 7.48–(139.65, 130.43), 7.44–(133.66, 128.29), 7.04–(147.54, 116.44), 7.04–(143.50, 130.35), 7.03–(147.54, 121.13), 6.91–(133.66, 128.35), 4.35–147.54, 4.31–143.50, 3.14–139.65. MS (EI): $[M]^+$ = 349. HRMS (ESI): m/z calcd. for $C_{16}H_{16}NO_6S$ $[M+H]^+$: 350.0693, found: 350.0694.

7-Methyl-2,3-dihydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12(7*H*)-one 6,6-dioxide (51). To the suspension of **50** (17.47 g, 50 mmol) in DCM (250 mL), $SOCl_2$ (8.93 g, 75 mmol, 5.5 mL) was added and the reaction mixture was refluxed for 8.5 h. The solution obtained was cooled to 0–5 °C, and anhydrous $AlCl_3$ (10.00 g, 75 mmol) was added. The solution was stirred at 0–5 °C for 1.5 h, then it was refluxed for 3 h. The brown solution was poured onto a mixture of crushed ice (300 g) and diluted aqueous hydrochloric acid (5 m/m %, 100 mL). After the ice melted the phases were separated, the aqueous phase was washed with DCM (100 mL), the combined organic phases were washed with water (100 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was subjected to dry-column flash

chromatography on a short silica gel column (thickness of the stationary phase: 30 mm, eluent: heptane/DCM 2:1, 1:1, 1:2, DCM, DCM/MeOH 100:1, 100:2). After evaporation of the solvents, the solid residue was triturated with Et_2O (20 mL) to give pure **51** (4.26 g, 26%) as pale yellow crystals. M. p. 194–196 °C (CH_3CN). IR (KBr): 1648, 1350, 1299, 1159, 1066, 894 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 8.29 (m, 1H), 7.61 (m, 1H), 7.55 (s, 1H), 7.48 (s, 1H), 7.36 (m, 1H), 7.34 (m, 1H), 4.36 (m, 2H), 4.34 (m, 2H), 3.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 188.81, 147.09, 146.39, 141.32, 134.49, 132.13, 131.70, 130.42, 129.60, 126.18, 125.32, 121.32, 115.48, 64.63, 64.36, 39.19. NOE: 3.30–(7.48, 7.34). COSY: 8.29–7.36–7.61–7.34, 4.36–4.34. HSQC (140 Hz): 8.29–132.13, 7.61–134.49, 7.55–121.32, 7.48–115.48, 7.36–126.18, 7.34–125.32, 4.36–64.36, 4.34–64.63, 3.30–39.19. HMQC (140 Hz, 8 Hz): 8.29–(188.81, 141.32, 134.49), 7.61–(141.32, 132.13), 7.55–(188.81, 146.39, 130.42), 7.48–(147.09, 129.60), 7.36–(131.70, 125.32), 7.34–(131.70, 126.18), 4.36–(146.39, 64.63), 4.34–(147.09, 64.36), 3.30–141.32. MS (EI): $[M]^+$ = 331. HRMS (ESI): m/z calcd. for $C_{16}H_{14}NO_5S$ $[M+H]^+$: 332.0587, found: 332.0582.

7-Methyl-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-ol 6,6-dioxide (52). To a suspension of **51** (4.10 g, 12.4 mmol) in DMF (25 mL) and abs. EtOH (25 mL), $NaBH_4$ (0.91 g, 24 mmol) was added, and the reaction mixture was stirred at room temperature for 4 h. To the solution obtained water (400 mL) was added dropwise. The product separated was filtered, washed with water, air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 200:1). After evaporation of solvents, the residue was triturated with DIPE (30 mL) to afford **52** (3.86 g, 93%) as colorless crystals. M. p. decomp. from 180 °C. IR (KBr): 3485, 1570, 1493, 1291, 1134, 1061 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): 7.58 (m, 1H), 7.46 (m, 1H), 7.36 (m, 1H), 7.34 (m, 1H), 7.28 (d, ^4J = 0.9 Hz, 1H), 7.19 (s, 1H), 6.44 (d, ^3J = 5.1 Hz, 1H), 6.18 (d, ^3J = 5.1 Hz, 1H), 4.30 (m, 2H), 4.27 (m, 2H), 3.32 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6): 146.54, 143.21, 142.67, 136.92, 134.90, 129.73, 128.71, 128.04, 127.55, 125.62, 116.13, 114.37, 67.70, 64.75, 64.36, 37.07. MS (EI): $[M]^+$ = 333. HRMS (ESI): m/z calcd. for $C_{16}H_{16}NO_5S$ $[M+H]^+$: 334.0744, found: 334.0741.

12-Chloro-7-methyl-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepine 6,6-dioxide (53). To a vigorously stirred suspension of **52** (3.50 g, 10.5 mmol) in DCM (25 mL), $SOCl_2$ (1.50 g, 12.6 mmol, 0.92 mL) was added dropwise at room temperature. The solution obtained turned to a thick suspension. It was stirred at room temperature for 2 h, then hexane (50 mL) was added, the product was filtered, washed with hexane (2 × 10 mL) and dried in vacuo to give crude **53** (3.50 g, 95%) as colorless crystals. M. p. decomp. from 175 °C. The

product was suitable for the next reaction step without further purification. IR (KBr): 1499, 1325, 1299, 1134, 1064, 926, 890 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.51 (s, 1H), 7.50 (m, 1H), 7.47 (m, 1H), 7.39 (m, 1H), 7.32 (m, 1H), 7.03 (s, 1H), 6.06 (s, 1H), 4.29 (m, 4H), 3.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): 146.22, 144.50, 139.38, 137.89, 133.03, 131.16, 129.74, 129.21, 128.57, 128.49, 119.78, 117.25, 64.56, 64.36, 64.15, 38.90. MS (ESI): $[M\text{-}Cl\text{-}OH\text{-}H]^-$ = 332, $[M+CH_3CN+Na]^+$ = 397 (after a rapid hydrolysis of **53**, compound **52** was detected). HRMS (TOF MS EI): m/z calcd. for $[C_{16}H_{14}ClNO_4S]^+$: 351.0332, found: 351.0331.

***N*,7-Dimethyl-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-amine 6,6-dioxide (54a).** To the solution of methylamine (0.78 g, 25 mmol) in dioxane (23 mL) crude **53** (1.76 g, 5 mmol) was added, and the suspension obtained was stirred at room temperature for 1.5 h. Water (75 mL) was added dropwise, the product separated was filtered, washed with water (2 × 10 mL), air-dried and purified by dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1). After evaporation of solvents, the residue was triturated with DIPE (10 mL), filtered and recrystallized from CH_3CN (9 mL) to afford **54a** (1.29 g, 75%) as colorless crystals. M. p. 182–184 °C (CH_3CN). IR (KBr): 3362, 1573, 1494, 1287, 1066, 895, 562 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.51 (s, 1H), 7.39 (m, 1H), 7.32 (m, 2H), 7.26 (m, 1H), 6.96 (s, 1H), 4.78 (s, 1H), 4.29 (m, 2H), 4.27 (m, 2H), 3.27 (s, 3H), 2.35 (s, 3H), 2.30 (br s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): 146.30, 142.65, 139.19, 138.07, 131.82, 130.47, 130.41, 128.89, 127.50, 127.48, 118.72, 118.30, 67.97, 64.61, 64.20, 38.55, 34.80. MS (ESI): $[M+H]^+$ = 347. HRMS (ESI): m/z calcd. for $C_{17}H_{19}N_2O_4S$ $[M+H]^+$: 347.1060, found: 347.1060.

7-Methyl-12-pyrrolidin-1-yl-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepine 6,6-dioxide (54b). To the solution of pyrrolidine (0.78 g, 11 mmol) in CH_3CN (15 mL) crude **53** (1.76 g, 5 mmol) was added. The suspension obtained was stirred at room temperature for 1 h. Water (30 mL) was added dropwise, the product separated was filtered, washed with water (2 × 5 mL), air-dried, and purified by dry-column chromatography on a short aluminum oxide column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 1:1, DCM). After evaporation of solvents, the residue was triturated with DIPE (10 mL) to afford TLC-pure **54b** (1.53 g, 79%) as colorless crystals. M. p. decomp. from 210 °C (CH_3CN). IR (KBr): 1503, 1311, 1293, 1135, 1066, 562 cm^{-1}.^1H NMR (500 MHz, $CDCl_3$): 7.47 (s, 1H), 7.43 (m, 1H), 7.34 (m, 1H), 7.29 (m, 1H), 7.25 (m, 1H), 6.89 (s, 1H), 4.27 (m, 1H), 4.24 (m, 1H), 4.23 (m, 2H), 4.11 (s, 1H), 3.50 (s, 3H), 2.25 (m, 4H), 1.69 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 145.36, 143.45, 142.18, 138.27, 133.73, 131.56, 130.38, 129.74, 129.51, 128.40,

119.27, 117.50, 75.80, 64.59, 64.21, 53.67 (2C), 39.44, 23.26 (2C). MS (ESI): $[M+H]^+$ = 387. HRMS (ESI): m/z calcd. for $C_{20}H_{23}N_2O_4S$ $[M+H]^+$: 387.1373, found: 387.1376.

7-Methyl-*N*-(2-morpholin-4-ylethyl)-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-amine 6,6-dioxide (54c). To the solution of 4-(2-aminoethyl)morpholine (1.15 g, 8.8 mmol) in CH_3CN (15 mL) crude **53** (1.41 g, 4 mmol) was added. The suspension formed was stirred at room temperature for 1.5 h. Water (50 mL) was added dropwise, and an oily product separated. Water (20 mL) and DCM (20 mL) were added, and stirring was continued for 10 min. The phases were separated, the aqueous phase was washed with DCM (20 mL), the combined organic phase was washed with water (20 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by dry-column flash chromatography first on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1, 100:2). After evaporation of solvents, the residue was purified again by dry-column flash chromatography on a short aluminum oxide column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 1:1, 1:2, DCM, DCM/MeOH 100:1). After evaporation of solvents, the residue was crystallized from CH_3CN to afford **54c** (1.31 g, 74%) as colorless crystals. M. p. 142–144 °C (CH_3CN). IR (KBr): 3347, 1575, 1333, 1308, 1287, 1118, 1066, 896 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 7.49 (s, 1H), 7.36 (m, 2H), 7.32 (m, 1H), 7.25 (m, 1H), 6.97 (s, 1H), 4.92 (s, 1H), 4.28 (m, 2H), 4.25 (m, 2H), 3.67 (m, 4H), 3.36 (s, 3H), 2.73 (br s, 1H), 2.62 (m, 2H), 2.52 (m, 1H), 2.46 (m, 1H), 2.35 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 146.21, 142.72, 139.51, 138.84, 132.63, 130.77, 129.33, 128.84, 127.65, 127.40, 118.06, 117.86, 66.87 (2C), 65.39, 64.60, 64.16, 58.19, 53.63 (2C), 44.11, 37.95. MS (EI): $[M]^+$ = 445. HRMS (ESI): m/z cald. for $C_{22}H_{28}N3O_5S$ $[M+H]^+$: 446.1744, found: 446.1740.

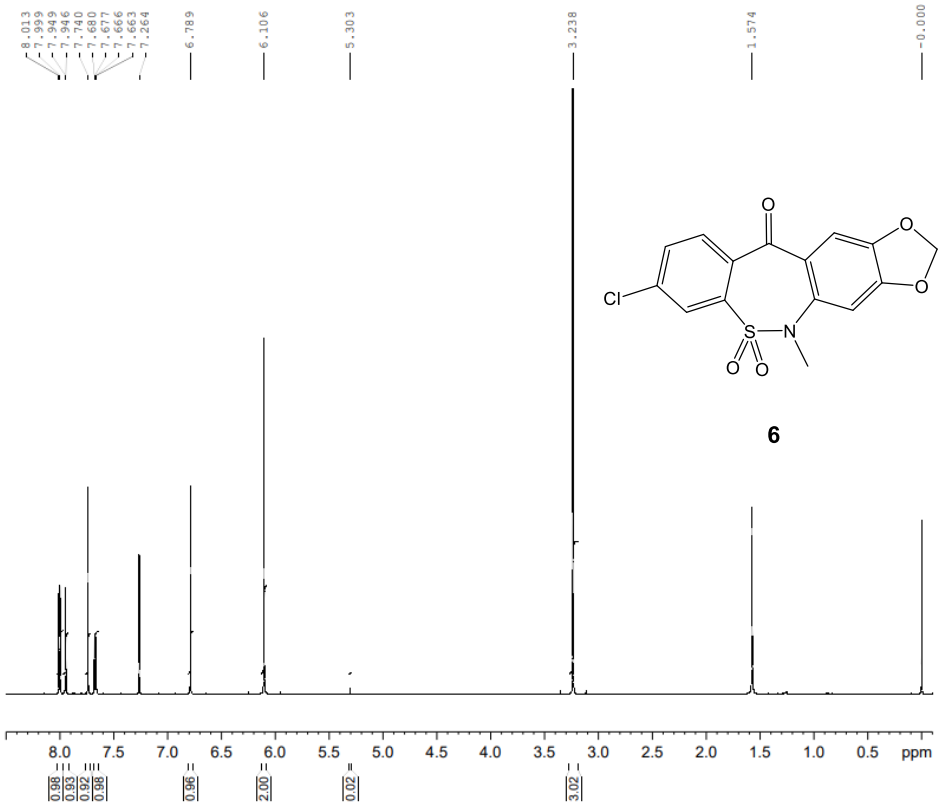
7-Methyl-*N*-(3-morpholin-4-ylpropyl)-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-amine 6,6-dioxide (54d). To the solution of 4-(3-aminopropyl)morpholine (1.27 g, 8.8 mmol) in CH_3CN (15 mL) crude **53** (1.41 g, 4 mmol) was added. The solution obtained was stirred at room temperature for 1 h, then it was evaporated in vacuo. The residue was dissolved in DCM (30 mL), the solution was washed with water (2 × 20 mL), dried over Na_2SO_4, and evaporated in vacuo. The residue was purified by dry-column flash chromatography firstly on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:1, 100:2, 100:3). After evaporation of solvents, the residue was purified again by dry-column flash chromatography on a short aluminum oxide column (thickness of stationary phase: 25 mm, eluent: heptane/DCM 1:1, DCM, DCM/MeOH 100:1). After evaporation of solvents, the residue was triturated with CH_3CN to afford **54d** (1.51 g, 82%) as colorless crystals. M. p. 149–151 °C (CH_3CN). IR (KBr): 3354, 1574, 1493, 1333,

1060, 896, 708 cm^{-1}. ^{1}H NMR (500 MHz, CDCl3): 7.49 (s, 1H), 7.37 (m, 1H), 7.35 (m, 1H), 7.31 (m, 1H), 7.27 (m, 1H), 7.00 (m, 1H), 4.99 (s, 1H), 4.28 (m, 2H), 4.24 (m, 2H), 3.67 (m, 4H), 3.32 (s, 3H), 2.58 (m, 3H), 2.42 (m, 6H), 1.70 (~qn, ^{3}J = 6.7 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): 146.32, 142.58, 139.55, 138.83, 132.92, 130.39, 129.07, 128.67, 127.53, 127.35, 118.13, 117.39, 66.88 (2C), 64.59, 64.13, 57.24, 53.71 (2C), 46.61, 37.92, 26.47. MS (ESI): $[M+H]^+$ = 460. HRMS (ESI): m/z calcd. for $C_{23}H_{30}N_3O_5S$ $[M+H]^+$: 460.1901, found: 460.1896.

Ethyl 7-[(7-methyl-6,6-dioxido-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-yl)amino]heptanoate (54e). To a solution of ethyl 7-aminoheptanoate (3.47 g, 20 mmol) in CH_3CN (25 mL) crude **53** (3.17 g, 9 mmol) was added which led to a slightly exothermic reaction. The solution obtained was stirred at room temperature for 1 h, then it was evaporated in vacuo. The residue was dissolved in DCM (50 mL), washed with water (2 × 25 mL), dried over Na_2SO_4, and partially evaporated in vacuo. The solution was purified by dry-column flash chromatography on a short aluminum oxide column (thickness of stationary phase: 40 mm, eluent: heptane/DCM 1:1, DCM). After evaporation of solvents in vacuo **54e** (4.16 g, 94%) was obtained as a pale yellow oil. IR (film): 2933, 1732, 1574, 1495, 1295, 1068, 895, 712 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): 7.50 (s, 1H), 7.36 (m, 1H), 7.34 (m, 1H), 7.32 (m, 1H), 7.26 (m, 1H), 6.95 (s, 1H), 4.91 (s, 1H), 4.29 (m, 2H), 4.27 (m, 2H), 4.11 (q, ^{3}J = 7.1 Hz, 2H), 3.31 (s, 3H), 2.48 (m, 2H), 2.27 (t, ^{3}J = 7.5 Hz, 2H), 2.06 (br s, 1H), 1.60 (m, 2H), 1.49 (m, 2H), 1.31 (m, 2H), 1.30 (m, 2H), 1.24 (t, ^{3}J = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): 173.77, 146.30, 142.65, 138.96 (2C), 132.57, 130.56, 129.85, 128.83, 127.60, 127.48, 118.17 (2C), 65.71, 64.60, 64.17, 60.15, 47.92, 38.27, 34.24, 29.89, 28.96, 26.92, 24.82, 14.22. COSY: 7.36–7.26–7.32–7.34, 4.29–4.27, 4.11–1.24, 2.48–1.49–1.31–1.30–1.60–2.27. HSQC (140 Hz): 7.50–118.17, 7.36–129.85, 7.34–127.48, 7.32–128.83, 7.26–127.60, 6.95–118.17, 4.91–65.71, 4.29–64.60, 4.27–64.17, 4.11–60.15, 3.31–38.27, 2.48–47.92, 2.27–34.24, 1.60–24.82, 1.49–29.89, 1.31–26.92, 1.30–28.96, 1.24–14.22. HMBC (8 Hz, 140 Hz): 7.50–(146.30, 132.57), 7.36–(138.96, 128.83), 7.34–(138.96, 127.60), 7.32–(138.96, 129.85), 7.26–(138.96, 127.48), 6.95–(142.65, 130.56), 4.91–(138.96, 132.57, 130.56, 129.85, 118.17, 47.92), 4.29–146.30, 4.27–142.65, 4.11–(173.77, 14.22), 3.31–138.96, 2.27–(173.77, 28.96, 24.82), 1.60–(173.77, 34.24, 28.96, 26.92), 1.49–(47.92, 26.92), 1.31–28.96, 1.30–26.92, 1.24–60.15. HRMS (ESI): m/z calcd. for $C_{25}H_{33}N_2O_6S$ $[M+H]^+$: 489.2054, found: 489.2055.

7-[(7-Methyl-6,6-dioxido-2,3,7,12-tetrahydrobenzo[*c*][1,4]benzodioxino[6,7-*f*][1,2]thiazepin-12-yl)amino]heptanoic acid (54f). To a solution of ester **54e** (3.91 g, 8 mmol) in EtOH (40 mL), NaOH (0.384 g, 9.6 mmol) dissolved in water (10 mL) was added at room temperature and the solution was stirred at room temperature for 20 h. Water (30 mL) was

added, and the reaction mixture was partly evaporated in vacuo to remove ethanol. The solution obtained was neutralized with aqueous HCl solution (1.00 g of cc. HCl dissolved in 9 mL of water, containing 10 mmol of HCl). DCM (50 mL) was added to the reaction mixture, after a short stirring the phases were separated, the aqueous phase was washed with DCM (50 mL), the combined organic phases were dried over Na_2SO_4 and partially evaporated in vacuo. The solution obtained was subjected to dry-column flash chromatography on a short silica gel column (thickness of stationary phase: 25 mm, eluent: DCM, DCM/MeOH 100:2, 100:4). After evaporation of solvents the oily residue was triturated with water (40 mL) to afford **54f** (2.58 g, 70%) as a colorless amorphous solid. Melting range (glass-transition range): 80–95 °C (Kofler–Boëtius, 2 °C/min), 63–84 °C (DSC, 10 °C/min). IR (KBr): 2931, 1716, 1500, 1296, 1137, 1064 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): 8.10 (br s, 2H), 7.49 (s, 1H), 7.47 (m, 1H), 7.34 (m, 1H), 7.30 (m, 1H), 7.24 (m, 1H), 7.07 (s, 1H), 5.23 (s, 1H), 4.28 (m, 4H), 3.21 (s, 3H), 2.55 (m, 1H), 2.41 (m, 1H), 2.20 (t, ^3J = 7.3 Hz, 2H), 1.54 (m, 2H), 1.48 (m, 2H), 1.25 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): 178.16, 146.61, 143.19, 139.78, 134.16, 131.69, 130.39, 129.64, 128.82, 127.40, 127.14, 120.35, 118.13, 65.58, 64.51, 64.20, 46.82, 38.83, 35.16, 28.93, 28.58, 26.79, 25.12. MS (ESI): $[M+H]^+$ = 461. HRMS (ESI): m/z calcd. for $C_{23}H_{29}N_2O_6S$ $[M+H]^+$: 461.1741, found: 461.1739.



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Berecz Gabor
2024.09.17. (DA)

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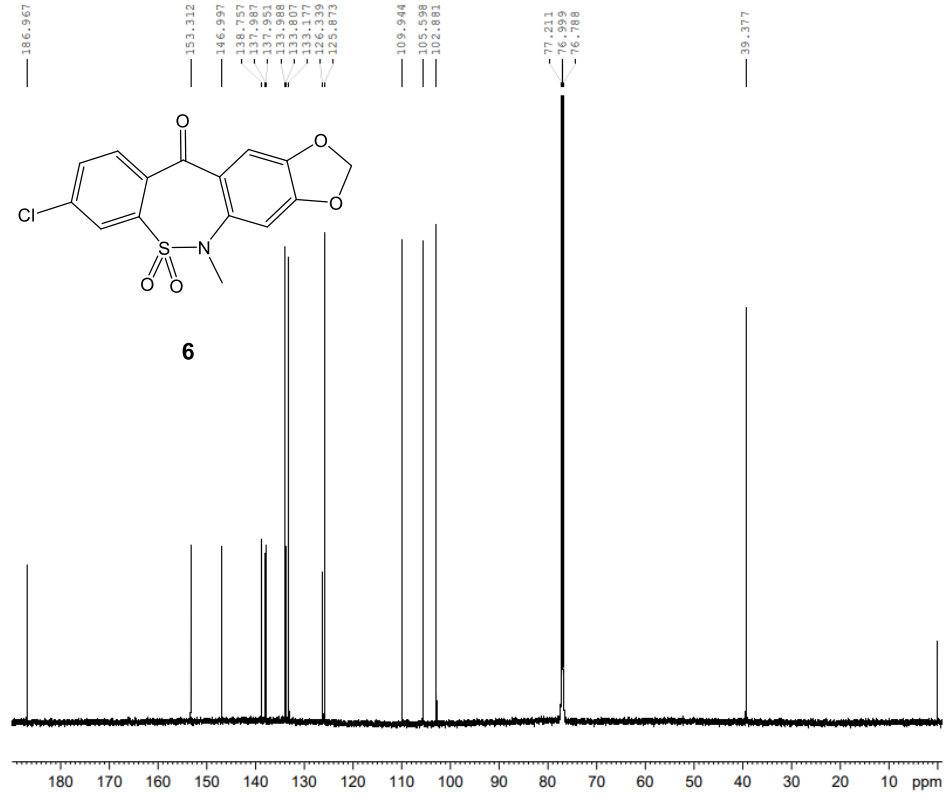

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Berecz Gabor
2024.09.17. (DA)

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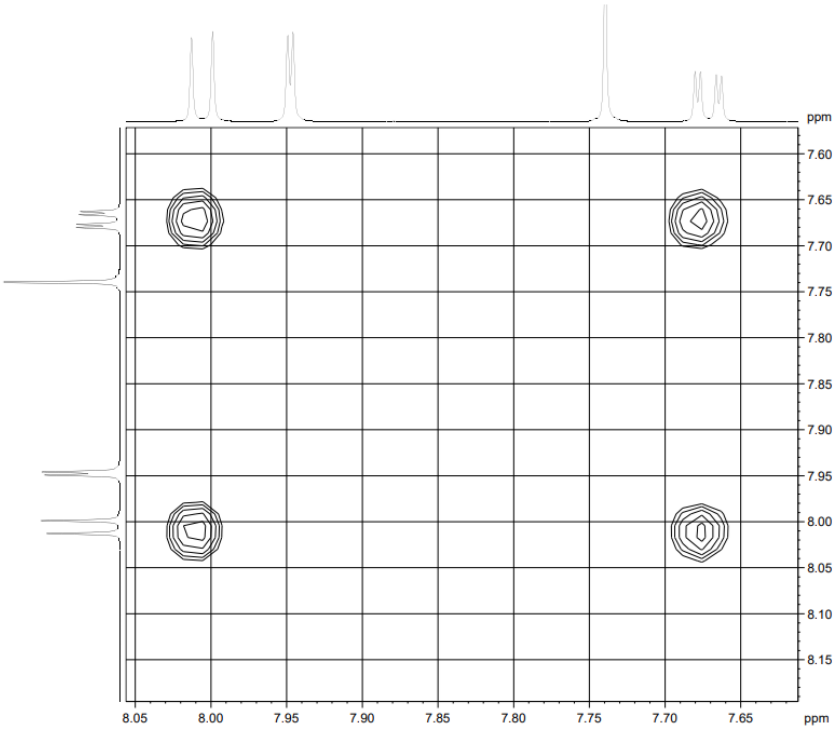

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1801-BGE
Berecz Gabor
2024.09.17. (DA)

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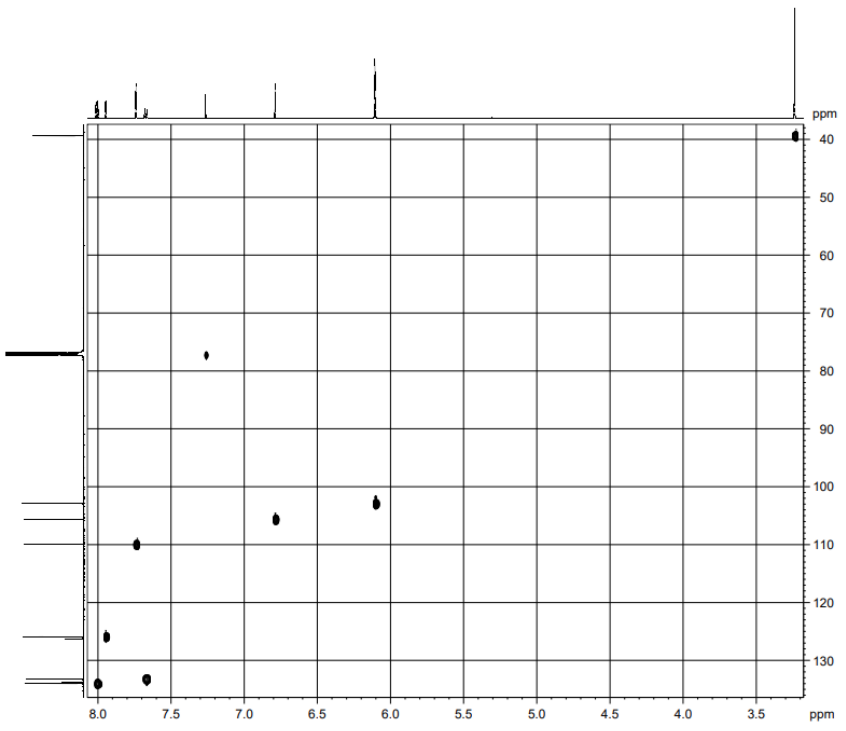
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000126 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000126 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



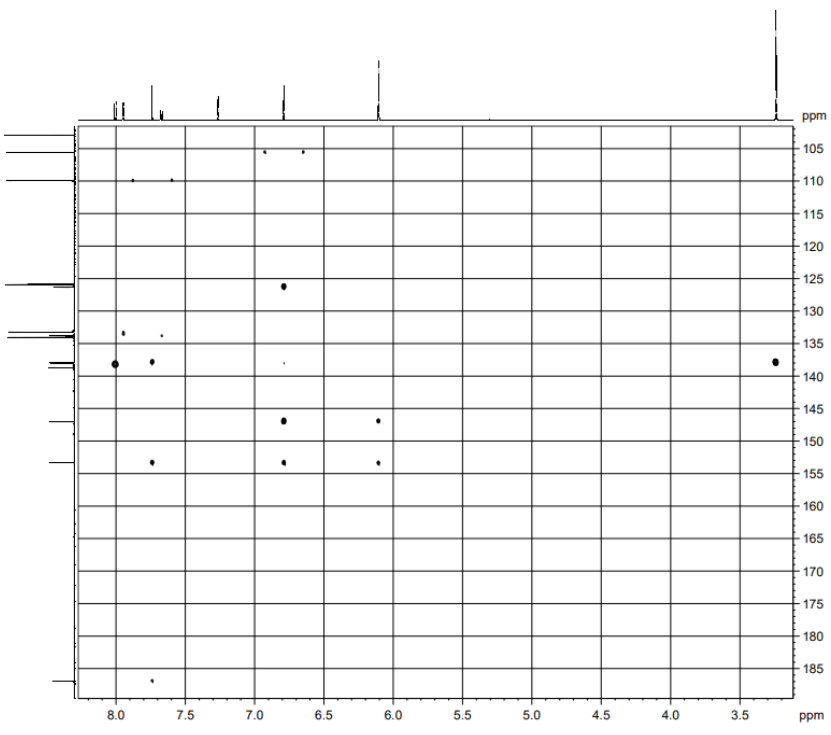
HSQC (140 Hz) **6**
143529
1801-BGE
Berecz Gabor
2024.09.17. (DA)

Current Data Parameters
NAME 143529
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240918
Time 7.19 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.3000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 7.90 usec
P14 500.00 usec
P24 2000.00 usec
P25 1500.00 usec
PLW0 0 W
PLW2 71.00000000 W
PLW12 2.30040002 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFF3 0 Hz
SPW3 10.63199997 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFF7 0 Hz
SPW7 10.63199997 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFF14 0 Hz
SPW14 5.95400000 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFF31 0 Hz
SPW31 1.48850000 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000126 MHz
WDW QSINE



HMBC (8 Hz, 140 Hz) **6**
143529
1801-BGE
Berecz Gabor
2024.09.17. (DA)

Current Data Parameters
NAME 143529
EXPNO 15
PROCNO 1

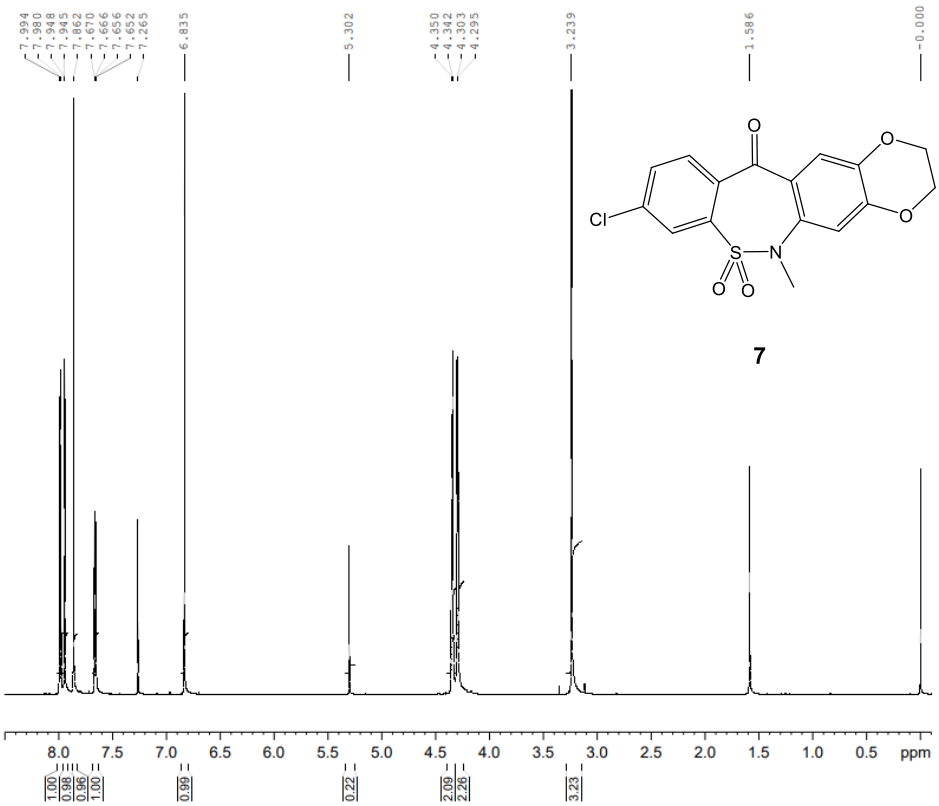
F2 - Acquisition Parameters
Date_ 20240918
Time 7.49 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.90 usec
PLW2 71.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000126 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701265 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

BRUKER



Standard 1H
144361
bge1721-1721-BGE_1
Berecz Gabor
2025.03.07. (KP)

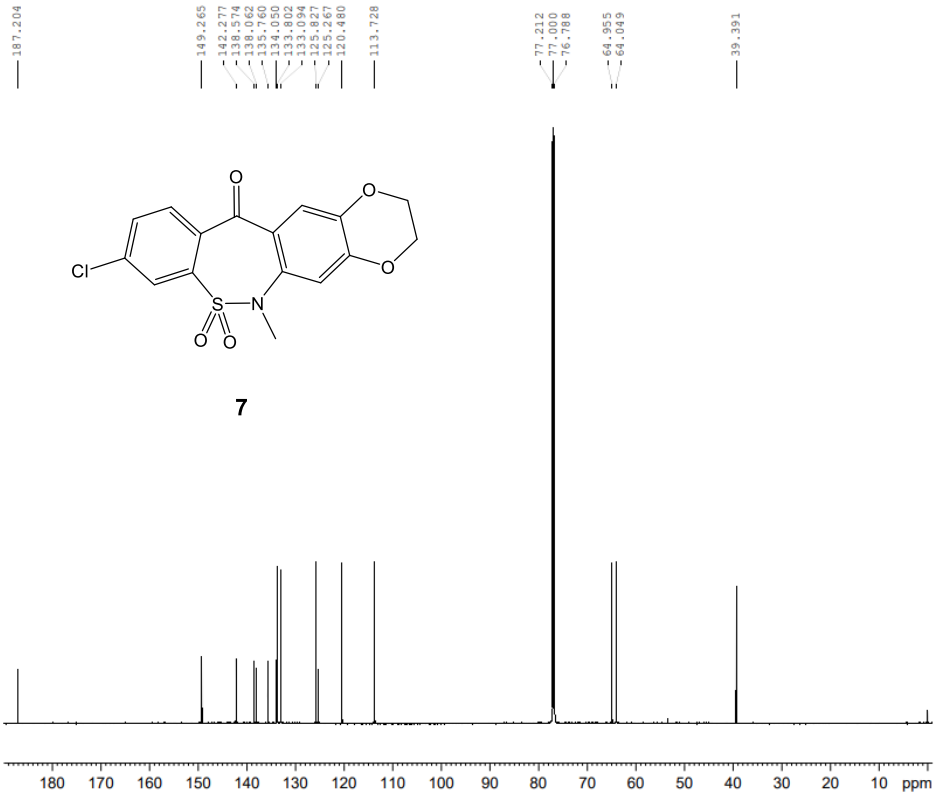
7

Current Data Parameters
NAME 144361
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250308
Time 3.23 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

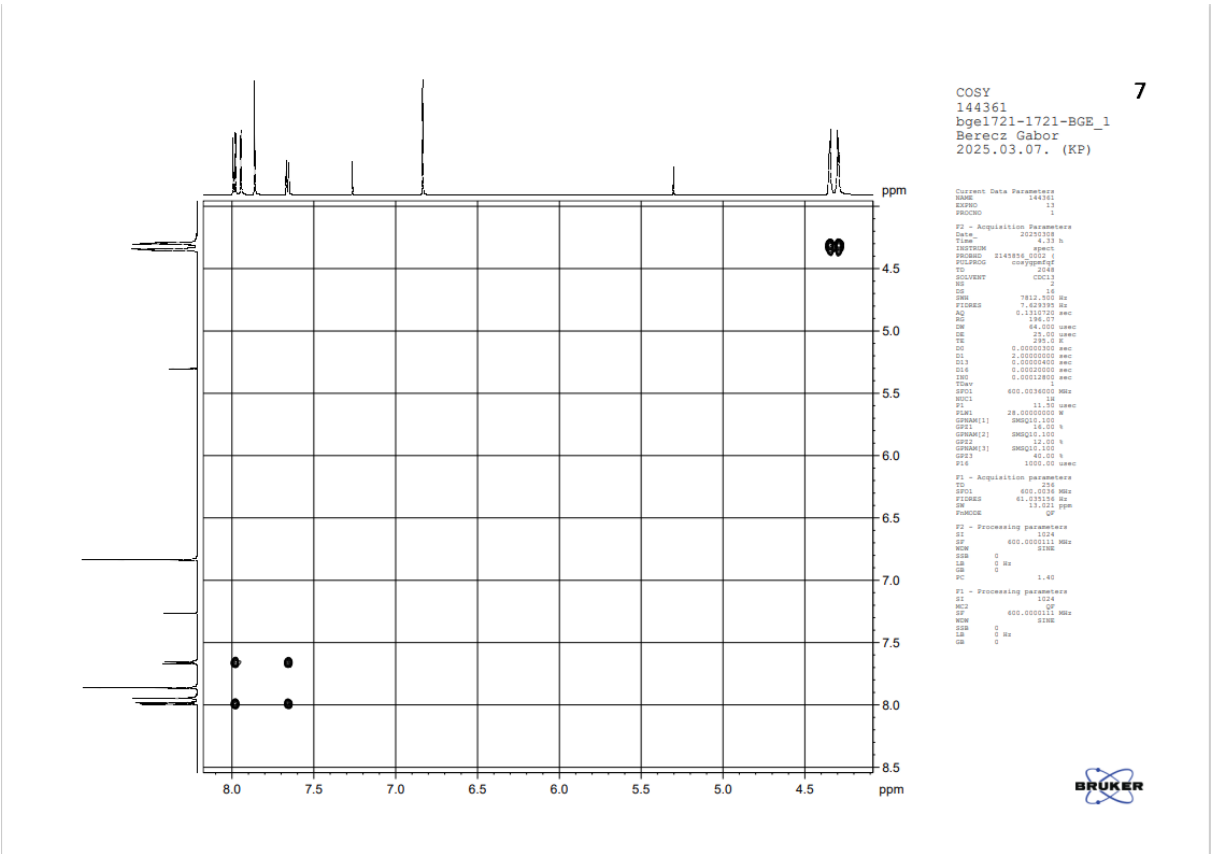
F2 - Processing parameters
SI 65536
SF 600.0000111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

BRUKER



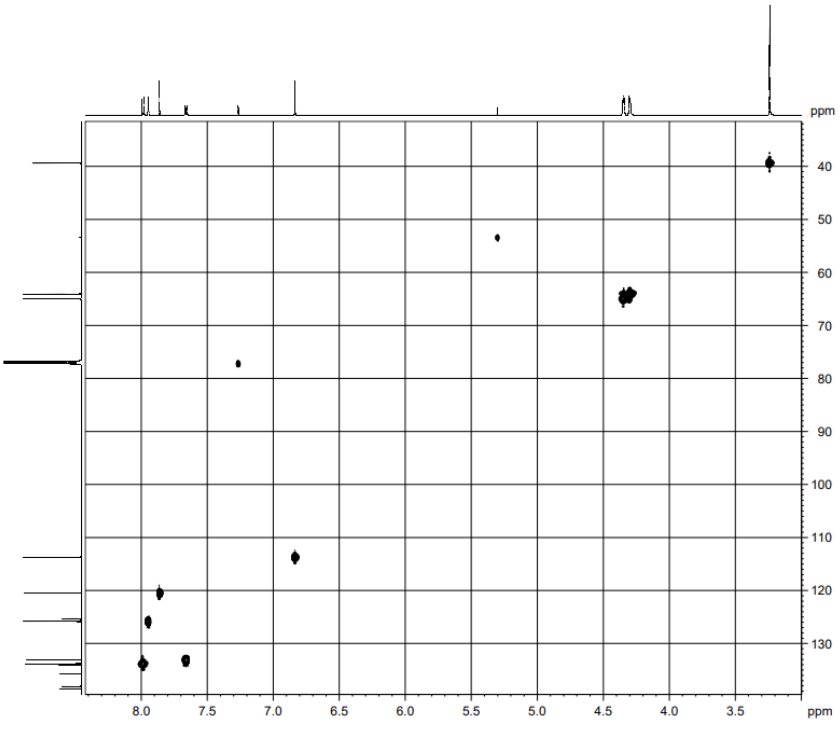
Standard 13C
144361
bge1721-1721-BGE_1
Berecz Gabor
2025.03.07. (KP)

```
Current Data Parameters
NAME                  144361
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250308
Time                   4.31 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        4
SWH               36231.883 Hz
FIDRES             1.105709 Hz
AQ                 0.9043968 sec
RG                    196.07
DW                   13.800 usec
DE                   18.00 usec
TE                   295.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1           150.8852070 MHz
NUC1                     13C
P1                    9.80 usec
PLW1           72.69999695 W
SFO2           600.0024000 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                 80.00 usec
PLW2           32.50000000 W
PLW12           0.70708001 W
PLW13           0.35508999 W

F2 - Processing parameters
SI                   131072
SF           150.8701276 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



COSY
144361
bge1721-1721-BGE_1
Berecz Gabor
2025.03.07. (KP)

```
Current Data Parameters
NAME                  144361
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20250308
Time                   4.33 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG          cosygpmfqf
TD                     2048
SOLVENT               CDCl3
NS                       16
DS                       16
SWH                7812.500 Hz
FIDRES             7.629395 Hz
AQ                 0.1310720 sec
RG                    196.07
DW                   64.000 usec
DE                   25.00 usec
TE                   295.0 K
D0              0.00000300 sec
D1              2.00000000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00012800 sec
TDav                     1
SFO1           600.0036000 MHz
NUC1                     1H
P1                   11.50 usec
PLW1           28.00000000 W
GPWAM[1]      SMSQ10.100
GPZ1                 16.00 %
GPWAM[2]      SMSQ10.100
GPZ2                 12.00 %
GPWAM[3]      SMSQ10.100
GPZ3                 40.00 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                     256
SFO1           600.0036 MHz
FIDRES           61.035156 Hz
SW                 13.021 ppm
FnMODE                   QF

F2 - Processing parameters
SI                    1024
SF           600.0000111 MHz
WDW                    SINE
SSB       0
LB        0 Hz
GB        0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF           600.0000111 MHz
WDW                    SINE
SSB       0
LB        0 Hz
GB        0
```



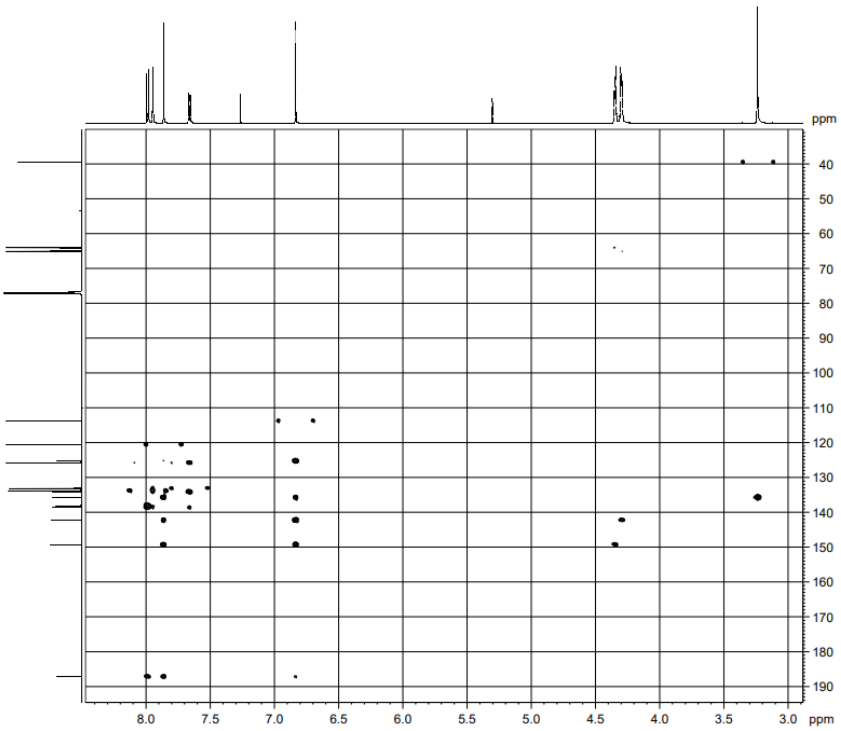
HSQC (140Hz) **7**
144361
bge1721-1721-BGE_1
Berecz Gabor
2025.03.07. (KP)

Current Data Parameters
NAME 144361
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250308
Time 4.53 h
INSTRUM spect
PROBHD 5145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.35803999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000111 MHz
WDW QSINE



HMBC (8Hz, 140Hz) **7**
144361
bge1721-1721-BGE_1
Berecz Gabor
2025.03.07. (KP)

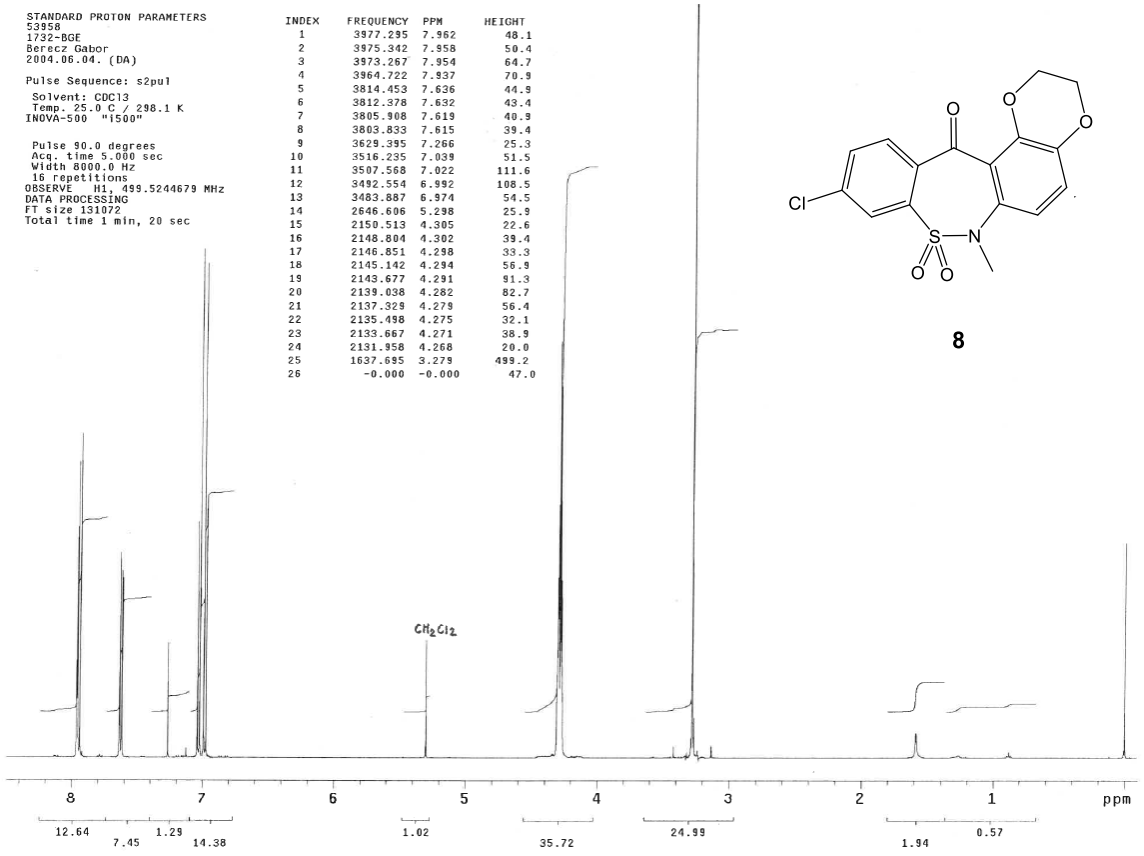
Current Data Parameters
NAME 144361
EXPNO 15
PROCNO 1

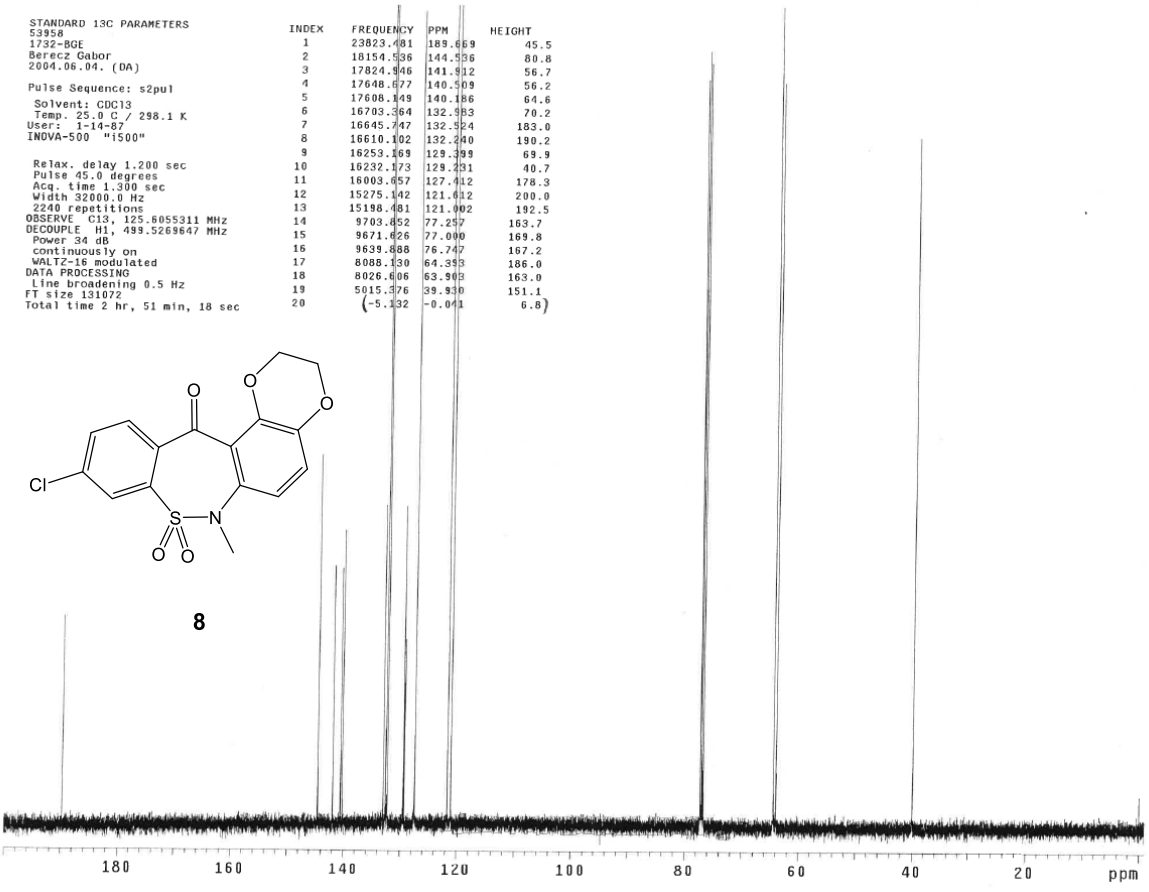
F2 - Acquisition Parameters
Date_ 20250308
Time 5.23 h
INSTRUM spect
PROBHD 5145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

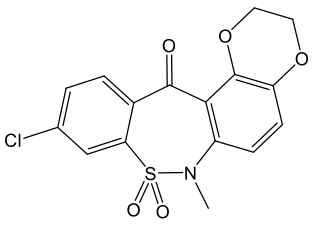
F2 - Processing parameters
SI 2048
SF 600.0000111 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701276 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

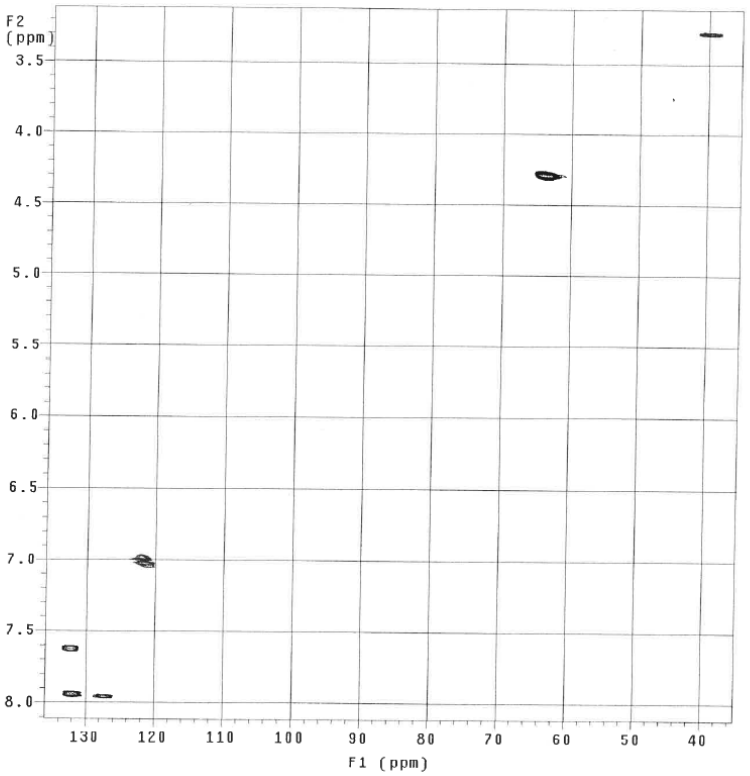

STANDARD PROTON PARAMETERS
53958
1732-BGE
Berecz Gabor
2004.06.04. (DA)
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244679 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 20 sec
INDEX FREQUENCY PPM HEIGHT
1 3977.295 7.962 48.1
2 3975.342 7.958 50.4
3 3973.267 7.954 64.7
4 3964.722 7.937 70.9
5 3814.453 7.636 44.9
6 3812.378 7.632 43.4
7 3805.908 7.619 40.9
8 3803.833 7.615 39.4
9 3629.395 7.266 25.3
10 3516.235 7.039 51.5
11 3507.568 7.022 111.6
12 3492.554 6.992 108.5
13 3483.887 6.974 54.5
14 2646.606 5.298 25.9
15 2150.513 4.305 22.6
16 2148.804 4.302 39.4
17 2146.851 4.298 33.3
18 2145.142 4.294 56.9
19 2143.677 4.291 91.3
20 2139.038 4.282 82.7
21 2137.329 4.278 56.4
22 2135.498 4.275 32.1
23 2133.667 4.271 38.9
24 2131.958 4.268 20.0
25 1637.695 3.278 499.2
26 -0.000 -0.000 47.0
Cl
O
O
O
S
N
O
O
8
CH2Cl2
8
7
6
5
4
3
2
1
ppm
12.64
1.29
7.45
14.38
1.02
35.72
24.99
1.94
0.57


STANDARD 13C PARAMETERS
53958
1732-BGE
Berecz Gabor
2004.06.04. (DA)
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
Relax. delay 1.200 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
2240 repetitions
OBSERVE C13, 125.6055311 MHz
DECOUPLE H1, 499.5269647 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 2 hr, 51 min, 18 sec
INDEX FREQUENCY PPM HEIGHT
1 23823.481 189.669 45.5
2 18154.536 144.536 80.8
3 17824.946 141.912 56.7
4 17648.677 140.509 56.2
5 17608.149 140.186 64.6
6 16703.364 132.983 70.2
7 16645.747 132.524 183.0
8 16610.102 132.240 190.2
9 16253.169 129.399 69.9
10 16232.173 129.231 40.7
11 16003.657 127.412 178.3
12 15275.142 121.612 200.0
13 15198.481 121.002 192.5
14 9703.852 77.257 163.7
15 9671.626 77.000 169.8
16 9639.888 76.747 167.2
17 8088.130 64.393 186.0
18 8026.606 63.903 163.0
19 5015.376 39.930 151.1
20 -5.132 -0.041 6.8
Cl
O
O
O
S
N
O
O
8
180
160
140
120
100
80
60
40
20
ppm

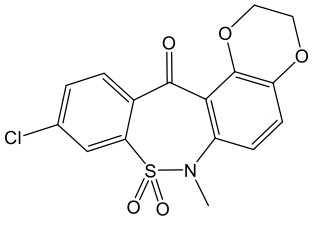
```
GHSQC_DA (140 Hz)
53958
1732-BGE
Berecz Gabor
2004.06.04. (DA)

Pulse Sequence: ghsqc_da
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"

 Relax. delay 1.500 sec
 Acq. time 0.098 sec
 Width    5219.9 Hz
 2D Width 26367.8 Hz
 2 repetitions
 2 x 256 increments
OBSERVE    H1, 499.5244683 MHz
DECOUPLE C13, 125.6174881 MHz
 Power 50 dB
 on during acquisition
 off during delay
 GARP-1 modulated
DATA PROCESSING
 Sq. sine bell 0.200 sec
  Shifted by -0.200 sec
F1 DATA PROCESSING
 Line broadening 0.3 Hz
 Sq. sine bell 0.005 sec
  Shifted by -0.005 sec
FT size 2048 x 512
Total time 28 min, 35 sec
```



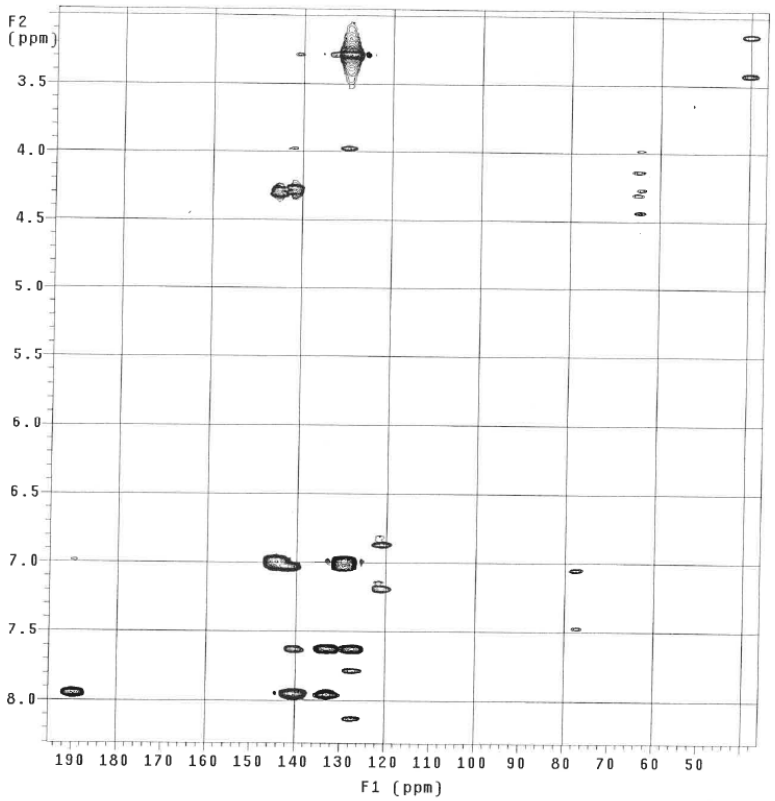
8

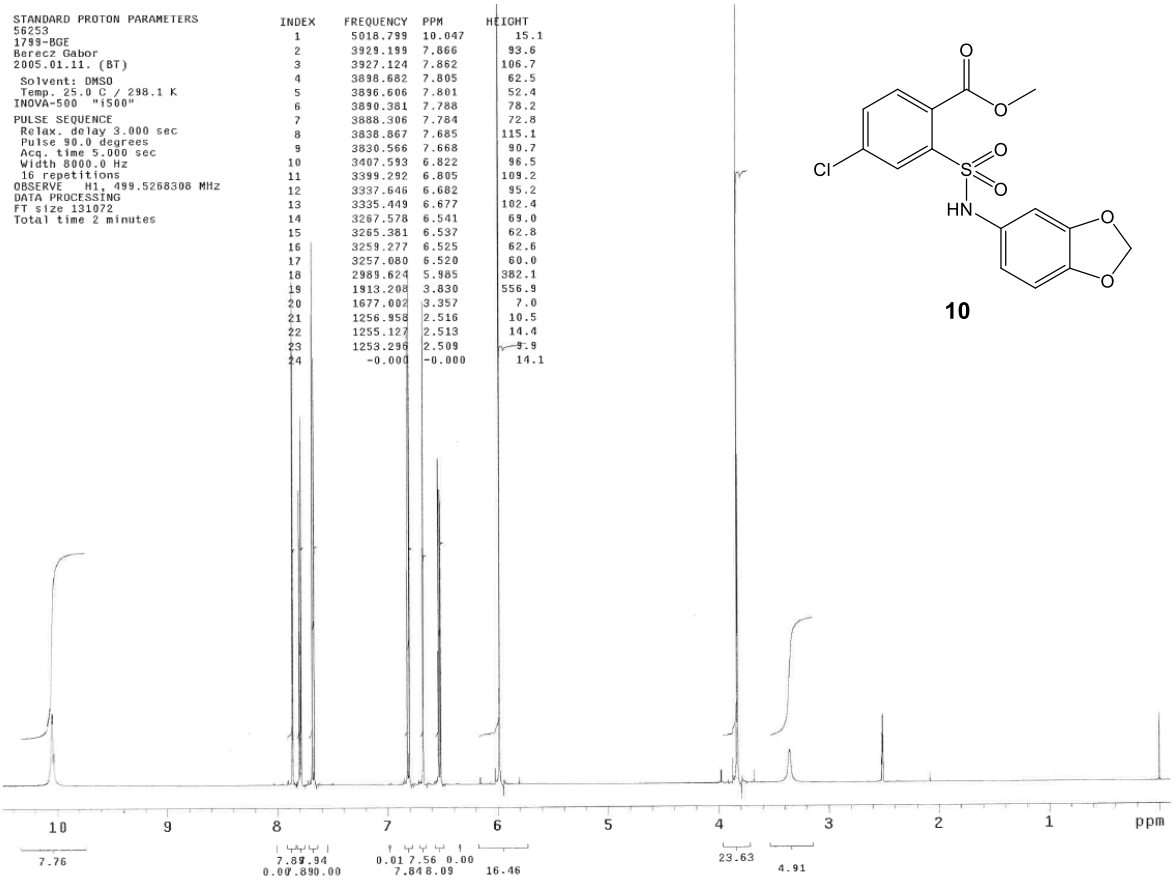


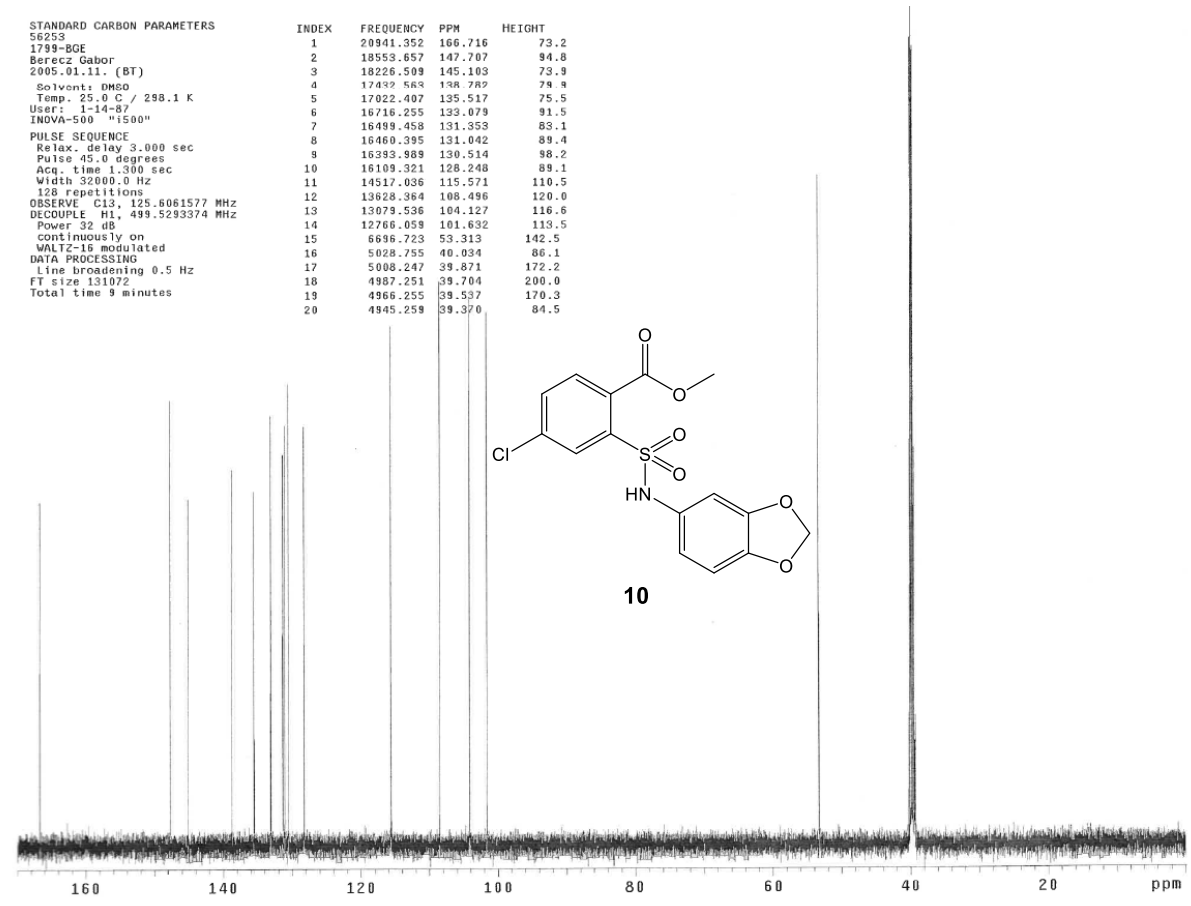

```
GHMQC_DA (140 Hz, 8 Hz)
53958
1732-BGE
Berecz Gabor
2004.06.04. (DA)

Pulse Sequence: ghmqc_da
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"

 Relax. delay 1.500 sec
 Acq. time 0.098 sec
 Width    5219.9 Hz
 2D Width 26367.8 Hz
 4 repetitions
 256 increments
OBSERVE    H1, 499.5244681 MHz
DATA PROCESSING
 Sine bell 0.098 sec
F1 DATA PROCESSING
 Sine bell 0.002 sec
FT size 2048 x 512
Total time 29 min, 9 sec
```



8




STANDARD PROTON PARAMETERS
56253
1799-BGE
Berecz Gabor
2005.01.11. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268308 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 5018.799 10.047 15.1
2 3929.199 7.866 93.6
3 3927.124 7.862 106.7
4 3898.682 7.805 62.5
5 3896.606 7.801 52.4
6 3890.381 7.788 78.2
7 3888.306 7.784 72.8
8 3838.867 7.685 115.1
9 3830.566 7.668 90.7
10 3407.593 6.822 96.5
11 3399.292 6.805 109.2
12 3337.646 6.682 95.2
13 3335.449 6.677 102.4
14 3267.578 6.541 69.0
15 3265.381 6.537 62.8
16 3259.277 6.525 62.6
17 3257.080 6.520 60.0
18 2989.624 5.985 382.1
19 1913.208 3.830 556.9
20 1677.002 3.357 7.0
21 1256.958 2.516 10.5
22 1255.127 2.513 14.4
23 1253.296 2.509 9.9
24 -0.000 -0.000 14.1
O
O
Cl
S
O
O
HN
O
O
10
10
9
8
7
6
5
4
3
2
1
ppm
7.76
7.89
7.94
0.00
7.89
0.01
7.56
0.00
7.84
8.09
16.46
23.63
4.91

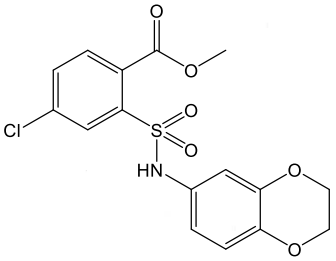

STANDARD CARBON PARAMETERS
56253
1799-BGE
Berecz Gabor
2005.01.11. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
128 repetitions
OBSERVE C13, 125.6061577 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 9 minutes
INDEX FREQUENCY PPM HEIGHT
1 20941.352 166.716 73.2
2 18553.657 147.707 94.8
3 18226.509 145.103 73.9
4 17432.583 138.782 79.9
5 17022.407 135.517 75.5
6 16716.255 133.079 91.5
7 16499.458 131.353 83.1
8 16460.395 131.042 89.4
9 16393.989 130.514 98.2
10 16109.321 128.248 89.1
11 14517.036 115.571 110.5
12 13628.384 108.496 120.0
13 13079.536 104.127 116.6
14 12766.059 101.632 113.5
15 6696.723 53.313 142.5
16 5028.755 40.034 86.1
17 5008.247 39.871 172.2
18 4987.251 39.704 200.0
19 4966.255 39.537 170.3
20 4945.259 39.370 84.5
O
O
Cl
S
O
O
HN
O
O
10
160
140
120
100
80
60
40
20
ppm

STANDARD 1H OBSERVE
52613
1699-BGE
Berecz Gabor
04/03/09(NM)

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"

PULSE SEQUENCE
Relax. delay 5.000 sec
Pulse 31.5 degrees
Acq. time 1.993 sec
Width 3003.0 Hz
16 repetitions
OBSERVE H1, 200.0557670 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	1592.779	7.962	30.1
2	1566.752	7.832	52.7
3	1564.919	7.822	78.5
4	1557.221	7.784	59.6
5	1512.865	7.562	39.8
6	1510.666	7.551	38.6
7	1504.434	7.520	29.1
8	1502.235	7.509	24.3
9	1453.480	7.265	18.6
10	1344.973	6.723	31.1
11	1342.040	6.708	42.5
12	1339.474	6.696	53.1
13	1336.542	6.681	70.9
14	1323.345	6.615	43.6
15	1320.779	6.602	31.0
16	1314.547	6.571	17.8
17	1312.348	6.560	16.0
18	1059.409	5.296	8.6
19	839.463	4.196	419.7
20	804.638	4.022	321.8
21	325.521	1.627	20.2
22	0.000	0.000	23.1



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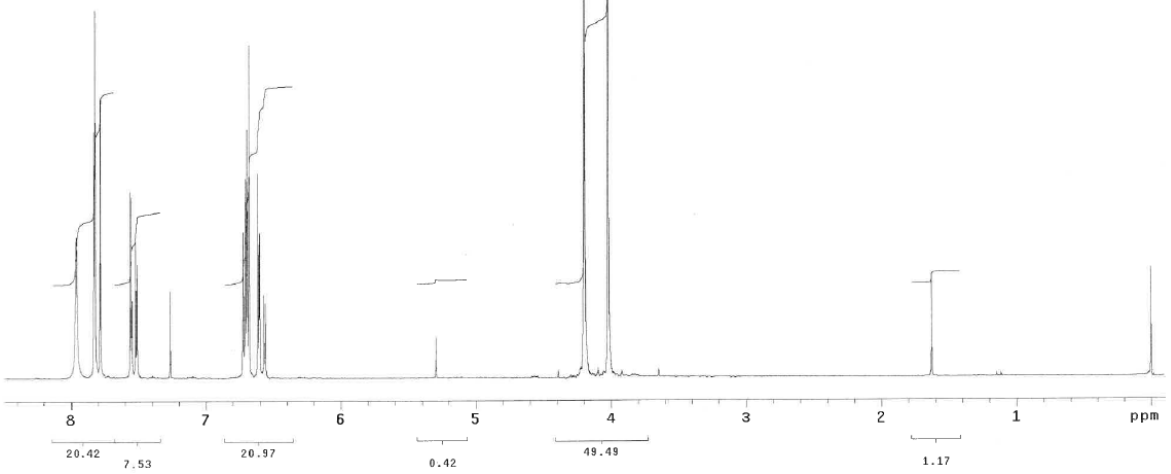
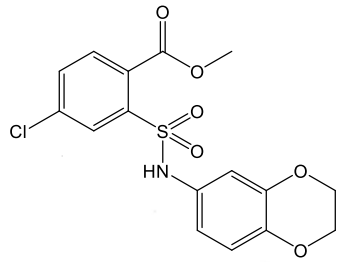


STANDARD 13C OBSERVE
52613
1699-BGE
Berecz Gabor
04/03/09(NM)

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 60.0 degrees
Acq. time 1.497 sec
Width 12484.4 Hz
144 repetitions
OBSERVE C13, 50.3040647 MHz
DECOUPLE H1, 200.0567131 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 10 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	8414.392	167.258	35.2
2	7224.168	143.599	52.3
3	7156.351	142.251	44.1
4	7051.578	140.168	43.0
5	6951.377	138.177	49.5
6	6661.822	132.421	86.8
7	6648.106	132.148	76.9
8	6572.288	130.641	80.9
9	6503.328	129.270	56.4
10	6461.800	128.445	38.0
11	5910.121	117.479	80.0
12	5885.738	116.994	76.8
13	5691.050	113.124	67.0
14	3905.715	77.636	157.3
15	3873.711	77.000	162.0
16	3841.708	76.364	157.7
17	3230.213	64.209	77.0
18	3225.260	64.110	76.0
19	2697.965	53.629	65.4



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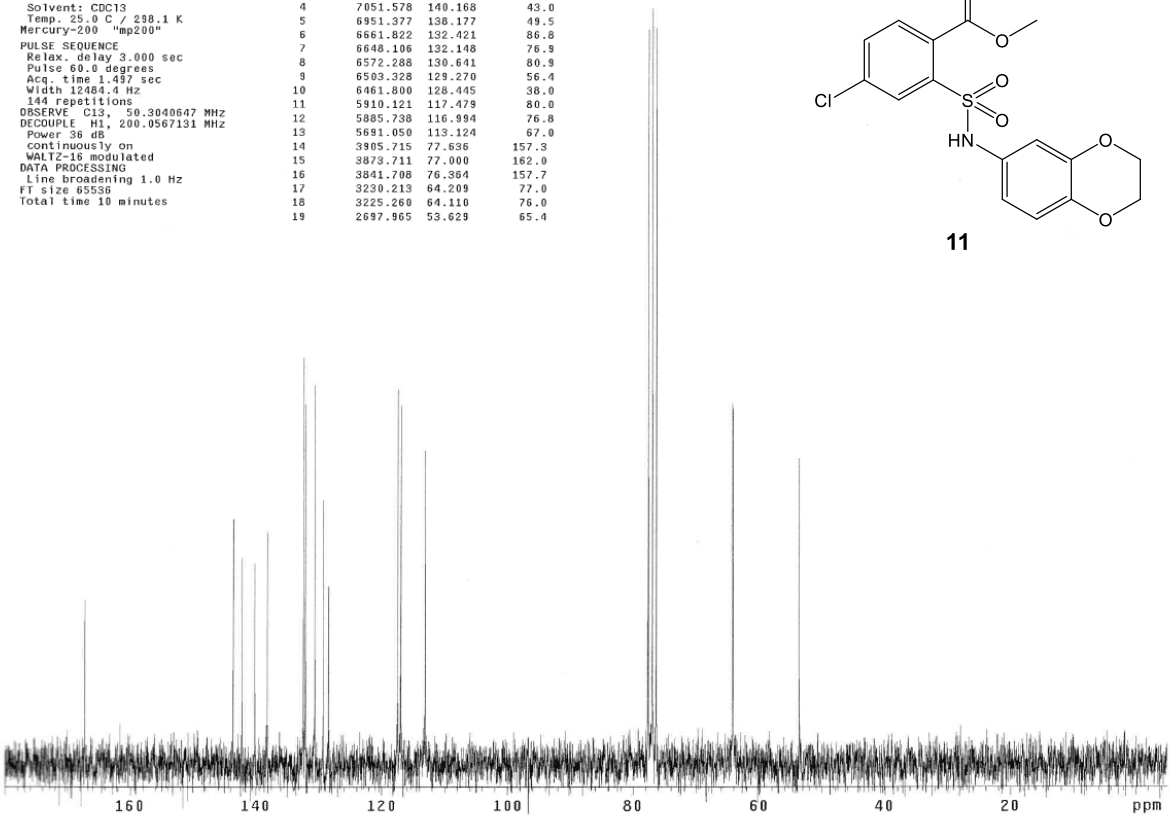
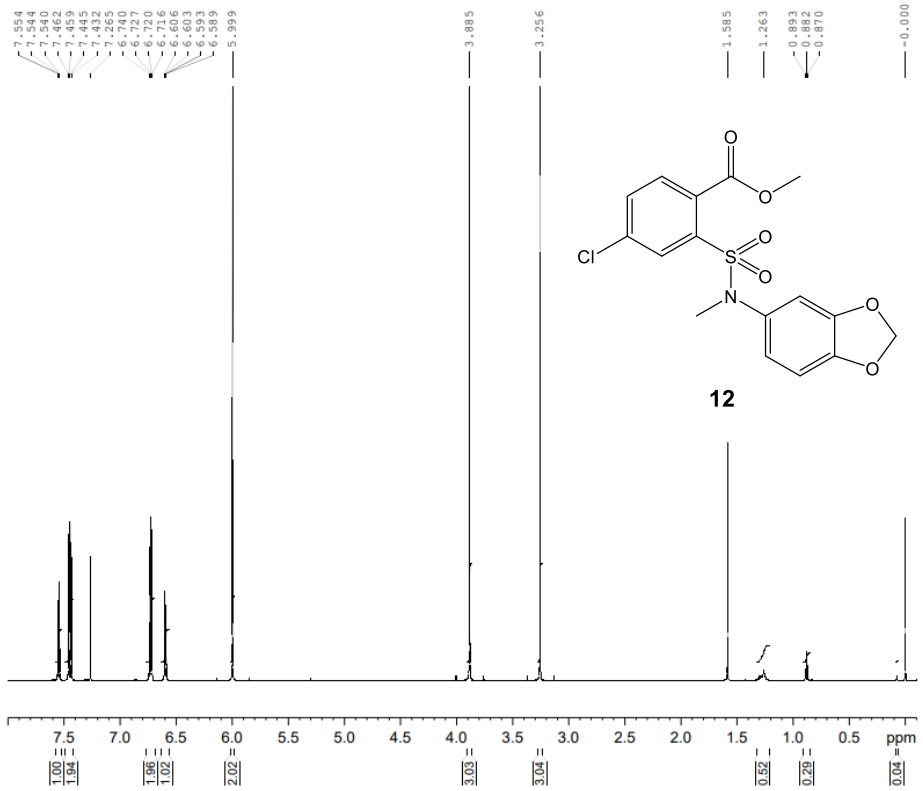


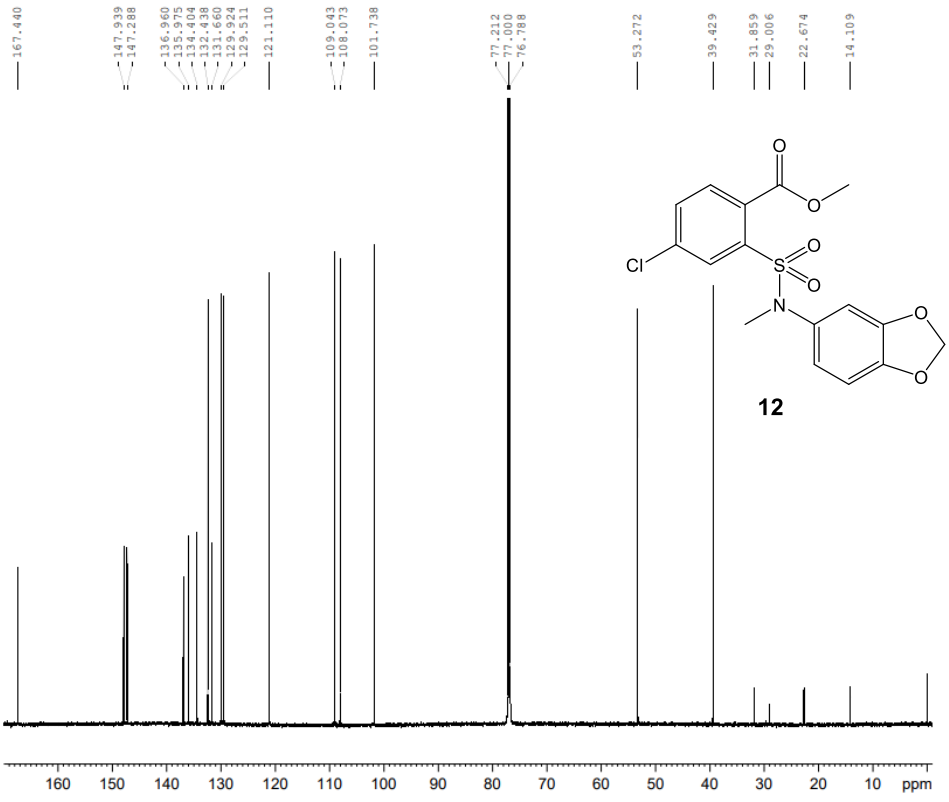


Standard 1H
143511
BEG0702_1
Berecz Gabor
2024.09.13. (KP)

Current Data Parameters
NAME 143511
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240913
Time 21.39 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

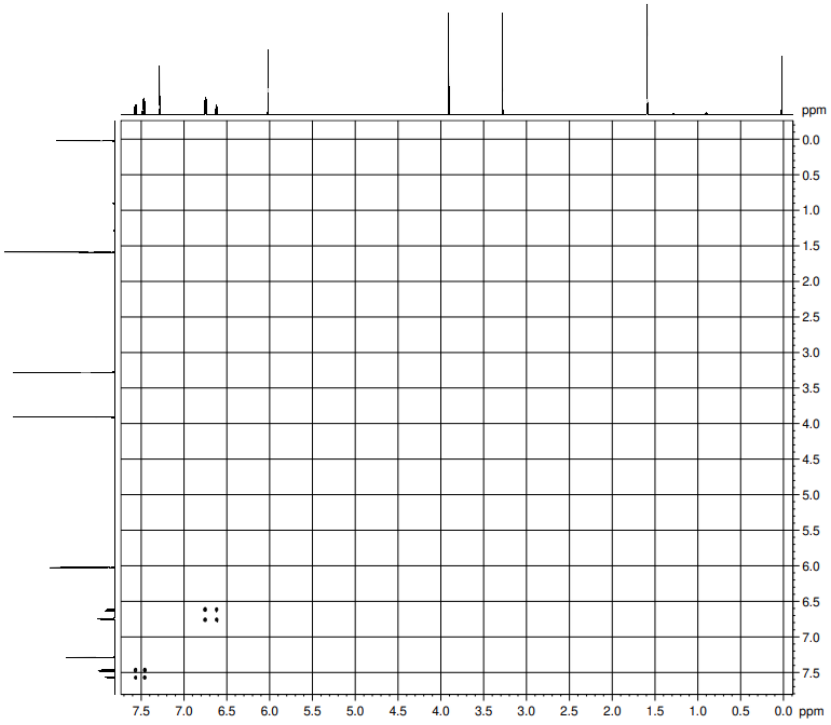


Standard 13C
143511
BEG0702_1
Berecz Gabor
2024.09.13. (KP)

Current Data Parameters
NAME 143511
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240913
Time 22.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701269 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



COSY **12**
143511
BEG0702_1
Berecz Gabor
2024.09.17. (DA)

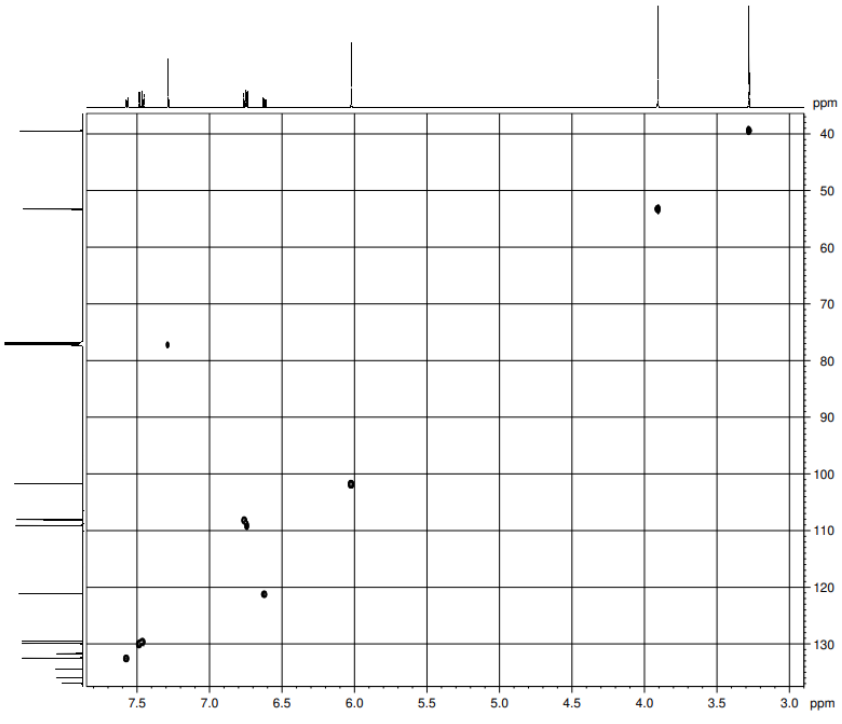
```
Current Data Parameters
NAME                  143511
EXPNO                     23
PROCNO                     1

F2 - Acquisition Parameters
Date_              20240917
Time                 21.00 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG       cosygpmfqf
TD                      2048
SOLVENT              CDCl3
NS                         2
DS                        16
SWH                7812.500 Hz
FIDRES             7.629395 Hz
AQ                 0.1310720 sec
RG                    196.07
DW                   64.000 usec
DE                   25.00 usec
TE                   295.0 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
INO                0.00012800 sec
TDav                       1
SFO1            600.0036000 MHz
NUC1                      1H
P1                   11.50 usec
PLW1           28.00000000 W
SPNAM[1]         SMSQ10.100
SPF1                 16.00 %
SPNAM[2]         SMSQ10.100
SPF2                 12.00 %
SPNAM[3]         SMSQ10.100
SPF3                 40.00 %
P16                1000.00 usec

F1 - Acquisition parameters
TD                       256
SFO1            600.0036 MHz
FIDRES          61.035156 Hz
SW                  13.021 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF              600.0000000 MHz
WDW                     SINE
SSB                     0
LB                      0 Hz
GB                      0
PC                      1.40

F1 - Processing parameters
SI                      1024
WDW                     SINE
SSB                     0
LB                      0 Hz
GB                      0
```



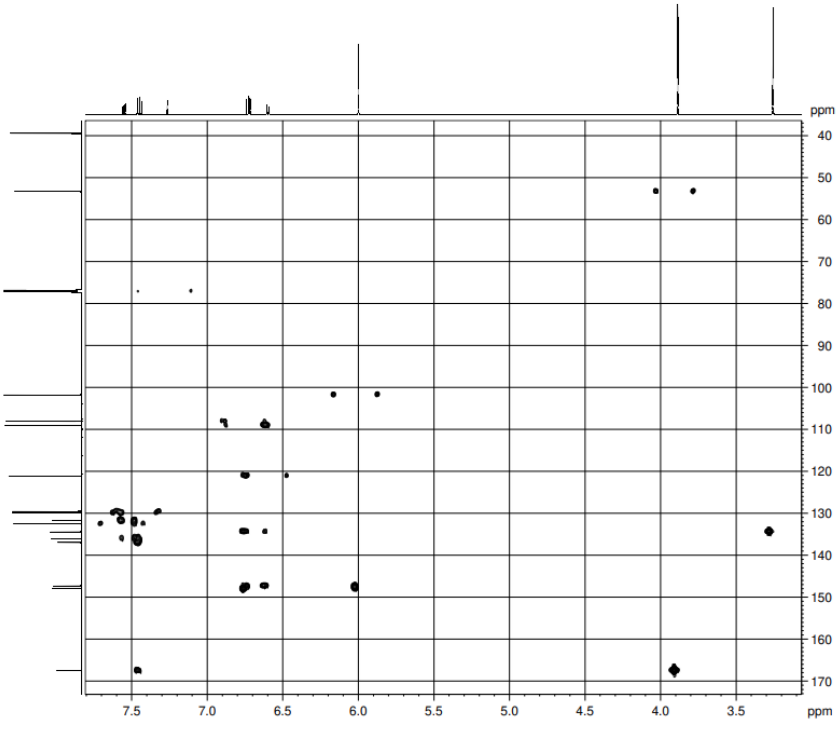
HSQC (140 Hz) **12**
143511
BEG0702_1
Berecz Gabor
2024.09.17. (DA)

```
Current Data Parameters
NAME                  143511
EXPNO                     24
PROCNO                     1

F2 - Acquisition Parameters
Date_              20240917
Time                 21.21 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG  hsqcetgpsisp2.2
TD                      2048
SOLVENT              CDCl3
NS                         4
DS                        32
SWH                7812.500 Hz
FIDRES             7.629395 Hz
AQ                 0.1310720 sec
RG                    196.07
DW                   64.000 usec
DE                   25.00 usec
TE                   295.0 K
CNST2         140.00000000
CNST17         -0.5000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00178571 sec
D11                0.03000000 sec
D16                0.00020000 sec
D24                0.00089000 sec
INO                0.00001510 sec
TDav                       1
SFO1            600.0036000 MHz
NUC1                      1H
P1                   11.50 usec
P2                   23.00 usec
P28         0 usec
PLW1           28.00000000 W
SFO2           150.8867157 MHz
NUC2                     13C
CPDPRG[2 ba_p5m4sp_4sp.2
P3                    9.90 usec
P14                 500.00 usec
P24                2000.00 usec
P63                1500.00 usec
PLW0        0 W
PLW1          71.00000000 W
PLW12          2.30040002 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3              0.500
SPOFFS3  0 Hz
SPW3           10.63199997 W
SPNAM[7]    Crp60comp.4
SPOAL7              0.500
SPOFFS7  0 Hz
SPW13          10.63199997 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14             0.500
SPOFFS14 0 Hz
SPW14           5.95400000 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31             0.500
SPOFFS31 0 Hz
SPW31           1.48850000 W
SPNAM[1]         SMSQ10.100
SPF1                 80.00 %
SPNAM[2]         SMSQ10.100
SPF2                 20.10 %
SPNAM[3]         SMSQ10.100
SPF3                 11.00 %
SPNAM[4]         SMSQ10.100
SPF4                 -5.00 %
P16                1000.00 usec
P19                 600.00 usec

F1 - Acquisition parameters
TD                       256
SFO1           150.8867 MHz
FIDRES         258.692047 Hz
SW                 219.453 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF              600.0000000 MHz
WDW                    QSINE
```



HMBC (8 Hz, 140 Hz) **12**
143511
BEG0702_1
Berecz Gabor
2024.09.17. (DA)

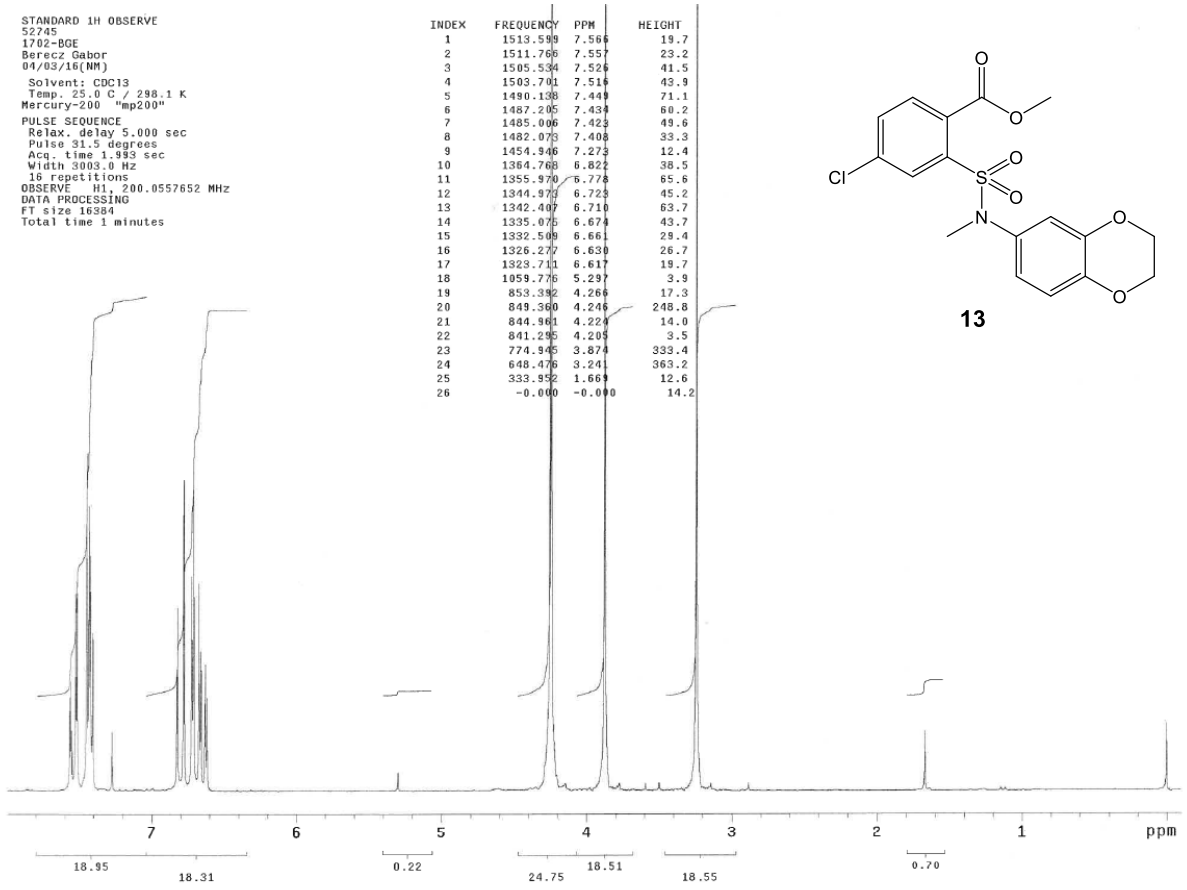
Current Data Parameters
NAME 143511
EXPNO 25
PROCNO 1

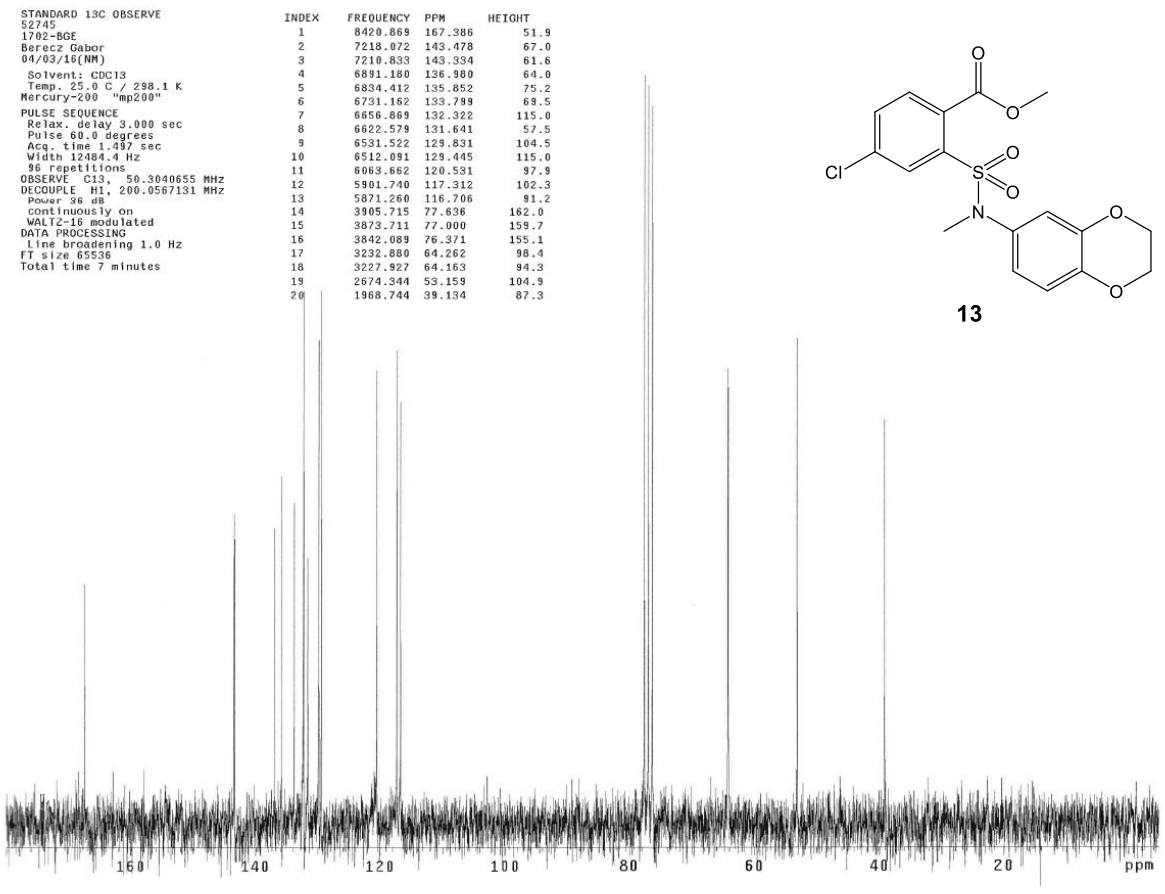
F2 - Acquisition Parameters
Date_ 20240917
Time 21.51 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.90 usec
PLW2 71.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

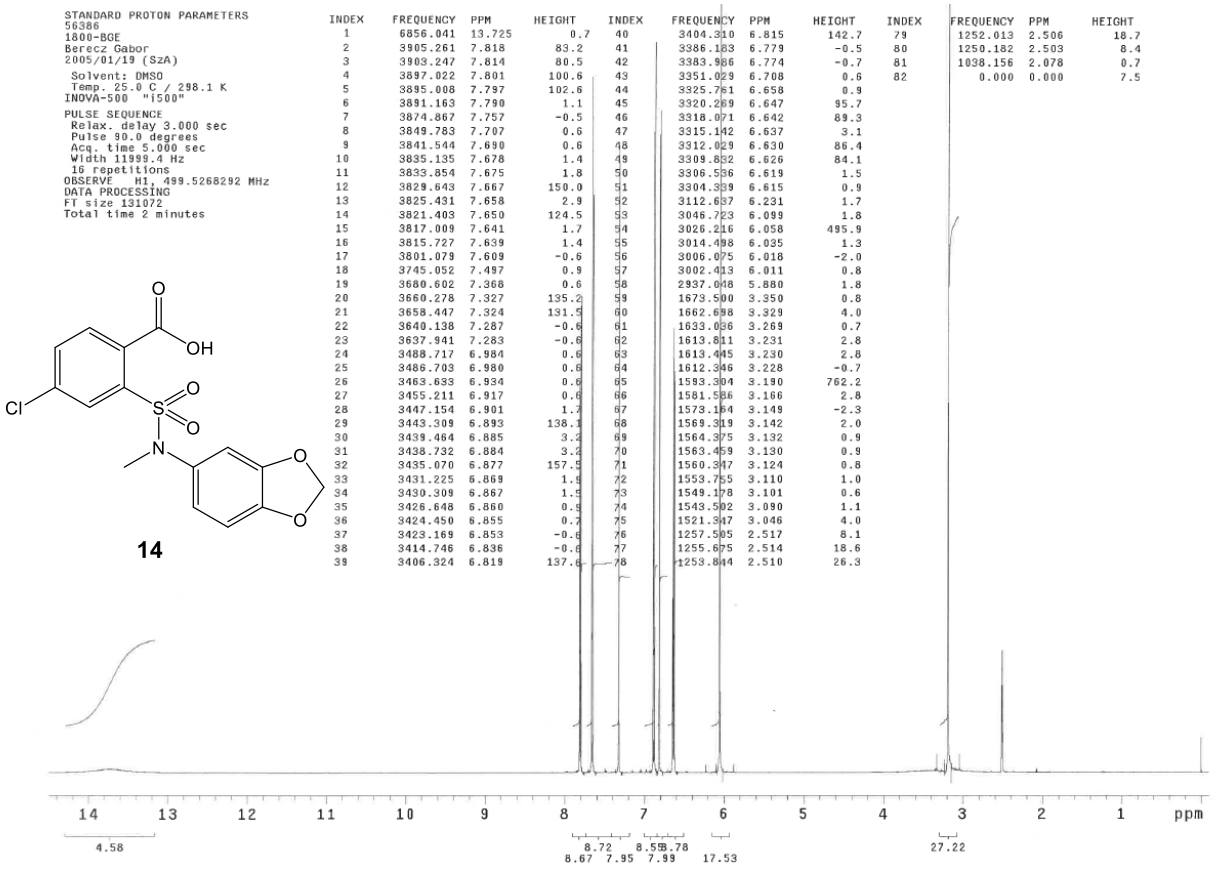
F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

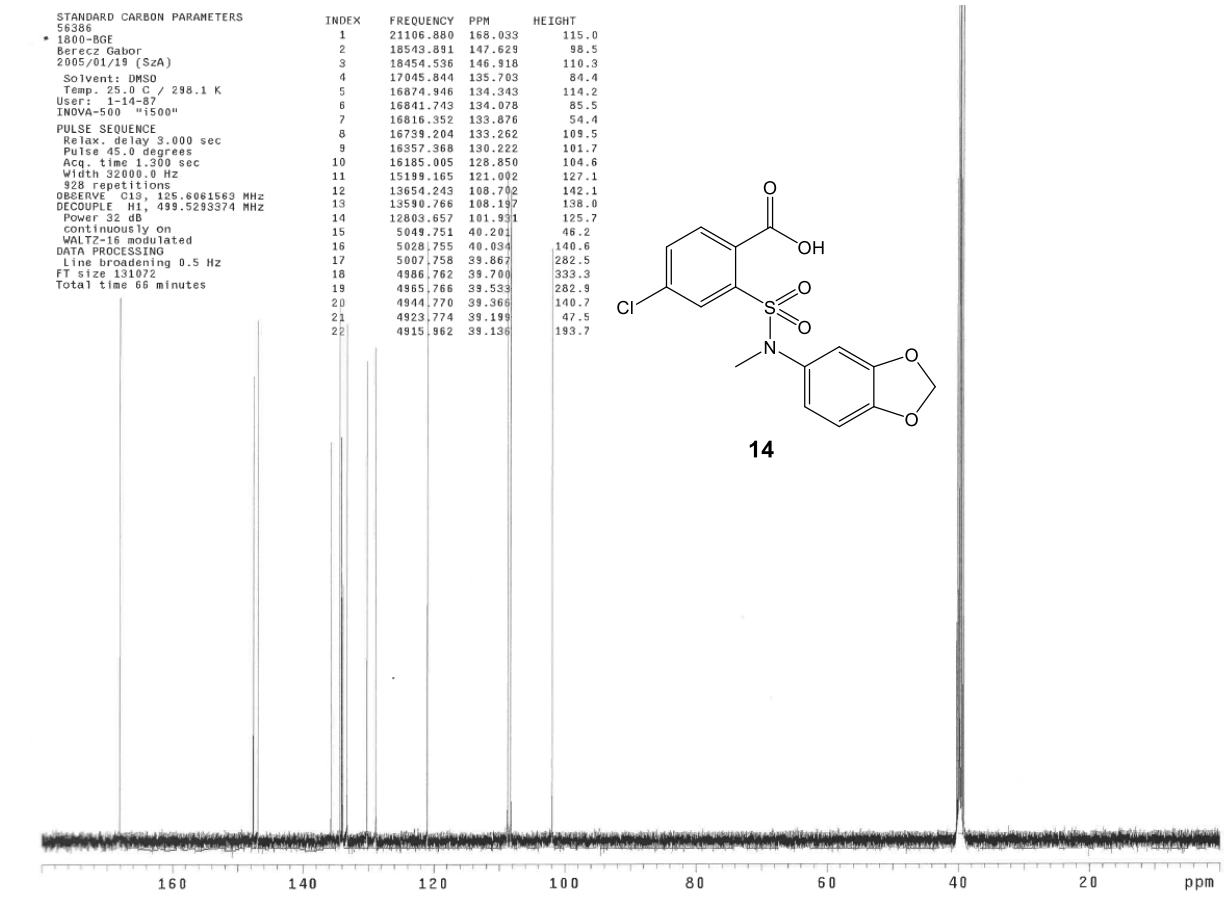
F2 - Processing parameters
SI 2048
SF 600.0000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

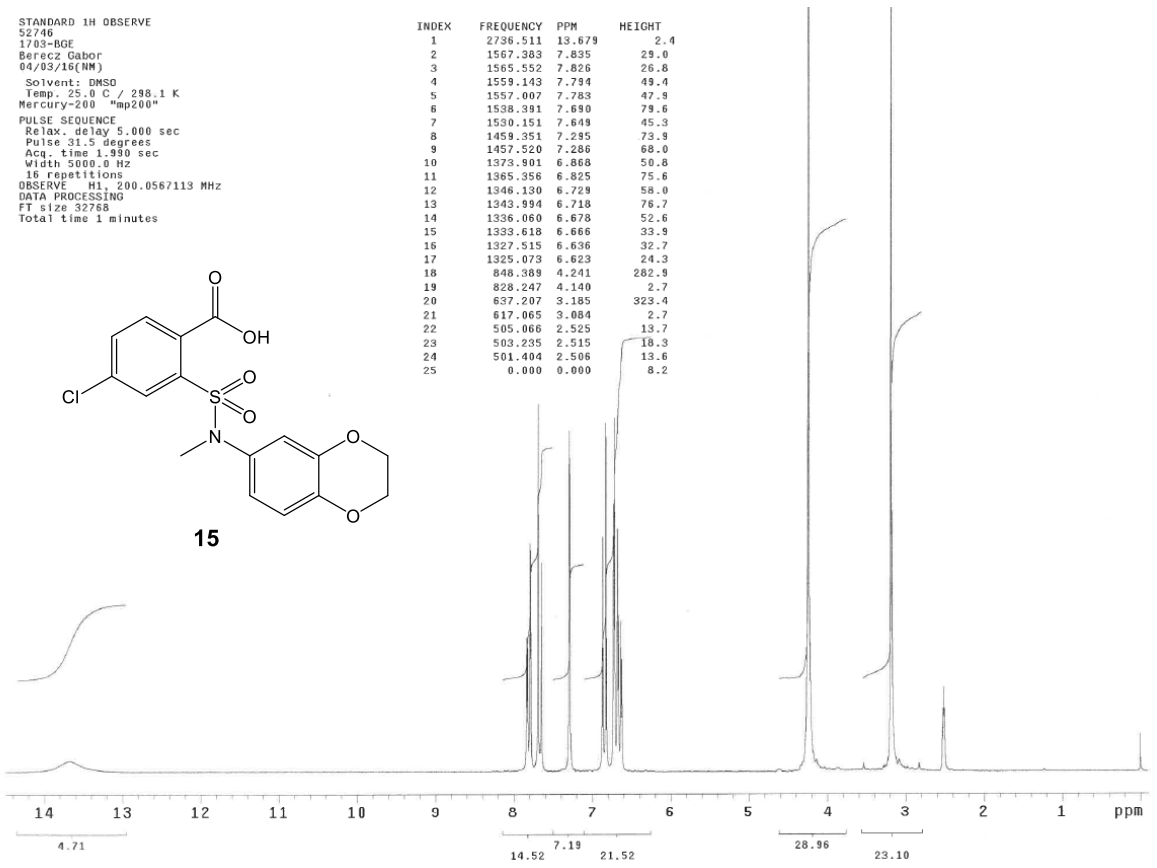
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701200 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

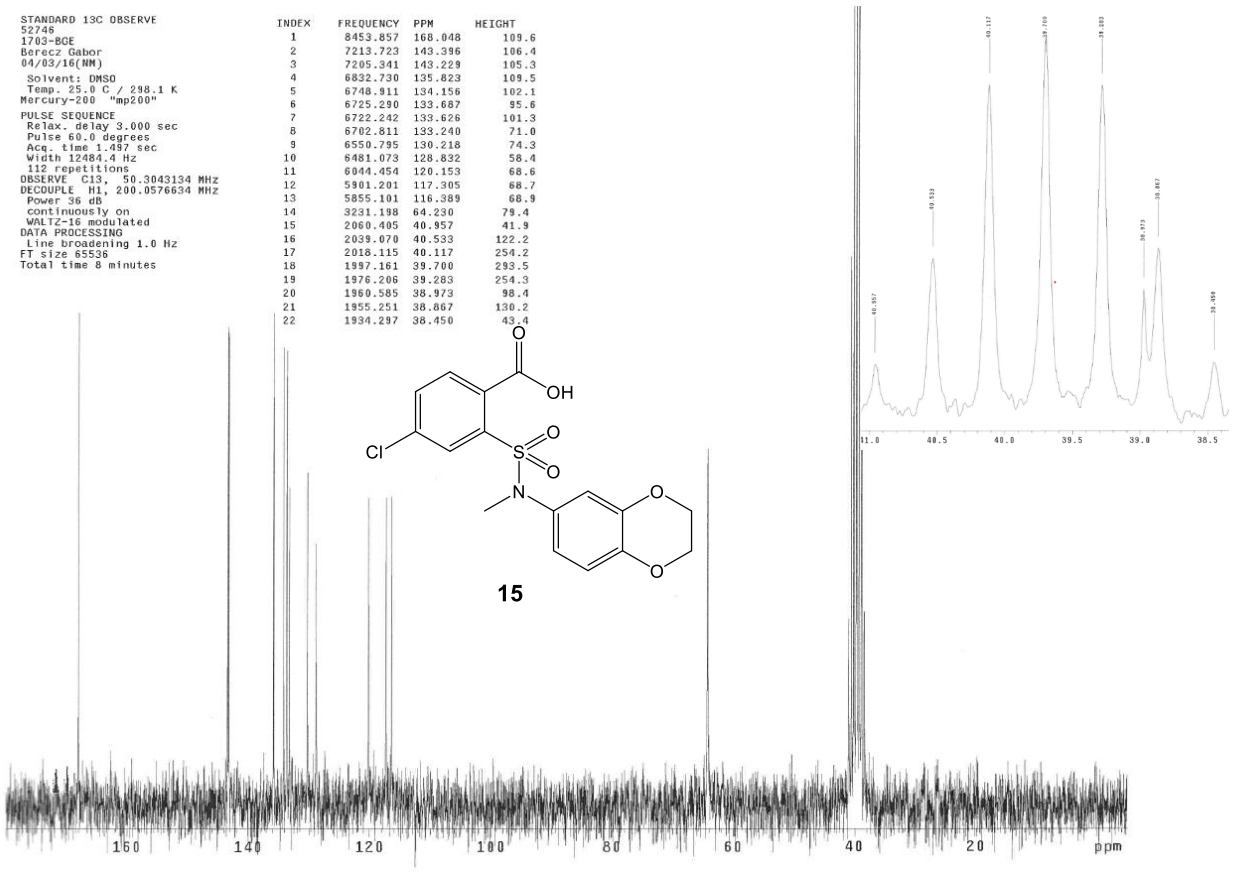

STANDARD 1H OBSERVE
52745
1702-BGE
Berecz Gabor
04/03/16(NM)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 5.000 sec
Pulse 31.5 degrees
Acq. time 1.993 sec
Width 3003.0 Hz
16 repetitions
OBSERVE H1, 200.0557652 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 1513.599 7.566 19.7
2 1511.766 7.557 23.2
3 1505.534 7.526 41.5
4 1503.701 7.516 43.9
5 1490.138 7.449 71.1
6 1487.205 7.434 60.2
7 1485.006 7.423 49.6
8 1482.073 7.408 33.3
9 1454.946 7.273 12.4
10 1364.768 6.822 38.5
11 1355.970 6.778 65.6
12 1344.971 6.723 45.2
13 1342.407 6.710 63.7
14 1335.075 6.674 43.7
15 1332.509 6.661 29.4
16 1326.277 6.630 26.7
17 1323.711 6.617 19.7
18 1059.776 5.297 3.9
19 853.392 4.266 17.3
20 849.360 4.246 248.8
21 844.961 4.224 14.0
22 841.295 4.205 3.5
23 774.945 3.874 333.4
24 648.476 3.241 363.2
25 333.952 1.669 12.6
26 -0.000 -0.000 14.2
Cl
O
S
N
13
7
6
5
4
3
2
1
ppm
18.95
18.31
0.22
24.75
18.51
18.55
0.70

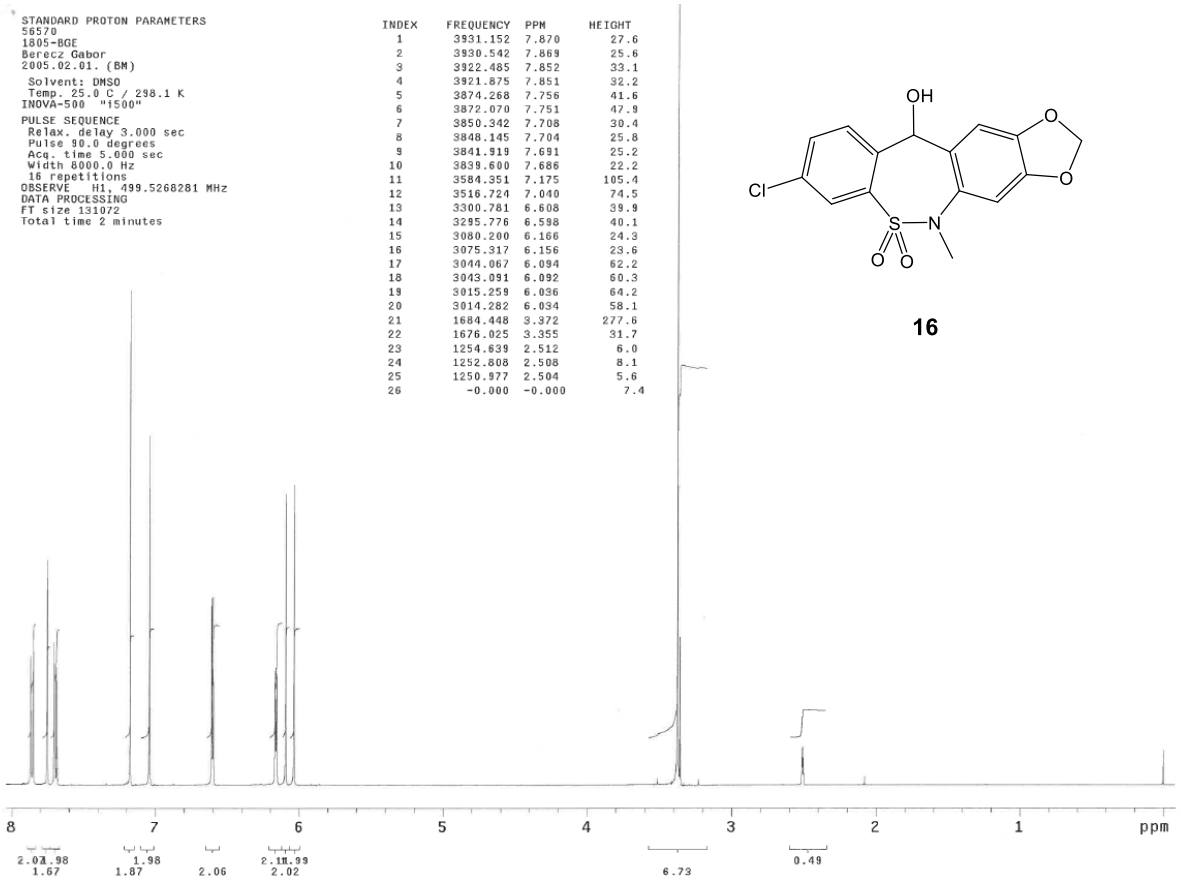

STANDARD 13C OBSERVE
52745
1702-BGE
Berecz Gabor
04/03/16(NM)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 60.0 degrees
Acq. time 1.497 sec
Width 12484.4 Hz
96 repetitions
OBSERVE C13, 50.3040655 MHz
DECOUPLE H1, 200.0567131 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 7 minutes
INDEX FREQUENCY PPM HEIGHT
1 8420.869 167.386 51.9
2 7218.072 143.478 67.0
3 7210.833 143.334 61.6
4 6891.180 136.980 64.0
5 6834.412 135.852 75.2
6 6731.162 133.799 69.5
7 6656.869 132.322 115.0
8 6622.579 131.641 57.5
9 6531.522 129.831 104.5
10 6512.091 129.445 115.0
11 6063.662 120.531 97.9
12 5901.740 117.312 102.3
13 5871.260 116.706 91.2
14 3905.715 77.636 162.0
15 3873.711 77.000 159.7
16 3842.089 76.371 155.1
17 3232.880 64.262 98.4
18 3227.927 64.163 94.3
19 2674.344 53.159 104.9
20 1968.744 39.134 87.3
Cl
O
S
N
13
160
140
120
100
80
60
40
20
ppm

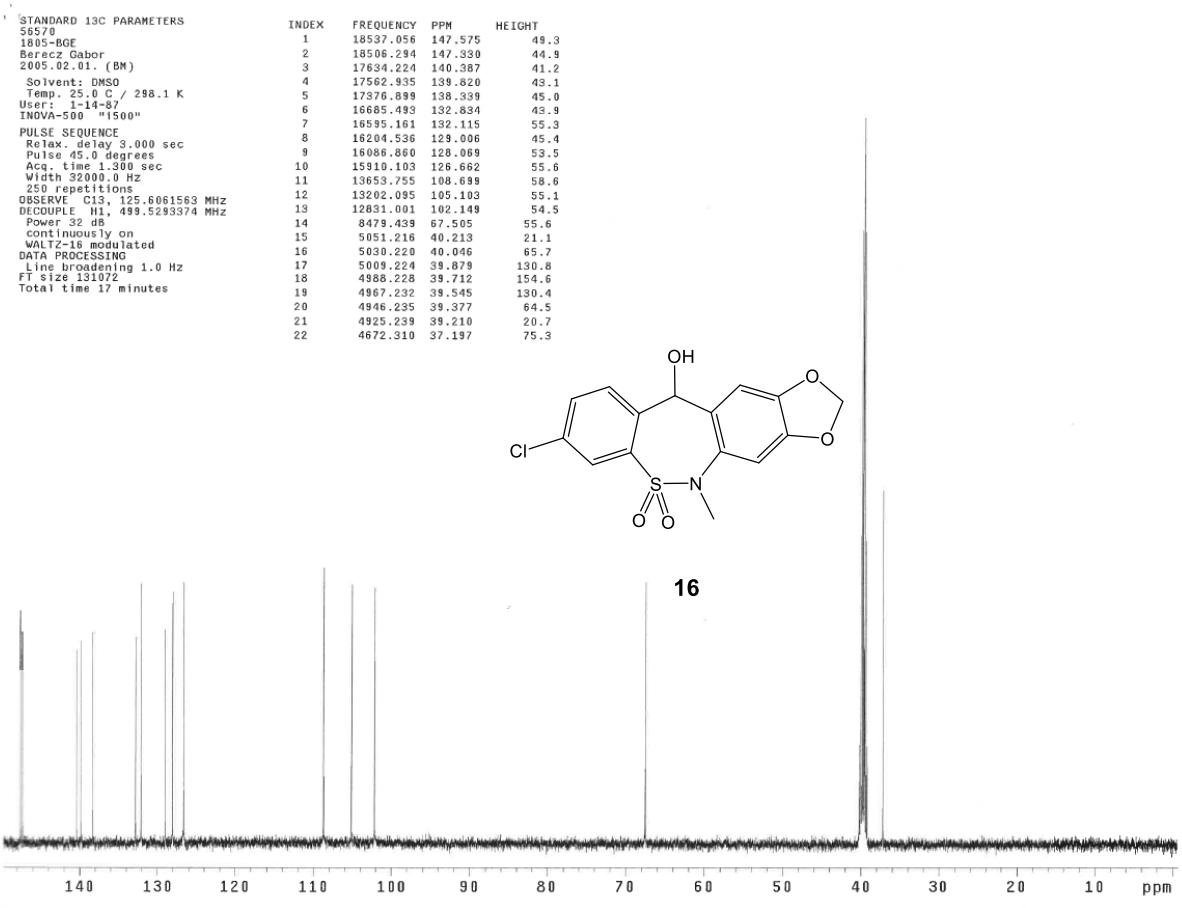

STANDARD PROTON PARAMETERS
56386
1800-BGE
Berecz Gabor
2005/01/19 (SzA)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 11999.4 Hz
16 repetitions
OBSERVE H1, 499.5268292 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 6856.041 13.725 0.7
2 3905.261 7.818 83.2
3 3903.247 7.814 80.5
4 3897.022 7.801 100.6
5 3895.008 7.797 102.6
6 3891.163 7.790 1.1
7 3874.867 7.757 -0.5
8 3849.783 7.707 0.6
9 3841.544 7.690 0.6
10 3835.135 7.678 1.4
11 3833.854 7.675 1.8
12 3829.643 7.667 150.0
13 3825.431 7.658 2.9
14 3821.403 7.650 124.5
15 3817.009 7.641 1.7
16 3815.727 7.639 1.4
17 3801.079 7.609 -0.6
18 3745.052 7.497 0.9
19 3680.602 7.368 0.6
20 3660.278 7.327 135.2
21 3658.447 7.324 131.5
22 3640.138 7.287 -0.6
23 3637.941 7.283 -0.6
24 3488.717 6.984 0.6
25 3486.703 6.980 0.6
26 3463.633 6.934 0.6
27 3455.211 6.917 0.6
28 3447.154 6.901 1.7
29 3443.309 6.893 138.1
30 3439.464 6.885 3.2
31 3438.732 6.884 3.2
32 3435.070 6.877 157.5
33 3431.225 6.869 1.5
34 3430.309 6.867 1.5
35 3426.648 6.860 0.9
36 3424.450 6.855 0.7
37 3423.169 6.853 -0.6
38 3414.746 6.836 -0.6
39 3406.324 6.819 137.6
40 3404.310 6.815 142.7
41 3386.183 6.779 -0.5
42 3383.986 6.774 -0.7
43 3351.029 6.708 0.6
44 3325.761 6.658 0.9
45 3320.269 6.647 95.7
46 3318.071 6.642 89.3
47 3315.142 6.637 3.1
48 3312.029 6.630 86.4
49 3309.832 6.626 84.1
50 3306.536 6.619 1.5
51 3304.339 6.615 0.9
52 3112.637 6.231 1.7
53 3046.723 6.099 1.8
54 3026.216 6.058 495.9
55 3014.498 6.035 1.3
56 3006.075 6.018 -2.0
57 3002.413 6.011 0.8
58 2937.048 5.880 1.8
59 1673.500 3.350 0.8
60 1662.698 3.329 4.0
61 1633.036 3.269 0.7
62 1613.811 3.231 2.8
63 1613.445 3.230 2.8
64 1612.346 3.228 -0.7
65 1593.304 3.190 762.2
66 1581.586 3.166 2.8
67 1573.154 3.149 -2.3
68 1569.319 3.142 2.0
69 1564.375 3.132 0.9
70 1563.459 3.130 0.9
71 1560.347 3.124 0.8
72 1553.755 3.110 1.0
73 1549.178 3.101 0.6
74 1543.502 3.090 1.1
75 1521.347 3.046 4.0
76 1257.505 2.517 8.1
77 1255.675 2.514 18.6
78 1253.844 2.510 26.3
79 1252.013 2.506 18.7
80 1250.182 2.503 8.4
81 1038.156 2.078 0.7
82 0.000 0.000 7.5
OH
O
S
N
Cl
14
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
4.58
8.72
8.67 7.95 8.55 7.99 8.78
17.53
27.22

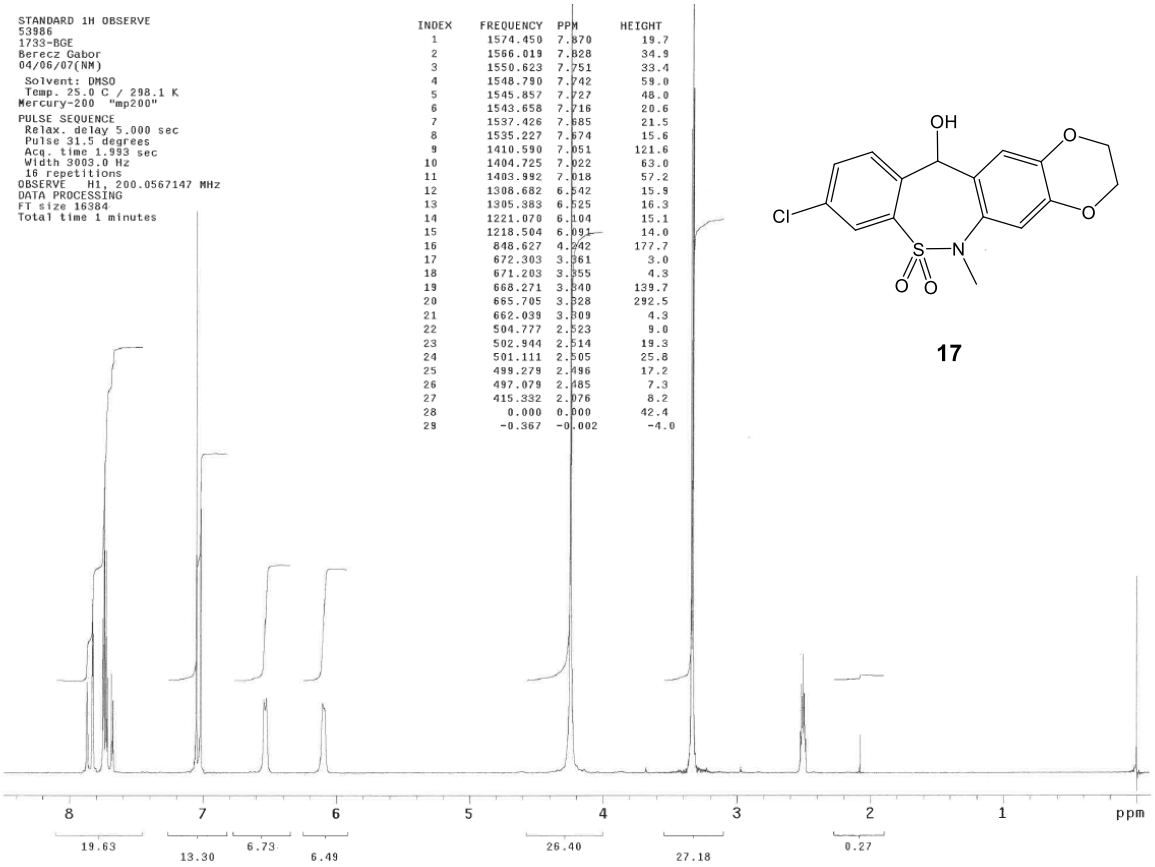

STANDARD CARBON PARAMETERS
56386
* 1800-BGE
Berecz Gabor
2005/01/19 (SzA)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
928 repetitions
OBSERVE C13, 125.6061569 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 66 minutes
INDEX FREQUENCY PPM HEIGHT
1 21106.880 168.033 115.0
2 18543.891 147.629 98.5
3 18454.536 146.918 110.3
4 17045.844 135.703 84.4
5 16874.946 134.343 114.2
6 16841.743 134.078 85.5
7 16816.352 133.876 54.4
8 16739.204 133.262 109.5
9 16357.368 130.222 101.7
10 16185.005 128.850 104.6
11 15199.165 121.002 127.1
12 13654.243 108.702 142.1
13 13590.766 108.197 138.0
14 12803.657 101.931 125.7
15 5049.751 40.201 46.2
16 5028.755 40.034 140.6
17 5007.758 39.867 282.5
18 4986.762 39.700 333.3
19 4965.766 39.533 282.9
20 4944.770 39.366 140.7
21 4923.774 39.199 47.5
22 4915.962 39.136 193.7
OH
O
S
N
Cl
14
160 140 120 100 80 60 40 20 ppm


STANDARD 1H OBSERVE
52746
1703-BGE
Berecz Gabor
04/03/16(NM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 5.000 sec
Pulse 31.5 degrees
Acq. time 1.990 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 200.0567113 MHz
DATA PROCESSING
FT size 32768
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 2736.511 13.679 2.4
2 1567.383 7.835 29.0
3 1565.552 7.826 26.8
4 1559.143 7.794 49.4
5 1557.007 7.783 47.9
6 1538.391 7.690 79.6
7 1530.151 7.649 45.3
8 1459.351 7.295 73.9
9 1457.520 7.286 68.0
10 1373.901 6.868 50.8
11 1365.356 6.825 75.6
12 1346.130 6.729 58.0
13 1343.994 6.718 76.7
14 1336.060 6.678 52.6
15 1333.618 6.666 33.9
16 1327.515 6.636 32.7
17 1325.073 6.623 24.3
18 848.389 4.241 282.9
19 828.247 4.140 2.7
20 637.207 3.185 323.4
21 617.065 3.084 2.7
22 505.066 2.525 13.7
23 503.235 2.515 18.3
24 501.404 2.506 13.6
25 0.000 0.000 8.2
O
OH
Cl
S
O
O
N
O
O
15
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
4.71
14.52
7.19
21.52
28.96
23.10

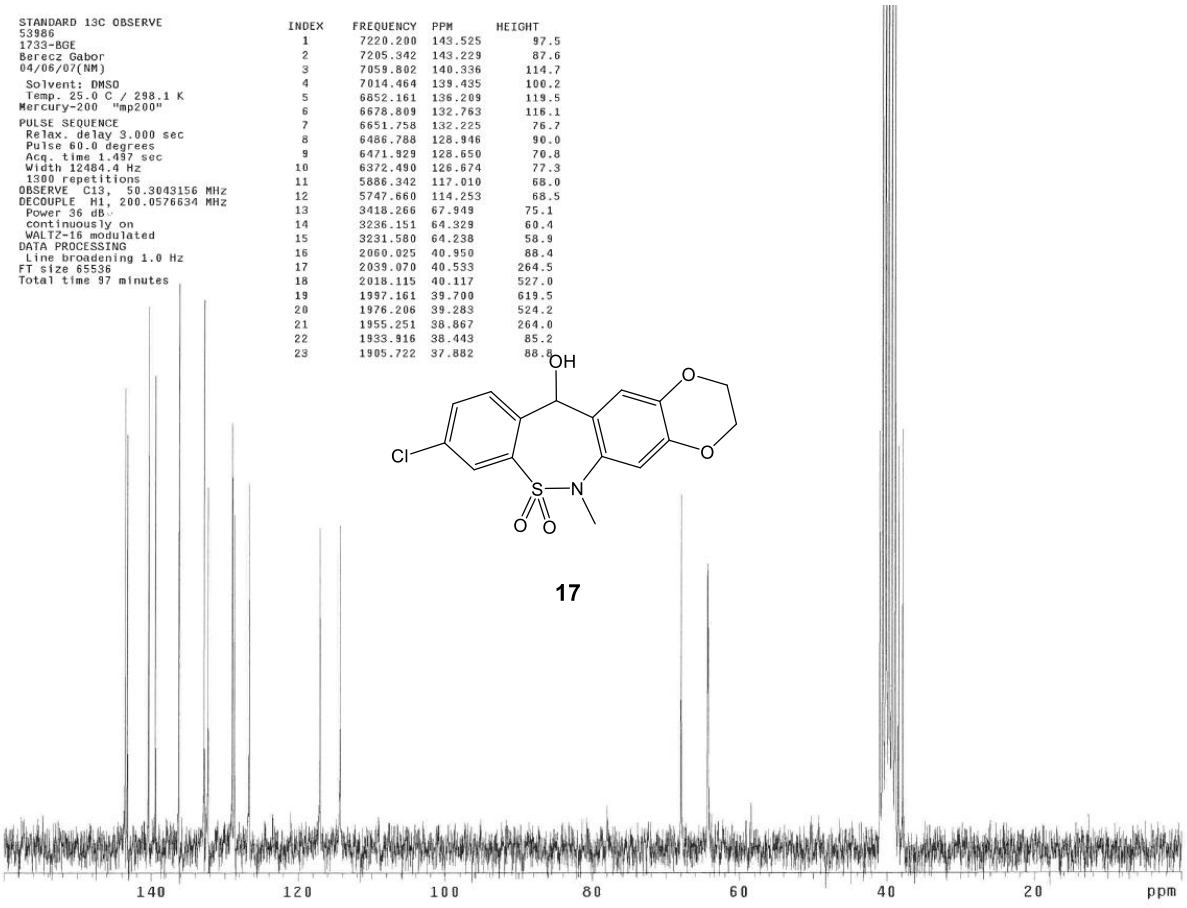

STANDARD 13C OBSERVE
52746
1703-BGE
Berecz Gabor
04/03/16(NM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 60.0 degrees
Acq. time 1.497 sec
Width 12484.4 Hz
112 repetitions
OBSERVE C13, 50.3043134 MHz
DECOUPLE H1, 200.0576634 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 minutes
INDEX FREQUENCY PPM HEIGHT
1 8453.857 168.048 109.6
2 7213.723 143.396 106.4
3 7205.341 143.229 105.3
4 6832.730 135.823 109.5
5 6748.911 134.156 102.1
6 6725.290 133.687 95.6
7 6722.242 133.626 101.3
8 6702.811 133.240 71.0
9 6550.795 130.218 74.3
10 6481.073 128.832 58.4
11 6044.454 120.153 68.6
12 5901.201 117.305 68.7
13 5855.101 116.389 68.9
14 3231.198 64.230 79.4
15 2060.405 40.957 41.9
16 2039.070 40.533 122.2
17 2018.115 40.117 254.2
18 1997.161 39.700 293.5
19 1976.206 39.283 254.3
20 1960.585 38.973 98.4
21 1955.251 38.867 130.2
22 1934.297 38.450 43.4
O
OH
Cl
S
O
O
N
O
O
15
160 140 120 100 80 60 40 20 ppm
41.0 40.5 40.0 39.5 39.0 38.5


STANDARD PROTON PARAMETERS
56570
1805-BGE
Berecz Gabor
2005.02.01. (BM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268281 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3931.152 7.870 27.6
2 3930.542 7.869 25.6
3 3922.485 7.852 33.1
4 3921.875 7.851 32.2
5 3874.268 7.756 41.6
6 3872.070 7.751 47.9
7 3850.342 7.708 30.4
8 3848.145 7.704 25.8
9 3841.919 7.691 25.2
10 3839.600 7.686 22.2
11 3584.351 7.175 105.4
12 3516.724 7.040 74.5
13 3300.781 6.608 39.9
14 3295.776 6.598 40.1
15 3080.200 6.166 24.3
16 3075.317 6.156 23.6
17 3044.067 6.094 62.2
18 3043.091 6.092 60.3
19 3015.259 6.036 64.2
20 3014.282 6.034 58.1
21 1684.448 3.372 277.6
22 1676.025 3.355 31.7
23 1254.639 2.512 6.0
24 1252.808 2.508 8.1
25 1250.977 2.504 5.6
26 -0.000 -0.000 7.4
OH
O
O
Cl
S
N
O
O
16
8
7
6
5
4
3
2
1
ppm
2.01 1.98
1.67
1.98
1.87
2.06
2.11 1.99
2.02
6.73
0.49

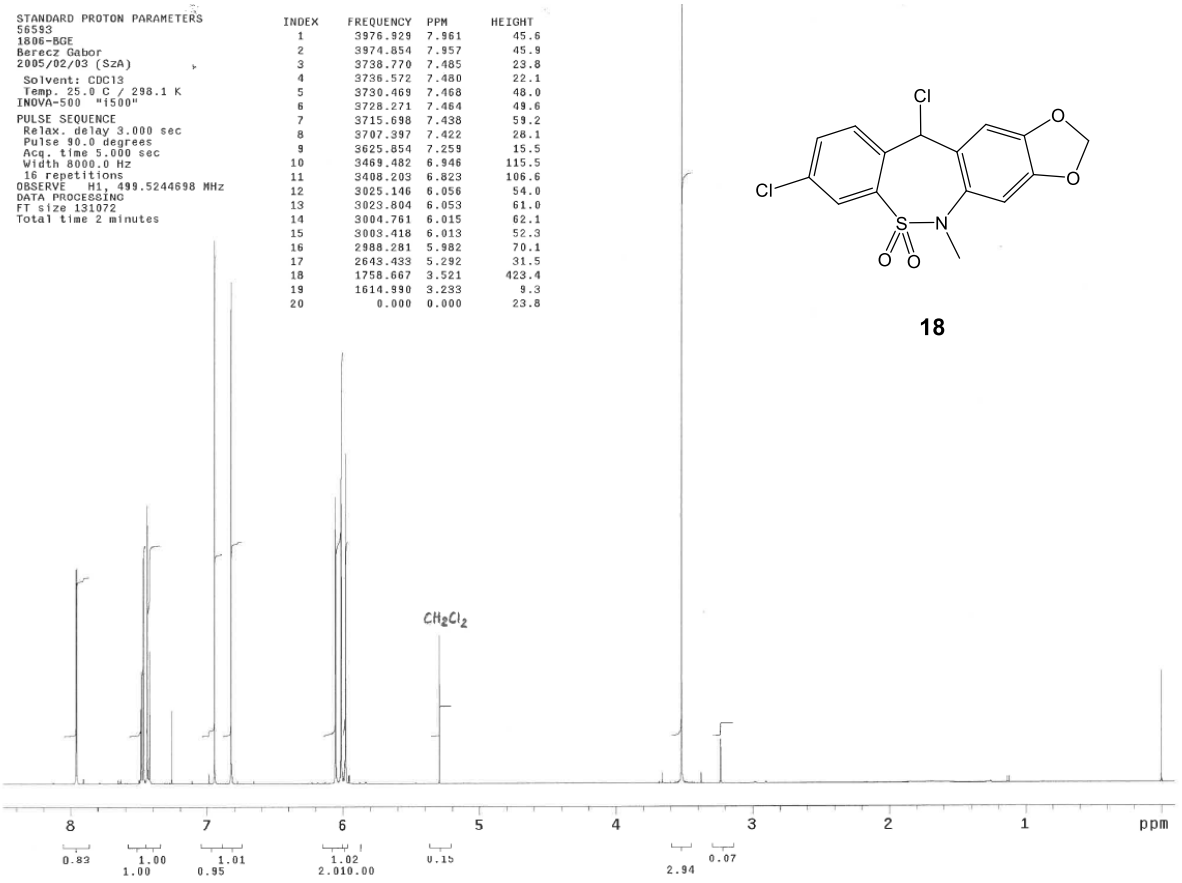

STANDARD 13C PARAMETERS
56570
1805-BGE
Berecz Gabor
2005.02.01. (BM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
250 repetitions
OBSERVE C13, 125.6061563 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 17 minutes
INDEX FREQUENCY PPM HEIGHT
1 18537.056 147.575 48.3
2 18506.294 147.330 44.9
3 17634.224 140.387 41.2
4 17562.935 139.820 43.1
5 17376.899 138.339 45.0
6 16685.493 132.834 43.9
7 16595.161 132.115 55.3
8 16204.536 129.006 45.4
9 16086.860 128.069 53.5
10 15910.103 126.662 55.6
11 13653.755 108.699 58.6
12 13202.095 105.103 55.1
13 12831.001 102.149 54.5
14 8479.439 67.505 55.6
15 5051.216 40.213 21.1
16 5030.220 40.046 65.7
17 5009.224 39.879 130.8
18 4988.228 39.712 154.6
19 4967.232 39.545 130.4
20 4946.235 39.377 64.5
21 4925.239 39.210 20.7
22 4672.310 37.197 75.3
OH
O
O
Cl
S
N
O
O
16
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


STANDARD 1H OBSERVE
53986
1733-BGE
Berecz Gabor
04/06/07(NM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 5.000 sec
Pulse 31.5 degrees
Acq. time 1.993 sec
Width 3003.0 Hz
16 repetitions
OBSERVE H1, 200.0567147 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 1574.450 7.870 19.7
2 1566.018 7.828 34.9
3 1550.823 7.751 33.4
4 1548.790 7.742 58.0
5 1545.857 7.727 48.0
6 1543.658 7.716 20.6
7 1537.426 7.685 21.5
8 1535.227 7.674 15.6
9 1410.590 7.051 121.6
10 1404.725 7.022 63.0
11 1403.992 7.018 57.2
12 1308.682 6.542 15.9
13 1305.383 6.525 16.3
14 1221.070 6.104 15.1
15 1218.504 6.091 14.0
16 848.627 4.242 177.7
17 672.303 3.361 3.0
18 671.203 3.355 4.3
19 668.271 3.340 139.7
20 665.705 3.328 292.5
21 662.039 3.309 4.3
22 504.777 2.523 9.0
23 502.944 2.514 19.3
24 501.111 2.505 25.8
25 499.279 2.496 17.2
26 497.079 2.485 7.3
27 415.332 2.076 8.2
28 0.000 0.000 42.4
29 -0.367 -0.002 -4.0
OH
Cl
S
N
O
8
7
6
5
4
3
2
1
ppm
19.63
13.30
6.73
6.49
26.40
27.18
0.27

17


STANDARD 13C OBSERVE
53986
1733-BGE
Berecz Gabor
04/06/07(NM)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
Mercury-200 "mp200"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 60.0 degrees
Acq. time 1.497 sec
Width 12484.4 Hz
1300 repetitions
OBSERVE C13, 50.3043156 MHz
DECOUPLE H1, 200.0576634 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 97 minutes
INDEX FREQUENCY PPM HEIGHT
1 7220.200 143.525 97.5
2 7205.342 143.229 87.6
3 7059.802 140.336 114.7
4 7014.464 139.435 100.2
5 6852.161 136.209 119.5
6 6678.809 132.763 116.1
7 6651.758 132.225 76.7
8 6486.788 128.946 90.0
9 6471.929 128.650 70.8
10 6372.490 126.674 77.3
11 5886.342 117.010 68.0
12 5747.660 114.253 68.5
13 3418.266 67.949 75.1
14 3236.151 64.329 60.4
15 3231.580 64.238 58.9
16 2060.025 40.950 88.4
17 2039.070 40.533 264.5
18 2018.115 40.117 527.0
19 1997.161 39.700 619.5
20 1976.206 39.283 524.2
21 1955.251 38.867 264.0
22 1933.916 38.443 85.2
23 1905.722 37.882 88.8
OH
Cl
S
N
O
140
120
100
80
60
40
20
ppm

17


STANDARD PROTON PARAMETERS
56593
1806-BGE
Berecz Gabor
2005/02/03 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244698 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3976.929 7.961 45.6
2 3974.854 7.957 45.9
3 3738.770 7.485 23.8
4 3736.572 7.480 22.1
5 3730.469 7.468 48.0
6 3728.271 7.464 49.6
7 3715.698 7.438 59.2
8 3707.397 7.422 28.1
9 3625.854 7.259 15.5
10 3469.482 6.946 115.5
11 3408.203 6.823 106.6
12 3025.146 6.056 54.0
13 3023.804 6.053 61.0
14 3004.761 6.015 62.1
15 3003.418 6.013 52.3
16 2988.281 5.982 70.1
17 2643.433 5.292 31.5
18 1758.667 3.521 423.4
19 1614.990 3.233 9.3
20 0.000 0.000 23.8
Cl
Cl
O
O
S
N
O
O
18
CH2Cl2
8
7
6
5
4
3
2
1
ppm
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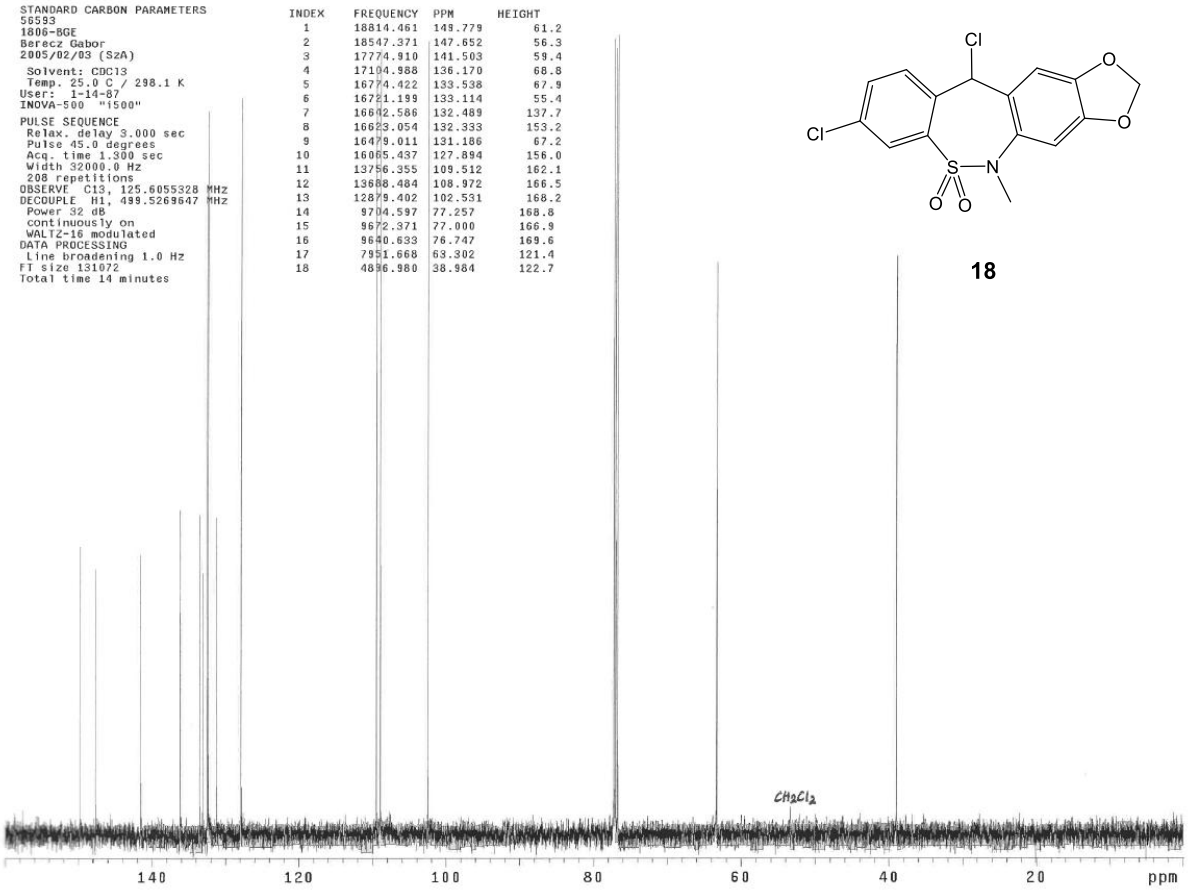
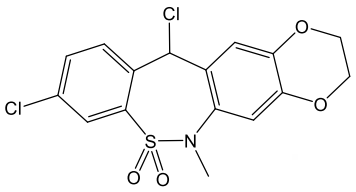
1.00
1.01
0.95
1.02
2.010.00
0.15
2.94
0.07

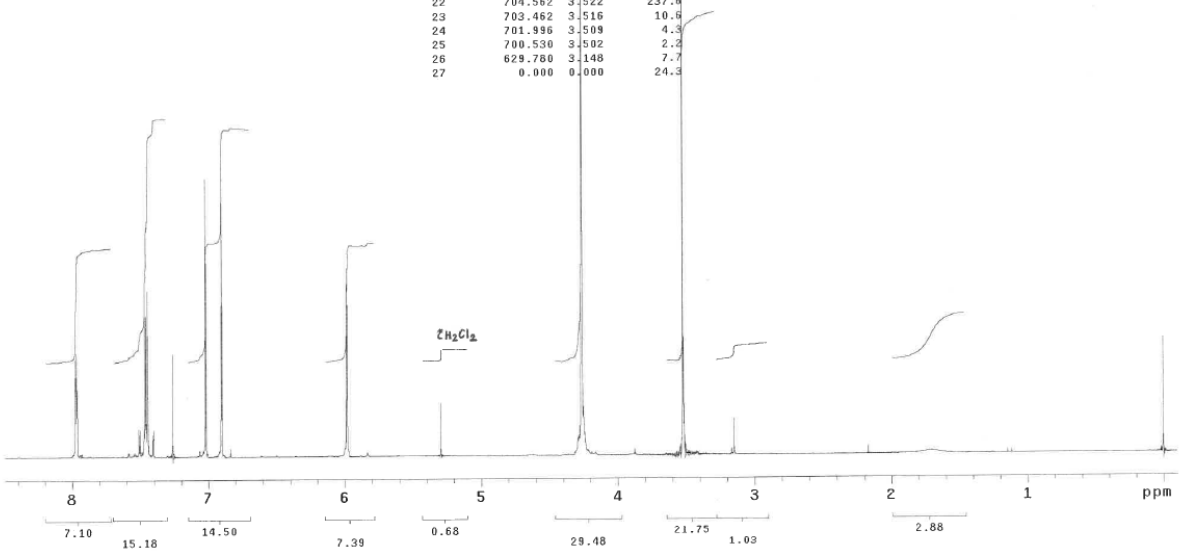

STANDARD CARBON PARAMETERS
56593
1806-BGE
Berecz Gabor
2005/02/03 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
208 repetitions
OBSERVE C13, 125.6055328 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 14 minutes
INDEX FREQUENCY PPM HEIGHT
1 18814.461 149.779 61.2
2 18547.371 147.652 56.3
3 17774.910 141.503 59.4
4 17104.988 136.170 68.8
5 16774.422 133.538 67.9
6 16721.199 133.114 55.4
7 16602.586 132.489 137.7
8 16623.054 132.333 153.2
9 16479.011 131.186 67.2
10 16065.437 127.894 156.0
11 13756.355 109.512 162.1
12 13688.484 108.972 166.5
13 12879.402 102.531 168.2
14 9704.597 77.257 168.8
15 9672.371 77.000 166.9
16 9640.633 76.747 169.6
17 7951.668 63.302 121.4
18 4896.980 38.984 122.7
Cl
Cl
O
O
S
N
O
O
18
CH2Cl2
140
120
100
80
60
40
20
ppm

```
STANDARD 1H OBSERVE
54080
1734-BGE
Berecz Gabor
04/06/10(NM)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
Mercury-200  "mp200"
PULSE SEQUENCE
 Relax. delay 5.000 sec
 Pulse 31.5 degrees
 Acq. time 1.993 sec
 Width 3003.0 Hz
 16 repetitions
OBSERVE   H1, 200.0557681 MHz
DATA PROCESSING
FT size 16384
Total time 1 minutes
```

INDEX	FREQUENCY	PPM	HEIGHT
1	1595.712	7.976	20.7
2	1593.879	7.967	22.0
3	1502.601	7.511	5.9
4	1500.402	7.500	5.7
5	1494.170	7.469	36.0
6	1491.970	7.458	29.7
7	1489.771	7.447	35.0
8	1481.340	7.405	5.7
9	1452.380	7.260	21.7
10	1404.358	7.020	58.8
11	1380.897	6.903	53.9
12	1197.242	5.985	36.3
13	1059.042	5.294	11.2
14	857.791	4.288	3.9
15	856.325	4.280	6.3
16	852.659	4.262	134.8
17	850.093	4.249	10.3
18	848.994	4.244	5.3
19	847.527	4.236	3.6
20	708.228	3.540	2.2
21	706.395	3.531	4.6
22	704.562	3.522	237.6
23	703.462	3.516	10.6
24	701.996	3.509	4.3
25	700.530	3.502	2.2
26	629.780	3.148	7.7
27	0.000	0.000	24.3



19

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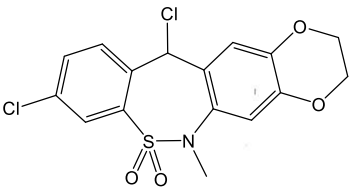
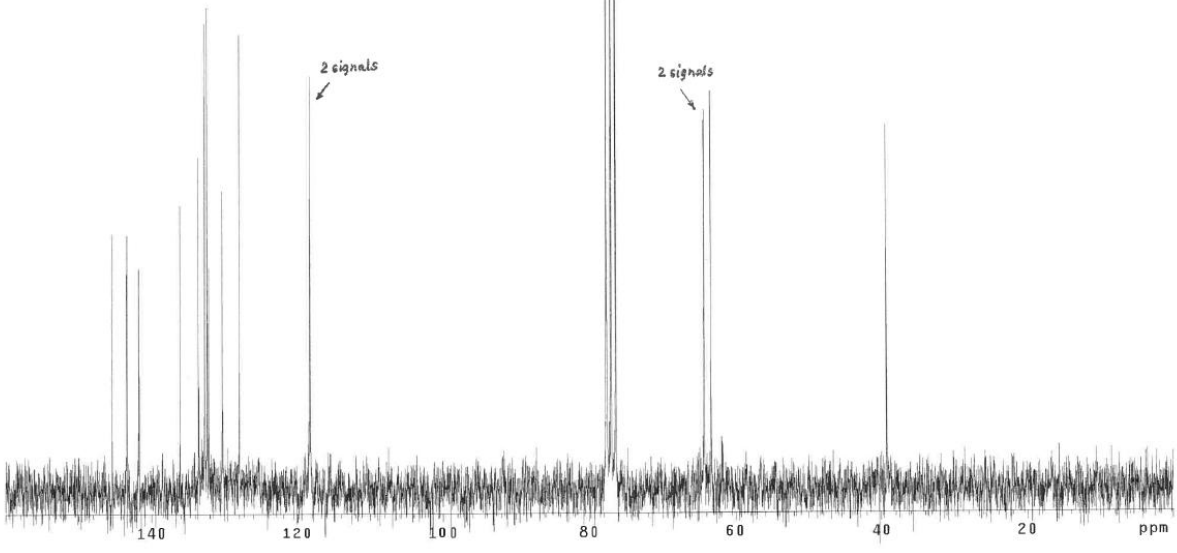
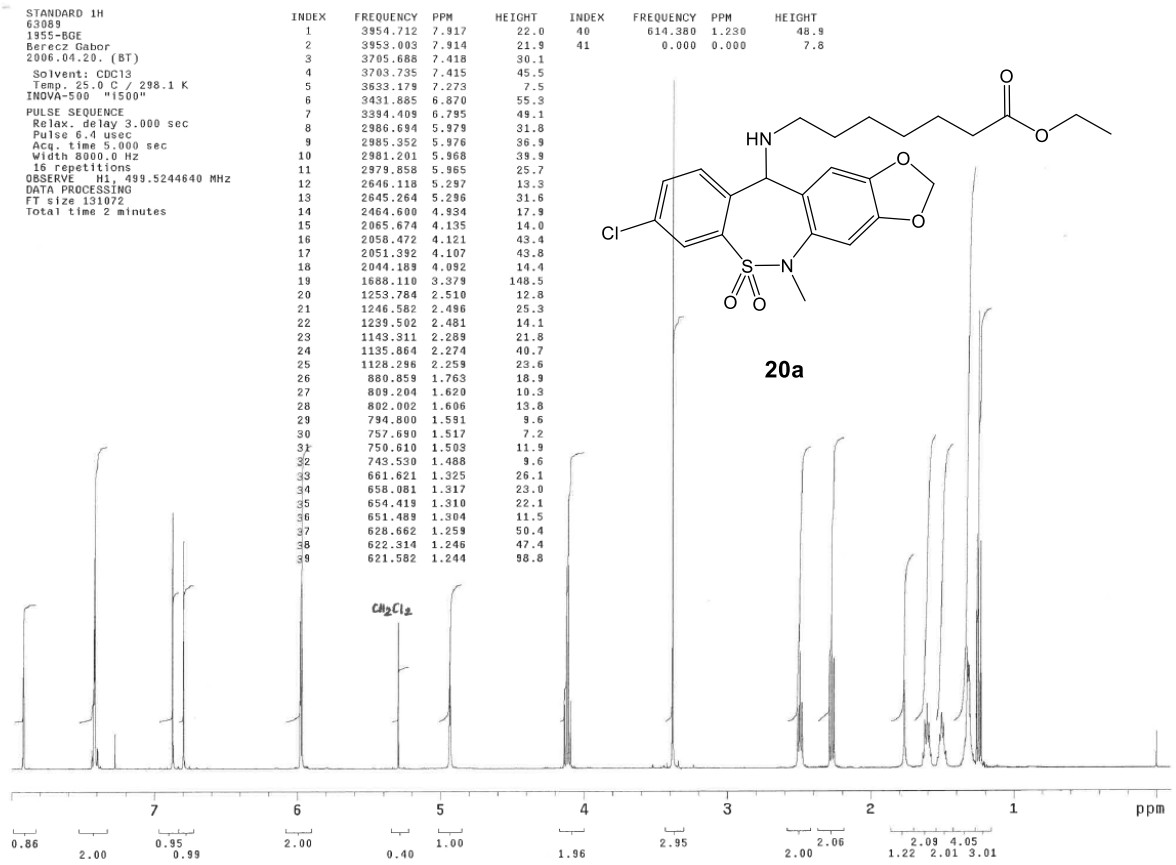
STANDARD 13C OBSERVE
54080
1734-BGE
Berecz Gabor
04/06/10(NM)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
Mercury-200  "mp200"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 60.0 degrees
 Acq. time 1.497 sec
 Width 12484.4 Hz
 265 repetitions
OBSERVE  C13,  50.3040643 MHz
DECOUPLE  H1, 200.0567131 MHz
 Power 36 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 65536
Total time 19 minutes
```

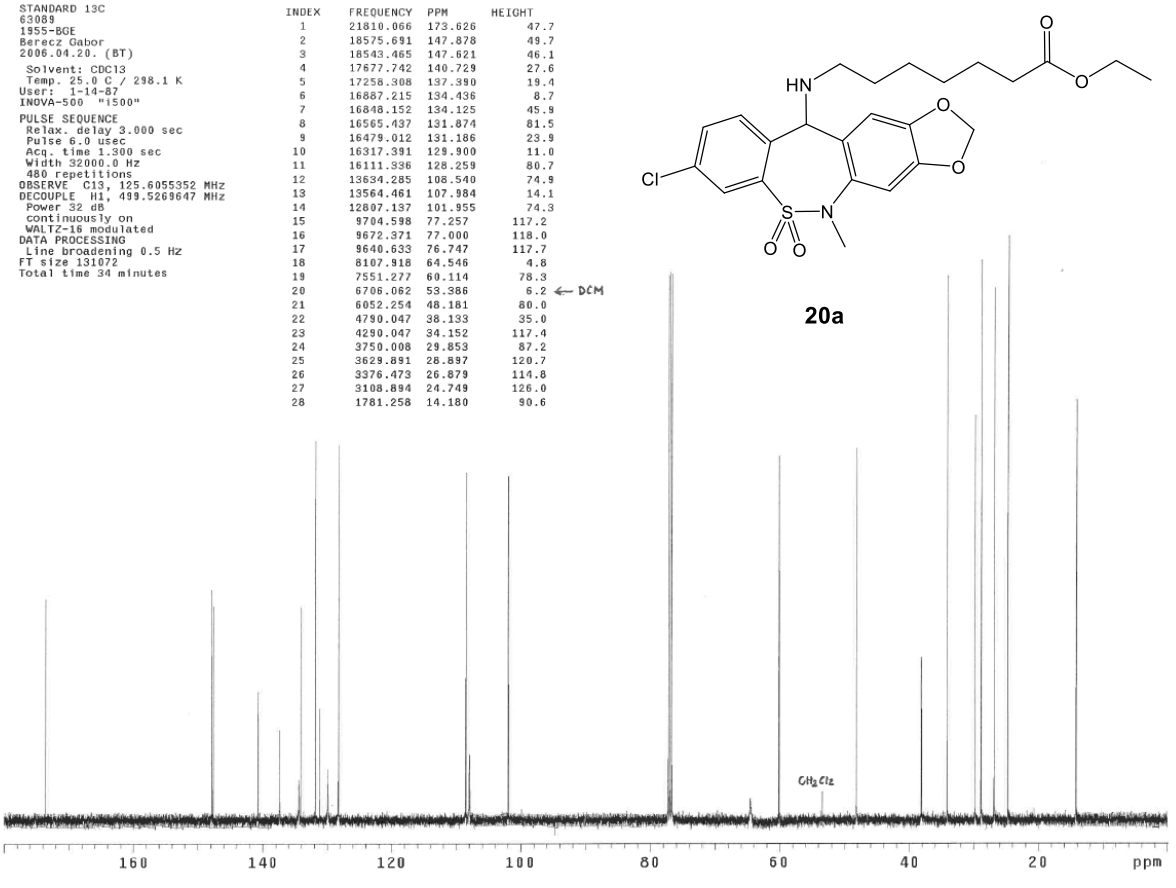
INDEX	FREQUENCY	PPM	HEIGHT
1	7315.606	145.417	54.8
2	7213.119	143.378	54.5
3	7128.920	141.706	47.6
4	6845.841	136.079	61.0
5	6717.066	133.519	71.2
6	6675.156	132.686	99.7
7	6656.869	132.322	103.2
8	6646.201	132.110	47.7
9	6553.619	130.270	63.9
10	6438.559	127.983	97.3
11	5951.269	118.297	88.4
12	5948.983	118.251	81.2
13	3905.715	77.636	256.9
14	3873.711	77.000	263.2
15	3841.708	76.364	249.8
16	3235.928	64.322	78.6
17	3232.499	64.254	80.9
18	3189.066	63.391	84.9
19	1974.840	39.255	77.8

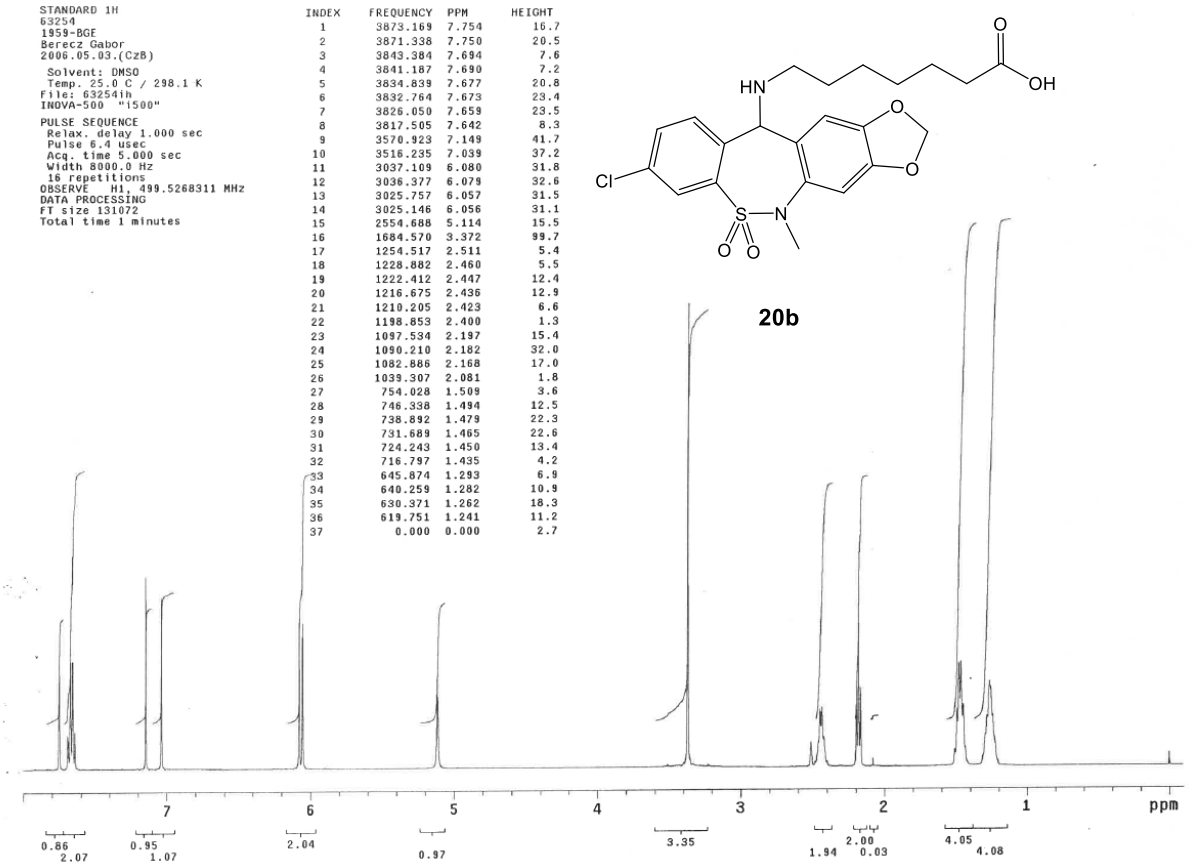


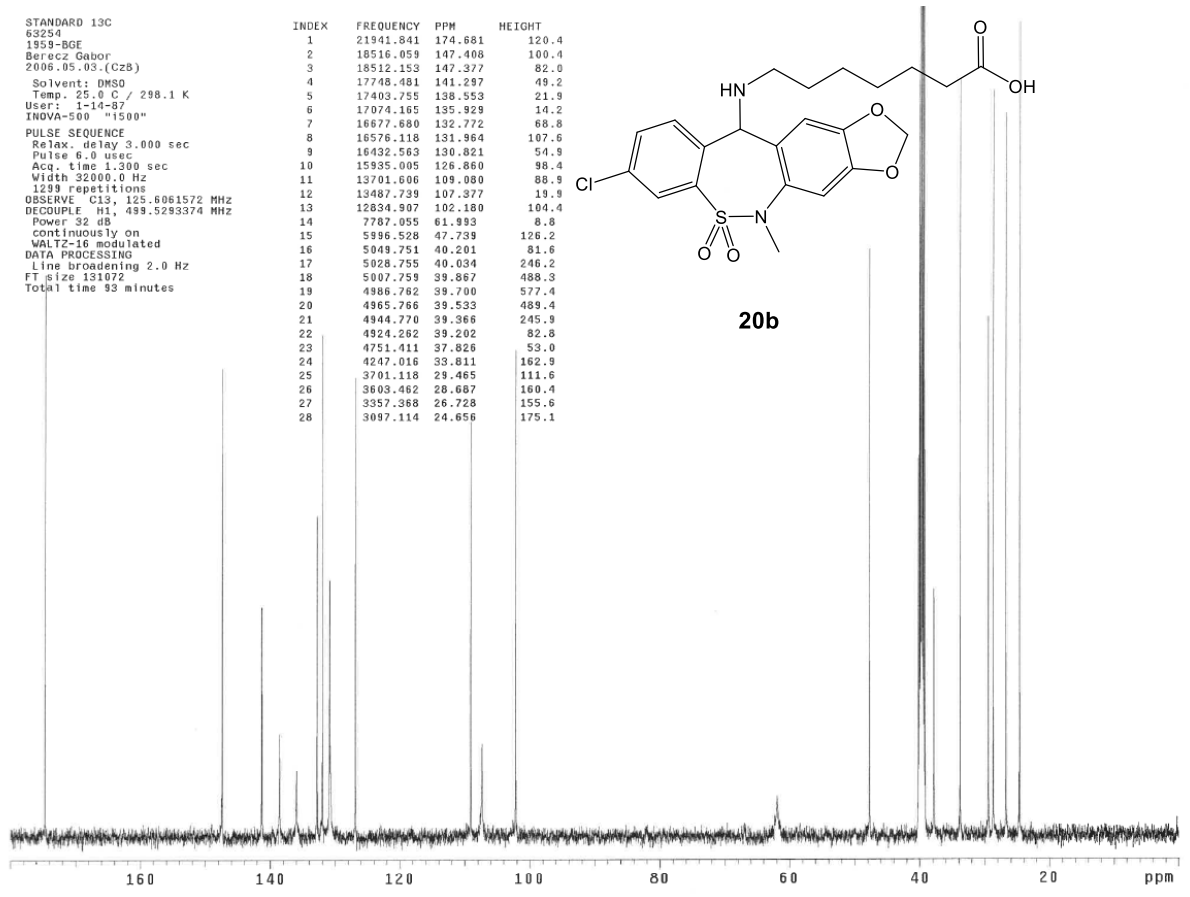
19




STANDARD 1H
63089
1955-BGE
Berecz Gabor
2006.04.20. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244640 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3954.712 7.917 22.0 40 614.380 1.230 48.9
2 3953.003 7.914 21.9 41 0.000 0.000 7.8
3 3705.688 7.418 30.1
4 3703.735 7.415 45.5
5 3633.179 7.273 7.5
6 3431.885 6.870 55.3
7 3394.409 6.795 49.1
8 2986.694 5.979 31.8
9 2985.352 5.976 36.9
10 2981.201 5.968 39.9
11 2979.858 5.965 25.7
12 2646.118 5.297 13.3
13 2645.264 5.296 31.6
14 2464.600 4.934 17.9
15 2065.674 4.135 14.0
16 2058.472 4.121 43.4
17 2051.392 4.107 43.8
18 2044.189 4.092 14.4
19 1688.110 3.379 148.5
20 1253.784 2.510 12.8
21 1246.582 2.496 25.3
22 1239.502 2.481 14.1
23 1143.311 2.289 21.8
24 1135.864 2.274 40.7
25 1128.296 2.259 23.6
26 880.859 1.763 18.9
27 809.204 1.620 10.3
28 802.002 1.606 13.8
29 794.800 1.591 9.6
30 757.690 1.517 7.2
31 750.610 1.503 11.9
32 743.530 1.488 9.6
33 661.621 1.325 26.1
34 658.081 1.317 23.0
35 654.419 1.310 22.1
36 651.489 1.304 11.5
37 628.662 1.259 50.4
38 622.314 1.246 47.4
39 621.582 1.244 98.8
HN
O
O
O
O
Cl
S
N
O
O
20a
CH2Cl2
7
6
5
4
3
2
1
ppm
0.86
2.00
0.95
0.99
2.00
0.40
1.00
1.96
2.95
2.00
2.06
2.09
4.05
1.22
2.01
3.01

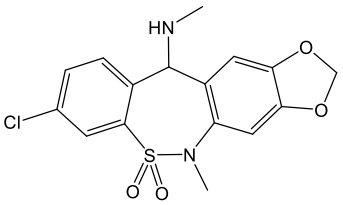

STANDARD 13C
63089
1955-BGE
Berecz Gabor
2006.04.20. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
480 repetitions
OBSERVE C13, 125.6055352 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 34 minutes
INDEX FREQUENCY PPM HEIGHT
1 21810.066 173.626 47.7
2 18575.691 147.878 49.7
3 18543.465 147.621 46.1
4 17677.742 140.729 27.6
5 17258.308 137.390 19.4
6 16887.215 134.436 8.7
7 16848.152 134.125 45.9
8 16565.437 131.874 81.5
9 16479.012 131.186 23.9
10 16317.391 129.900 11.0
11 16111.336 128.259 80.7
12 13634.285 108.540 74.9
13 13564.461 107.984 14.1
14 12807.137 101.955 74.3
15 9704.598 77.257 117.2
16 9672.371 77.000 118.0
17 9640.633 76.747 117.7
18 8107.918 64.546 4.8
19 7551.277 60.114 78.3
20 6706.062 53.386 6.2 ← DCM
21 6052.254 48.181 80.0
22 4790.047 38.133 35.0
23 4290.047 34.152 117.4
24 3750.008 29.853 87.2
25 3629.891 28.897 120.7
26 3376.473 26.879 114.8
27 3108.894 24.749 126.0
28 1781.258 14.180 90.6
HN
O
O
O
O
Cl
S
N
O
O
20a
CH2Cl2
160
140
120
100
80
60
40
20
ppm


STANDARD 1H
63254
1959-BGE
Berecz Gabor
2006.05.03.(CzB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
File: 63254ih
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 8.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268311 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3873.169 7.754 16.7
2 3871.338 7.750 20.5
3 3843.384 7.694 7.6
4 3841.187 7.690 7.2
5 3834.839 7.677 20.8
6 3832.764 7.673 23.4
7 3826.050 7.659 23.5
8 3817.505 7.642 8.3
9 3570.923 7.149 41.7
10 3516.235 7.039 37.2
11 3037.109 6.080 31.8
12 3036.377 6.079 32.6
13 3025.757 6.057 31.5
14 3025.146 6.056 31.1
15 2554.688 5.114 15.5
16 1684.570 3.372 99.7
17 1254.517 2.511 5.4
18 1228.882 2.460 5.5
19 1222.412 2.447 12.4
20 1216.675 2.436 12.9
21 1210.205 2.423 6.6
22 1198.853 2.400 1.3
23 1097.534 2.197 15.4
24 1090.210 2.182 32.0
25 1082.886 2.168 17.0
26 1039.307 2.081 1.8
27 754.028 1.509 3.6
28 746.338 1.494 12.5
29 738.892 1.479 22.3
30 731.689 1.465 22.6
31 724.243 1.450 13.4
32 716.797 1.435 4.2
33 645.874 1.293 6.9
34 640.259 1.282 10.9
35 630.371 1.262 18.3
36 619.751 1.241 11.2
37 0.000 0.000 2.7
HN
O
OH
O
O
Cl
S
N
O
O
20b
7
6
5
4
3
2
1
ppm
0.86
2.07
0.95
1.07
2.04
0.97
3.35
1.94
2.00
0.03
4.05
4.08

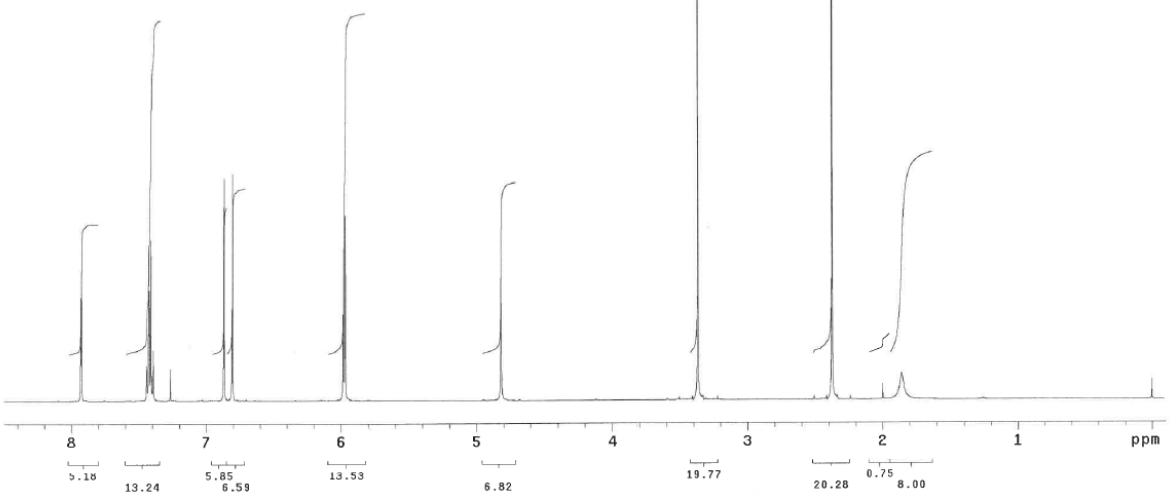

STANDARD 13C
63254
1959-BGE
Berecz Gabor
2006.05.03.(CzB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
1299 repetitions
OBSERVE C13, 125.6061572 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 93 minutes
INDEX FREQUENCY PPM HEIGHT
1 21941.841 174.681 120.4
2 18516.059 147.408 100.4
3 18512.153 147.377 82.0
4 17748.481 141.297 49.2
5 17403.755 138.553 21.9
6 17074.165 135.929 14.2
7 16677.680 132.772 68.8
8 16576.118 131.964 107.6
9 16432.563 130.821 54.9
10 15935.005 126.860 98.4
11 13701.606 109.080 88.9
12 13487.739 107.377 19.9
13 12834.907 102.180 104.4
14 7787.055 61.993 8.8
15 5996.528 47.739 126.2
16 5049.751 40.201 81.6
17 5028.755 40.034 246.2
18 5007.759 39.867 488.3
19 4986.762 39.700 577.4
20 4965.766 39.533 489.4
21 4944.770 39.366 245.9
22 4924.262 39.202 82.8
23 4751.411 37.826 53.0
24 4247.016 33.811 162.9
25 3701.118 29.465 111.6
26 3603.462 28.687 160.4
27 3357.368 26.728 155.6
28 3097.114 24.656 175.1
HN
O
OH
O
O
Cl
S
N
O
O
20b
160
140
120
100
80
60
40
20
ppm

STANDARD 1H
59563
1887-BGE
Berecz Gabor
2005.09.12. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244691 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3960.571	7.929	22.2
2	3958.496	7.925	21.6
3	3717.529	7.442	7.6
4	3715.454	7.438	6.8
5	3709.106	7.425	23.5
6	3707.153	7.421	23.7
7	3701.294	7.410	34.6
8	3692.993	7.393	10.9
9	3629.150	7.265	6.9
10	3431.152	6.869	47.8
11	3399.902	6.806	48.8
12	2987.915	5.982	32.8
13	2986.816	5.979	37.6
14	2981.445	5.969	40.0
15	2980.225	5.966	28.4
16	2406.982	4.819	29.7
17	1681.396	3.366	151.2
18	1186.157	2.375	143.2
19	998.047	1.998	3.4
20	928.711	1.859	5.7
21	928.955	1.860	5.7
22	0.000	0.000	4.2

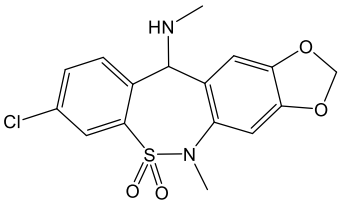


20c

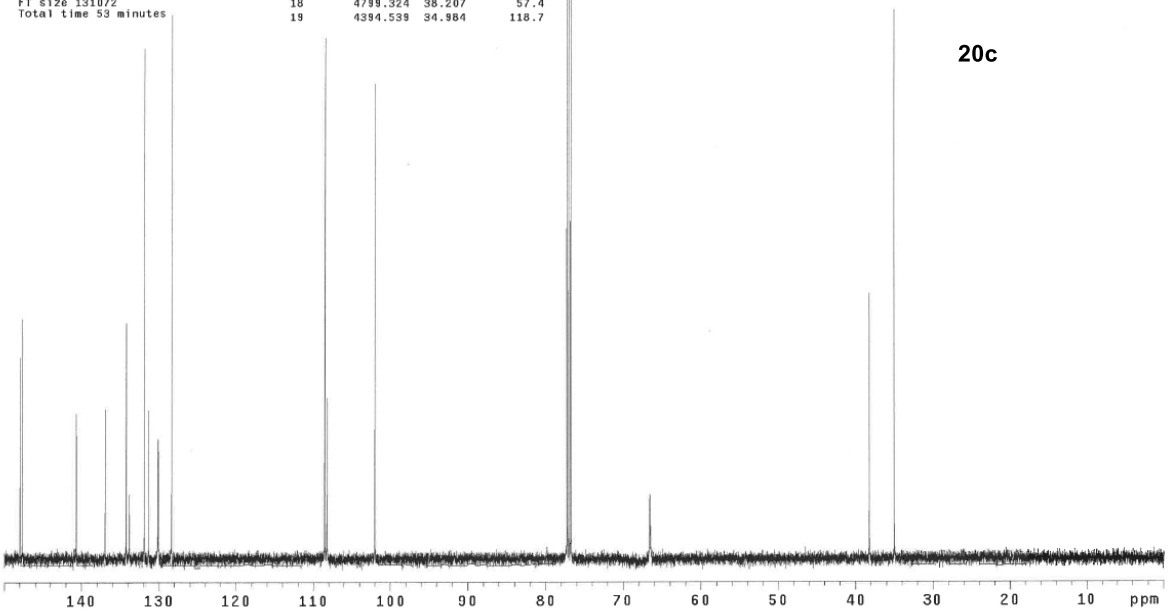


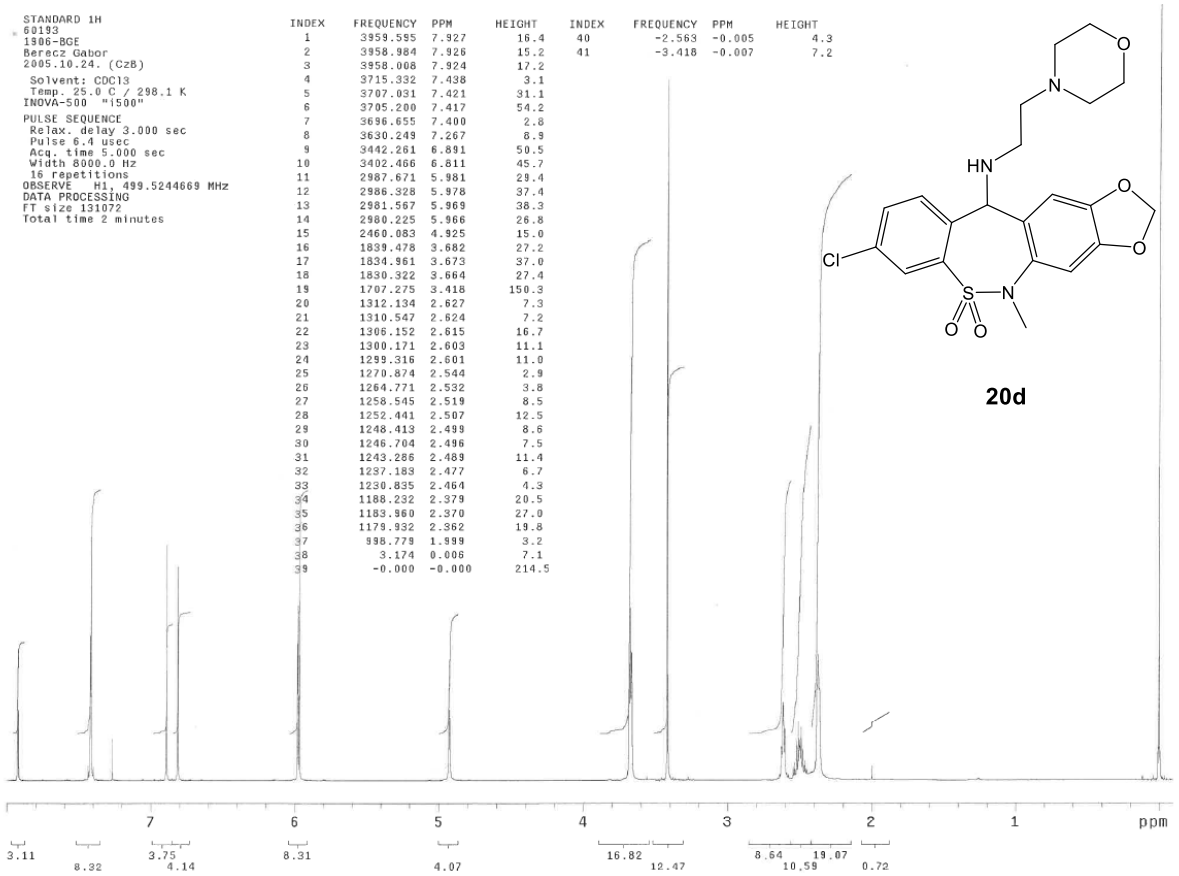
STANDARD 13C
59563
1887-BGE
Berecz Gabor
2005.09.12. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
752 repetitions
OBSERVE C13, 125.6055328 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 53 minutes

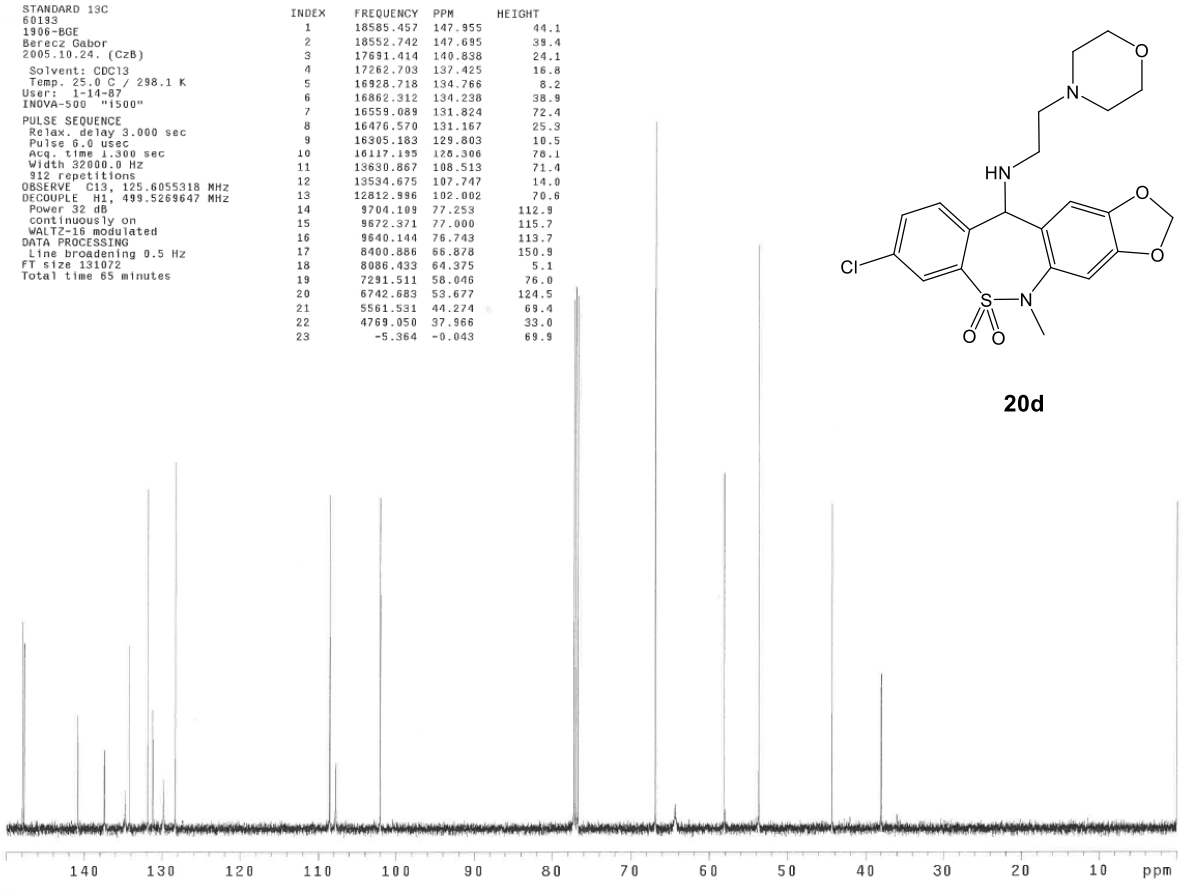
INDEX	FREQUENCY	PPM	HEIGHT
1	18586.433	147.963	43.6
2	18545.906	147.641	51.9
3	17672.371	140.687	31.4
4	17204.109	136.959	32.4
5	16862.800	134.242	51.1
6	16810.066	133.822	14.0
7	16568.367	131.898	110.4
8	16498.543	131.342	32.1
9	16343.269	130.106	26.0
10	16123.054	128.353	117.5
11	13629.890	108.505	112.6
12	13595.222	108.229	34.8
13	12811.531	101.990	102.8
14	9704.597	77.257	123.3
15	9672.859	77.004	122.4
16	9640.633	76.747	124.2
17	8355.476	66.516	13.9
18	4799.324	38.207	57.4
19	4394.539	34.984	118.7

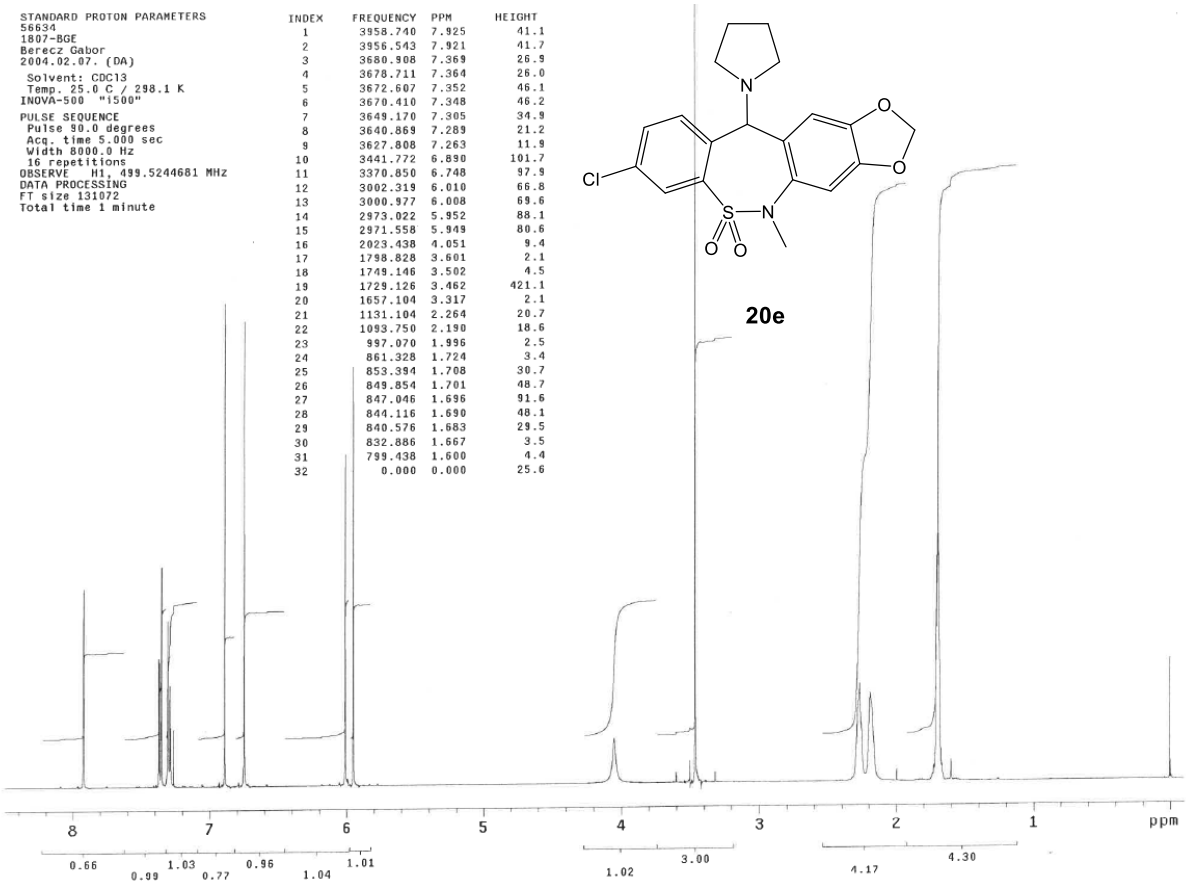


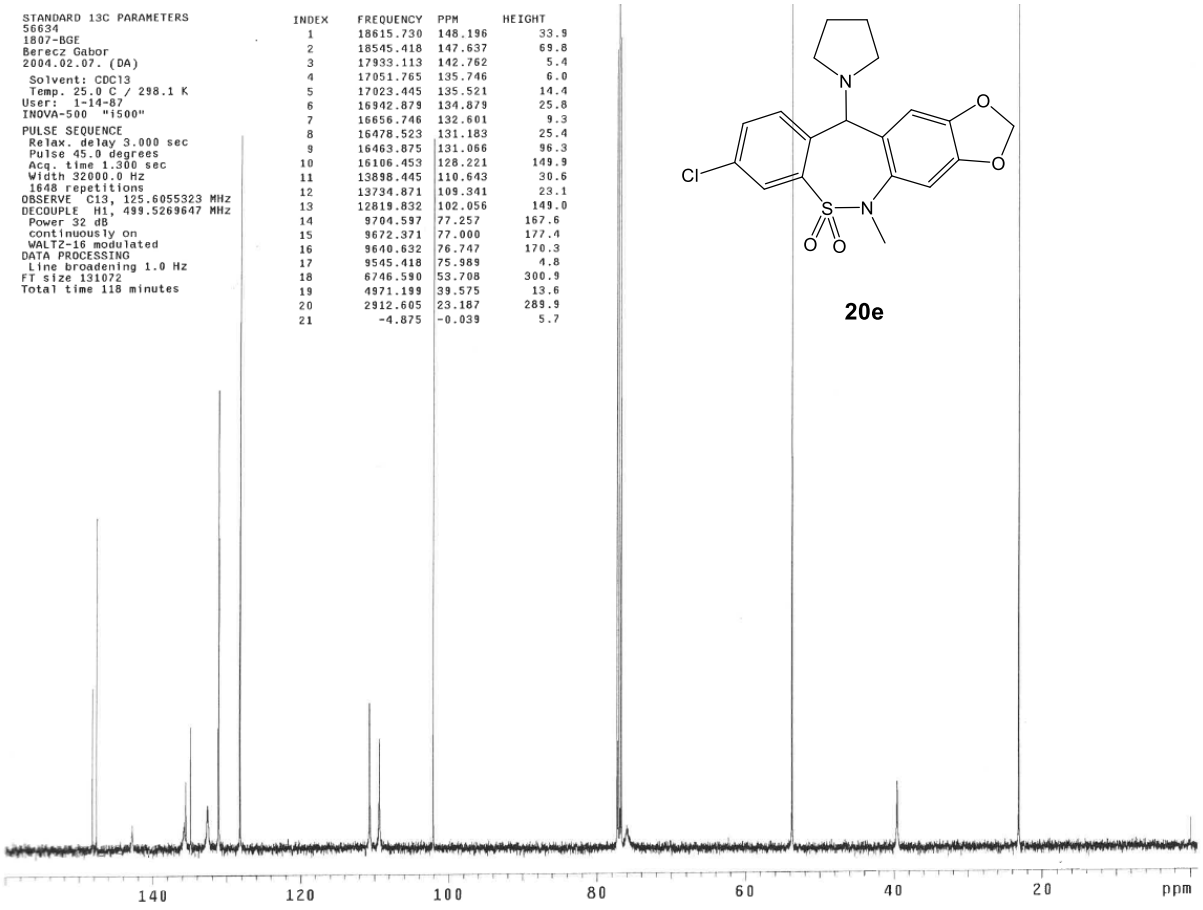
20c

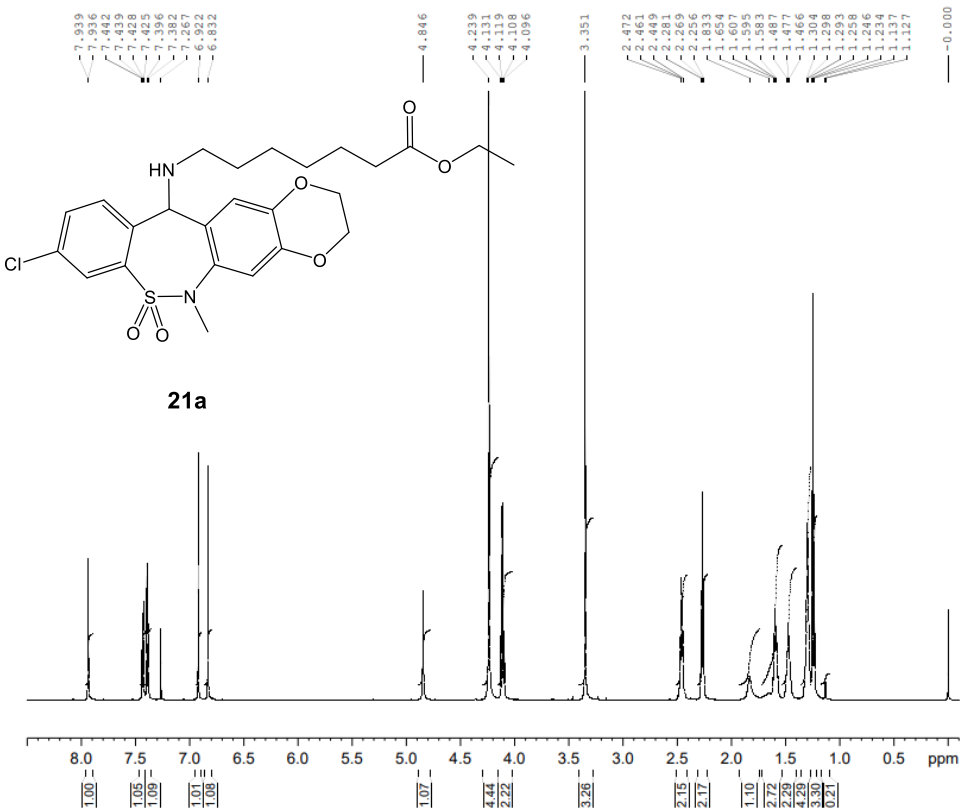



STANDARD 1H
60193
1906-BGE
Berecz Gabor
2005.10.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244669 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3959.595 7.927 16.4 40 -2.563 -0.005 4.3
2 3958.984 7.926 15.2 41 -3.418 -0.007 7.2
3 3958.008 7.924 17.2
4 3715.332 7.438 3.1
5 3707.031 7.421 31.1
6 3705.200 7.417 54.2
7 3696.655 7.400 2.8
8 3630.249 7.267 8.9
9 3442.261 6.891 50.5
10 3402.466 6.811 45.7
11 2987.671 5.981 29.4
12 2986.328 5.978 37.4
13 2981.567 5.969 38.3
14 2980.225 5.966 26.8
15 2460.083 4.925 15.0
16 1839.478 3.682 27.2
17 1834.961 3.673 37.0
18 1830.322 3.664 27.4
19 1707.275 3.418 150.3
20 1312.134 2.627 7.3
21 1310.547 2.624 7.2
22 1306.152 2.615 16.7
23 1300.171 2.603 11.1
24 1299.316 2.601 11.0
25 1270.874 2.544 2.9
26 1264.771 2.532 3.8
27 1258.545 2.519 8.5
28 1252.441 2.507 12.5
29 1248.413 2.499 8.6
30 1246.704 2.496 7.5
31 1243.286 2.489 11.4
32 1237.183 2.477 6.7
33 1230.835 2.464 4.3
34 1188.232 2.379 20.5
35 1183.960 2.370 27.0
36 1179.932 2.362 19.8
37 998.779 1.999 3.2
38 3.174 0.006 7.1
39 -0.000 -0.000 214.5
O
N
HN
O
O
Cl
S
N
O
O
20d
7
6
5
4
3
2
1
ppm
3.11
8.32
3.75
4.14
8.31
4.07
16.82
12.47
8.64
19.07
10.58
0.72


STANDARD 13C
60193
1906-BGE
Berecz Gabor
2005.10.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
912 repetitions
OBSERVE C13, 125.6055318 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 65 minutes
INDEX FREQUENCY PPM HEIGHT
1 18585.457 147.955 44.1
2 18552.742 147.695 39.4
3 17691.414 140.838 24.1
4 17262.703 137.425 16.8
5 16928.718 134.766 8.2
6 16862.312 134.238 38.9
7 16559.089 131.824 72.4
8 16476.570 131.167 25.3
9 16305.183 129.803 10.5
10 16117.195 128.306 78.1
11 13630.867 108.513 71.4
12 13534.675 107.747 14.0
13 12812.996 102.002 70.6
14 9704.109 77.253 112.9
15 9672.371 77.000 115.7
16 9640.144 76.743 113.7
17 8400.886 66.878 150.9
18 8086.433 64.375 5.1
19 7291.511 58.046 76.0
20 6742.683 53.677 124.5
21 5561.531 44.274 69.4
22 4769.050 37.966 33.0
23 -5.364 -0.043 69.9
O
N
HN
O
O
Cl
S
N
O
O
20d
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


STANDARD PROTON PARAMETERS
56634
1807-BGE
Berecz Gabor
2004.02.07. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244681 MHz
DATA PROCESSING
FT size 131072
Total time 1 minute
INDEX FREQUENCY PPM HEIGHT
1 3958.740 7.925 41.1
2 3956.543 7.921 41.7
3 3680.908 7.369 26.9
4 3678.711 7.364 26.0
5 3672.607 7.352 46.1
6 3670.410 7.348 46.2
7 3649.170 7.305 34.9
8 3640.869 7.289 21.2
9 3627.808 7.263 11.9
10 3441.772 6.890 101.7
11 3370.850 6.748 97.9
12 3002.319 6.010 66.8
13 3000.977 6.008 69.6
14 2973.022 5.952 88.1
15 2971.558 5.949 80.6
16 2023.438 4.051 9.4
17 1798.828 3.601 2.1
18 1749.146 3.502 4.5
19 1729.126 3.462 421.1
20 1657.104 3.317 2.1
21 1131.104 2.264 20.7
22 1093.750 2.190 18.6
23 997.070 1.996 2.5
24 861.328 1.724 3.4
25 853.394 1.708 30.7
26 849.854 1.701 48.7
27 847.046 1.696 91.6
28 844.116 1.690 48.1
29 840.576 1.683 29.5
30 832.886 1.667 3.5
31 799.438 1.600 4.4
32 0.000 0.000 25.6
20e
8
7
6
5
4
3
2
1
ppm
0.66
1.03
0.99
0.77
0.96
1.04
1.01
1.02
3.00
4.17
4.30


STANDARD 13C PARAMETERS
56634
1807-BGE
Berecz Gabor
2004.02.07. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
1648 repetitions
OBSERVE C13, 125.6055323 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 118 minutes
INDEX FREQUENCY PPM HEIGHT
1 18615.730 148.196 33.9
2 18545.418 147.637 69.8
3 17933.113 142.762 5.4
4 17051.765 135.746 6.0
5 17023.445 135.521 14.4
6 16942.879 134.879 25.8
7 16656.746 132.601 9.3
8 16478.523 131.183 25.4
9 16463.875 131.066 96.3
10 16106.453 128.221 149.9
11 13898.445 110.643 30.6
12 13734.871 109.341 23.1
13 12819.832 102.056 149.0
14 9704.597 77.257 167.6
15 9672.371 77.000 177.4
16 9640.632 76.747 170.3
17 9545.418 75.989 4.8
18 6746.590 53.708 300.9
19 4971.199 39.575 13.6
20 2912.605 23.187 289.9
21 -4.875 -0.039 5.7
20e
140
120
100
80
60
40
20
ppm



Standard 1H
144404
bge-1768-1768-BGE_1
Berecz Gabor
2025.03.19. (KP)

Current Data Parameters

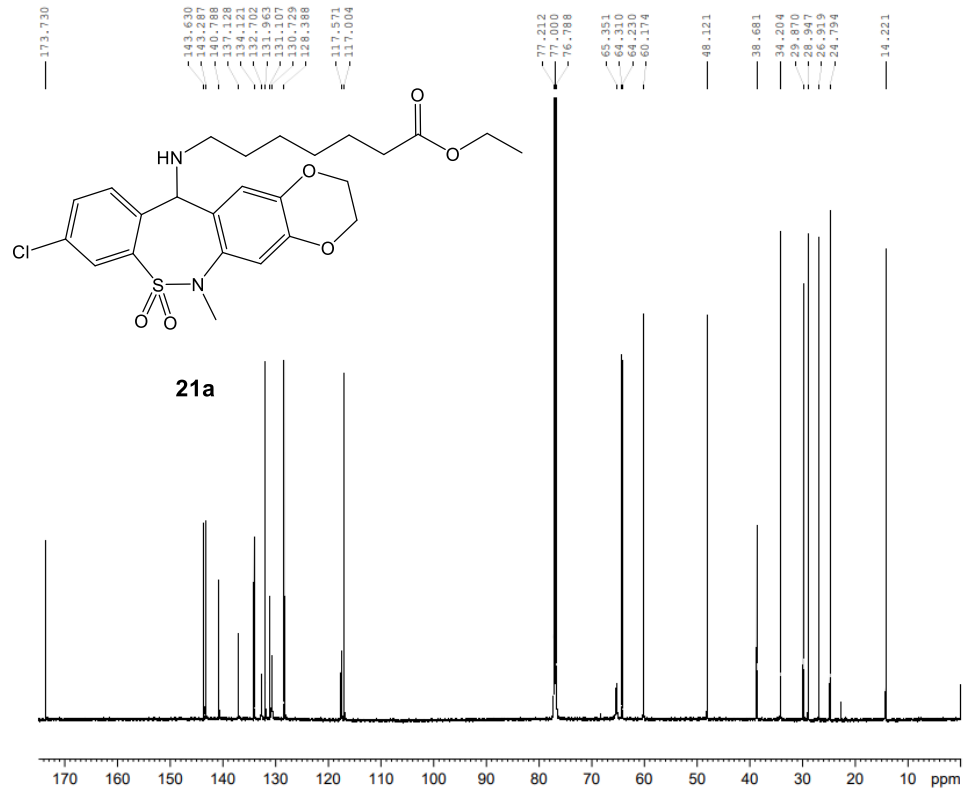
NAME	144404
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20250319
Time	19.08 h
INSTRUM	spect
PROBHD	Z145856_0002 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.366798 Hz
AQ	2.7262976 sec
RG	111.4
DW	41.600 usec
DE	25.00 usec
TE	295.0 K
D1	1.00000000 sec
TD0	1
SFO1	600.0037050 MHz
NUC1	1H
P1	11.50 usec
PLW1	28.00000000 W

F2 - Processing parameters

SI	65536
SF	600.0000098 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Standard 13C
144404
bge-1768-1768-BGE_1
Berecz Gabor
2025.03.19. (KP)

Current Data Parameters

NAME	144404
EXPNO	12
PROCNO	1

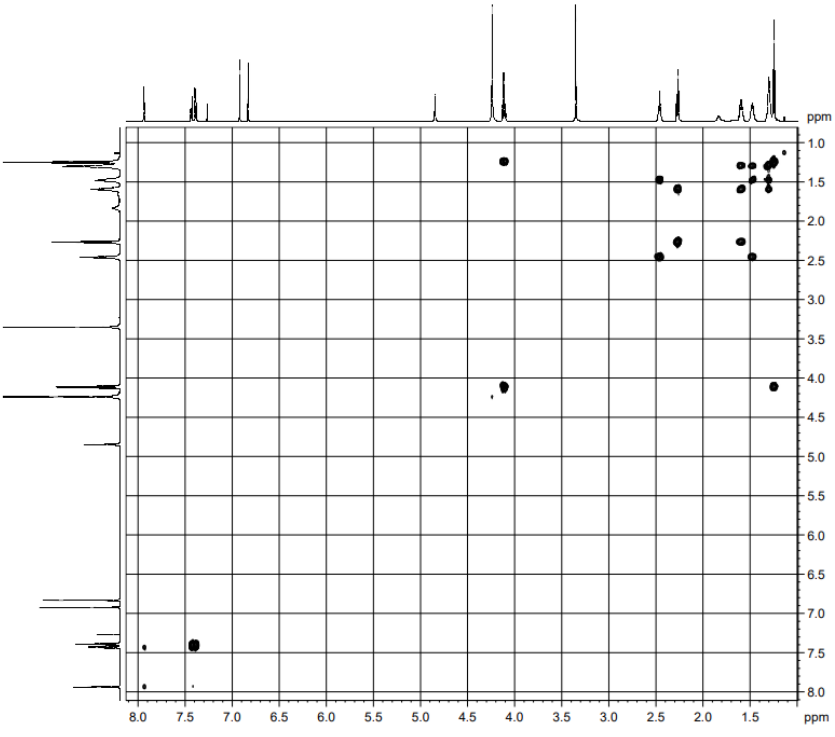
F2 - Acquisition Parameters

Date_	20250319
Time	20.16 h
INSTRUM	spect
PROBHD	Z145856_0002 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	36231.883 Hz
FIDRES	1.105709 Hz
AQ	0.9043968 sec
RG	196.07
DW	13.800 usec
DE	18.00 usec
TE	295.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	150.8852070 MHz
NUC1	13C
P1	9.80 usec
PLW1	72.69999695 W
SFO2	600.0024000 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	32.50000000 W
PLW12	0.70708001 W
PLW13	0.35508999 W

F2 - Processing parameters

SI	131072
SF	150.8701288 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

21a



COSY
144404
bge-1768-1768-BGE_1
Berecz Gabor
2025.03.19. (KP)

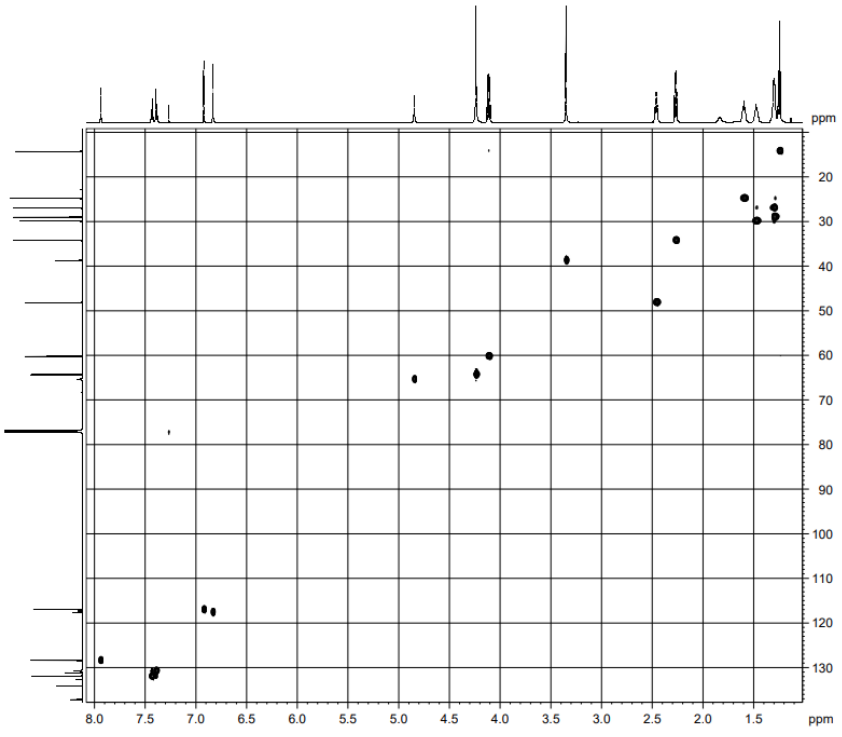
Current Data Parameters
NAME 144404
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250319
Time 20.18 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000098 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000098 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



21a

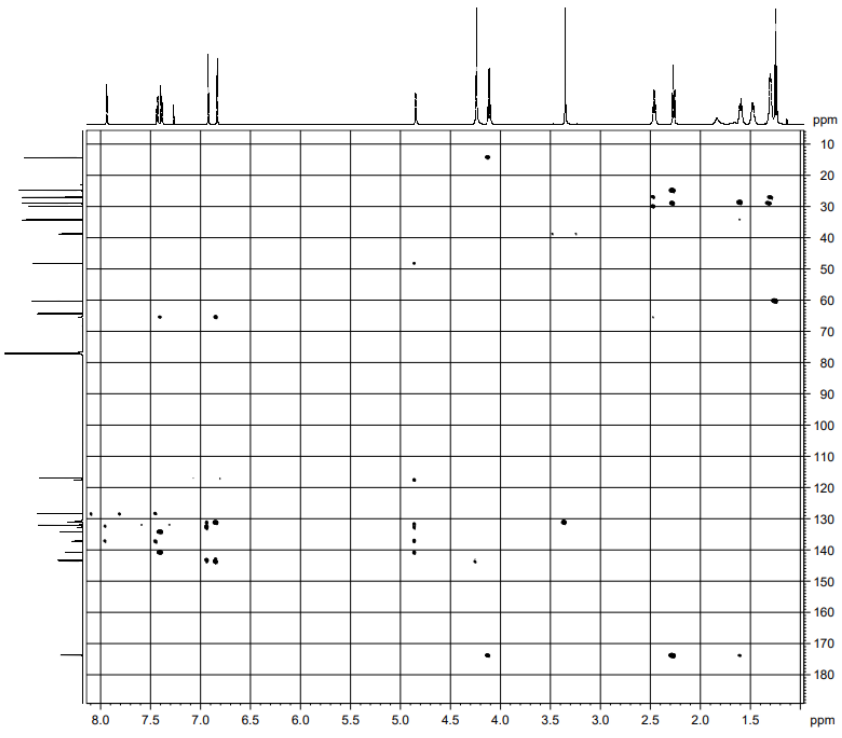
HSQC (140Hz)
144404
bge-1768-1768-BGE_1
Berecz Gabor
2025.03.19. (KP)

Current Data Parameters
NAME 144404
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250319
Time 20.38 h
INSTRUM spect
PROBHD 5145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp62,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[31 Crp62,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000098 MHz
WDW QSINE



21a

HMBC (8Hz, 140Hz)
144404
bge-1768-1768-BGE_1
Berecz Gabor
2025.03.19. (KP)

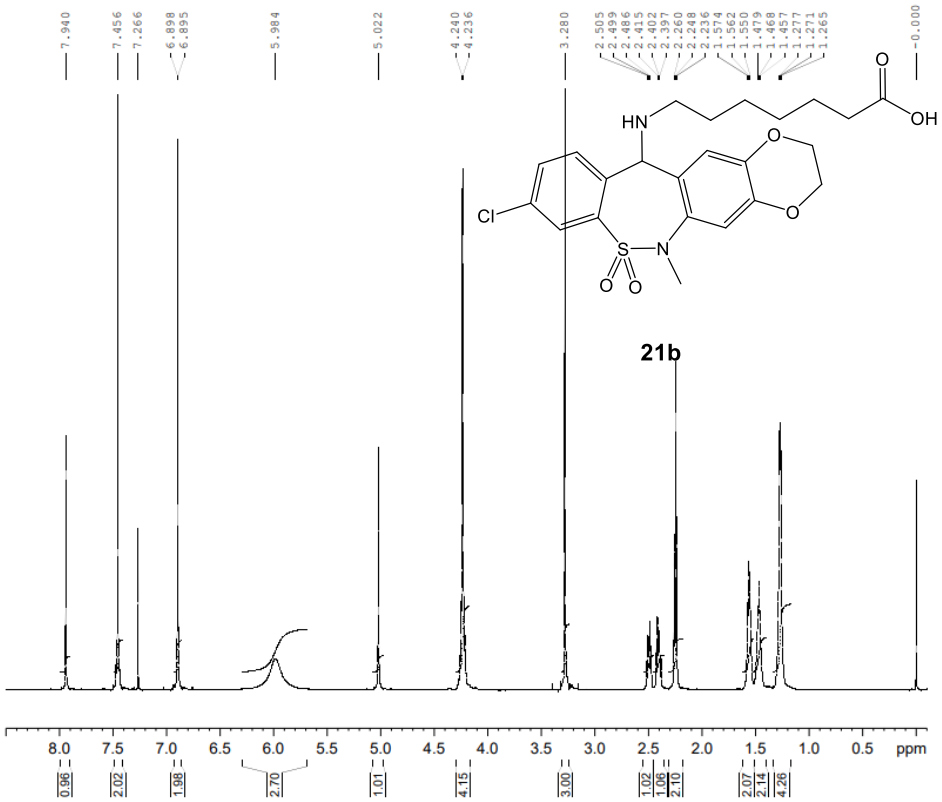
Current Data Parameters
NAME 144404
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250319
Time 21.08 h
INSTRUM spect
PROBHD 5145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701200 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

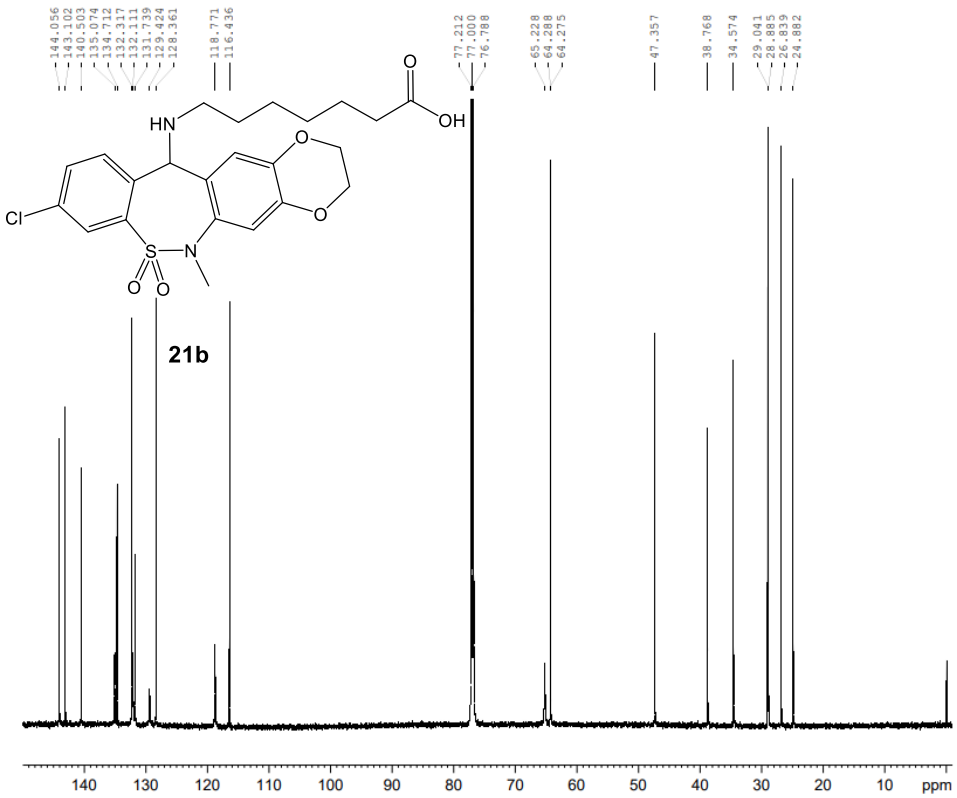


Standard 1H
144419
bge1778-1974-BGE_1
Berecz Gabor
2025.03.21. (KP)

Current Data Parameters
NAME 144419
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250321
Time 15.45 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 119.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

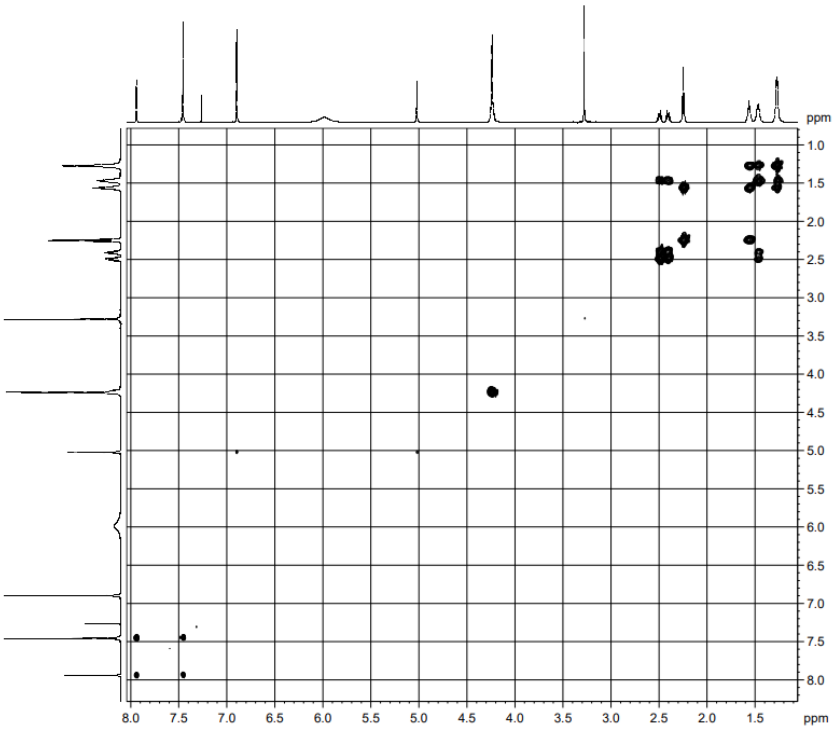


Standard 13C
144419
bge1778-1974-BGE_1
Berecz Gabor
2025.03.21. (KP)

Current Data Parameters
NAME 144419
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250321
Time 16.53 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.80 usec
PLW1 72.69999695 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.50000000 W
PLW12 0.70708001 W
PLW13 0.35508999 W

F2 - Processing parameters
SI 131072
SF 150.8701283 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



21b

COSY
144419
bge1778-1974-BGE_1
Berecz Gabor
2025.03.21. (KP)

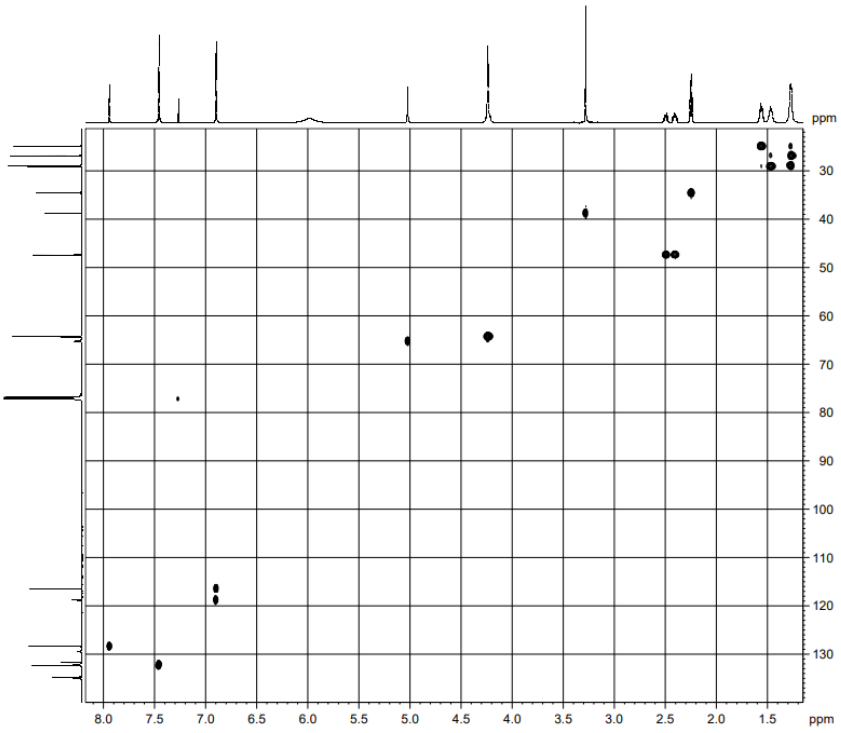
Current Data Parameters
NAME 144419
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250321
Time 16.55 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



21b

HSQC (140Hz)
144419
bge1778-1974-BGE_1
Berecz Gabor
2025.03.21. (KP)

Current Data Parameters
NAME 144419
EXPNO 14
PROCNO 1

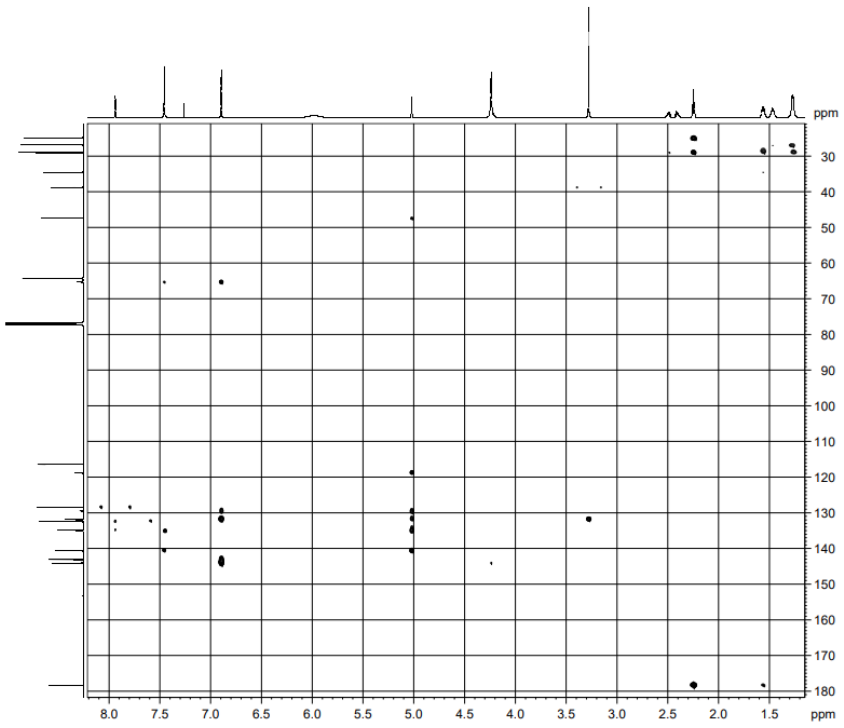
F2 - Acquisition Parameters
Date_ 20250321
Time 17.15 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001515 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.7,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp41.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[31 Crp41.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 -7.00 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000100 MHz
WDW QSINE

21b

HMBC (8Hz, 140Hz)
144419
bge1778-1974-BGE_1
Berecz Gabor
2025.03.21. (KP)



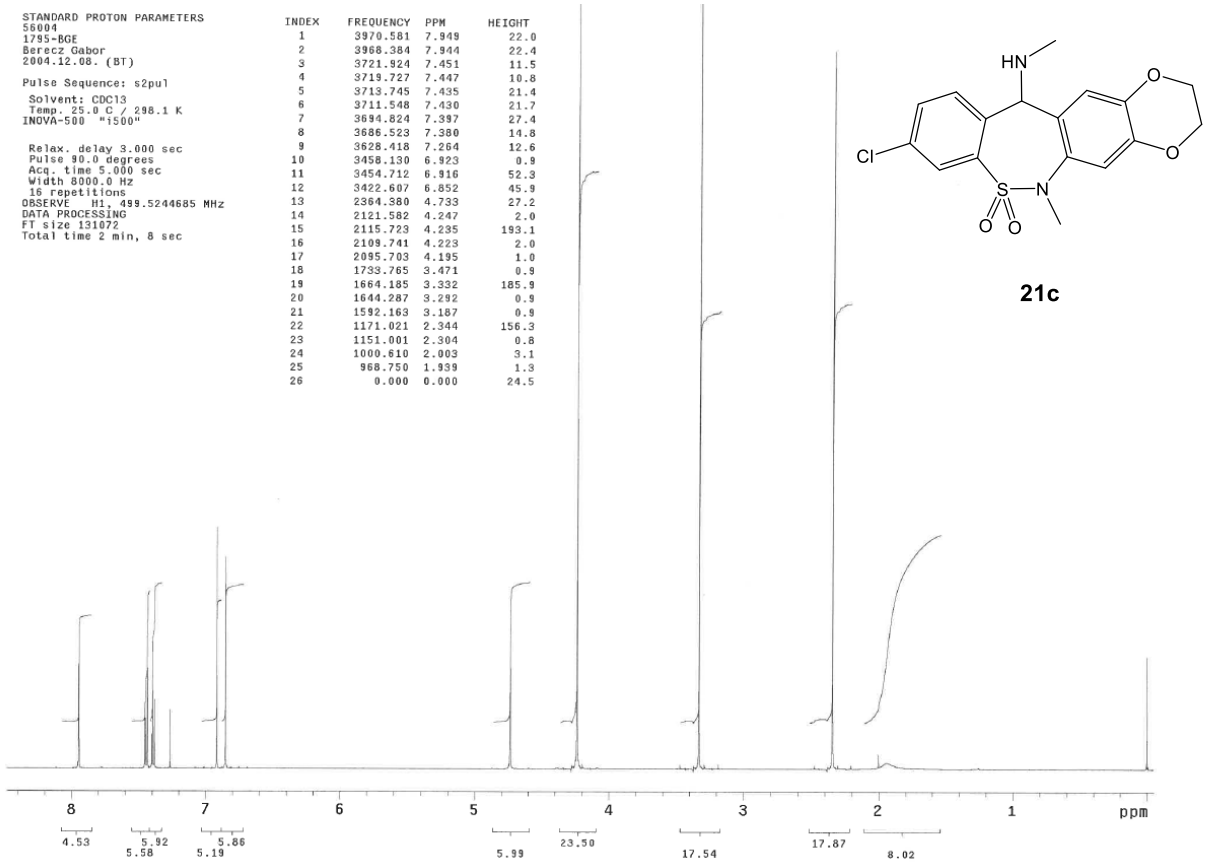
Current Data Parameters
NAME 144419
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250321
Time 17.45 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1315725 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

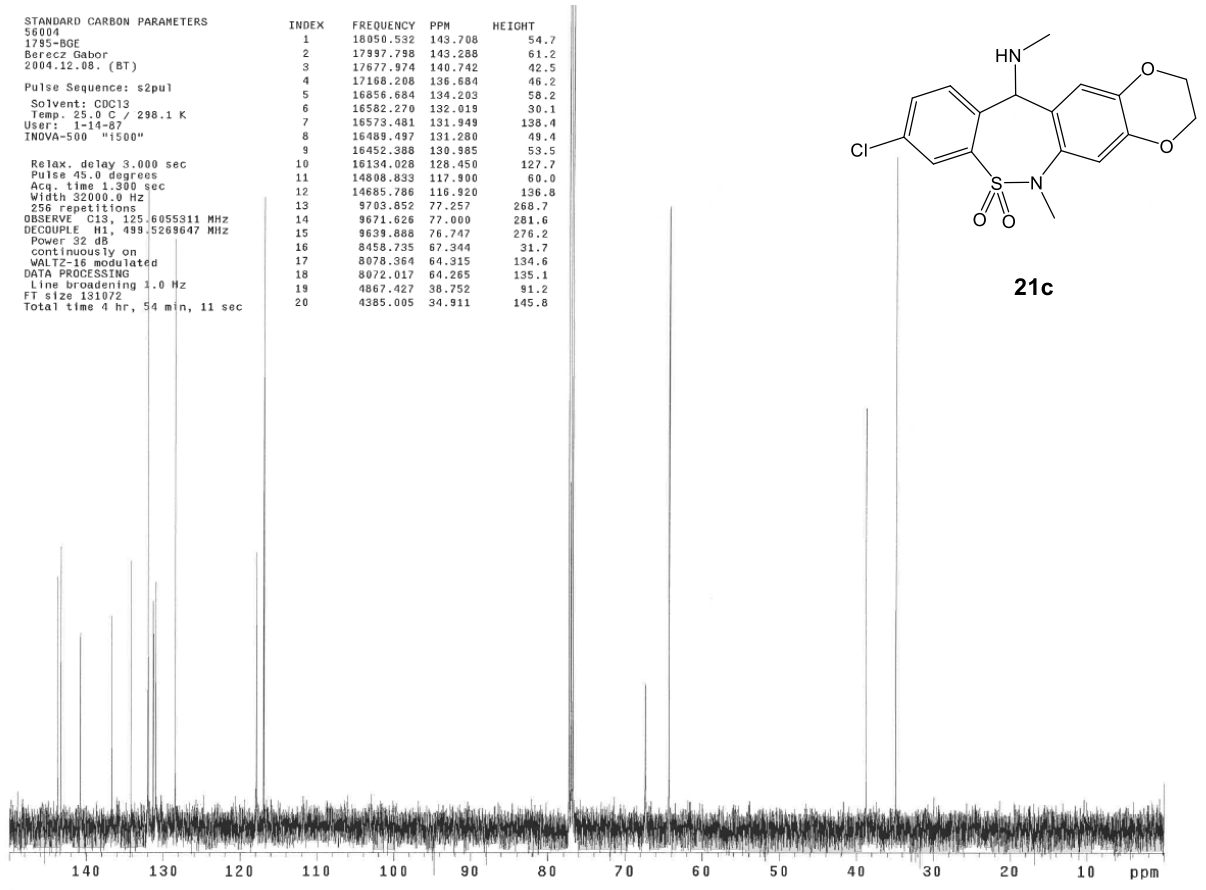
F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000100 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

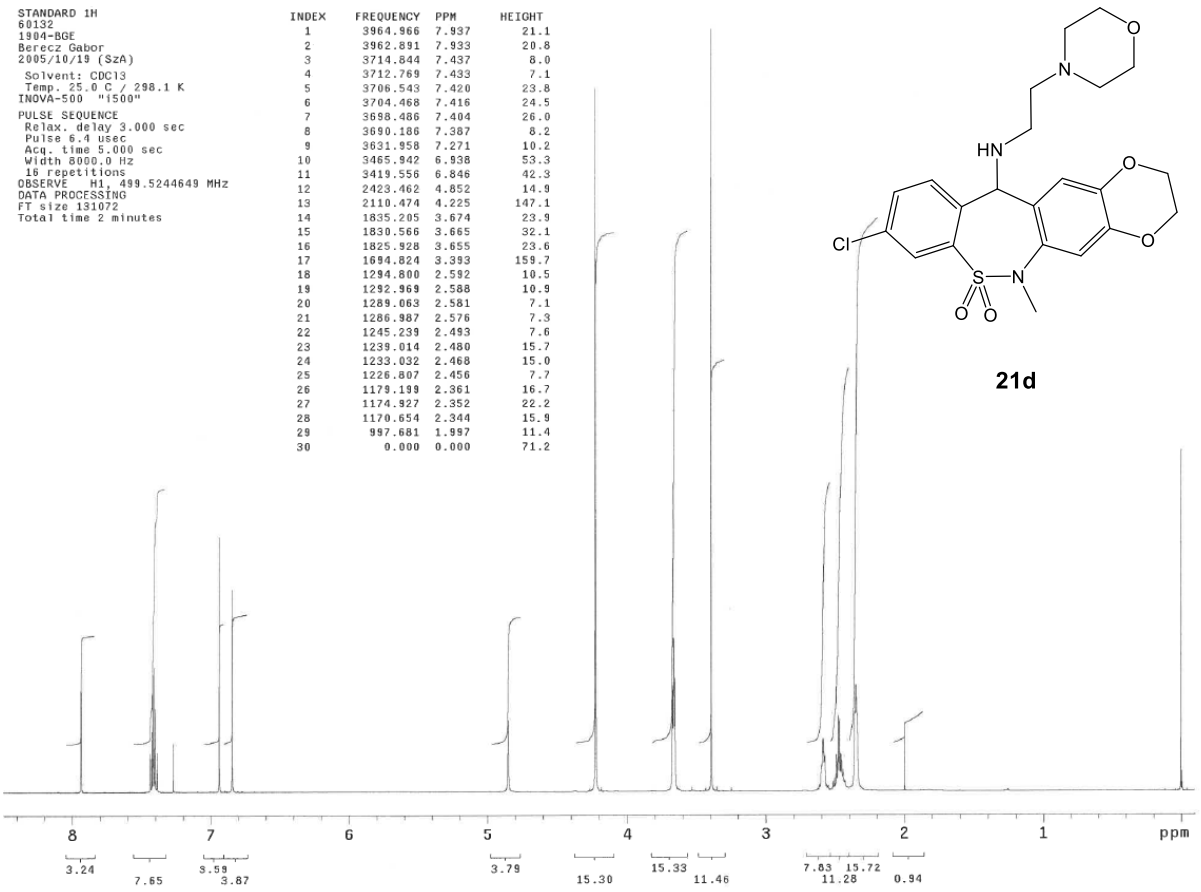
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701283 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

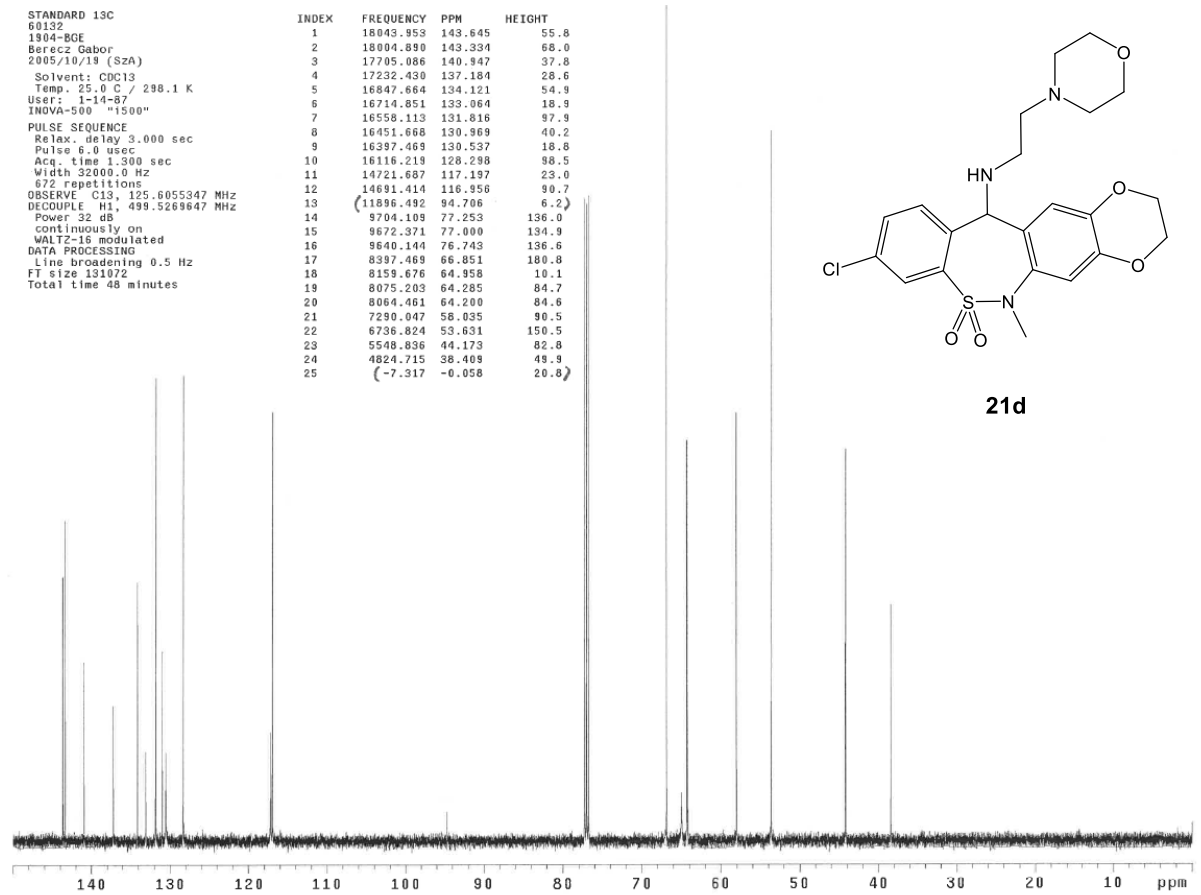

STANDARD PROTON PARAMETERS
56004
1795-BGE
Berecz Gabor
2004.12.08. (BT)
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244685 MHz
DATA PROCESSING
FT size 131072
Total time 2 min, 8 sec
INDEX FREQUENCY PPM HEIGHT
1 3970.581 7.949 22.0
2 3968.384 7.944 22.4
3 3721.924 7.451 11.5
4 3719.727 7.447 10.8
5 3713.745 7.435 21.4
6 3711.548 7.430 21.7
7 3694.824 7.397 27.4
8 3686.523 7.380 14.8
9 3628.418 7.264 12.6
10 3458.130 6.923 0.9
11 3454.712 6.916 52.3
12 3422.607 6.852 45.9
13 2364.380 4.733 27.2
14 2121.582 4.247 2.0
15 2115.723 4.235 193.1
16 2109.741 4.223 2.0
17 2095.703 4.195 1.0
18 1733.765 3.471 0.9
19 1664.185 3.332 185.9
20 1644.287 3.292 0.9
21 1592.163 3.187 0.9
22 1171.021 2.344 156.3
23 1151.001 2.304 0.8
24 1000.610 2.003 3.1
25 968.750 1.939 1.3
26 0.000 0.000 24.5
HN
O
O
Cl
S
N
O
O
8
7
6
5
4
3
2
1
ppm
4.53
5.92
5.58
5.86
5.19
5.99
23.50
17.54
17.87
8.02

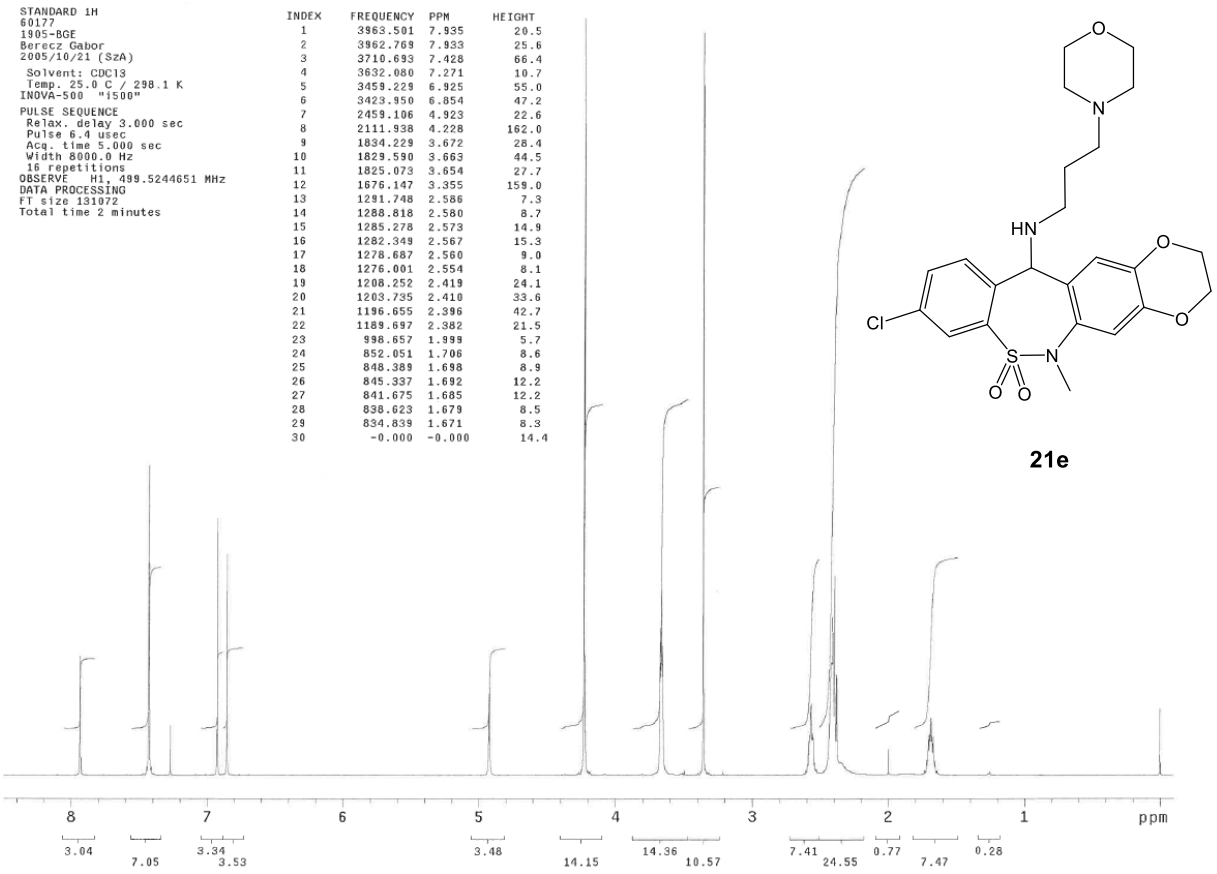
21c

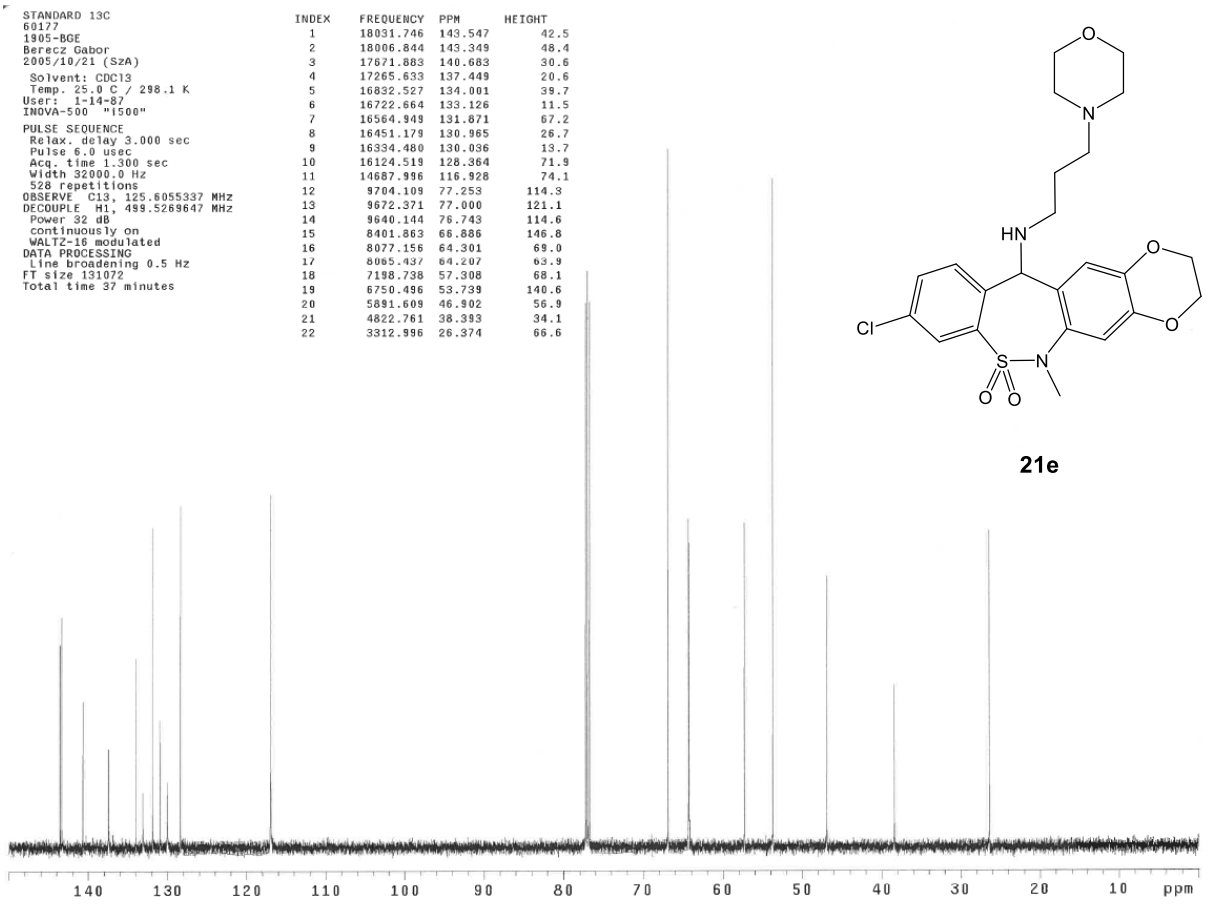

STANDARD CARBON PARAMETERS
56004
1795-BGE
Berecz Gabor
2004.12.08. (BT)
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
256 repetitions
OBSERVE C13, 125.6055311 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 4 hr, 54 min, 11 sec
INDEX FREQUENCY PPM HEIGHT
1 18050.532 143.708 54.7
2 17997.798 143.288 61.2
3 17677.974 140.742 42.5
4 17168.208 136.684 46.2
5 16856.684 134.203 58.2
6 16582.270 132.019 30.1
7 16573.481 131.949 138.4
8 16489.497 131.280 49.4
9 16452.388 130.985 53.5
10 16134.028 128.450 127.7
11 14808.833 117.900 60.0
12 14685.786 116.920 136.8
13 9703.852 77.257 268.7
14 9671.626 77.000 281.6
15 9639.888 76.747 276.2
16 8458.735 67.344 31.7
17 8078.364 64.315 134.6
18 8072.017 64.265 135.1
19 4867.427 38.752 91.2
20 4385.005 34.911 145.8
HN
O
O
Cl
S
N
O
O
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

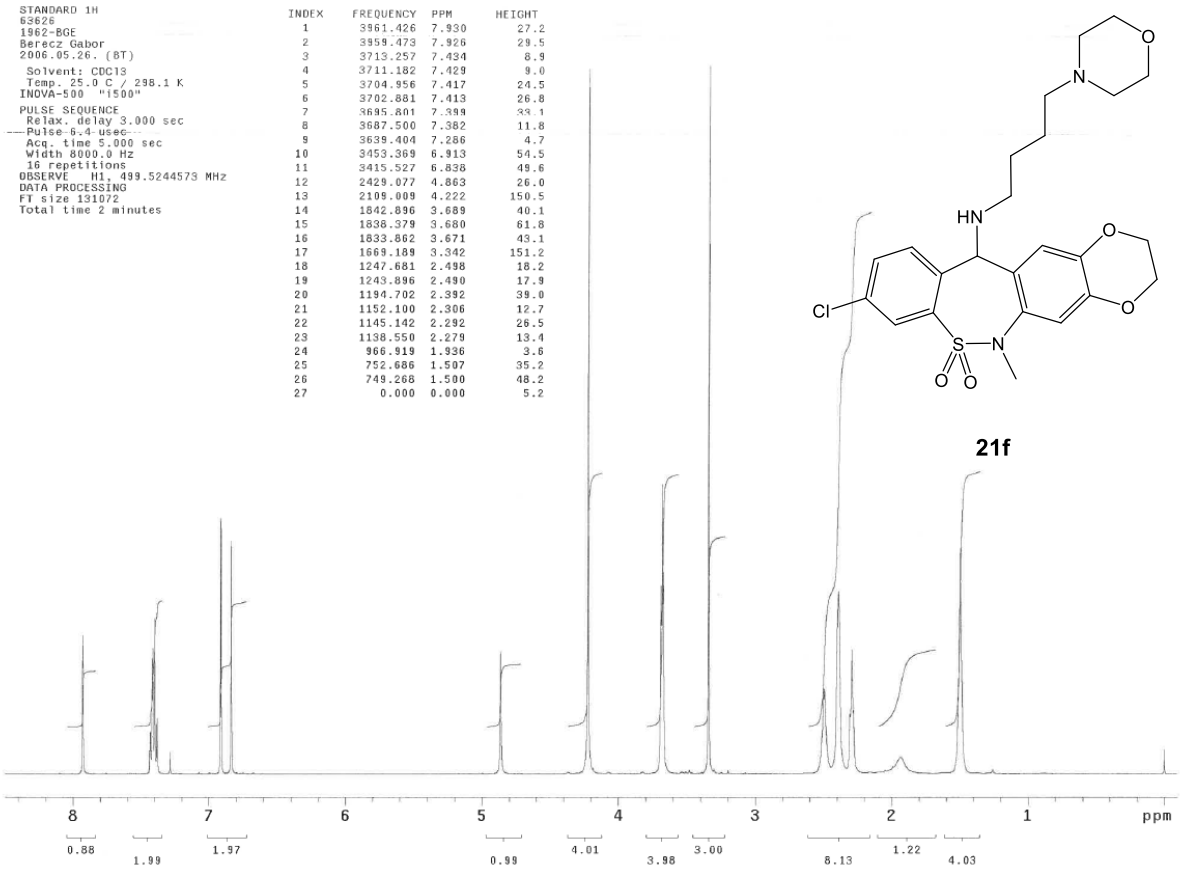
21c

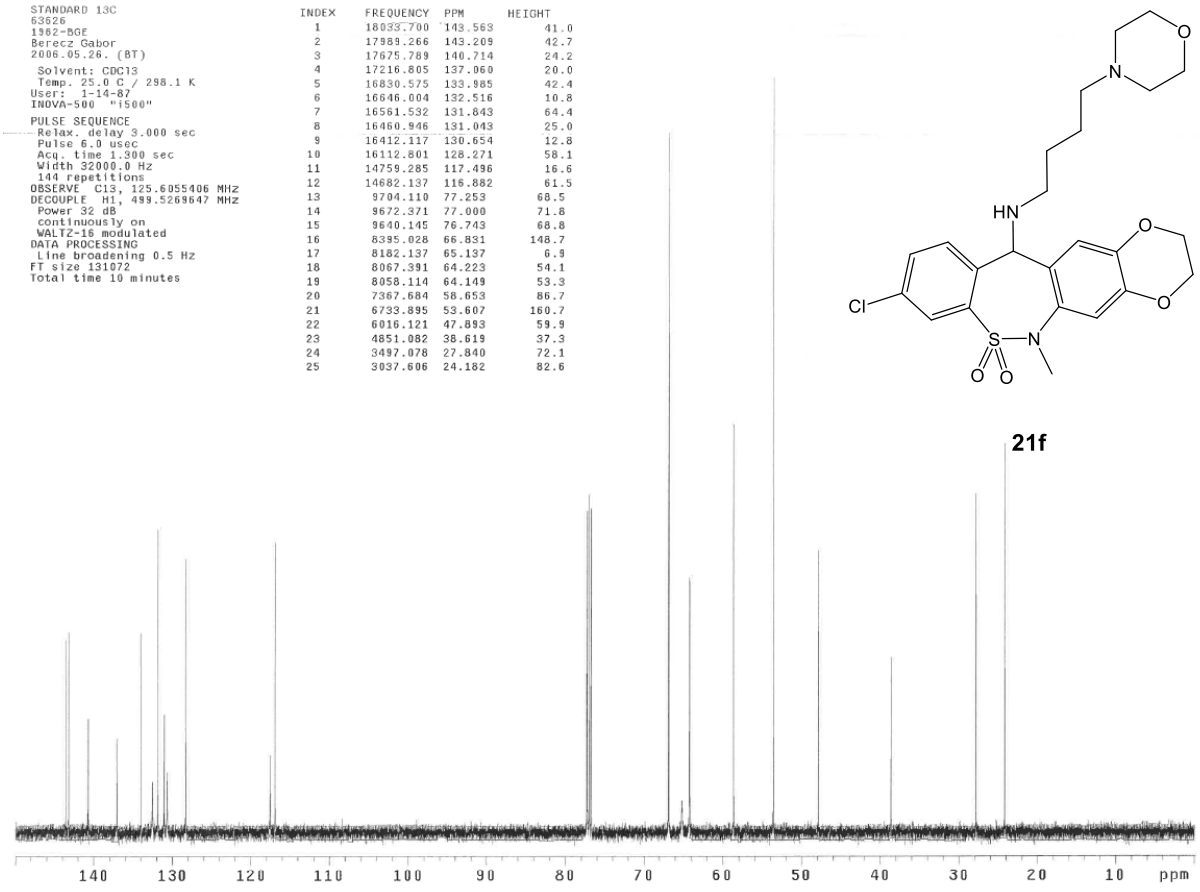

STANDARD 1H
60132
1904-BGE
Berecz Gabor
2005/10/19 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244649 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3964.966 7.937 21.1
2 3962.891 7.933 20.8
3 3714.844 7.437 8.0
4 3712.769 7.433 7.1
5 3706.543 7.420 23.8
6 3704.468 7.416 24.5
7 3698.486 7.404 26.0
8 3690.186 7.387 8.2
9 3631.958 7.271 10.2
10 3465.942 6.938 53.3
11 3419.556 6.846 42.3
12 2423.462 4.852 14.9
13 2110.474 4.225 147.1
14 1835.205 3.674 23.9
15 1830.566 3.665 32.1
16 1825.928 3.655 23.6
17 1694.824 3.393 159.7
18 1294.800 2.592 10.5
19 1292.969 2.588 10.9
20 1289.063 2.581 7.1
21 1286.987 2.576 7.3
22 1245.239 2.493 7.6
23 1239.014 2.480 15.7
24 1233.032 2.468 15.0
25 1226.807 2.456 7.7
26 1179.199 2.361 16.7
27 1174.927 2.352 22.2
28 1170.654 2.344 15.9
29 997.681 1.997 11.4
30 0.000 0.000 71.2
21d
8
7
6
5
4
3
2
1
ppm
3.24
7.65
3.59
3.87
3.79
15.30
15.33
11.46
7.83
15.72
11.28
0.94


STANDARD 13C
60132
1904-BGE
Berecz Gabor
2005/10/19 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
672 repetitions
OBSERVE C13, 125.6055347 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 48 minutes
INDEX FREQUENCY PPM HEIGHT
1 18043.953 143.645 55.8
2 18004.890 143.334 68.0
3 17705.086 140.947 37.8
4 17232.430 137.184 28.6
5 16847.664 134.121 54.9
6 16714.851 133.064 18.9
7 16558.113 131.816 97.9
8 16451.668 130.969 40.2
9 16397.469 130.537 18.8
10 16116.219 128.298 98.5
11 14721.687 117.197 23.0
12 14691.414 116.956 90.7
13 (11896.492 94.706 6.2)
14 9704.109 77.253 136.0
15 9672.371 77.000 134.9
16 9640.144 76.743 136.6
17 8397.469 66.851 180.8
18 8159.676 64.958 10.1
19 8075.203 64.285 84.7
20 8064.461 64.200 84.6
21 7290.047 58.035 90.5
22 6736.824 53.631 150.5
23 5548.836 44.173 82.8
24 4824.715 38.409 49.9
25 (-7.317 -0.058 20.8)
21d
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


STANDARD 1H
60177
1905-BGE
Berecz Gabor
2005/10/21 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244651 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3963.501 7.935 20.5
2 3962.769 7.933 25.6
3 3710.693 7.428 66.4
4 3632.080 7.271 10.7
5 3459.229 6.925 55.0
6 3423.950 6.854 47.2
7 2459.106 4.923 22.6
8 2111.938 4.228 162.0
9 1834.229 3.672 28.4
10 1829.590 3.663 44.5
11 1825.073 3.654 27.7
12 1676.147 3.355 159.0
13 1291.748 2.586 7.3
14 1288.818 2.580 8.7
15 1285.278 2.573 14.9
16 1282.349 2.567 15.3
17 1278.687 2.560 9.0
18 1276.001 2.554 8.1
19 1208.252 2.419 24.1
20 1203.735 2.410 33.6
21 1196.655 2.396 42.7
22 1189.697 2.382 21.5
23 998.657 1.999 5.7
24 852.051 1.706 8.6
25 848.389 1.698 8.9
26 845.337 1.692 12.2
27 841.675 1.685 12.2
28 838.623 1.679 8.5
29 834.839 1.671 8.3
30 -0.000 -0.000 14.4
21e
8
7
6
5
4
3
2
1
ppm
3.04
7.05
3.34
3.53
3.48
14.15
14.36
10.57
7.41
24.55
0.77
7.47
0.28


STANDARD 13C
60177
1905-BGE
Berecz Gabor
2005/10/21 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
528 repetitions
OBSERVE C13, 125.6055337 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 37 minutes
INDEX FREQUENCY PPM HEIGHT
1 18031.746 143.547 42.5
2 18006.844 143.349 48.4
3 17671.883 140.683 30.6
4 17265.633 137.449 20.6
5 16832.527 134.001 39.7
6 16722.664 133.126 11.5
7 16564.949 131.871 67.2
8 16451.179 130.965 26.7
9 16334.480 130.036 13.7
10 16124.519 128.364 71.9
11 14687.996 116.928 74.1
12 9704.109 77.253 114.3
13 9672.371 77.000 121.1
14 9640.144 76.743 114.6
15 8401.863 66.886 146.8
16 8077.156 64.301 69.0
17 8065.437 64.207 63.9
18 7198.738 57.308 68.1
19 6750.496 53.739 140.6
20 5891.609 46.902 56.9
21 4822.761 38.393 34.1
22 3312.996 26.374 66.6
21e
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


STANDARD 1H
63626
1362-BGE
Berecz Gabor
2006.05.26. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244573 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3961.426 7.930 27.2
2 3959.473 7.926 29.5
3 3713.257 7.434 8.9
4 3711.182 7.429 9.0
5 3704.956 7.417 24.5
6 3702.881 7.413 26.8
7 3695.801 7.399 39.1
8 3687.500 7.382 11.8
9 3639.404 7.286 4.7
10 3453.369 6.913 54.5
11 3415.527 6.838 49.6
12 2429.077 4.863 26.0
13 2109.009 4.222 150.5
14 1842.896 3.689 40.1
15 1838.379 3.680 61.8
16 1833.862 3.671 43.1
17 1669.189 3.342 151.2
18 1247.681 2.498 18.2
19 1243.896 2.490 17.9
20 1194.702 2.392 39.0
21 1152.100 2.306 12.7
22 1145.142 2.292 26.5
23 1138.550 2.279 13.4
24 966.919 1.936 3.6
25 752.686 1.507 35.2
26 749.268 1.500 48.2
27 0.000 0.000 5.2
21f
8
7
6
5
4
3
2
1
ppm
0.88
1.99
1.97
0.99
4.01
3.98
3.00
8.13
1.22
4.03

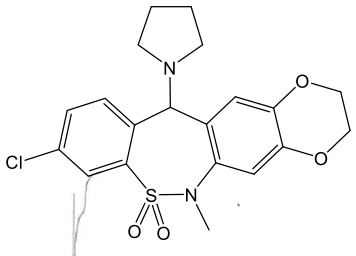

STANDARD 13C
63626
1362-BGE
Berecz Gabor
2006.05.26. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
144 repetitions
OBSERVE C13, 125.6055406 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 10 minutes
INDEX FREQUENCY PPM HEIGHT
1 18033.700 143.563 41.0
2 17989.266 143.209 42.7
3 17675.789 140.714 24.2
4 17216.805 137.060 20.0
5 16830.575 133.985 42.4
6 16646.004 132.516 10.8
7 16561.532 131.843 64.4
8 16460.946 131.043 25.0
9 16412.117 130.654 12.8
10 16112.801 128.271 58.1
11 14759.285 117.496 16.6
12 14682.137 116.882 61.5
13 9704.110 77.253 68.5
14 9672.371 77.000 71.8
15 9640.145 76.743 68.8
16 8395.028 66.831 148.7
17 8182.137 65.137 6.9
18 8067.391 64.223 54.1
19 8058.114 64.149 53.3
20 7367.684 58.653 86.7
21 6733.895 53.607 160.7
22 6016.121 47.893 59.9
23 4851.082 38.619 37.3
24 3497.078 27.840 72.1
25 3037.606 24.182 82.6
21f
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD PROTON PARAMETERS
54081
1735-BGE
Berecz Gabor
2004.06.10. (DA)

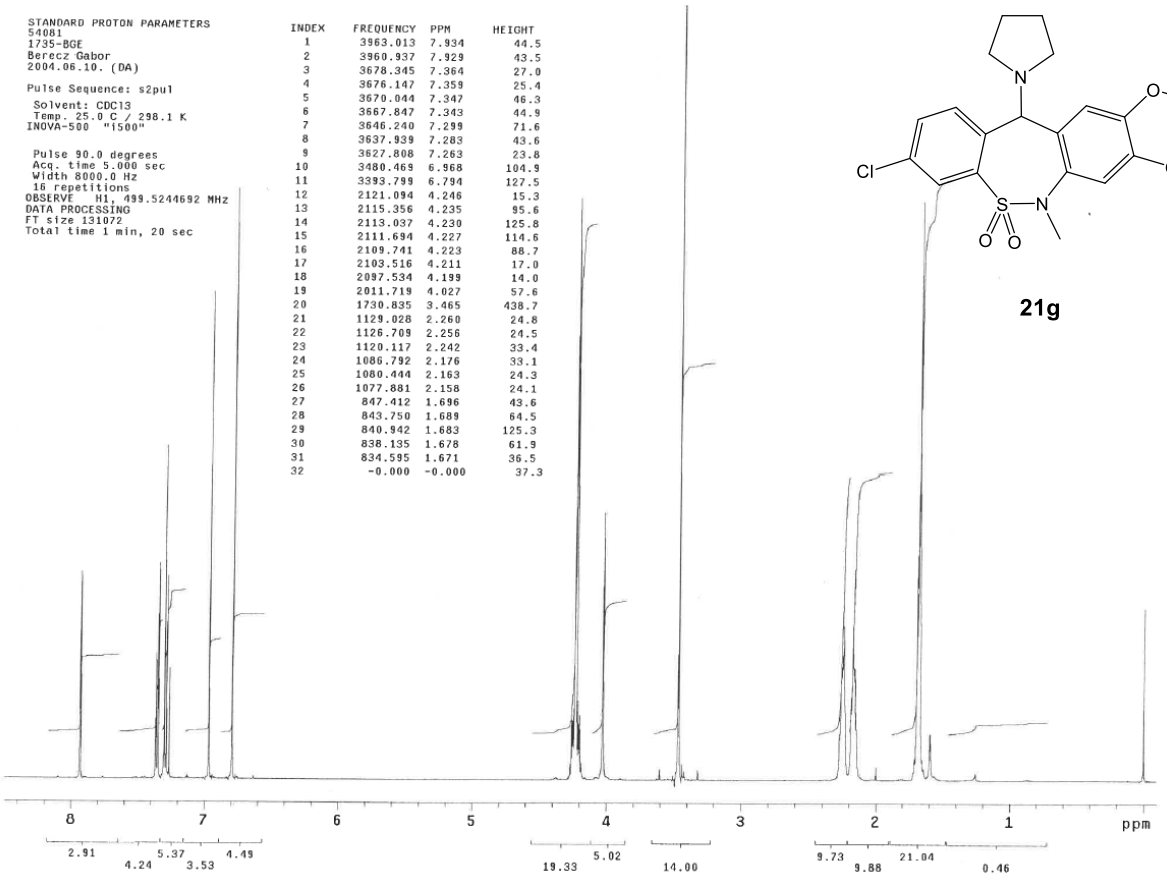
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"

Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244692 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 20 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	3963.013	7.934	44.5
2	3960.937	7.929	43.5
3	3678.345	7.364	27.0
4	3676.147	7.359	25.4
5	3670.044	7.347	46.3
6	3667.847	7.343	44.9
7	3646.240	7.299	71.6
8	3637.939	7.283	43.6
9	3627.808	7.263	23.8
10	3480.469	6.968	104.9
11	3393.799	6.794	127.5
12	2121.094	4.246	15.3
13	2115.356	4.235	95.6
14	2113.037	4.230	125.8
15	2111.694	4.227	114.6
16	2109.741	4.223	88.7
17	2103.516	4.211	17.0
18	2097.534	4.199	14.0
19	2011.719	4.027	57.6
20	1730.835	3.465	438.7
21	1129.028	2.260	24.8
22	1126.709	2.256	24.5
23	1120.117	2.242	33.4
24	1086.792	2.176	33.1
25	1080.444	2.163	24.3
26	1077.881	2.158	24.1
27	847.412	1.696	43.6
28	843.750	1.689	64.5
29	840.942	1.683	125.3
30	838.135	1.678	61.9
31	834.595	1.671	36.5
32	-0.000	-0.000	37.3



21g



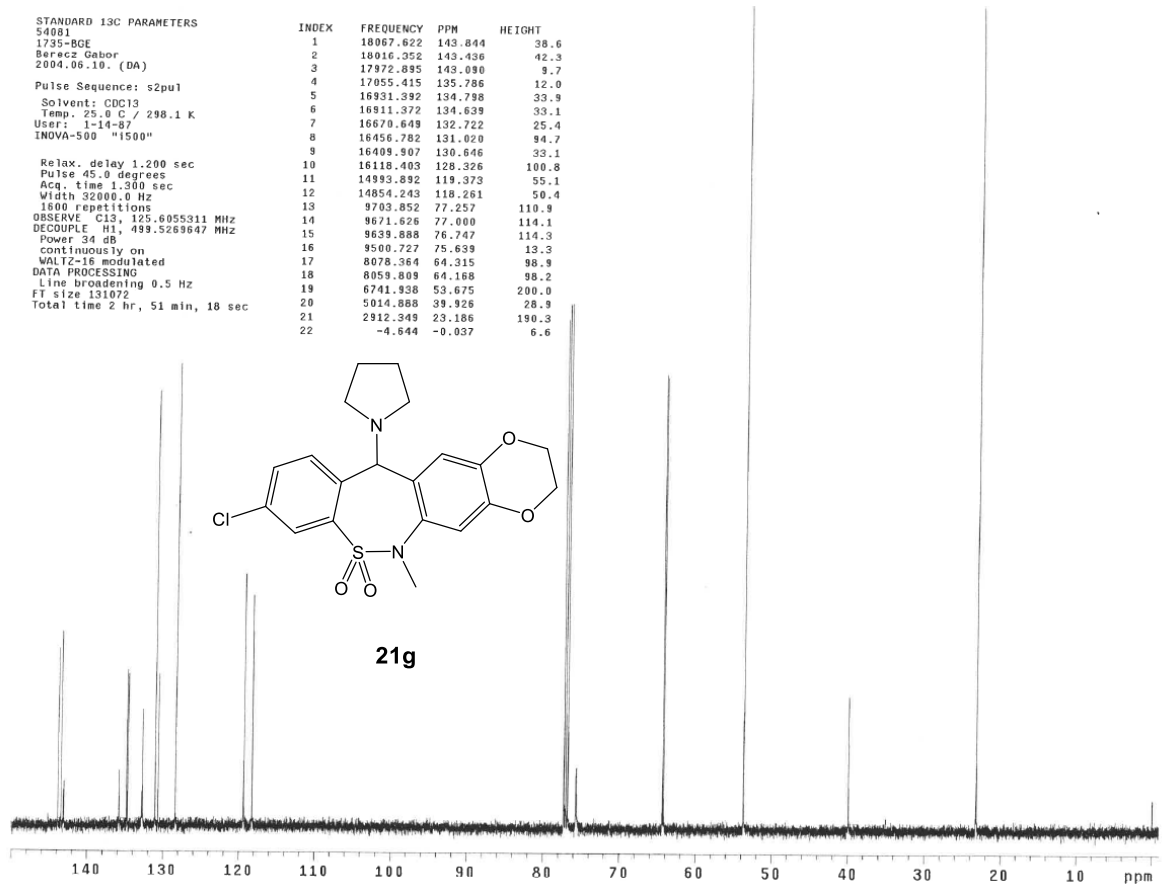
STANDARD 13C PARAMETERS
54081
1735-BGE
Berecz Gabor
2004.06.10. (DA)

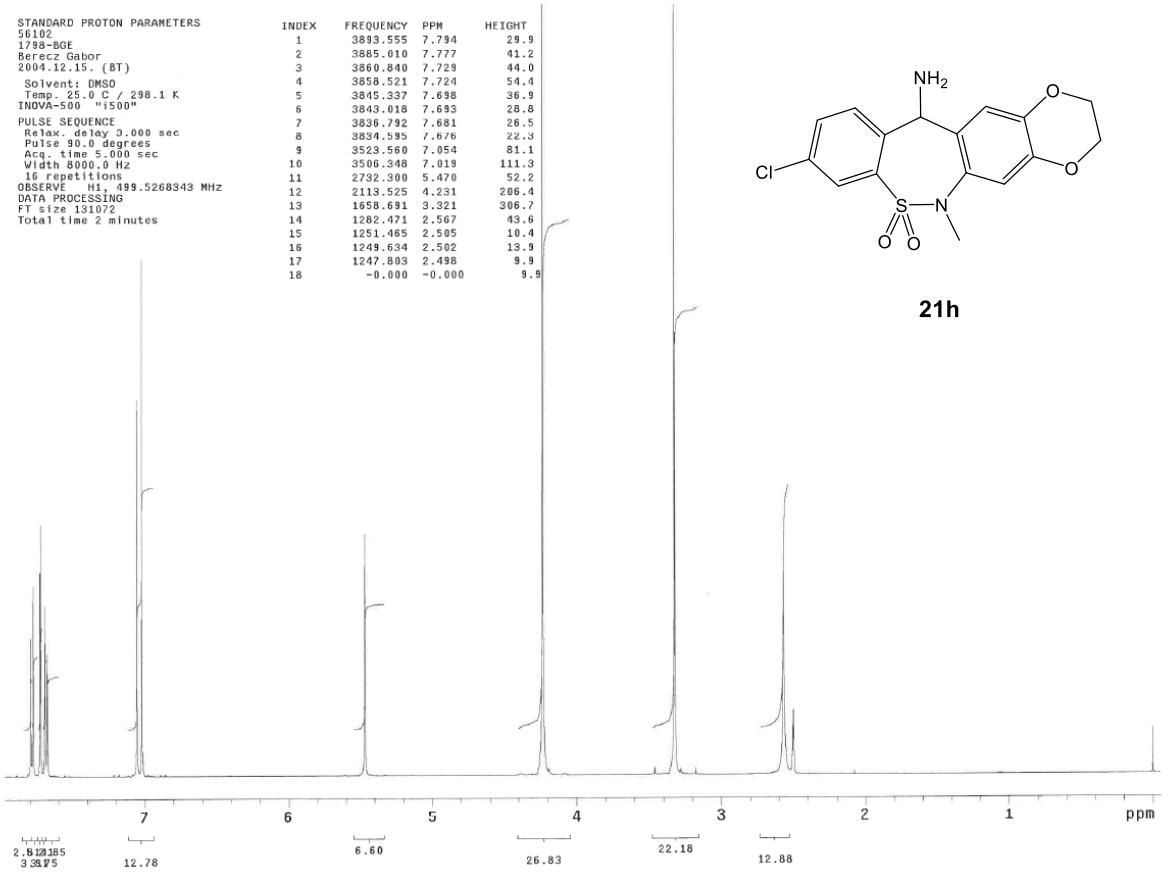
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"

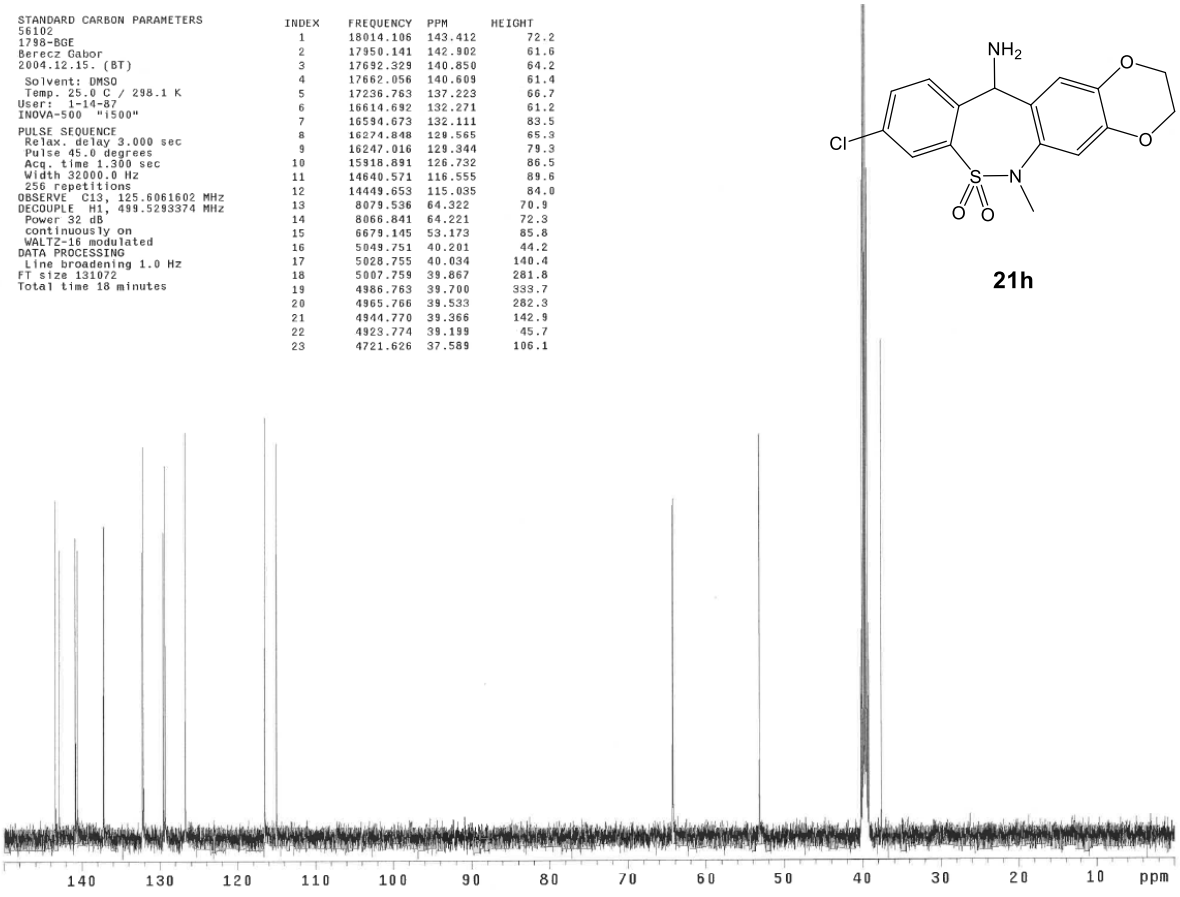
Relax. delay 1.200 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
1600 repetitions
OBSERVE C13, 125.6055311 MHz
DECOUPLE H1, 499.5269647 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 2 hr, 51 min, 18 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	18067.622	143.844	38.6
2	18016.352	143.436	42.3
3	17972.895	143.090	9.7
4	17055.415	135.786	12.0
5	16931.392	134.798	33.9
6	16911.372	134.639	33.1
7	16670.649	132.722	25.4
8	16456.782	131.020	94.7
9	16409.907	130.646	33.1
10	16118.403	128.326	100.8
11	14993.892	119.373	55.1
12	14854.243	118.261	50.4
13	9703.852	77.257	110.9
14	9671.626	77.000	114.1
15	9639.888	76.747	114.3
16	9500.727	75.639	13.3
17	8078.364	64.315	98.9
18	8059.809	64.168	98.2
19	6741.938	53.675	200.0
20	5014.888	39.926	28.9
21	2912.349	23.186	190.3
22	-4.644	-0.037	6.6

21g

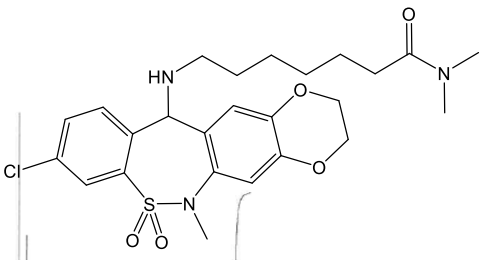



STANDARD PROTON PARAMETERS
56102
1798-BGE
Berecz Gabor
2004.12.15. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268343 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3893.555 7.794 29.9
2 3885.010 7.777 41.2
3 3860.840 7.729 44.0
4 3858.521 7.724 54.4
5 3845.337 7.698 36.9
6 3843.018 7.693 28.8
7 3836.792 7.681 26.5
8 3834.595 7.676 22.3
9 3523.560 7.054 81.1
10 3506.348 7.019 111.3
11 2732.300 5.470 52.2
12 2113.525 4.231 206.4
13 1658.691 3.321 306.7
14 1282.471 2.567 43.6
15 1251.465 2.505 10.4
16 1249.634 2.502 13.9
17 1247.803 2.498 9.9
18 -0.000 -0.000 9.9
NH2
Cl
S
N
O
O
O
O
21h
7
6
5
4
3
2
1
ppm
12.78
6.60
26.83
22.18
12.88

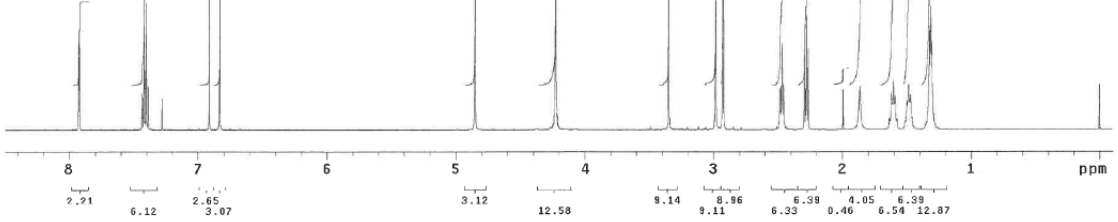

STANDARD CARBON PARAMETERS
56102
1798-BGE
Berecz Gabor
2004.12.15. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
256 repetitions
OBSERVE C13, 125.6061602 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 18 minutes
INDEX FREQUENCY PPM HEIGHT
1 18014.106 143.412 72.2
2 17950.141 142.902 61.6
3 17692.329 140.850 64.2
4 17662.056 140.609 61.4
5 17236.763 137.223 66.7
6 16614.692 132.271 61.2
7 16594.673 132.111 83.5
8 16274.848 129.565 65.3
9 16247.016 129.344 79.3
10 15918.891 126.732 86.5
11 14640.571 116.555 89.6
12 14449.653 115.035 84.0
13 8079.536 64.322 70.9
14 8066.841 64.221 72.3
15 6679.145 53.173 85.8
16 5049.751 40.201 44.2
17 5028.755 40.034 140.4
18 5007.759 39.867 281.8
19 4986.763 39.700 333.7
20 4965.766 39.533 282.3
21 4944.770 39.366 142.9
22 4923.774 39.199 45.7
23 4721.626 37.589 106.1
NH2
Cl
S
N
O
O
O
O
21h
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
79981
2264-BGE
Berecz Gabor
2009.05.15. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 11999.4 Hz
16 repetitions
OBSERVE H1, 499.5244598 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3958.908	7.925	19.0
2	3956.894	7.921	18.5
3	3714.475	7.436	8.2
4	3712.461	7.432	7.2
5	3706.236	7.420	23.9
6	3705.137	7.417	10.0
7	3704.222	7.415	23.2
8	3697.630	7.402	28.5
9	3689.208	7.385	9.7
10	3636.859	7.280	7.1
11	3453.013	6.913	49.2
12	3412.732	6.832	43.9
13	2422.914	4.850	23.5
14	2111.100	4.226	130.2
15	2104.692	4.213	3.7
16	1673.134	3.349	155.3
17	1490.587	2.984	137.9
18	1461.658	2.926	110.4
19	1240.661	2.484	9.3
20	1239.379	2.481	8.8
21	1232.971	2.468	19.4
22	1226.379	2.455	10.3
23	1145.817	2.294	16.7
24	1138.493	2.279	25.7
25	1130.803	2.264	18.4
26	995.861	1.994	9.0
27	931.960	1.866	9.9
28	808.920	1.619	8.3
29	801.596	1.605	11.3
30	794.272	1.590	7.7
31	748.498	1.498	6.6
32	741.906	1.485	10.3
33	734.949	1.471	7.9
34	660.428	1.322	23.4
35	656.766	1.315	27.8
36	653.105	1.307	19.9
37	-0.000	-0.000	10.2

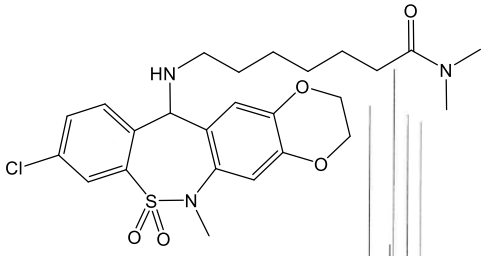


21i

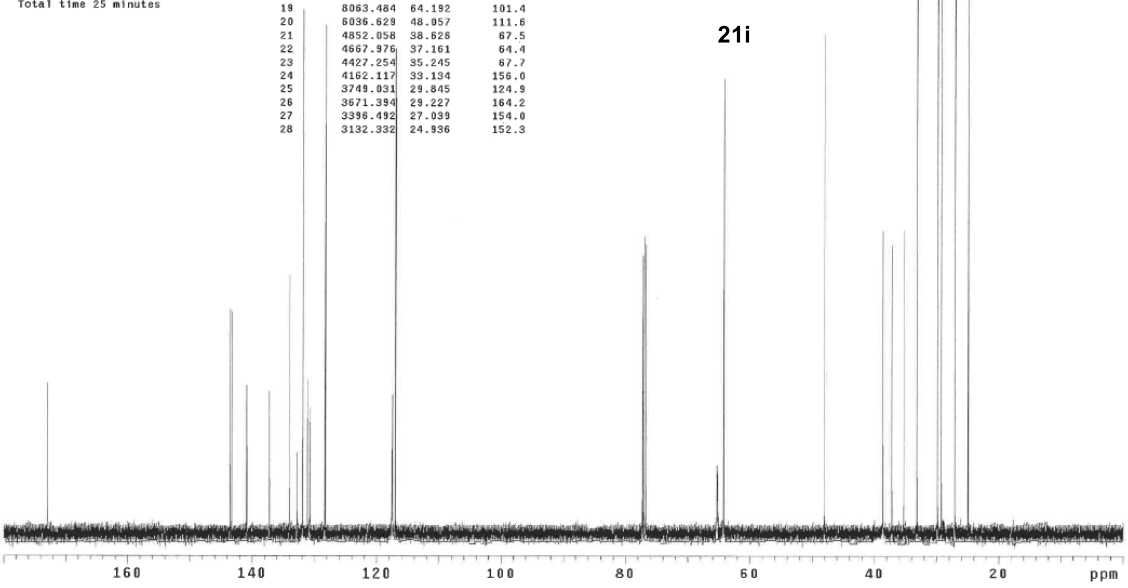


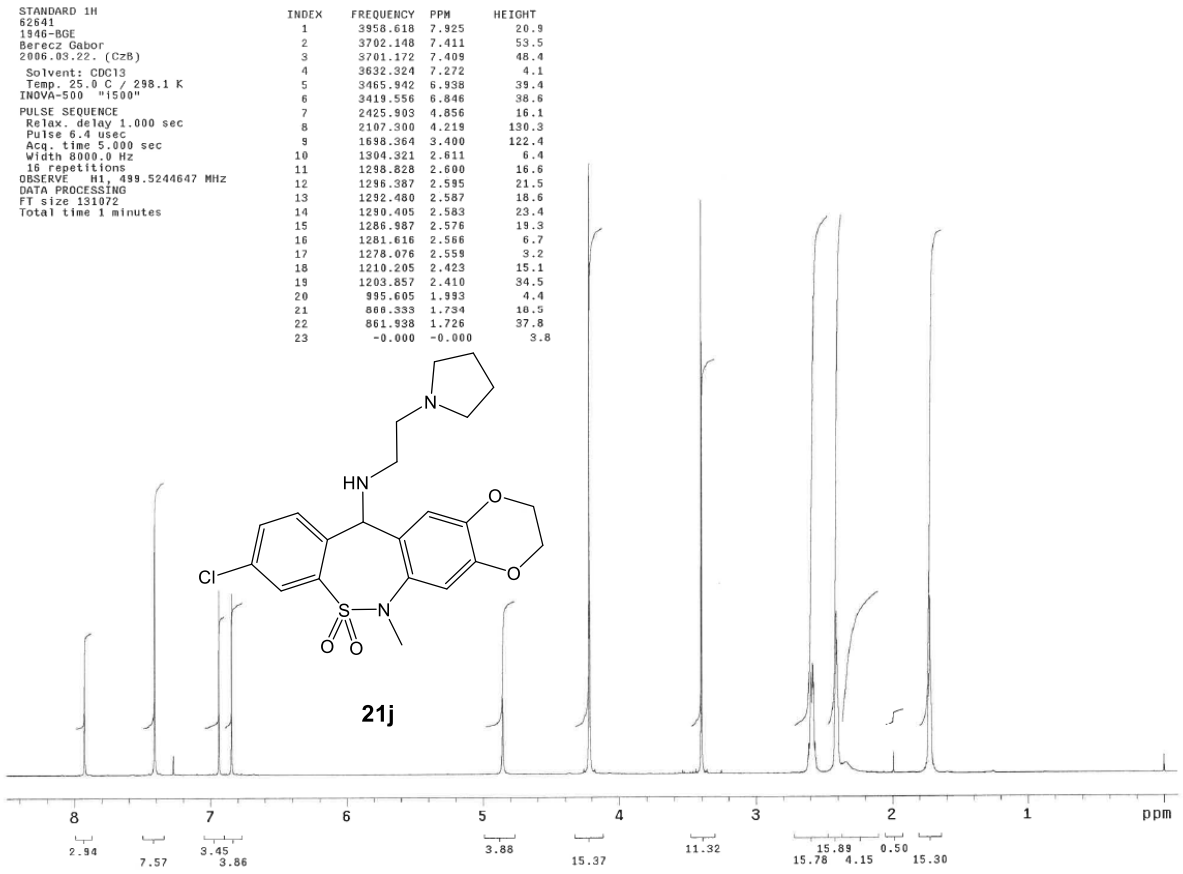
STANDARD 13C
79981
2264-BGE
Berecz Gabor
2009.05.15. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
352 repetitions
OBSERVE C13, 125.6055352 MHz
DECOUPLE H1, 499.5269647 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 25 minutes

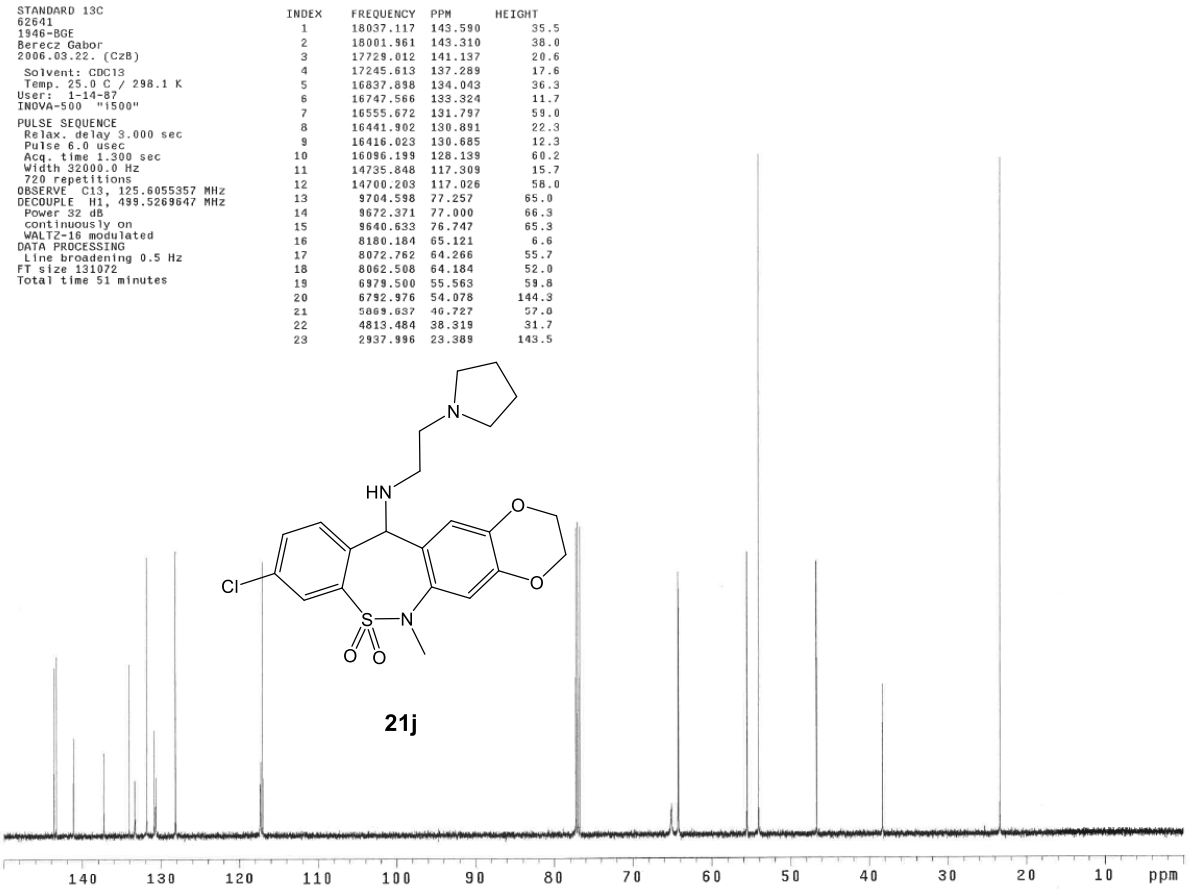
INDEX	FREQUENCY	PPM	HEIGHT
1	21721.687	172.922	33.7
2	18037.605	143.594	50.1
3	17997.078	143.271	49.6
4	17693.367	140.854	33.2
5	17234.383	137.200	31.8
6	16833.504	134.008	57.7
7	16677.254	132.765	18.2
8	16564.461	131.867	116.8
9	16465.340	131.078	34.3
10	16418.853	130.708	28.2
11	16112.801	128.271	113.4
12	14760.750	117.508	31.1
13	14693.855	116.975	108.1
14	9704.109	77.253	62.1
15	9672.371	77.000	66.3
16	9640.144	76.743	64.3
17	8196.297	65.249	15.4
18	8072.273	64.262	96.4
19	8063.484	64.192	101.4
20	6036.629	48.057	111.6
21	4852.058	38.628	67.5
22	4667.976	37.161	64.4
23	4427.254	35.245	67.7
24	4162.117	33.134	156.0
25	3749.031	29.845	124.9
26	3671.394	29.227	164.2
27	3396.492	27.039	154.0
28	3132.332	24.936	152.3



21i

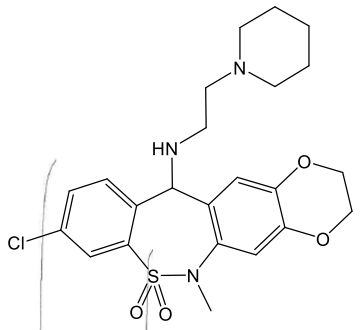



STANDARD 1H
62641
1346-BGE
Berecz Gabor
2006.03.22. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244647 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3958.618 7.925 20.9
2 3702.148 7.411 53.5
3 3701.172 7.409 48.4
4 3632.324 7.272 4.1
5 3465.942 6.938 39.4
6 3419.556 6.846 38.6
7 2425.903 4.856 16.1
8 2107.300 4.219 130.3
9 1698.364 3.400 122.4
10 1304.321 2.611 6.4
11 1298.828 2.600 16.6
12 1296.387 2.595 21.5
13 1292.480 2.587 18.6
14 1290.405 2.583 23.4
15 1288.987 2.576 18.3
16 1281.616 2.566 6.7
17 1278.076 2.559 3.2
18 1210.205 2.423 15.1
19 1203.857 2.410 34.5
20 995.605 1.993 4.4
21 868.333 1.734 10.5
22 861.538 1.726 37.8
23 -0.000 -0.000 3.8
N
HN
O
O
Cl
S
N
O
O
21j
8
7
6
5
4
3
2
1
ppm
2.94
7.57
3.45
3.86
3.88
15.37
11.32
15.89
15.78
4.15
0.50
15.30

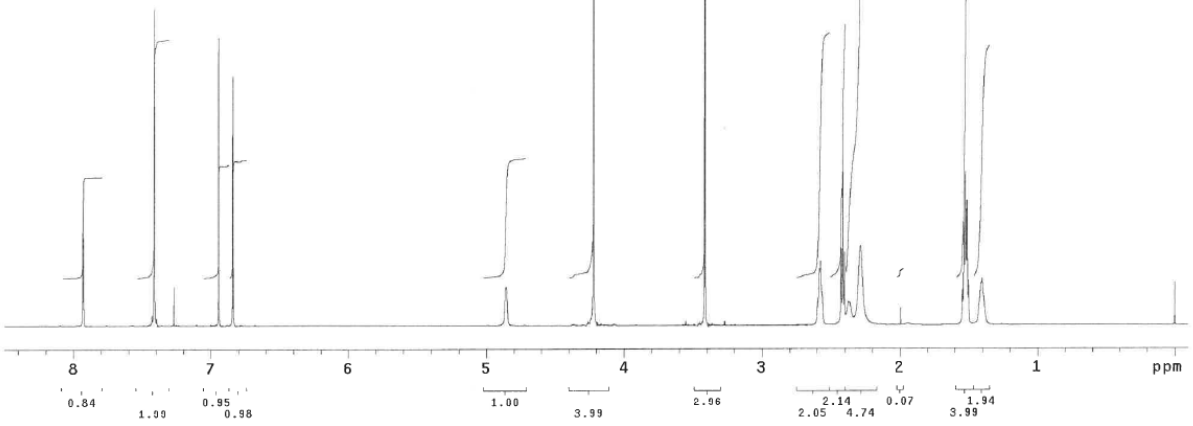

STANDARD 13C
62641
1346-BGE
Berecz Gabor
2006.03.22. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
720 repetitions
OBSERVE C13, 125.6055357 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 51 minutes
INDEX FREQUENCY PPM HEIGHT
1 18037.117 143.590 35.5
2 18001.961 143.310 38.0
3 17729.012 141.137 20.6
4 17245.613 137.289 17.6
5 16837.898 134.043 36.3
6 16747.566 133.324 11.7
7 16555.672 131.797 59.0
8 16441.902 130.891 22.3
9 16416.023 130.685 12.3
10 16096.199 128.139 60.2
11 14735.848 117.309 15.7
12 14700.203 117.026 58.0
13 9704.598 77.257 65.0
14 9672.371 77.000 66.3
15 9640.633 76.747 65.3
16 8180.184 65.121 6.6
17 8072.762 64.266 55.7
18 8062.508 64.184 52.0
19 6979.500 55.563 59.8
20 6792.976 54.078 144.3
21 5069.637 40.727 57.0
22 4813.484 38.319 31.7
23 2937.996 23.389 143.5
N
HN
O
O
Cl
S
N
O
O
21j
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
62615
1945-BGE
Berecz Gabor
2006.03.21. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244668 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3962.158	7.932	19.6
2	3960.937	7.929	25.3
3	3702.637	7.412	46.3
4	3701.294	7.410	66.9
5	3630.737	7.268	8.1
6	3467.896	6.942	60.8
7	3416.504	6.840	52.7
8	2428.223	4.861	8.0
9	2424.438	4.853	8.1
10	2108.032	4.220	177.2
11	1705.811	3.415	177.7
12	1290.527	2.584	12.1
13	1285.522	2.573	13.5
14	1211.914	2.426	22.1
15	1205.811	2.414	33.9
16	1199.829	2.402	15.4
17	1185.913	2.374	5.1
18	1180.420	2.363	4.9
19	1141.602	2.285	16.8
20	996.338	1.995	3.6
21	772.339	1.546	7.4
22	766.602	1.535	21.5
23	760.986	1.523	32.5
24	755.493	1.512	26.3
25	750.000	1.501	9.4
26	704.956	1.411	9.0
27	700.073	1.401	9.8
28	-0.000	-0.000	9.0

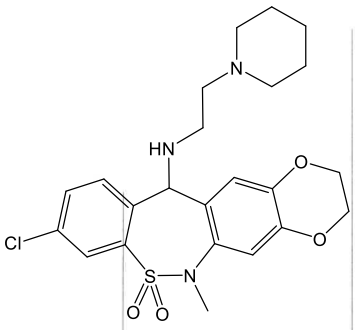


21k

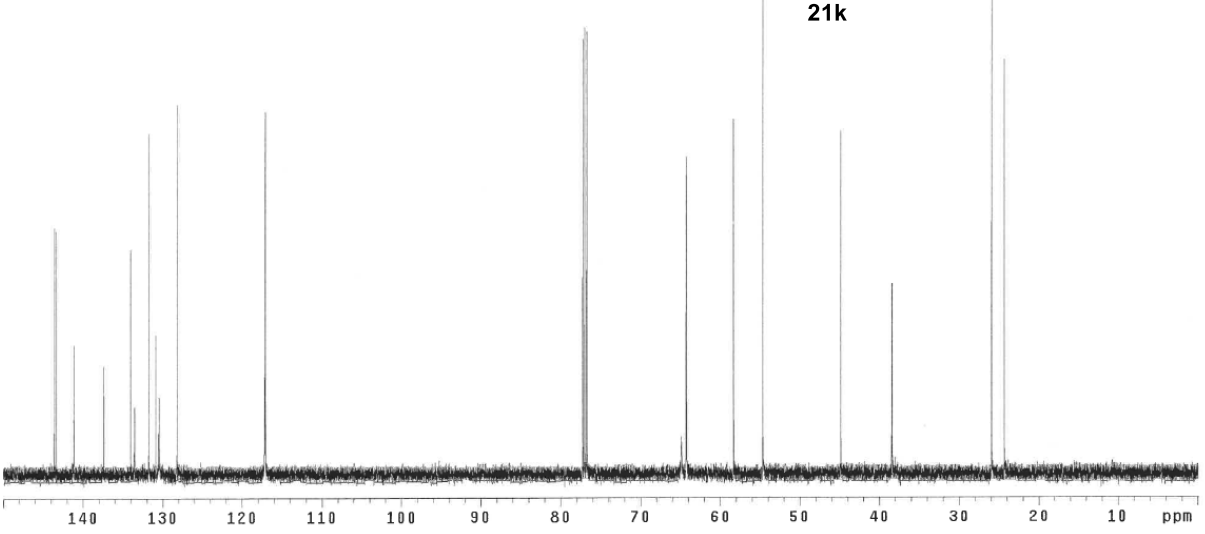


STANDARD 13C
62615
1945-BGE
Berecz Gabor
2006.03.21. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
256 repetitions
OBSERVE C13, 125.6055342 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 18 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18036.140	143.582	51.7
2	18008.797	143.365	50.9
3	17729.012	141.137	27.0
4	17257.332	137.383	22.6
5	16836.922	134.036	47.1
6	16774.422	133.538	14.1
7	16550.789	131.758	71.5
8	16440.437	130.879	29.2
9	16390.633	130.483	16.1
10	16103.523	128.197	77.6
11	14713.387	117.131	20.4
12	14707.039	117.080	76.1
13	9704.597	77.257	91.1
14	9672.371	77.000	93.5
15	9640.633	76.747	92.7
16	8145.515	64.845	7.9
17	8074.715	64.281	62.5
18	8063.484	64.192	66.5
19	7328.621	58.342	74.4
20	6870.613	54.696	136.1
21	5634.773	44.857	72.0
22	4825.203	38.413	39.9
23	3259.773	25.950	170.3
24	3059.090	24.353	86.7

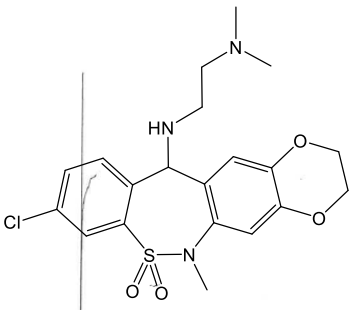


21k

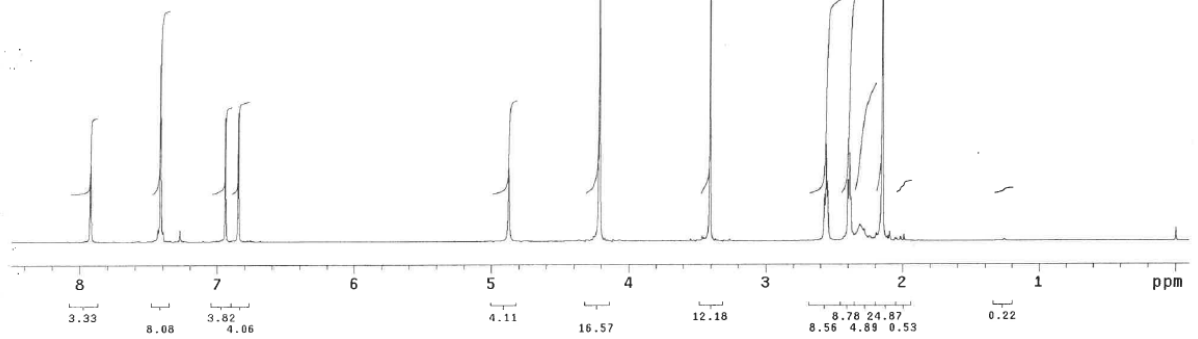


STANDARD 1H
62658
1947-BGE
Berecz Gabor
2006.03.23. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244637 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3957.764	7.923	16.5
2	3712.769	7.433	2.7
3	3704.224	7.415	37.4
4	3695.190	7.397	2.1
5	3694.092	7.395	2.1
6	3632.812	7.273	2.4
7	3468.384	6.943	26.2
8	3420.410	6.847	27.2
9	2434.570	4.874	15.5
10	2106.079	4.216	96.6
11	1703.003	3.409	82.0
12	1285.034	2.573	9.9
13	1279.297	2.561	20.4
14	1273.560	2.550	12.7
15	1206.787	2.416	1.6
16	1199.707	2.402	12.9
17	1193.848	2.390	18.6
18	1188.477	2.379	9.4
19	1181.152	2.365	1.8
20	1155.396	2.313	3.5
21	1140.015	2.282	2.5
22	1094.727	2.192	1.7
23	1074.341	2.151	151.5
24	1047.119	2.096	2.0
25	-0.000	-0.000	2.7

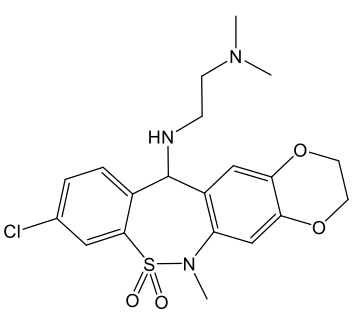


21l

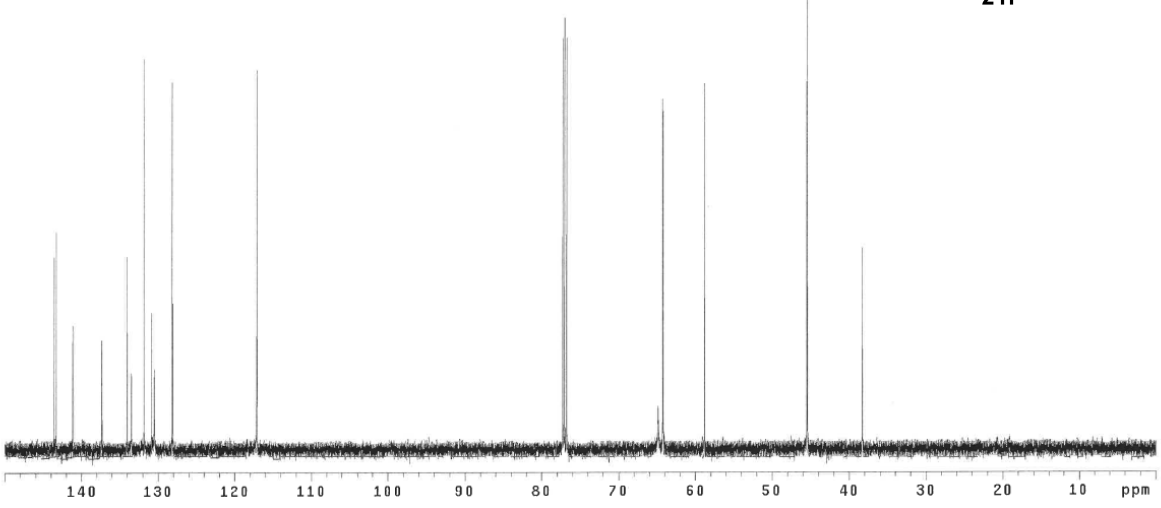


STANDARD 13C
62658
1947-BGE
Berecz Gabor
2006.03.23. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
256 repetitions
OBSERVE C13, 125.6055362 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 18 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18034.676	143.571	41.9
2	18002.937	143.318	47.3
3	17729.500	141.141	26.9
4	17252.449	137.344	23.8
5	16835.457	134.024	42.0
6	16764.656	133.460	16.7
7	16557.137	131.808	84.8
8	16435.555	130.840	29.8
9	16391.609	130.491	17.5
10	16093.758	128.120	79.8
11	14714.363	117.138	24.6
12	14706.551	117.076	82.3
13	9704.598	77.257	89.3
14	9672.371	77.000	93.8
15	9640.633	76.747	89.4
16	8146.980	64.857	9.4
17	8072.273	64.262	76.3
18	8060.555	64.169	73.6
19	7385.750	58.797	79.4
20	5717.781	45.518	79.9
21	5704.109	45.409	200.0
22	4809.090	38.284	43.8

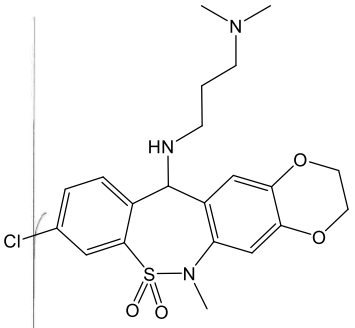


21l

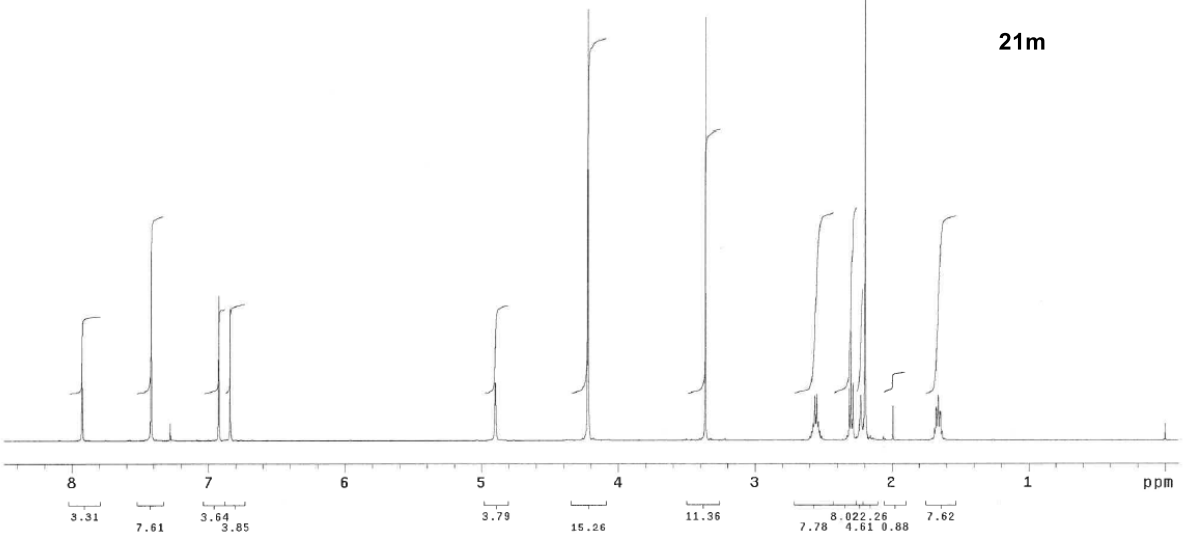


STANDARD 1H
62678
1948-BGE
Berecz Gabor
2006/03/24 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244625 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3958.374	7.924	16.8
2	3705.811	7.419	40.2
3	3704.834	7.417	33.6
4	3458.496	6.924	30.8
5	3417.114	6.841	28.1
6	2446.777	4.898	12.2
7	2108.032	4.220	91.7
8	1679.932	3.363	90.0
9	1280.029	2.562	9.4
10	1273.560	2.550	9.8
11	1155.273	2.313	11.0
12	1148.193	2.299	23.1
13	1141.235	2.285	12.1
14	1113.647	2.229	9.5
15	1097.412	2.197	161.8
16	995.728	1.993	7.4
17	836.670	1.675	7.1
18	835.083	1.672	6.6
19	829.956	1.661	9.6
20	828.125	1.658	9.1
21	822.998	1.648	6.2
22	821.167	1.644	6.1

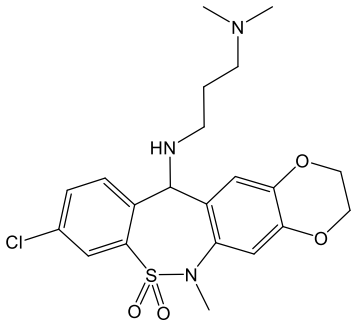


21m

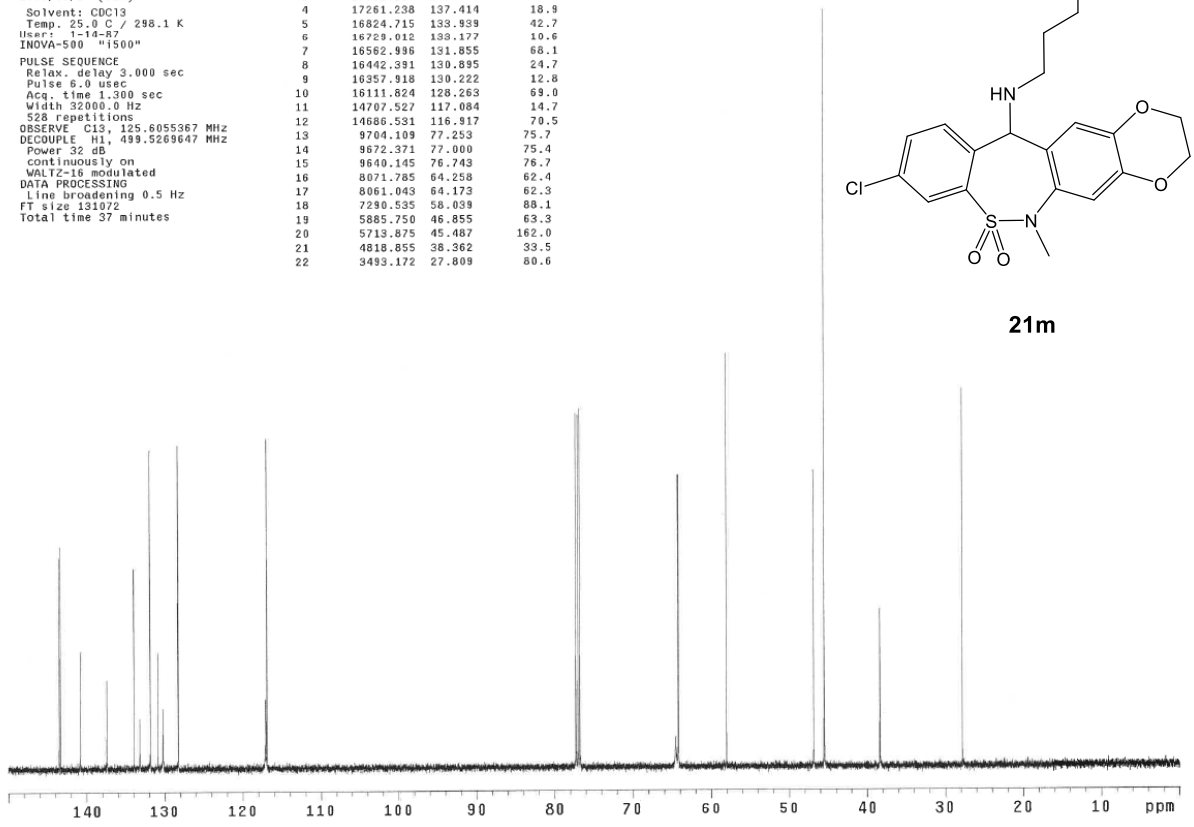


STANDARD 13C
62678
1948-BGE
Berecz Gabor
2006/03/24 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-R7
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
528 repetitions
OBSERVE C13, 125.6055367 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 37 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18028.816	143.524	45.2
2	18004.402	143.330	47.5
3	17682.137	140.764	25.0
4	17261.238	137.414	18.9
5	16824.715	133.939	42.7
6	16729.012	133.177	10.6
7	16562.996	131.855	68.1
8	16442.391	130.895	24.7
9	16357.918	130.222	12.8
10	16111.824	128.263	69.0
11	14707.527	117.084	14.7
12	14686.531	116.917	70.5
13	9704.109	77.253	75.7
14	9672.371	77.000	75.4
15	9640.145	76.743	76.7
16	8071.785	64.258	62.4
17	8061.043	64.173	62.3
18	7290.535	58.039	88.1
19	5885.750	46.855	63.3
20	5713.875	45.487	162.0
21	4818.855	38.362	33.5
22	3493.172	27.809	80.6



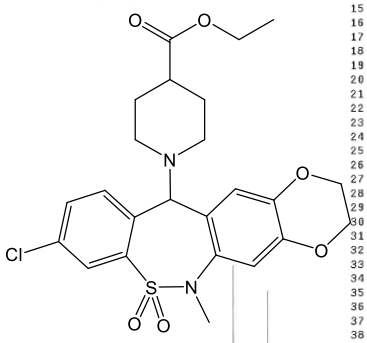
21m



STANDARD 1H
65651
2014-BGE
Berecz Gabor
2006/10/05 (SzA)

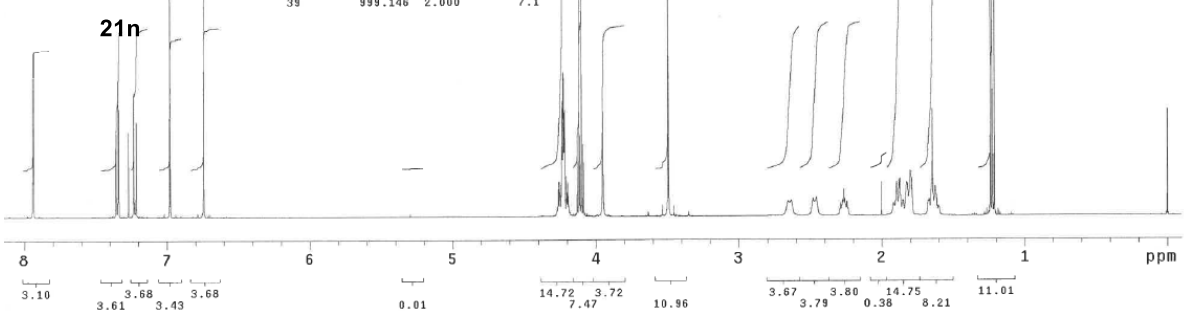
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244663 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes



21n

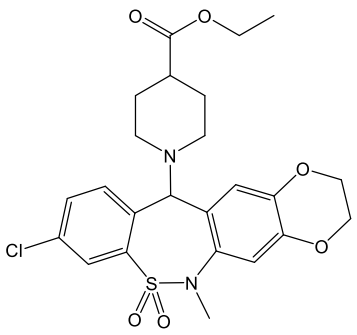
INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3965.698	7.939	29.4	40	946.411	1.895	7.2
2	3963.501	7.935	28.5	41	935.059	1.872	7.8
3	3675.537	7.358	18.4	42	925.171	1.852	3.3
4	3673.218	7.353	17.6	43	923.706	1.849	3.3
5	3667.236	7.341	24.0	44	912.109	1.826	7.1
6	3664.917	7.337	22.9	45	910.645	1.823	7.0
7	3630.615	7.268	17.9	46	908.569	1.819	6.7
8	3612.183	7.231	26.2	47	903.320	1.808	5.0
9	3603.882	7.215	20.2	48	898.804	1.799	9.5
10	3486.450	6.980	63.2	49	897.339	1.796	9.3
11	3368.652	6.744	57.7	50	835.693	1.673	3.2
12	2127.197	4.258	7.3	51	832.642	1.667	3.5
13	2124.268	4.253	5.0	52	820.801	1.643	22.5
14	2122.192	4.248	7.3	53	811.279	1.624	6.4
15	2120.972	4.246	6.2	54	619.629	1.240	57.0
16	2115.601	4.235	24.3	55	612.549	1.226	122.3
17	2114.014	4.232	12.5	56	605.347	1.212	54.1
18	2112.305	4.229	22.8	57	1.099	0.002	3.3
19	2110.962	4.226	30.4	58	0.000	0.000	22.3
20	2108.765	4.222	18.8				
21	2106.445	4.217	22.4				
22	2105.347	4.215	17.4				
23	2099.976	4.204	8.6				
24	2097.290	4.199	5.0				
25	2094.604	4.193	7.0				
26	2062.012	4.128	14.8				
27	2054.932	4.114	47.5				
28	2047.729	4.099	48.6				
29	2040.649	4.085	15.2				
30	1973.145	3.950	22.7				
31	1744.507	3.492	197.3				
32	1326.660	2.656	3.2				
33	1315.796	2.634	3.4				
34	1238.892	2.480	3.7				
35	1227.783	2.458	4.0				
36	1135.986	2.274	3.4				
37	1131.958	2.266	5.8				
38	1127.930	2.258	3.5				
39	999.146	2.000	7.1				



STANDARD 13C
65651
2014-BGE
Berecz Gabor
2006/10/05 (SzA)

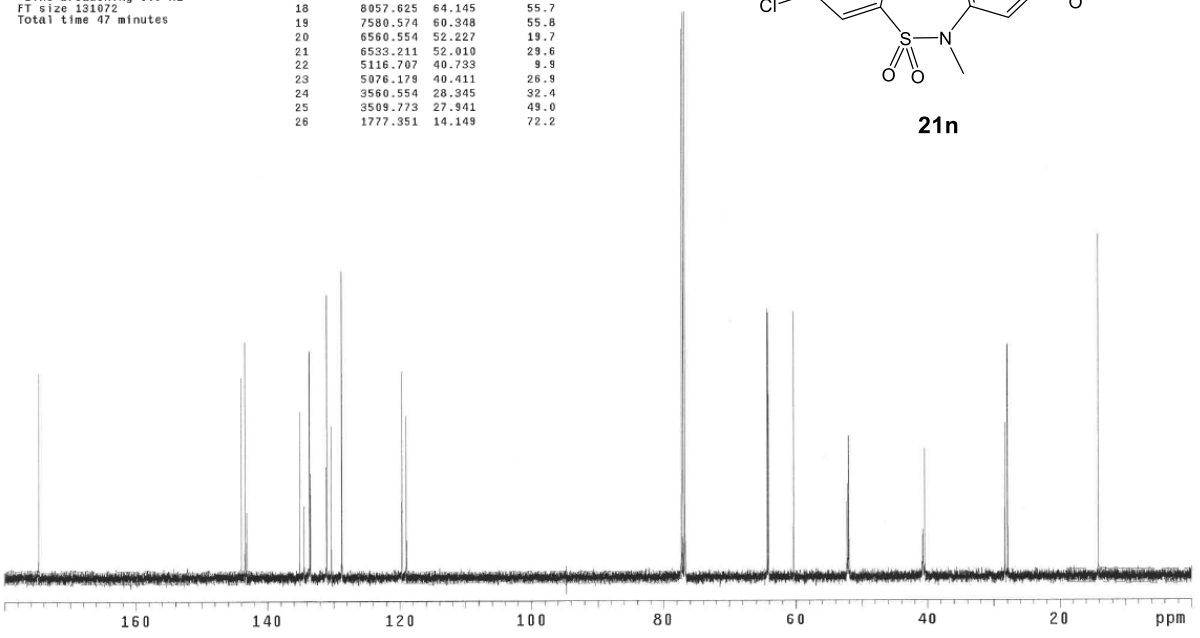
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"

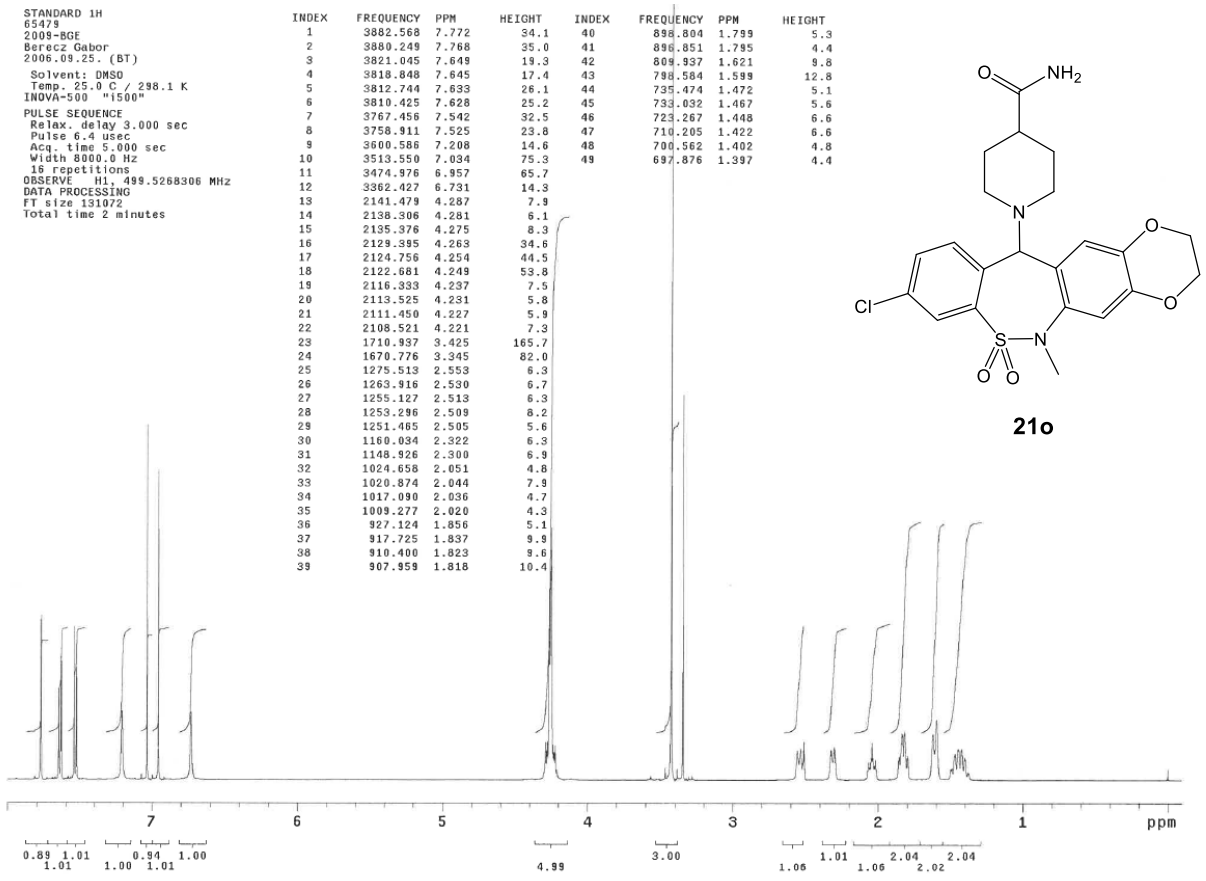
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
666 repetitions
OBSERVE C13, 125.6055323 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 47 minutes



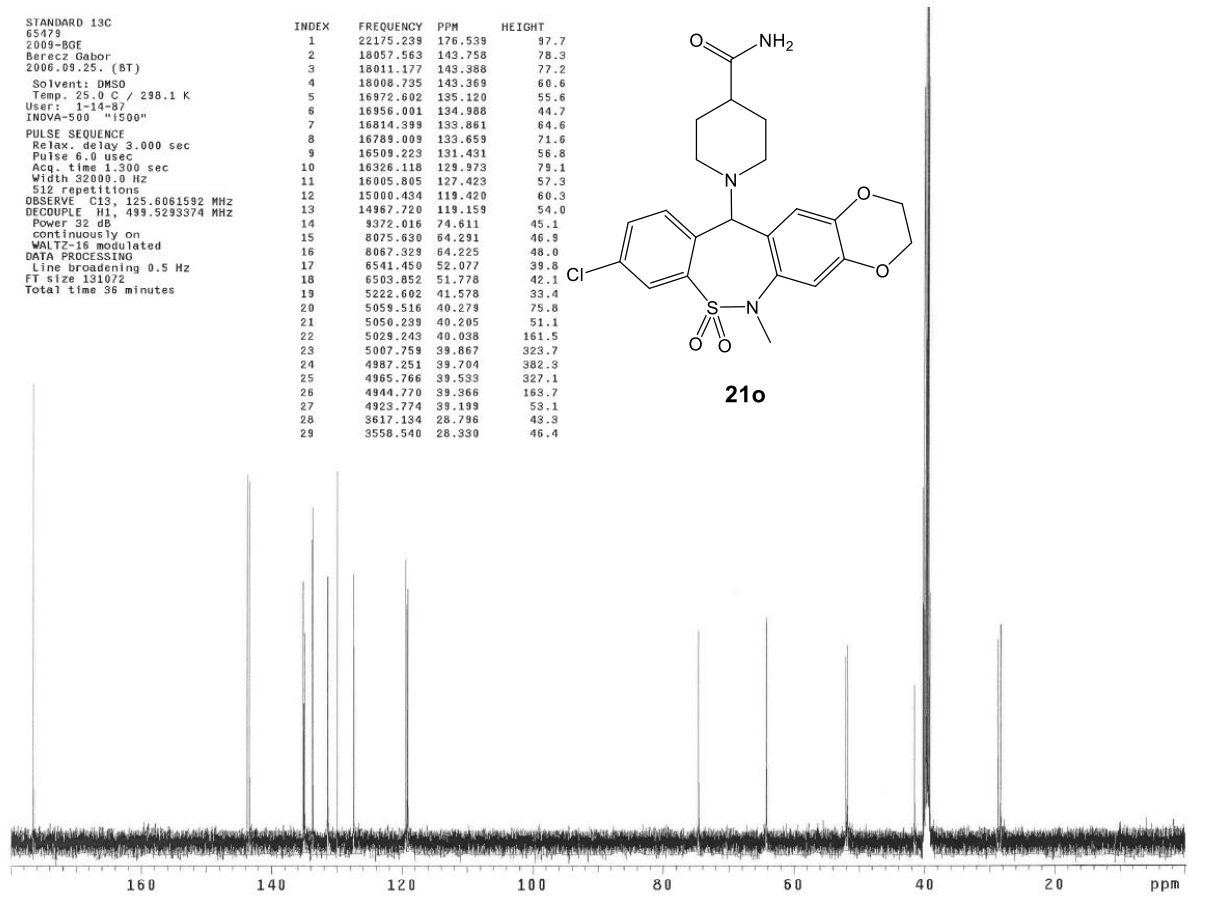
21n

INDEX	FREQUENCY	PPM	HEIGHT
1	21956.062	174.788	43.2
2	18088.875	144.002	42.1
3	18021.980	143.470	49.7
4	17983.406	143.163	13.8
5	16969.734	135.093	34.9
6	16883.308	134.405	15.2
7	16783.699	133.612	47.7
8	16765.632	133.468	21.9
9	16457.527	131.015	59.7
10	16366.707	130.292	31.9
11	16169.929	128.726	64.6
12	15029.793	119.649	43.4
13	14948.738	119.004	34.0
14	9704.597	77.257	115.6
15	9672.371	77.000	119.0
16	9640.632	76.747	119.2
17	8076.179	64.293	56.4
18	8057.625	64.145	55.7
19	7580.574	60.348	55.8
20	6560.554	52.227	19.7
21	6533.211	52.010	29.6
22	5116.707	40.733	9.9
23	5076.179	40.411	26.9
24	3560.554	28.345	32.4
25	3509.773	27.941	49.0
26	1777.351	14.149	72.2

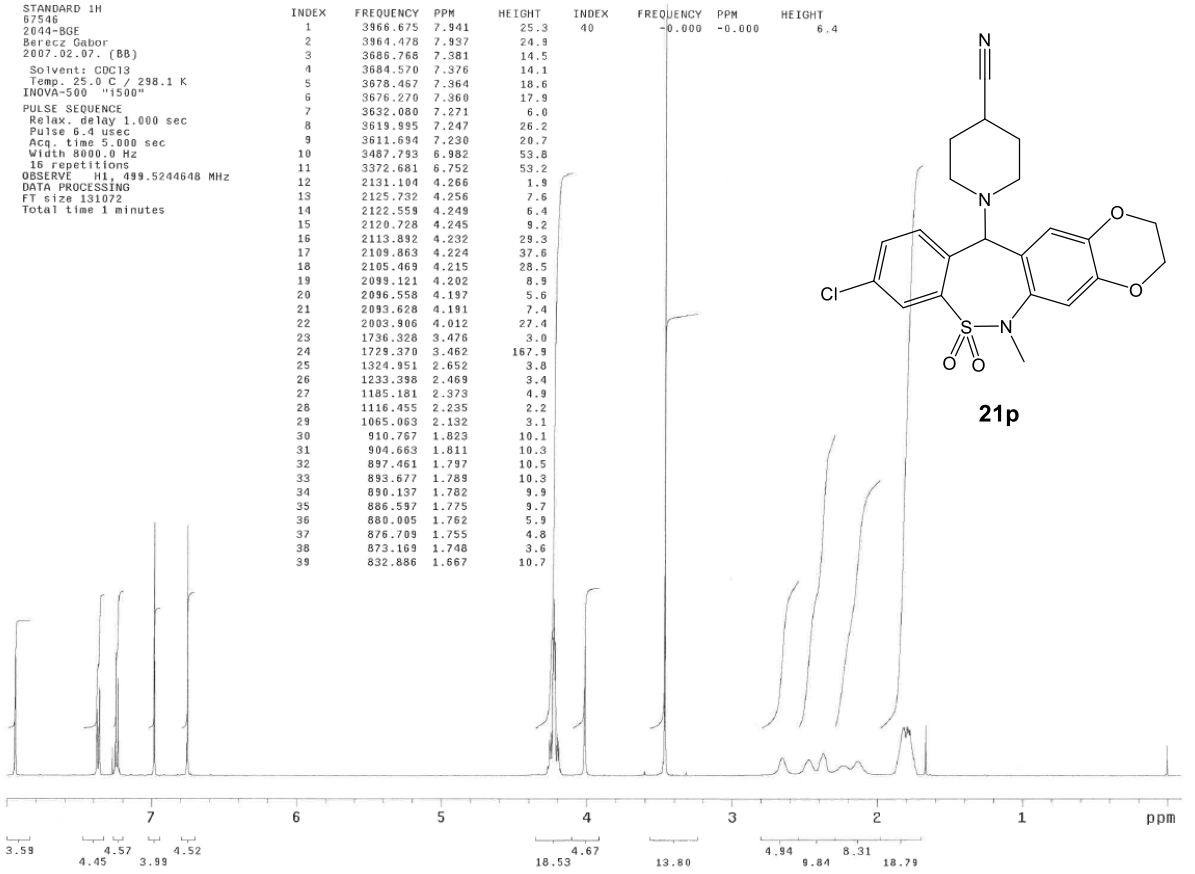


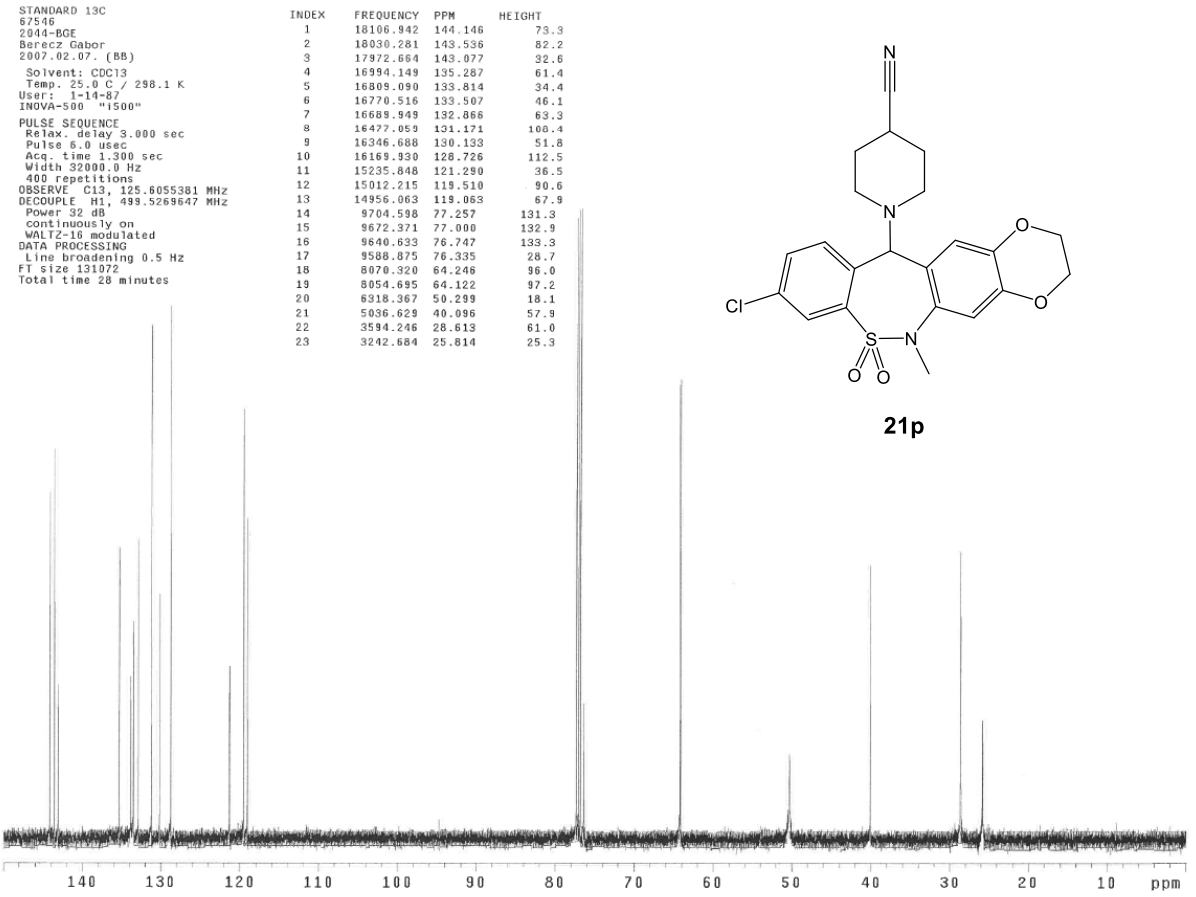

STANDARD 1H
65479
2009-BGE
Berecz Gabor
2006.09.25. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268306 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3882.568 7.772 34.1 40 898.804 1.799 5.3
2 3880.249 7.768 35.0 41 896.851 1.795 4.4
3 3821.045 7.649 19.3 42 809.937 1.621 9.8
4 3818.848 7.645 17.4 43 798.584 1.599 12.8
5 3812.744 7.633 26.1 44 735.474 1.472 5.1
6 3810.425 7.628 25.2 45 733.032 1.467 5.6
7 3767.456 7.542 32.5 46 723.267 1.448 6.6
8 3758.911 7.525 23.8 47 710.205 1.422 6.6
9 3600.586 7.208 14.6 48 700.562 1.402 4.8
10 3513.550 7.034 75.3 49 697.876 1.397 4.4
11 3474.976 6.957 65.7
12 3362.427 6.731 14.3
13 2141.479 4.287 7.9
14 2138.306 4.281 6.1
15 2135.376 4.275 8.3
16 2129.395 4.263 34.6
17 2124.756 4.254 44.5
18 2122.681 4.249 53.8
19 2116.333 4.237 7.5
20 2113.525 4.231 5.8
21 2111.450 4.227 5.9
22 2108.521 4.221 7.3
23 1710.937 3.425 165.7
24 1670.776 3.345 82.0
25 1275.513 2.553 6.3
26 1263.916 2.530 6.7
27 1255.127 2.513 6.3
28 1253.296 2.509 8.2
29 1251.465 2.505 5.6
30 1160.034 2.322 6.3
31 1148.926 2.300 6.9
32 1024.658 2.051 4.8
33 1020.874 2.044 7.9
34 1017.090 2.036 4.7
35 1009.277 2.020 4.3
36 927.124 1.856 5.1
37 917.725 1.837 9.9
38 910.400 1.823 9.6
39 907.959 1.818 10.4
O
NH2
N
O
O
Cl
S
N
O
O
7
6
5
4
3
2
1
ppm
0.89 1.01 1.01
0.94 1.01
1.00 1.00
4.99
3.00
1.06
1.01 1.06
2.04 2.02
2.04

21o


STANDARD 13C
65479
2009-BGE
Berecz Gabor
2006.09.25. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
512 repetitions
OBSERVE C13, 125.6061592 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 36 minutes
INDEX FREQUENCY PPM HEIGHT
1 22175.239 176.539 97.7
2 18057.563 143.758 78.3
3 18011.177 143.388 77.2
4 18008.735 143.369 60.6
5 16972.602 135.120 55.6
6 16956.001 134.988 44.7
7 16814.399 133.861 64.6
8 16789.009 133.659 71.6
9 16509.223 131.431 56.8
10 16326.118 129.973 79.1
11 16005.805 127.423 57.3
12 15000.434 119.420 60.3
13 14967.720 119.159 54.0
14 9372.016 74.611 45.1
15 8075.630 64.291 46.9
16 8067.329 64.225 48.0
17 6541.450 52.077 39.8
18 6503.852 51.778 42.1
19 5222.602 41.578 33.4
20 5059.516 40.279 75.8
21 5050.239 40.205 51.1
22 5029.243 40.038 161.5
23 5007.759 39.867 323.7
24 4987.251 39.704 382.3
25 4965.766 39.533 327.1
26 4944.770 39.366 163.7
27 4923.774 39.199 53.1
28 3617.134 28.796 43.3
29 3558.540 28.330 46.4
O
NH2
N
O
O
Cl
S
N
O
O
160
140
120
100
80
60
40
20
ppm

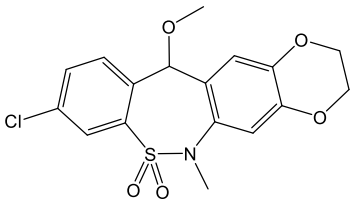
21o


STANDARD 1H
67546
2044-BGE
Berecz Gabor
2007.02.07. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244648 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3966.675 7.941 25.3
2 3964.478 7.937 24.9
3 3686.768 7.381 14.5
4 3684.570 7.376 14.1
5 3678.467 7.364 18.6
6 3676.270 7.360 17.9
7 3632.080 7.271 6.0
8 3619.995 7.247 26.2
9 3611.694 7.230 20.7
10 3487.793 6.982 53.8
11 3372.681 6.752 53.2
12 2131.104 4.266 1.9
13 2125.732 4.256 7.6
14 2122.559 4.249 6.4
15 2120.728 4.245 9.2
16 2113.892 4.232 29.3
17 2109.863 4.224 37.6
18 2105.469 4.215 28.5
19 2099.121 4.202 8.9
20 2096.558 4.197 5.6
21 2093.628 4.191 7.4
22 2003.906 4.012 27.4
23 1736.328 3.476 3.0
24 1729.370 3.462 167.9
25 1324.951 2.652 3.8
26 1233.398 2.469 3.4
27 1185.181 2.373 4.9
28 1116.455 2.235 2.2
29 1065.063 2.132 3.1
30 910.767 1.823 10.1
31 904.663 1.811 10.3
32 897.461 1.797 10.5
33 893.677 1.789 10.3
34 890.137 1.782 9.9
35 886.597 1.775 9.7
36 880.005 1.762 5.9
37 876.709 1.755 4.8
38 873.169 1.748 3.6
39 832.886 1.667 10.7
INDEX FREQUENCY PPM HEIGHT
40 -0.000 -0.000 6.4
N
N
O
O
Cl
S
N
O
O
21p
7
6
5
4
3
2
1
ppm
3.58
4.57
4.45
3.99
4.52
4.67
18.53
13.80
4.94
8.31
9.84
18.79

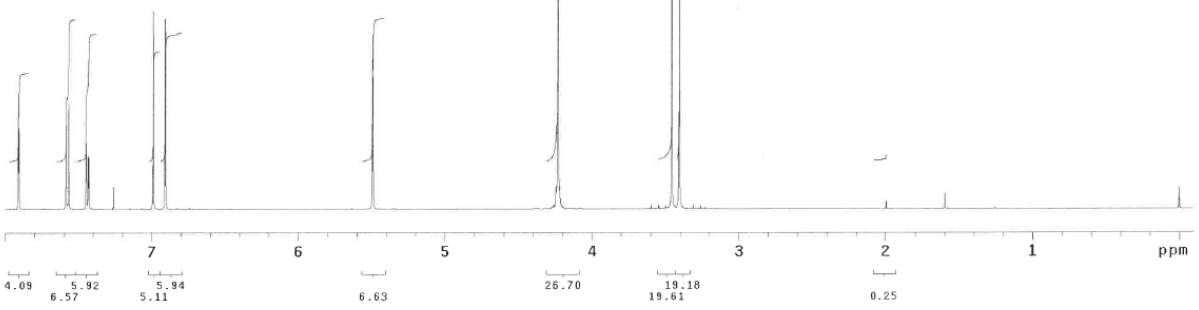

STANDARD 13C
67546
2044-BGE
Berecz Gabor
2007.02.07. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
400 repetitions
OBSERVE C13, 125.6055381 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 28 minutes
INDEX FREQUENCY PPM HEIGHT
1 18106.942 144.146 73.3
2 18030.281 143.536 82.2
3 17972.664 143.077 32.6
4 16994.149 135.287 61.4
5 16809.090 133.814 34.4
6 16770.516 133.507 46.1
7 16689.949 132.866 63.3
8 16477.059 131.171 108.4
9 16346.688 130.133 51.8
10 16169.930 128.726 112.5
11 15235.848 121.290 36.5
12 15012.215 119.510 90.6
13 14956.063 119.063 67.9
14 9704.598 77.257 131.3
15 9672.371 77.000 132.9
16 9640.633 76.747 133.3
17 9588.875 76.335 28.7
18 8070.320 64.246 96.0
19 8054.695 64.122 97.2
20 6318.367 50.299 18.1
21 5036.629 40.096 57.9
22 3594.246 28.613 61.0
23 3242.684 25.814 25.3
N
N
O
O
Cl
S
N
O
O
21p
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
68717
2068-BGE
Berecz Gabor
2007.04.10. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244691 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3950.317	7.908	16.9
2	3948.242	7.904	16.9
3	3787.598	7.582	17.6
4	3779.175	7.566	22.0
5	3720.581	7.448	14.2
6	3718.384	7.444	13.8
7	3712.036	7.431	11.0
8	3709.961	7.427	10.8
9	3626.953	7.261	4.8
10	3491.333	6.989	41.3
11	3450.195	6.907	39.7
12	2743.774	5.493	31.3
13	2119.507	4.243	4.9
14	2113.159	4.230	135.2
15	2106.812	4.218	4.9
16	1726.074	3.455	152.1
17	1700.439	3.404	153.4
18	997.070	1.996	1.7
19	797.729	1.597	3.2
20	0.000	0.000	4.5

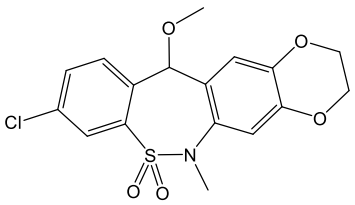


23a

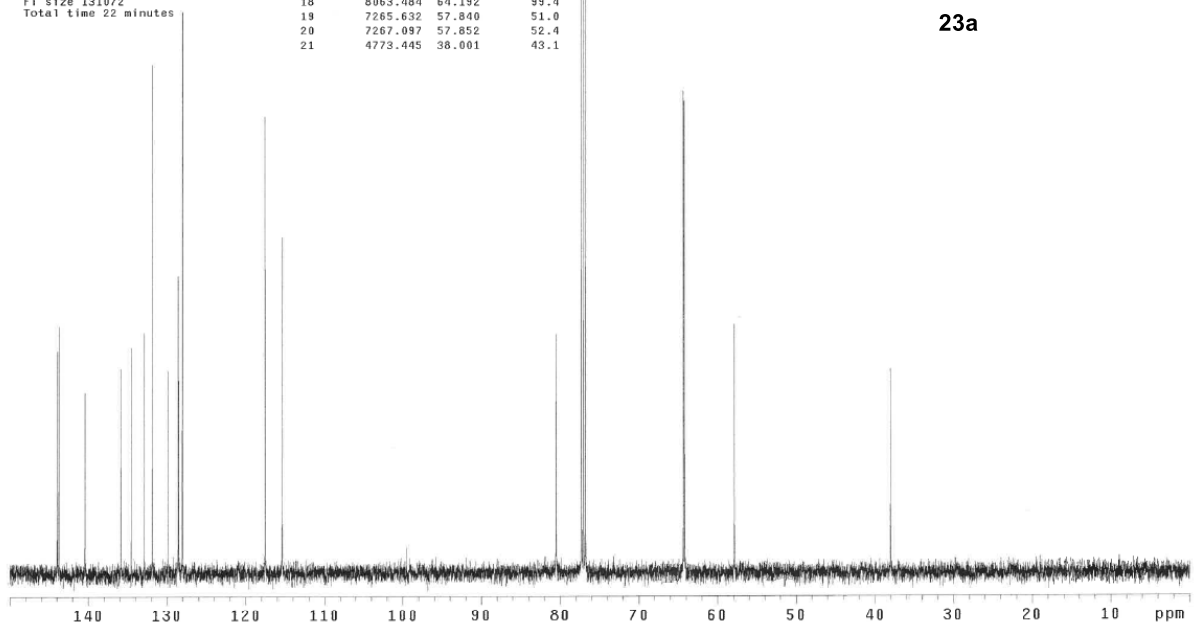


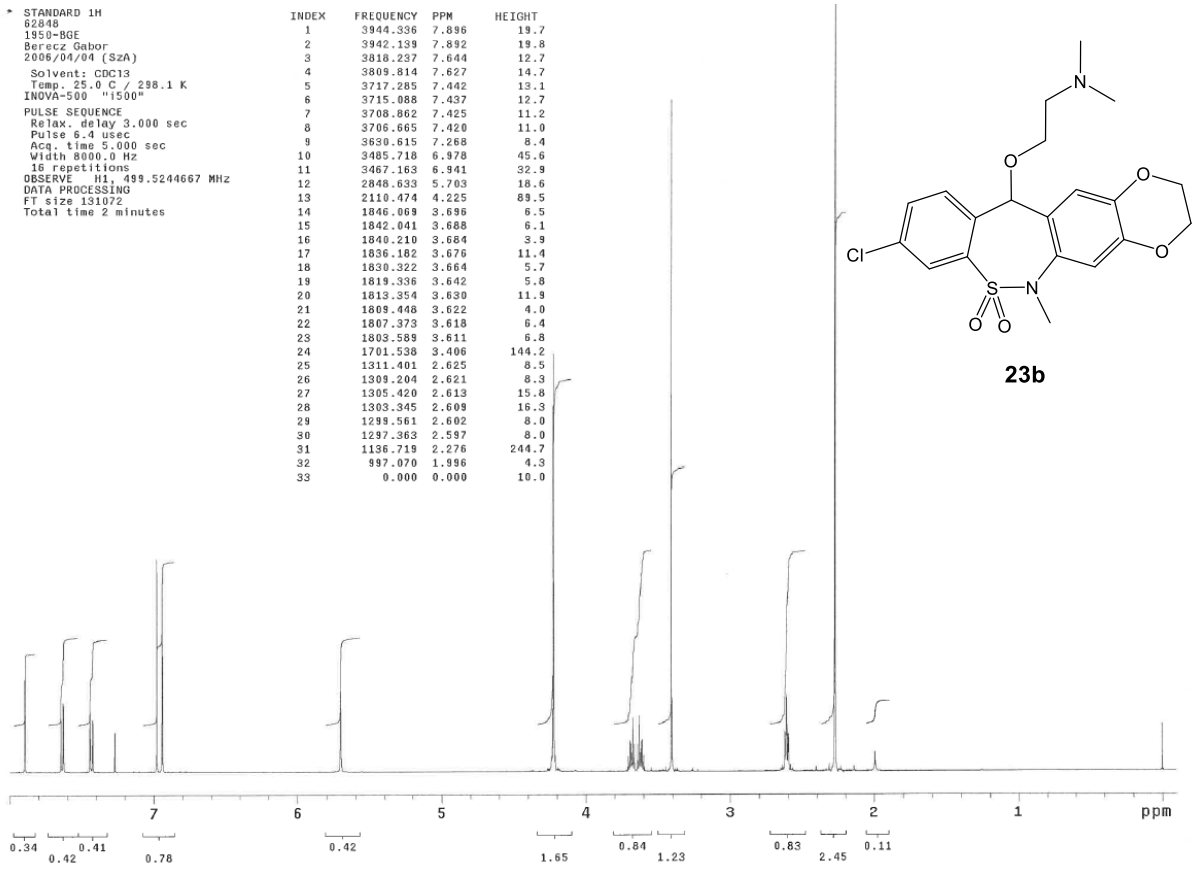
STANDARD 13C
68717
2068-BGE
Berecz Gabor
2007.04.10. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
318 repetitions
OBSERVE C13, 125.6055317 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 22 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18079.597	143.928	46.8
2	18055.183	143.734	51.9
3	17638.679	140.418	38.1
4	17063.972	135.843	43.1
5	16903.816	134.568	47.5
6	16691.414	132.877	50.6
7	16564.949	131.871	107.0
8	16313.972	129.873	42.7
9	16145.027	128.528	62.5
10	16079.109	128.003	118.0
11	14763.191	117.527	96.0
12	14491.218	115.362	70.9
13	10113.777	80.514	50.2
14	9704.109	77.253	139.9
15	9672.371	77.000	139.8
16	9640.144	76.743	139.3
17	8078.132	64.309	101.5
18	8063.484	64.192	99.4
19	7265.632	57.840	51.0
20	7267.097	57.852	52.4
21	4773.445	38.001	43.1



23a




* STANDARD 1H
62848
1950-BGE
Berecz Gabor
2006/04/04 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244667 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3944.336 7.896 19.7
2 3942.139 7.892 19.8
3 3818.237 7.644 12.7
4 3809.814 7.627 14.7
5 3717.285 7.442 13.1
6 3715.088 7.437 12.7
7 3708.862 7.425 11.2
8 3706.665 7.420 11.0
9 3630.615 7.268 8.4
10 3485.718 6.978 45.6
11 3467.163 6.941 32.9
12 2848.633 5.703 18.6
13 2110.474 4.225 89.5
14 1846.069 3.696 6.5
15 1842.041 3.688 6.1
16 1840.210 3.684 3.9
17 1836.182 3.676 11.4
18 1830.322 3.664 5.7
19 1819.336 3.642 5.8
20 1813.354 3.630 11.9
21 1809.448 3.622 4.0
22 1807.373 3.618 6.4
23 1803.589 3.611 6.8
24 1701.538 3.406 144.2
25 1311.401 2.625 8.5
26 1309.204 2.621 8.3
27 1305.420 2.613 15.8
28 1303.345 2.609 16.3
29 1299.561 2.602 8.0
30 1297.363 2.597 8.0
31 1136.719 2.276 244.7
32 997.070 1.996 4.3
33 0.000 0.000 10.0
7
6
5
4
3
2
1
ppm
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0.41
0.42
0.78
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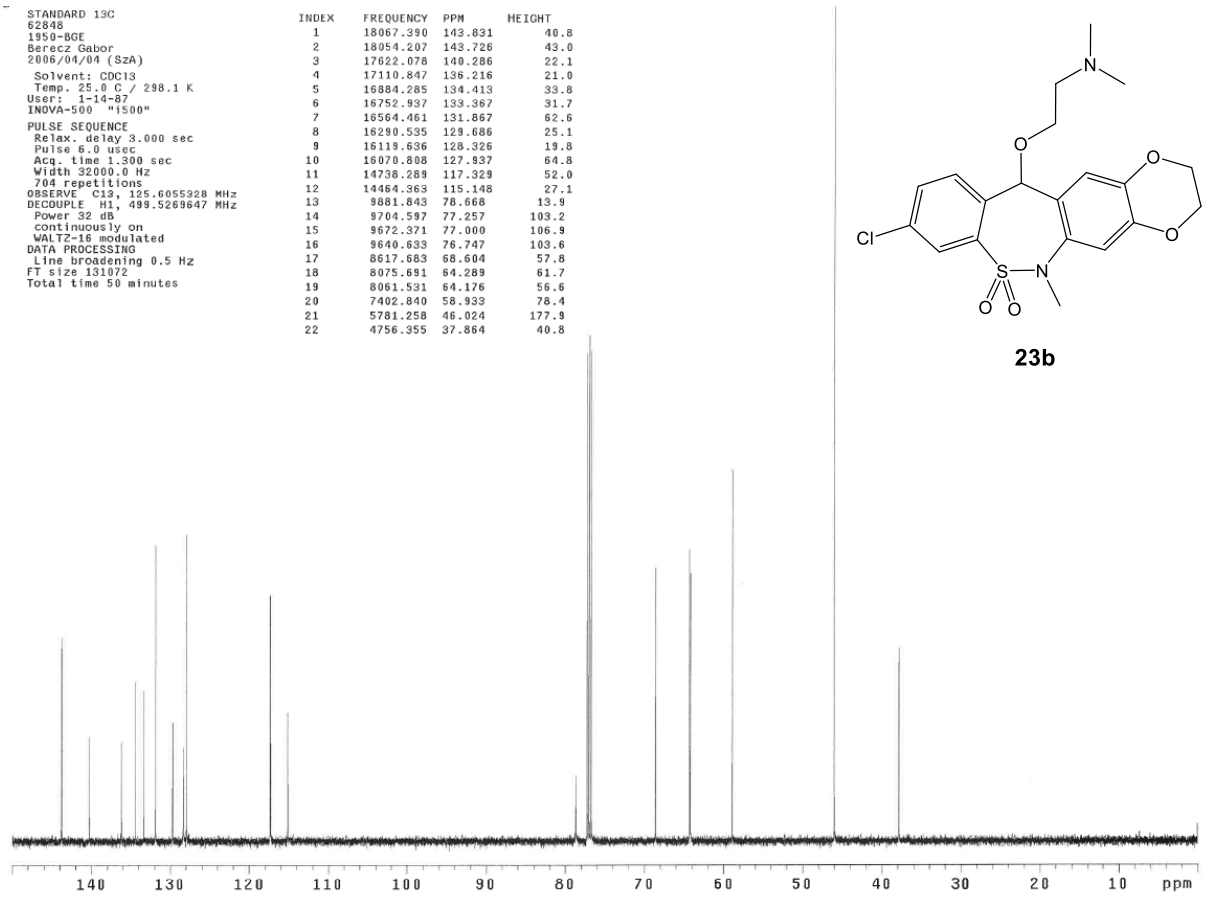
1.65
0.84
1.23
0.83
2.45
0.11

23b

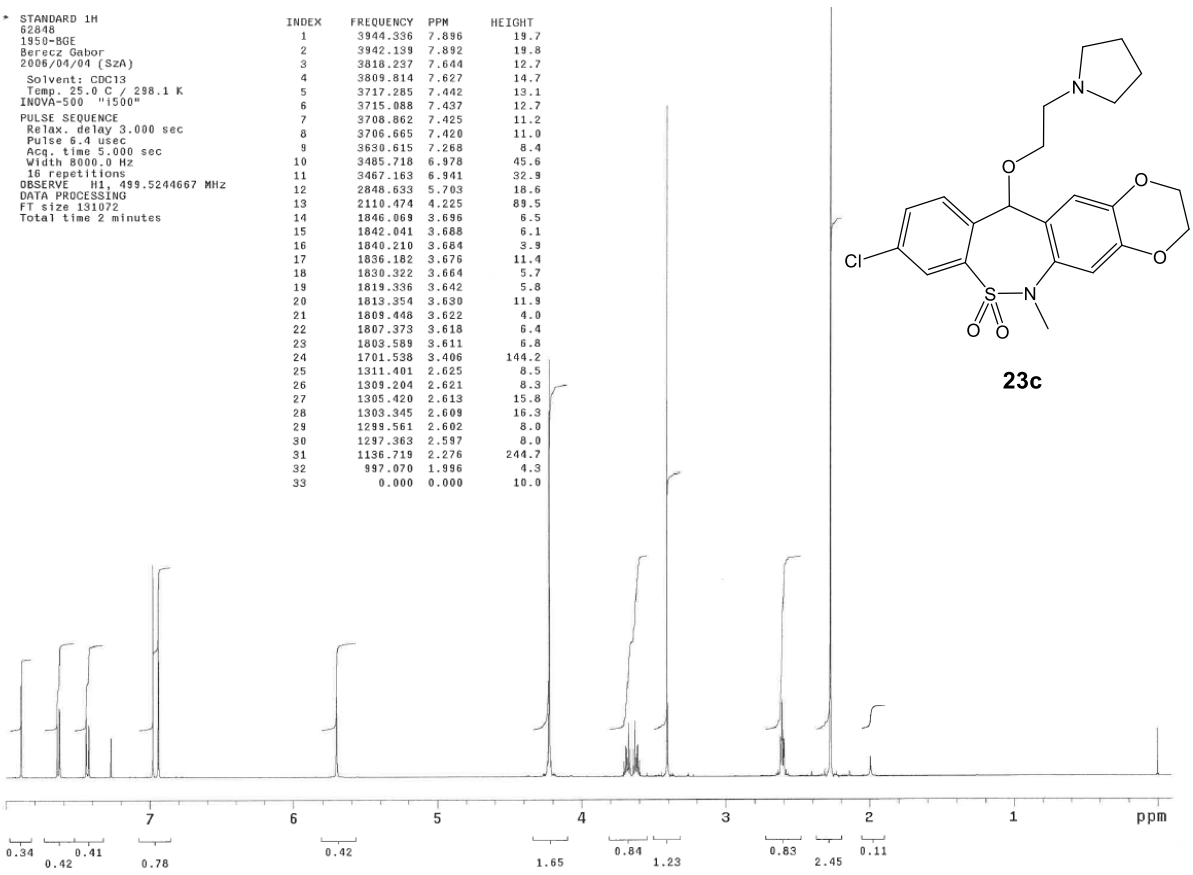

STANDARD 13C
62848
1950-BGE
Berecz Gabor
2006/04/04 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
704 repetitions
OBSERVE C13, 125.6055328 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 50 minutes
INDEX FREQUENCY PPM HEIGHT
1 18067.390 143.831 40.8
2 18054.207 143.726 43.0
3 17622.078 140.286 22.1
4 17110.847 136.216 21.0
5 16884.285 134.413 33.8
6 16752.937 133.367 31.7
7 16564.461 131.867 62.6
8 16290.535 129.686 25.1
9 16119.636 128.326 19.8
10 16070.808 127.937 64.8
11 14738.289 117.329 52.0
12 14464.363 115.148 27.1
13 9881.843 78.668 13.9
14 9704.597 77.257 103.2
15 9672.371 77.000 106.9
16 9640.633 76.747 103.6
17 8617.683 68.604 57.8
18 8075.691 64.289 61.7
19 8061.531 64.176 56.6
20 7402.840 58.933 78.4
21 5781.258 46.024 177.9
22 4756.355 37.864 40.8
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

23b

```
* STANDARD 1H
  62848
  1950-BGE
  Berecz Gabor
  2006/04/04 (SzA)
   Solvent: CDCl3
   Temp. 25.0 C / 298.1 K
  INOVA-500  "i500"
  PULSE SEQUENCE
   Relax. delay 3.000 sec
   Pulse 6.4 usec
   Acq. time 5.000 sec
   Width 8000.0 Hz
   16 repetitions
  OBSERVE    H1, 499.5244667 MHz
  DATA PROCESSING
  FT size 131072
  Total time 2 minutes
```

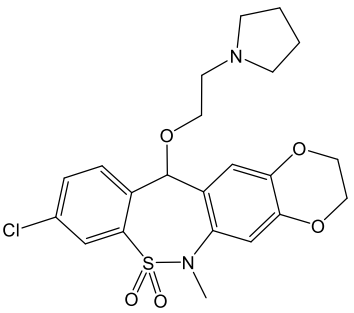
INDEX	FREQUENCY	PPM	HEIGHT
1	3944.336	7.896	19.7
2	3942.139	7.892	19.8
3	3818.237	7.644	12.7
4	3809.814	7.627	14.7
5	3717.285	7.442	13.1
6	3715.088	7.437	12.7
7	3708.862	7.425	11.2
8	3706.665	7.420	11.0
9	3630.615	7.268	8.4
10	3485.718	6.978	45.6
11	3467.163	6.941	32.9
12	2848.633	5.703	18.6
13	2110.474	4.225	89.5
14	1846.069	3.696	6.5
15	1842.041	3.688	6.1
16	1840.210	3.684	3.9
17	1836.182	3.676	11.4
18	1830.322	3.664	5.7
19	1819.336	3.642	5.8
20	1813.354	3.630	11.9
21	1809.448	3.622	4.0
22	1807.373	3.618	6.4
23	1803.589	3.611	6.8
24	1701.538	3.406	144.2
25	1311.401	2.625	8.5
26	1309.204	2.621	8.3
27	1305.420	2.613	15.8
28	1303.345	2.609	16.3
29	1299.561	2.602	8.0
30	1297.363	2.597	8.0
31	1136.719	2.276	244.7
32	997.070	1.996	4.3
33	0.000	0.000	10.0

23c

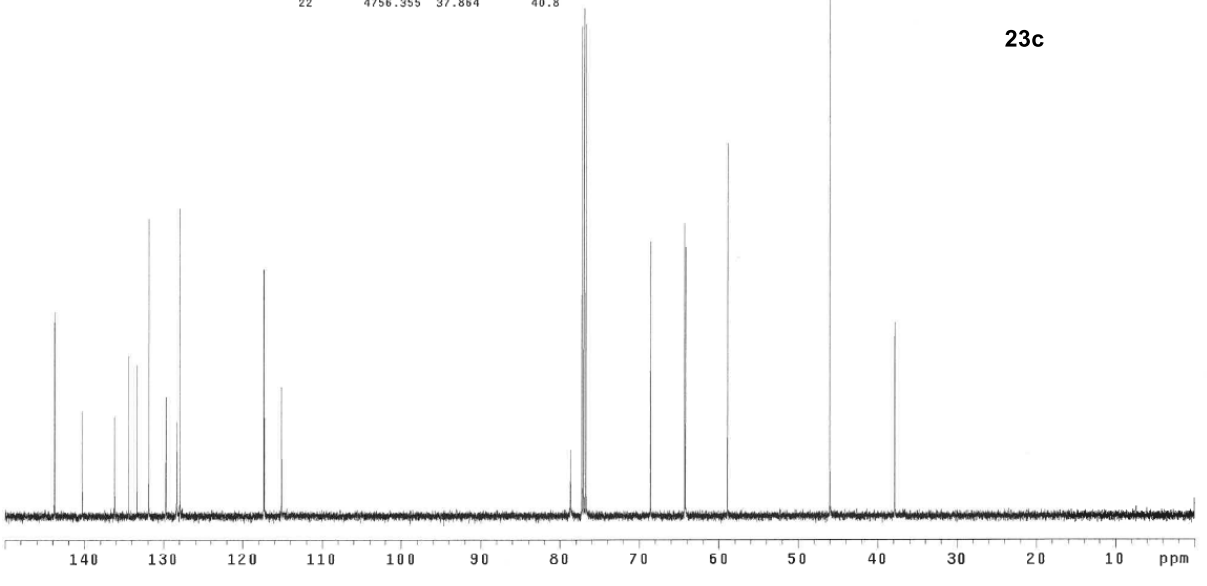


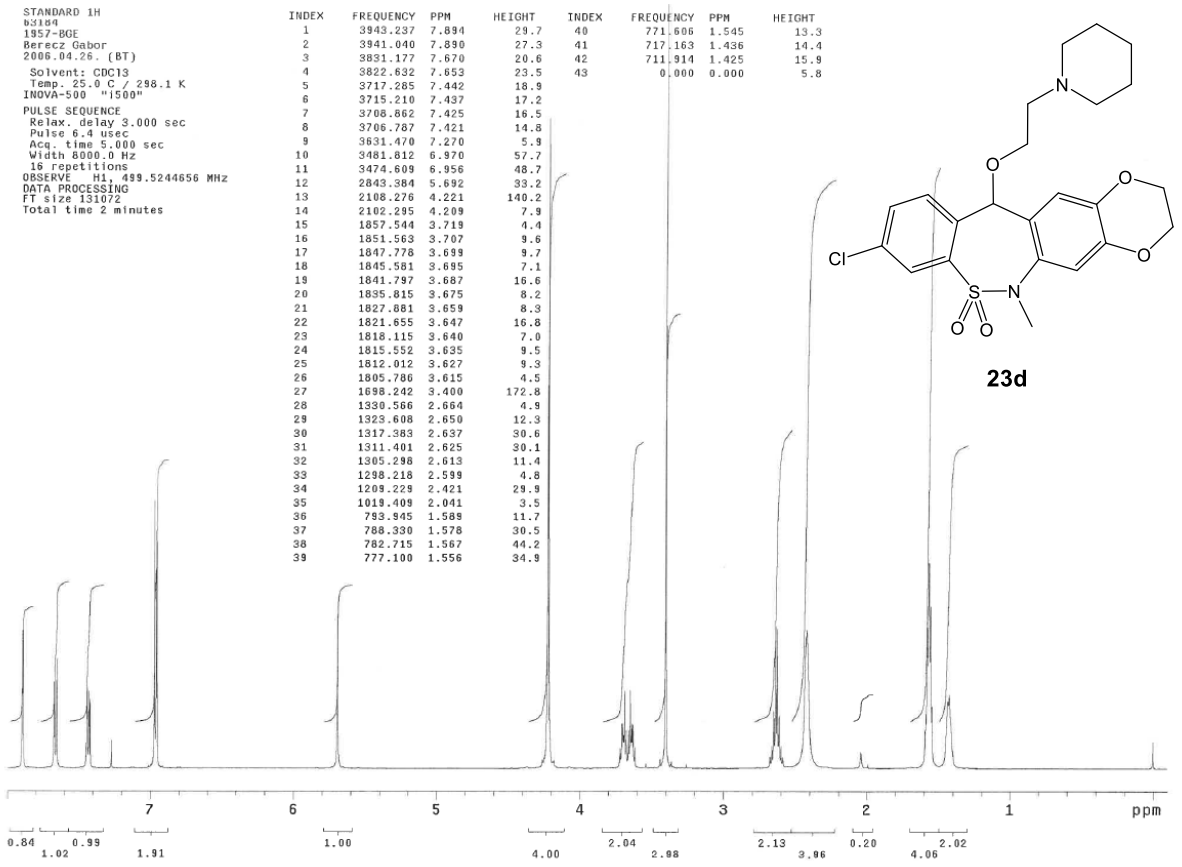

```
STANDARD 13C
62848
1950-BGE
Berecz Gabor
2006/04/04 (SzA)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
User:  1-14-87
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 6.0 usec
 Acq. time 1.300 sec
 Width 32000.0 Hz
 704 repetitions
OBSERVE  C13, 125.6055328 MHz
DECOUPLE  H1, 499.5269847 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 0.5 Hz
FT size 131072
Total time 50 minutes
```

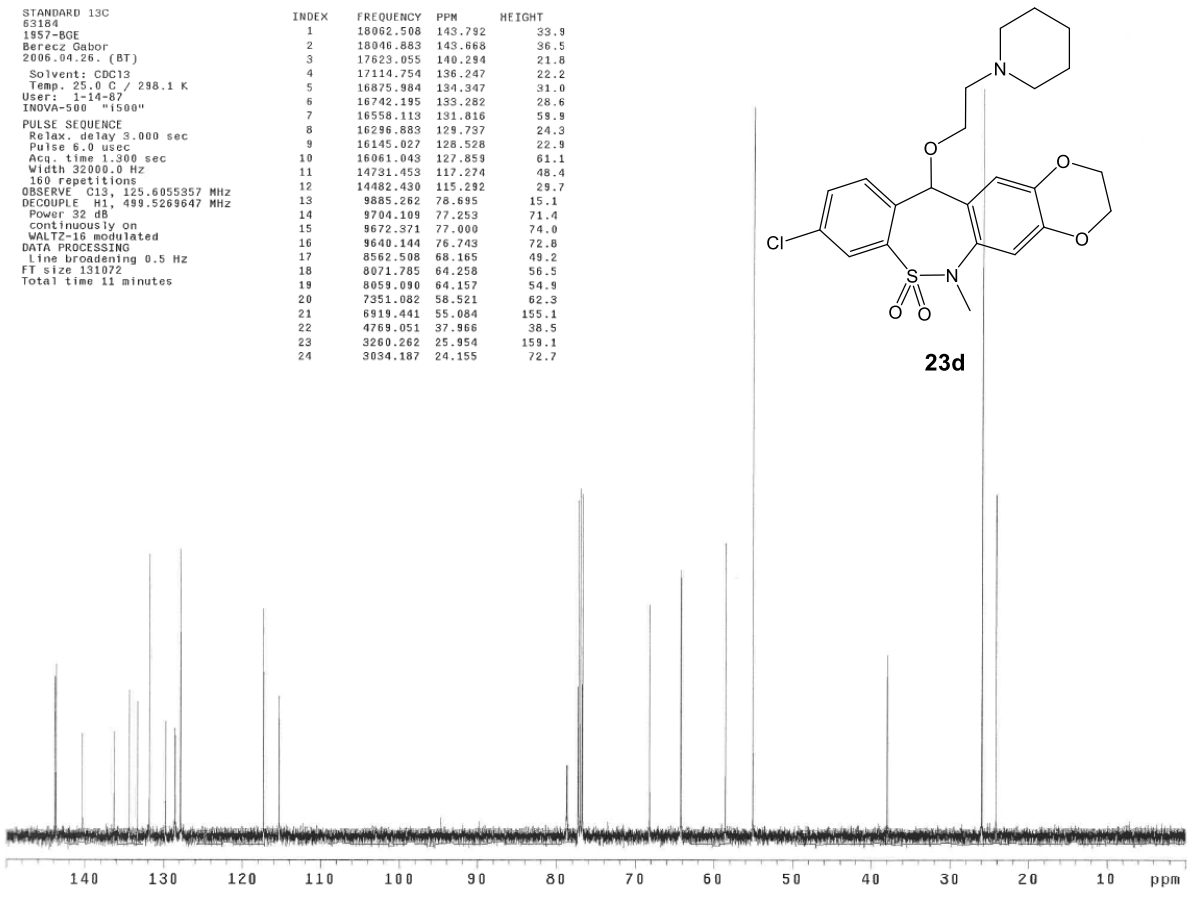
INDEX	FREQUENCY	PPM	HEIGHT
1	18067.390	143.831	40.8
2	18054.207	143.726	43.0
3	17622.078	140.286	22.1
4	17110.847	136.216	21.0
5	16884.285	134.413	33.8
6	16752.937	133.367	31.7
7	16564.461	131.867	62.6
8	16290.535	129.686	25.1
9	16119.636	128.326	19.8
10	16070.808	127.937	64.8
11	14738.289	117.329	52.0
12	14464.363	115.148	27.1
13	9881.843	78.668	13.9
14	9704.597	77.257	103.2
15	9672.371	77.000	106.9
16	9640.633	76.747	103.6
17	8617.683	68.604	57.8
18	8075.691	64.289	61.7
19	8061.531	64.176	56.6
20	7402.840	58.933	78.4
21	5781.258	46.024	177.9
22	4756.355	37.864	40.8



23c




STANDARD 1H
63184
1957-BGE
Berecz Gabor
2006.04.26. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "I500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244656 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3943.237 7.894 29.7 40 771.606 1.545 13.3
2 3941.040 7.890 27.3 41 717.163 1.436 14.4
3 3831.177 7.670 20.6 42 711.914 1.425 15.9
4 3822.632 7.653 23.5 43 0.000 0.000 5.8
5 3717.285 7.442 18.9
6 3715.210 7.437 17.2
7 3708.862 7.425 16.5
8 3706.787 7.421 14.8
9 3631.470 7.270 5.9
10 3481.812 6.970 57.7
11 3474.609 6.956 48.7
12 2843.384 5.692 33.2
13 2108.276 4.221 140.2
14 2102.295 4.209 7.9
15 1857.544 3.719 4.4
16 1851.563 3.707 9.6
17 1847.778 3.699 9.7
18 1845.581 3.695 7.1
19 1841.797 3.687 16.6
20 1835.815 3.675 8.2
21 1827.881 3.659 8.3
22 1821.655 3.647 16.8
23 1818.115 3.640 7.0
24 1815.552 3.635 9.5
25 1812.012 3.627 9.3
26 1805.786 3.615 4.5
27 1698.242 3.400 172.8
28 1330.566 2.664 4.9
29 1323.608 2.650 12.3
30 1317.383 2.637 30.6
31 1311.401 2.625 30.1
32 1305.298 2.613 11.4
33 1298.218 2.599 4.8
34 1209.229 2.421 29.9
35 1019.409 2.041 3.5
36 793.945 1.589 11.7
37 788.330 1.578 30.5
38 782.715 1.567 44.2
39 777.100 1.556 34.9
N
O
O
O
Cl
S
N
O
O
23d
7
6
5
4
3
2
1
ppm
0.84
0.99
1.02
1.91
1.00
4.00
2.04
2.98
2.13
3.96
0.20
2.02
4.06


STANDARD 13C
63184
1957-BGE
Berecz Gabor
2006.04.26. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "I500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
160 repetitions
OBSERVE C13, 125.6055357 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 11 minutes
INDEX FREQUENCY PPM HEIGHT
1 18062.508 143.792 33.9
2 18046.883 143.668 36.5
3 17623.055 140.294 21.8
4 17114.754 136.247 22.2
5 16875.984 134.347 31.0
6 16742.195 133.282 28.6
7 16558.113 131.816 59.9
8 16296.883 129.737 24.3
9 16145.027 128.528 22.9
10 16061.043 127.859 61.1
11 14731.453 117.274 48.4
12 14482.430 115.292 29.7
13 9885.262 78.695 15.1
14 9704.109 77.253 71.4
15 9672.371 77.000 74.0
16 9640.144 76.743 72.8
17 8562.508 68.165 49.2
18 8071.785 64.258 56.5
19 8059.090 64.157 54.9
20 7351.082 58.521 62.3
21 6919.441 55.084 155.1
22 4769.051 37.966 38.5
23 3260.262 25.954 159.1
24 3034.187 24.155 72.7
N
O
O
O
Cl
S
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O
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23d
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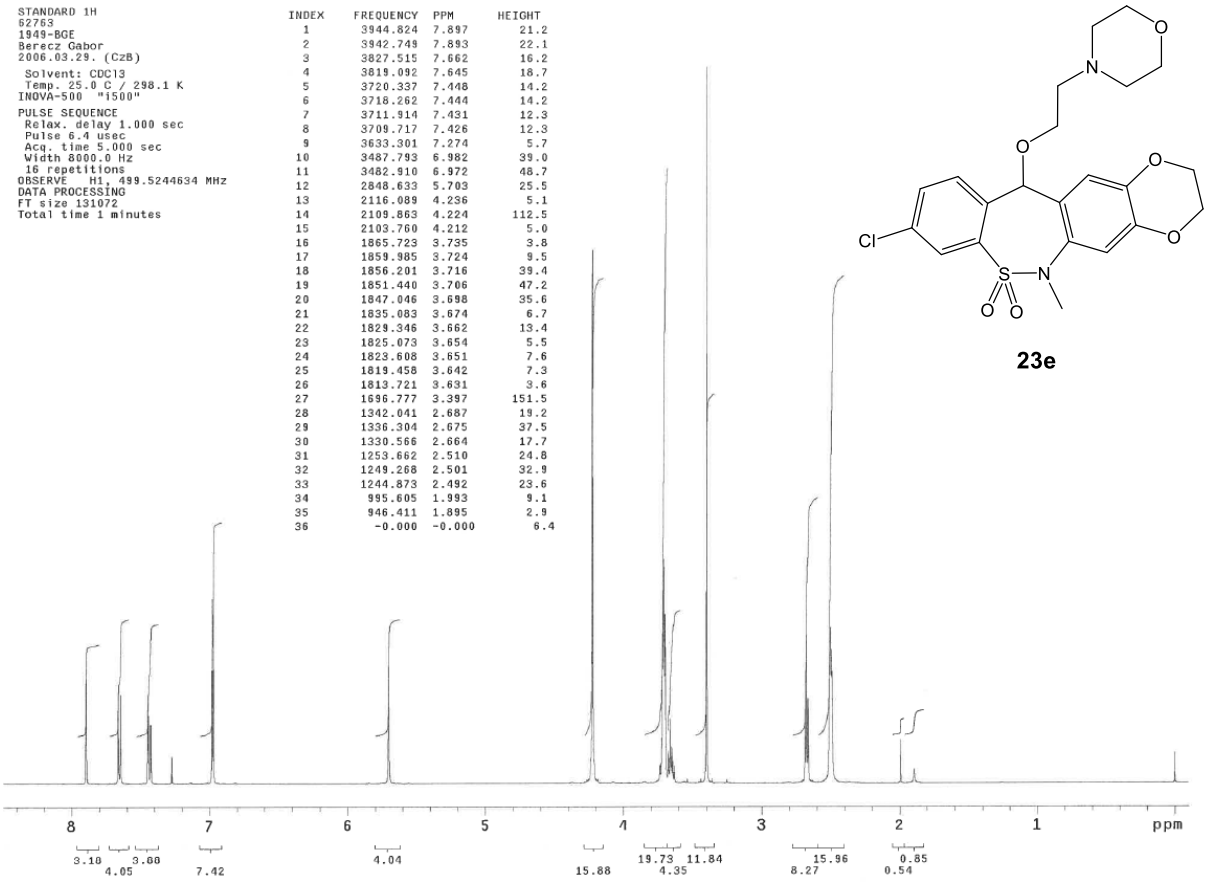
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


STANDARD 1H
62763
1949-BGE
Berecz Gabor
2006.03.29. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244634 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3944.824 7.897 21.2
2 3942.749 7.893 22.1
3 3827.515 7.662 16.2
4 3819.092 7.645 18.7
5 3720.337 7.448 14.2
6 3718.262 7.444 14.2
7 3711.914 7.431 12.3
8 3709.717 7.426 12.3
9 3633.301 7.274 5.7
10 3487.793 6.982 39.0
11 3482.910 6.972 48.7
12 2848.633 5.703 25.5
13 2116.089 4.236 5.1
14 2109.863 4.224 112.5
15 2103.760 4.212 5.0
16 1865.723 3.735 3.8
17 1859.985 3.724 9.5
18 1856.201 3.716 39.4
19 1851.440 3.706 47.2
20 1847.046 3.698 35.6
21 1835.083 3.674 6.7
22 1829.346 3.662 13.4
23 1825.073 3.654 5.5
24 1823.608 3.651 7.6
25 1819.458 3.642 7.3
26 1813.721 3.631 3.6
27 1696.777 3.397 151.5
28 1342.041 2.687 19.2
29 1336.304 2.675 37.5
30 1330.566 2.664 17.7
31 1253.662 2.510 24.8
32 1249.268 2.501 32.9
33 1244.873 2.492 23.6
34 995.605 1.993 9.1
35 946.411 1.895 2.9
36 -0.000 -0.000 6.4
O
N
O
O
O
Cl
S
N
O
O
23e
8
7
6
5
4
3
2
1
ppm
3.10
3.00
4.05
7.42
4.04
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19.73
11.84
4.35
15.96
8.27
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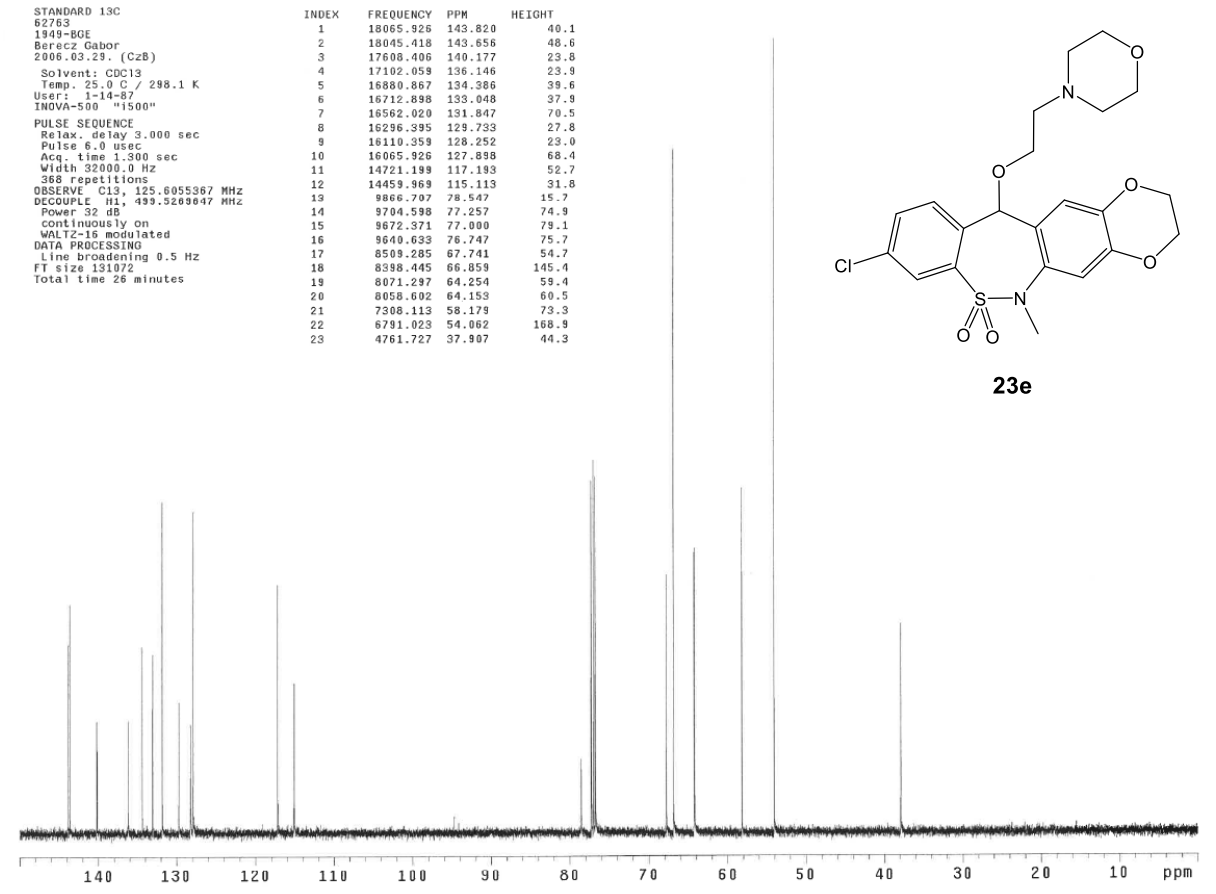
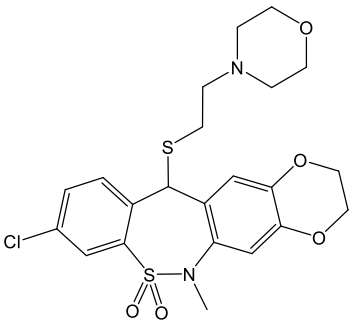
0.54


STANDARD 13C
62763
1949-BGE
Berecz Gabor
2006.03.29. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
368 repetitions
OBSERVE C13, 125.6055367 MHz
DECOUPLE H1, 499.5268647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 26 minutes
INDEX FREQUENCY PPM HEIGHT
1 18065.926 143.820 40.1
2 18045.418 143.656 48.6
3 17608.406 140.177 23.8
4 17102.059 136.146 23.9
5 16880.867 134.386 39.6
6 16712.898 133.048 37.9
7 16562.020 131.847 70.5
8 16296.395 129.733 27.8
9 16110.359 128.252 23.0
10 16065.926 127.898 68.4
11 14721.199 117.193 52.7
12 14459.969 115.113 31.8
13 9866.707 78.547 15.7
14 9704.598 77.257 74.9
15 9672.371 77.000 79.1
16 9640.633 76.747 75.7
17 8509.285 67.741 54.7
18 8398.445 66.859 145.4
19 8071.297 64.254 59.4
20 8058.602 64.153 60.5
21 7308.113 58.179 73.3
22 6791.023 54.062 168.9
23 4761.727 37.907 44.3
O
N
O
O
O
Cl
S
N
O
O
23e
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
63256
1960-BGE
Berecz Gabor
2006.05.03. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244696 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3964.844	7.937	20.8	40	1230.957	2.464	5.9
2	3962.646	7.933	20.6	41	1225.952	2.454	7.1
3	3703.979	7.415	12.7	42	1223.145	2.449	8.5
4	3701.782	7.411	12.3	43	1220.947	2.444	6.7
5	3695.679	7.398	18.2	44	1217.896	2.438	7.5
6	3693.481	7.394	18.0	45	1211.792	2.426	6.6
7	3655.273	7.318	25.3	46	1206.543	2.415	13.3
8	3646.973	7.301	18.2	47	1202.759	2.408	24.7
9	3628.174	7.263	23.5	48	1198.120	2.399	24.6
10	3492.554	6.992	48.4	49	1194.092	2.390	11.4
11	3373.169	6.753	48.7	50	1187.012	2.376	3.1
12	2470.215	4.945	30.9	51	1000.488	2.003	2.1
13	2133.911	4.272	3.4	52	816.895	1.635	4.5
14	2130.371	4.265	7.2	53	-0.000	-0.000	23.7
15	2128.418	4.261	10.8				
16	2126.587	4.257	26.0				
17	2124.512	4.253	88.4				
18	2119.263	4.243	8.4				
19	2115.112	4.234	3.5				
20	2112.915	4.230	1.9				
21	1845.703	3.695	32.9				
22	1841.064	3.686	52.1				
23	1836.304	3.676	32.4				
24	1753.540	3.510	168.5				
25	1312.378	2.627	3.3				
26	1307.495	2.617	6.5				
27	1301.270	2.605	6.3				
28	1298.950	2.600	8.2				
29	1296.875	2.596	6.3				
30	1292.358	2.587	8.3				
31	1284.546	2.572	5.7				
32	1264.404	2.531	3.9				
33	1259.033	2.520	4.3				
34	1256.470	2.515	8.2				
35	1250.977	2.504	18.7				
36	1245.972	2.494	6.6				
37	1243.530	2.489	17.3				
38	1238.892	2.480	11.5				
39	1235.718	2.474	15.0				



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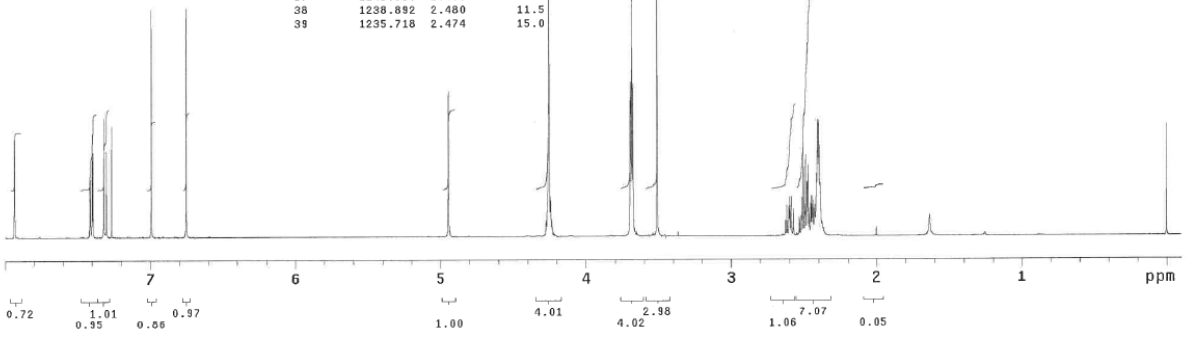
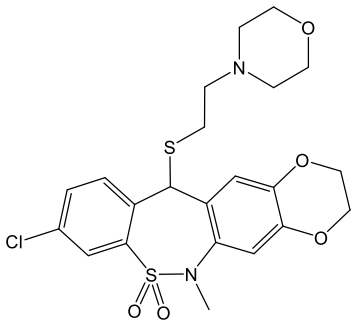


STANDARD 13C
63256
1960-BGE
Berecz Gabor
2006.05.03. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
14336 repetitions
OBSERVE C13, 125.6055293 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 17.1 hours

INDEX	FREQUENCY	PPM	HEIGHT
1	18128.425	144.317	29.4
2	17968.757	143.046	25.2
3	17875.984	142.307	21.2
4	16911.628	134.630	26.1
5	16901.863	134.553	23.6
6	16644.050	132.500	29.6
7	16566.902	131.886	22.7
8	16546.394	131.723	43.0
9	16511.238	131.443	21.3
10	16052.742	127.793	40.6
11	14835.456	118.102	40.4
12	14810.554	117.904	44.2
13	9704.597	77.257	171.4
14	9672.371	77.000	178.2
15	9640.632	76.747	174.4
16	8393.074	66.816	90.0
17	8080.574	64.328	37.7
18	8071.785	64.258	41.5
19	7313.484	58.221	56.6
20	6825.691	54.338	20.8
21	6725.593	53.541	113.2
22	4942.390	39.345	37.0
23	3803.230	30.277	46.5



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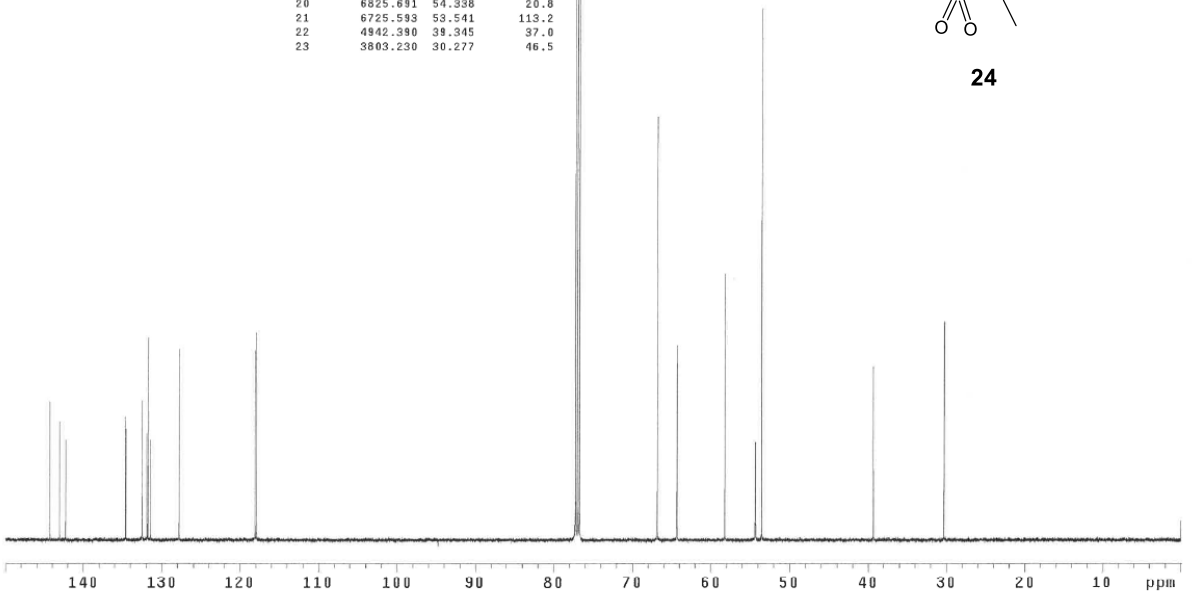
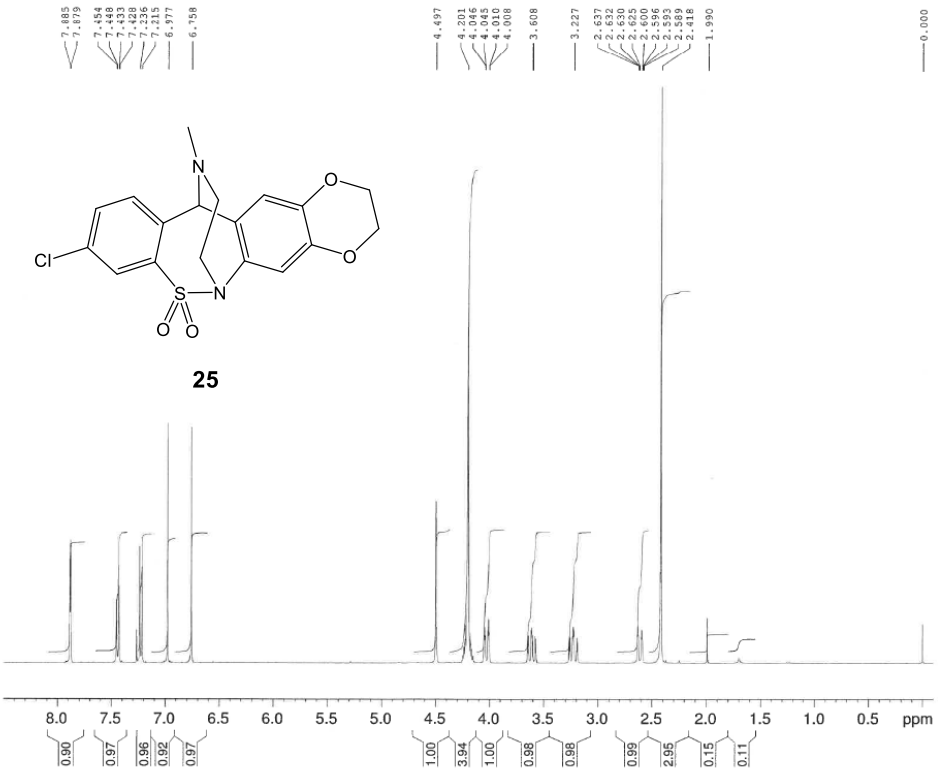
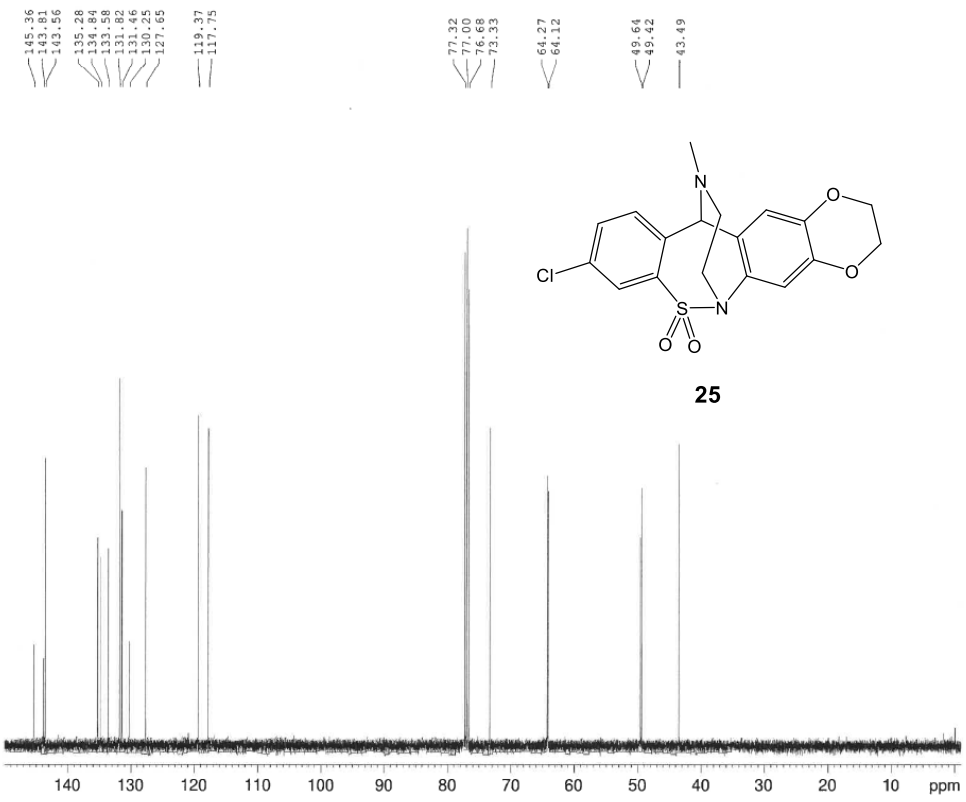




25

Standard 1H
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)

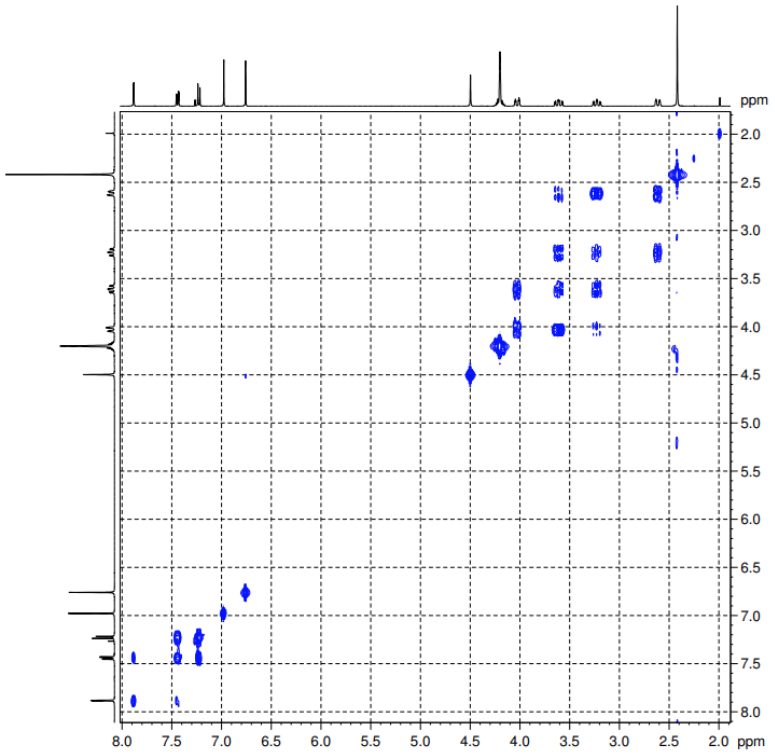
NAME	85376
EXPNO	1
PROCNO	1
Date_	20100319
Time	11.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	302.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	1.00 dB
PL1W	11.97157383 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300075 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



25

Standard 13C
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)

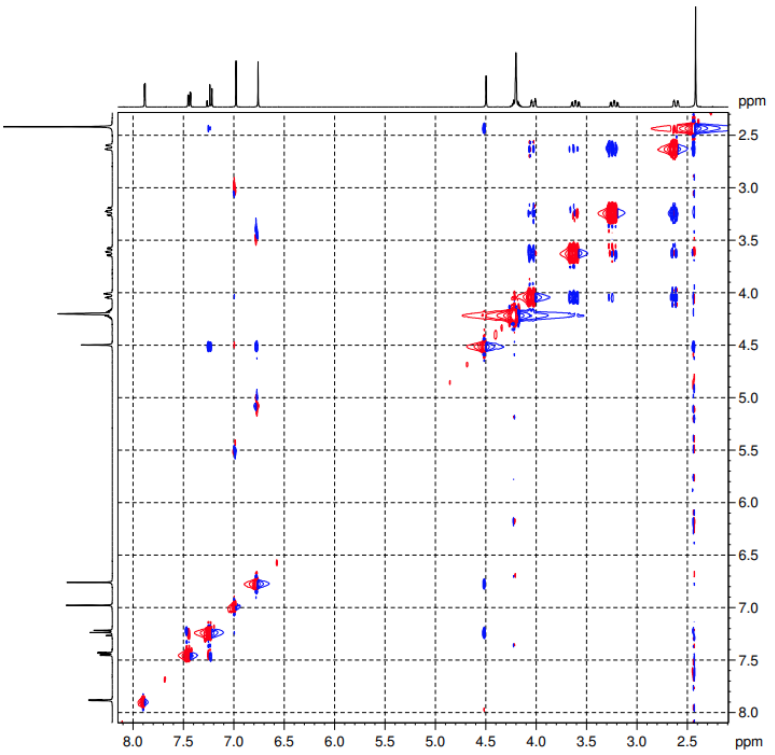
NAME	85376
EXPNO	2
PROCNO	1
Date_	20100319
Time	11.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	257
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	1620
DW	20.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.80 dB
PL1W	40.49391937 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	2.00 dB
PL12	20.00 dB
PL13	20.00 dB
PL2W	9.50935936 W
PL12W	0.15071319 W
PL13W	0.15071319 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127751 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



COSY
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)

25

NAME	85376
EXPNO	3
PROCNO	1
Date_	20100319
Time	12.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	cosygpqf
TD	2048
SOLVENT	CDCl3
NS	1
DS	8
SWH	3401.361 Hz
FIDRES	1.660821 Hz
AQ	0.3011060 sec
RG	36
DW	147.000 usec
DE	6.50 usec
TE	303.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00029400 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	12.50 usec
P1	12.50 usec
PL1	1.00 dB
PL1W	11.97157383 W
SFO1	400.1317006 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPZ1	10.00 %
P16	1000.00 usec
ND0	1
TD	128
SFO1	400.1317 MHz
FIDRES	26.571245 Hz
SW	8.500 ppm
FnMODE	QF
SI	1024
SF	400.1300059 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	400.1300051 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0

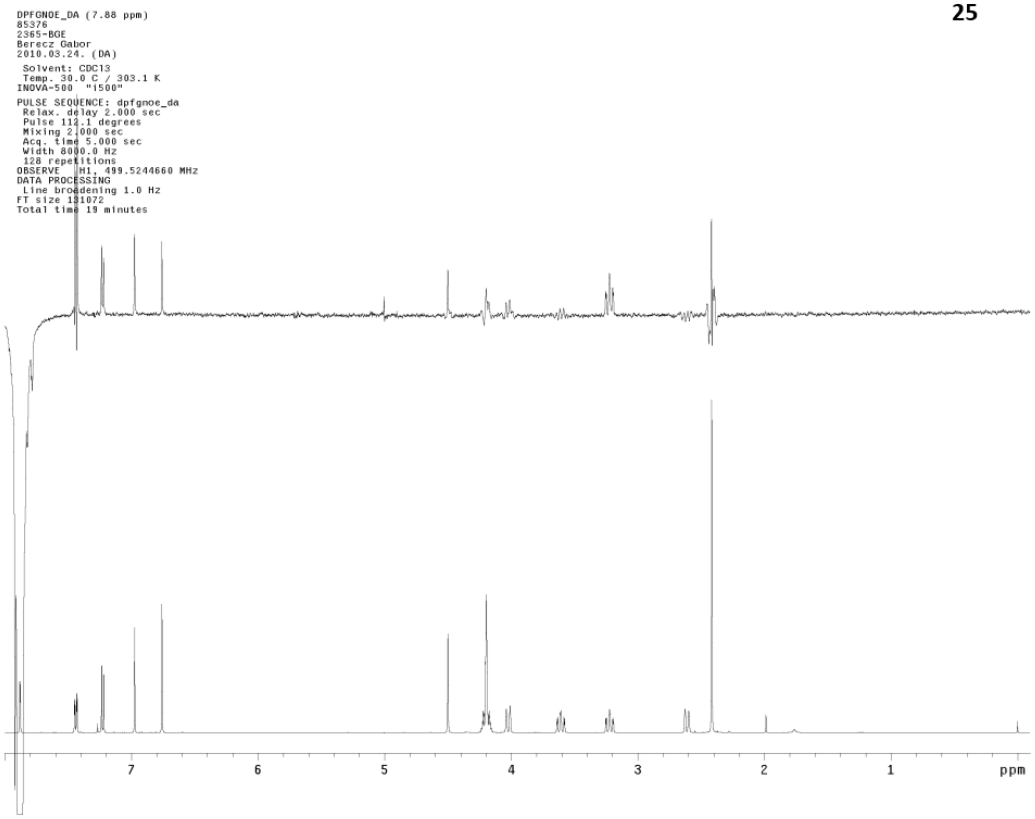


NOESY
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)

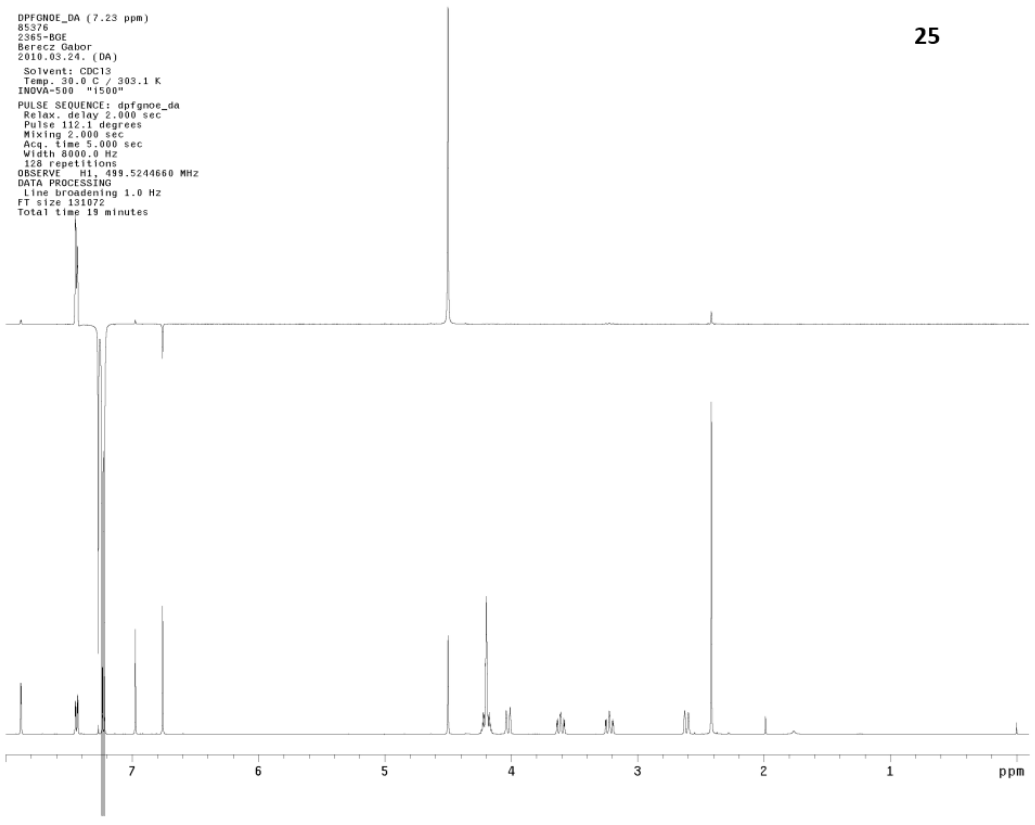
25

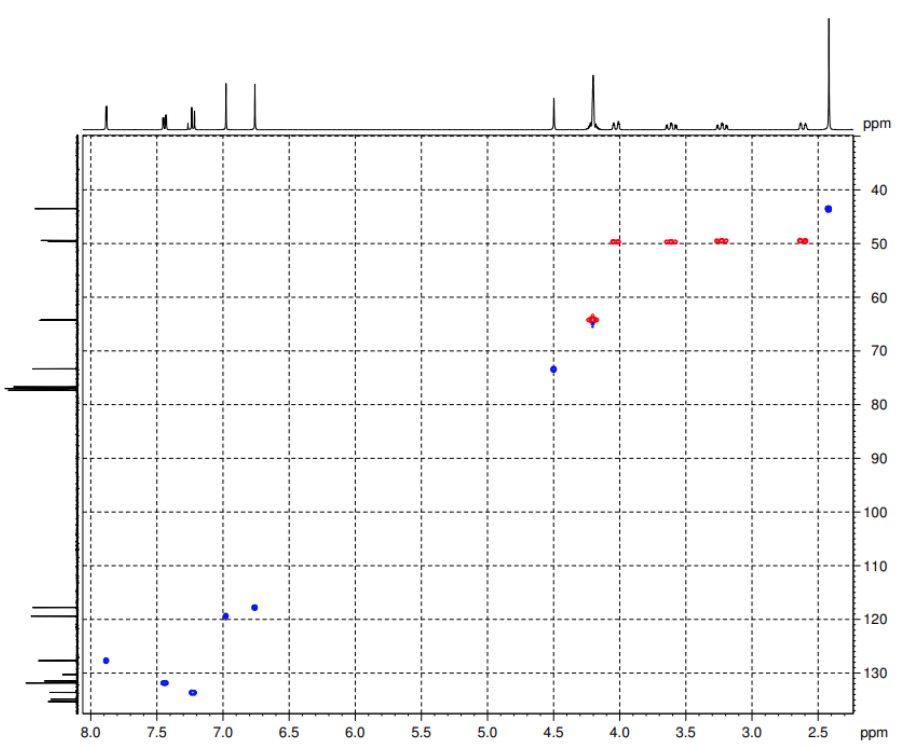
NAME	85376
EXPNO	6
PROCNO	1
Date_	20100319
Time	13.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	noesyph
TD	2048
SOLVENT	CDCl3
NS	4
DS	4
SWH	3401.361 Hz
FIDRES	1.660821 Hz
AQ	0.3011060 sec
RG	64
DW	147.000 usec
DE	6.50 usec
TE	303.0 K
D0	0.00013110 sec
D1	1.00000000 sec
D8	0.30000001 sec
IN0	0.00029400 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	1.00 dB
PL1W	11.97157383 W
SFO1	400.1317006 MHz
ND0	1
TD	142
SFO1	400.1317 MHz
FIDRES	23.951546 Hz
SW	8.500 ppm
FnMODE	States-TPPI
SI	1024
SF	400.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	400.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

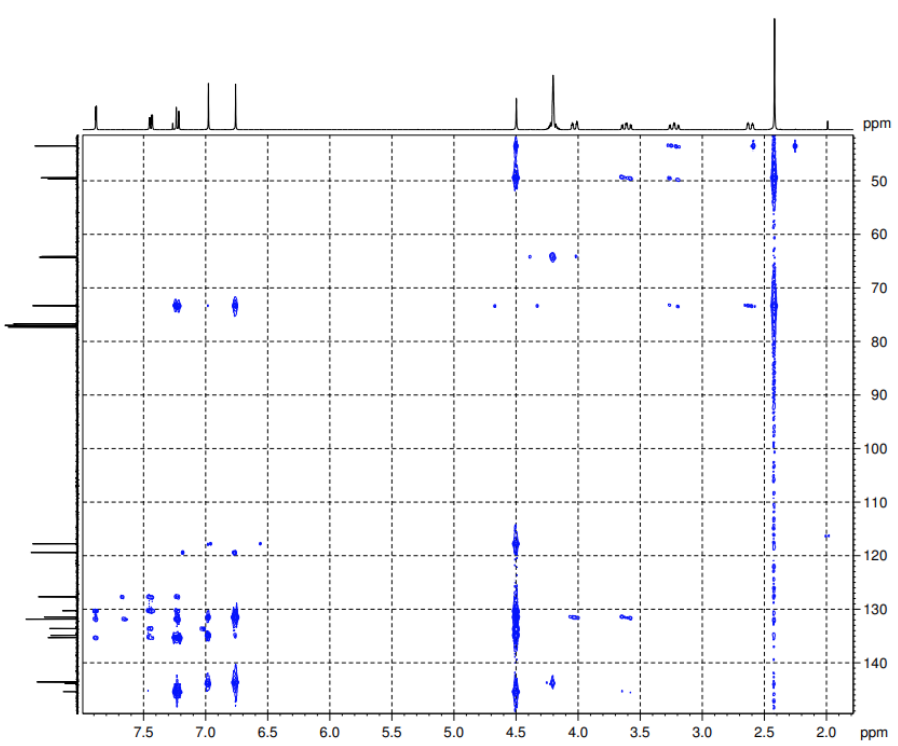
25

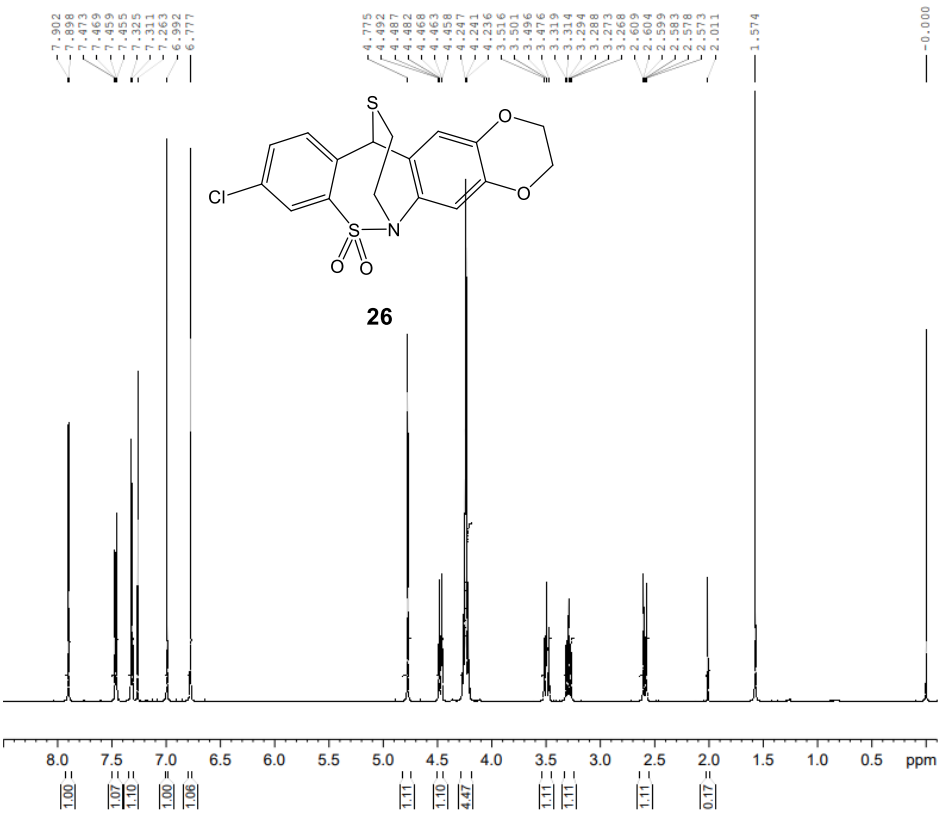

DPFGNOE_DA (7.88 ppm)
85376
2365-BGE
Berecz Gabor
2010.03.24. (DA)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE: dpfgnoe_da
Relax. delay 2.000 sec
Pulse 112.1 degrees
Mixing 2.000 sec
Acq. time 5.000 sec
Width 8000.0 Hz
128 repetitions
OBSERVE H1, 499.5244660 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 19 minutes
7
6
5
4
3
2
1
ppm

25


DPFGNOE_DA (7.23 ppm)
85376
2365-BGE
Berecz Gabor
2010.03.24. (DA)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE: dpfgnoe_da
Relax. delay 2.000 sec
Pulse 112.1 degrees
Mixing 2.000 sec
Acq. time 5.000 sec
Width 8000.0 Hz
128 repetitions
OBSERVE H1, 499.5244660 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 19 minutes
7
6
5
4
3
2
1
ppm


HSQC
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)
25
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
40
50
60
70
80
90
100
110
120
130


HMBC
85376
2365-BGE
Berecz Gabor
2010.03.19. (BB)
25
ppm
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
50
60
70
80
90
100
110
120
130
140

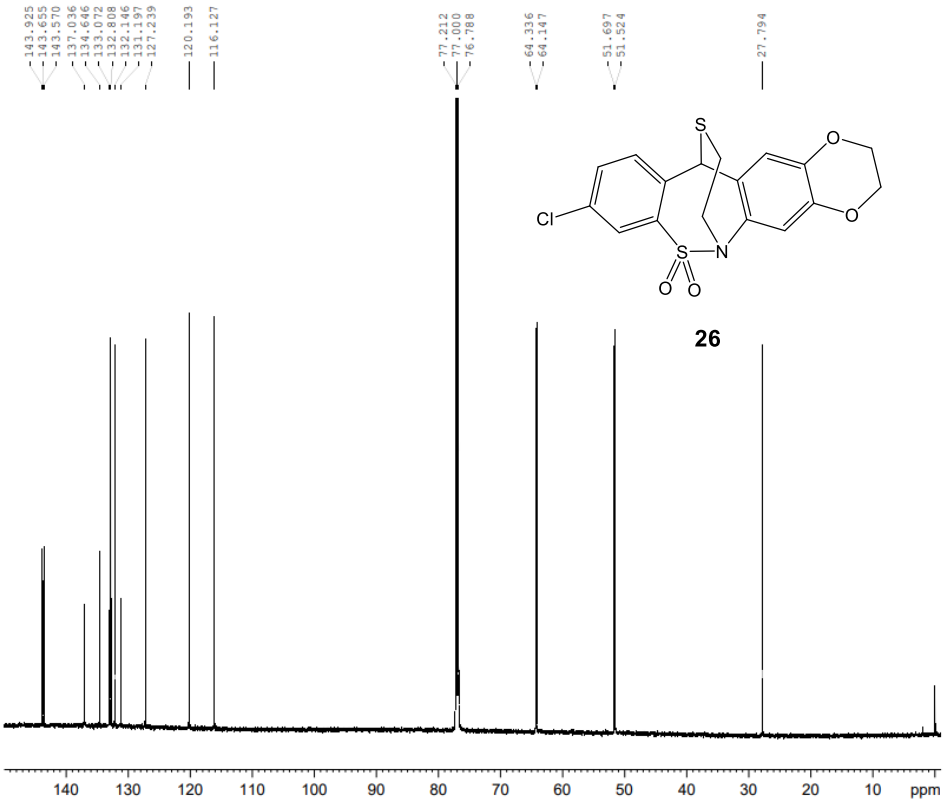


Standard 1H
143465
BEG0701_1B
Berecz Gábor
2024.09.06. (KP)

Current Data Parameters
NAME 143465
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240906
Time 15.41 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Standard 13C
143465
BEG0701_1B
Berecz Gábor
2024.09.06. (KP)

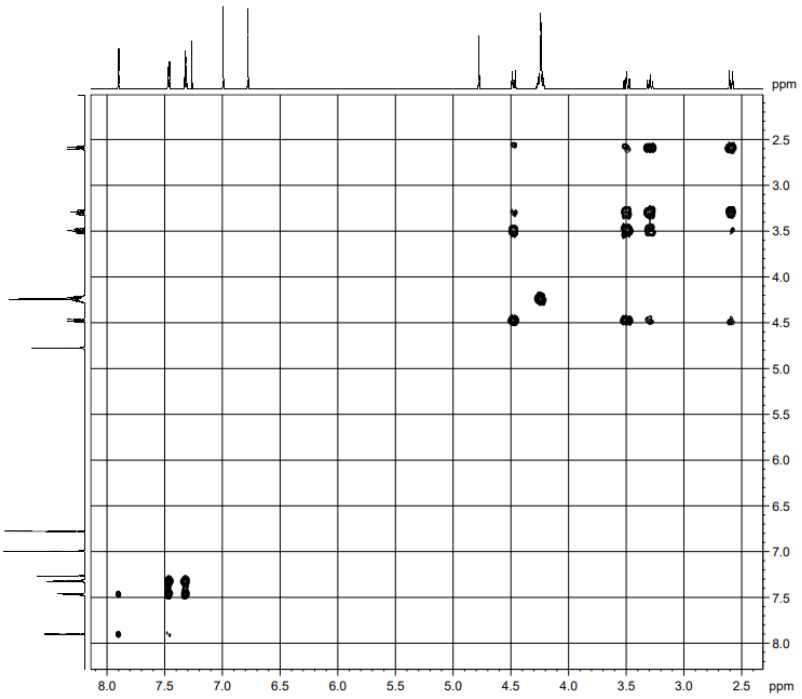
Current Data Parameters
NAME 143465
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240906
Time 16.50 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701274 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

COSY
143465
BEG0701_1B
Berecz Gábor
2024.09.06. (KP)

26



Current Data Parameters
NAME 143465
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240906
Time 16.51 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

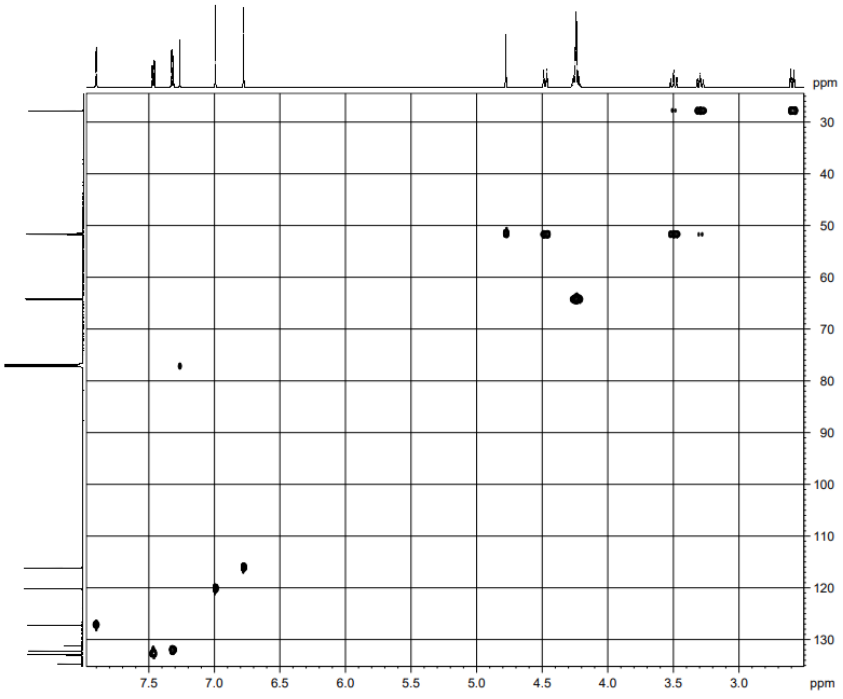
F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000132 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000132 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

HSQC (140Hz)
143465
BEG0701_1B
Berecz Gábor
2024.09.06. (KP)

26



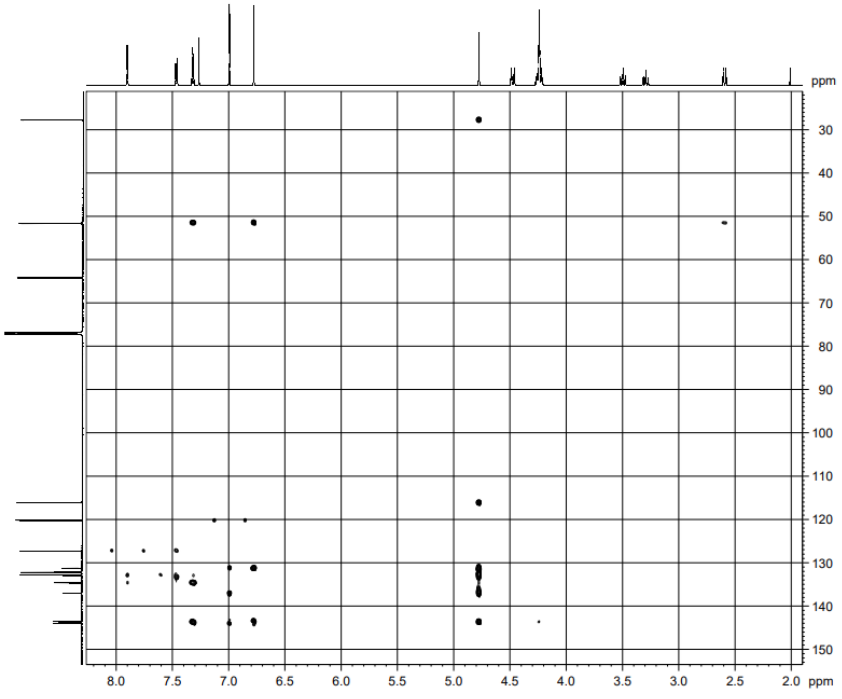
Current Data Parameters
NAME 143465
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240906
Time 17.12 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p3m4sp_4sp.2
P3 9.90 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 71.00000000 W
PLW12 2.30040002 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.63199997 W
SPNAM[7] Cap60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.63199997 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.95400000 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.48850000 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000132 MHz
WDW QSINE

HMBC (8Hz, 140Hz) **26**
143465
BEG0701_1B
Berecz Gábor
2024.09.06. (KP)



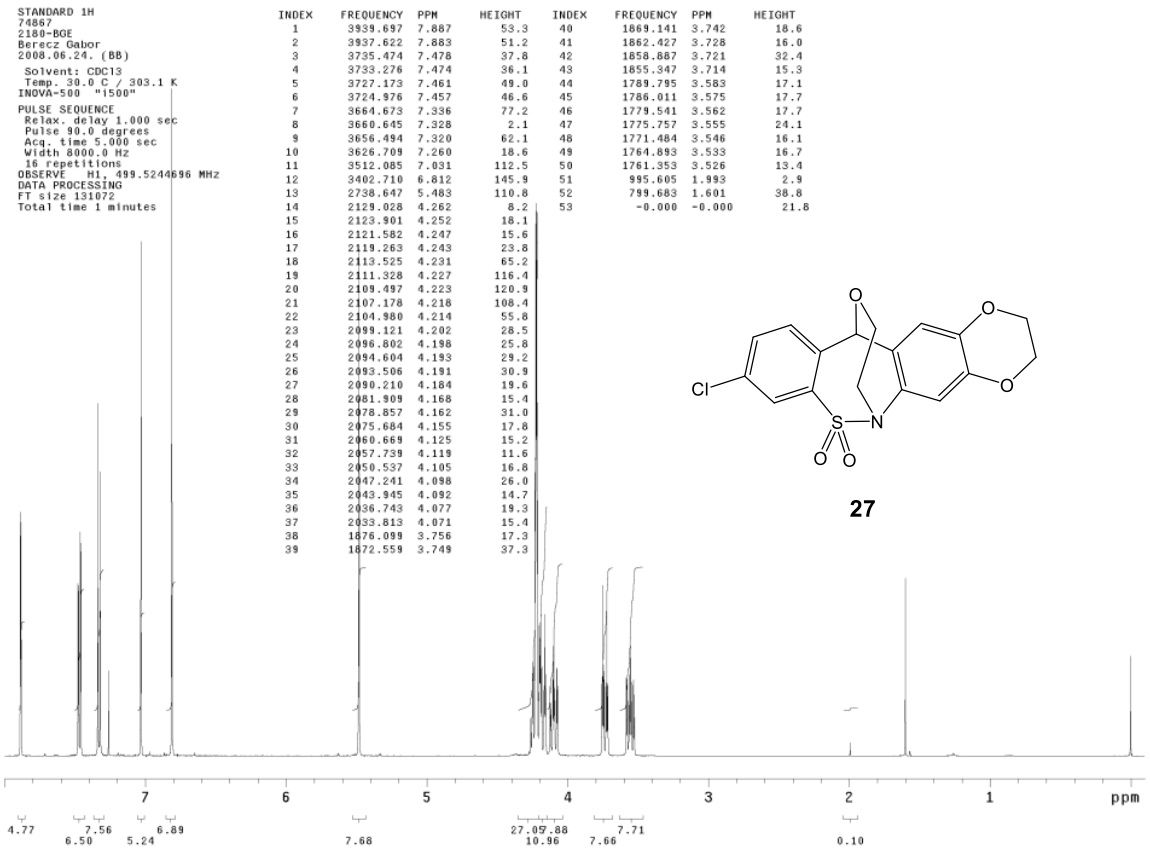
Current Data Parameters
NAME 143465
EXPNO 15
PROCNO 1

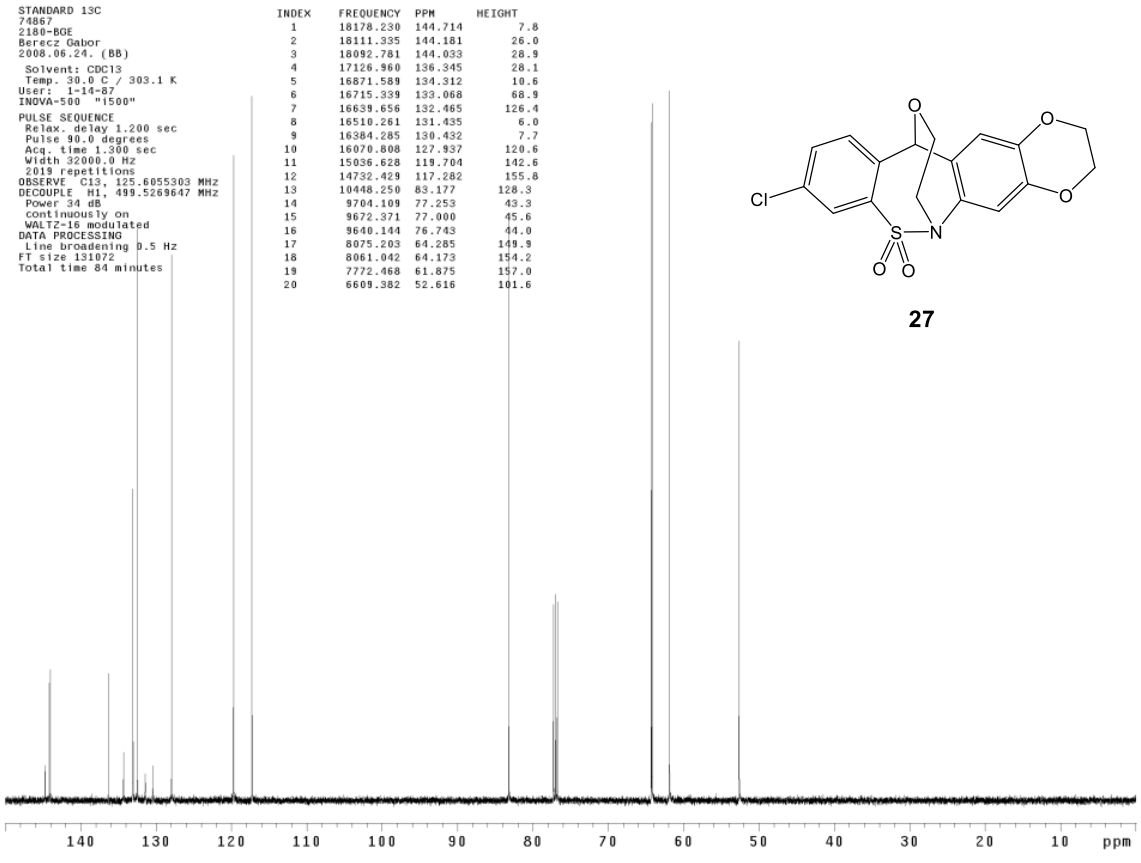
F2 - Acquisition Parameters
Date_ 20240906
Time 17.42 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.90 usec
PLW2 71.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000132 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

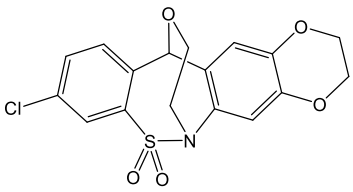
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701273 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0


STANDARD 1H
74867
2180-BGE
Berecz Gabor
2008.06.24. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244696 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3939.697 7.887 53.3 40 1869.141 3.742 18.6
2 3937.622 7.883 51.2 41 1862.427 3.728 16.0
3 3735.474 7.478 37.8 42 1858.887 3.721 32.4
4 3733.276 7.474 36.1 43 1855.347 3.714 15.3
5 3727.173 7.461 49.0 44 1789.795 3.583 17.1
6 3724.976 7.457 46.6 45 1786.011 3.575 17.7
7 3664.673 7.336 77.2 46 1779.541 3.562 17.7
8 3660.645 7.328 2.1 47 1775.757 3.555 24.1
9 3656.494 7.320 62.1 48 1771.484 3.546 16.1
10 3626.709 7.260 18.6 49 1764.893 3.533 16.7
11 3512.085 7.031 112.5 50 1761.353 3.526 13.4
12 3402.710 6.812 145.9 51 995.605 1.993 2.9
13 2738.647 5.483 110.8 52 799.683 1.601 38.8
14 2129.028 4.262 8.2 53 -0.000 -0.000 21.8
15 2123.901 4.252 18.1
16 2121.582 4.247 15.6
17 2119.263 4.243 23.8
18 2113.525 4.231 65.2
19 2111.328 4.227 116.4
20 2109.497 4.223 120.9
21 2107.178 4.218 108.4
22 2104.980 4.214 55.8
23 2099.121 4.202 28.5
24 2096.802 4.198 25.8
25 2094.604 4.193 29.2
26 2093.506 4.191 30.9
27 2090.210 4.184 19.6
28 2081.909 4.168 15.4
29 2078.857 4.162 31.0
30 2075.684 4.155 17.8
31 2060.669 4.125 15.2
32 2057.739 4.119 11.6
33 2050.537 4.105 16.8
34 2047.241 4.098 26.0
35 2043.945 4.092 14.7
36 2036.743 4.077 19.3
37 2033.813 4.071 15.4
38 1876.099 3.756 17.3
39 1872.559 3.749 37.3
Cl
S
N
O
27
7
6
5
4
3
2
1
ppm
4.77
7.56
6.50
6.89
5.24
7.68
27.05
27.88
10.96
7.71
7.66
0.10

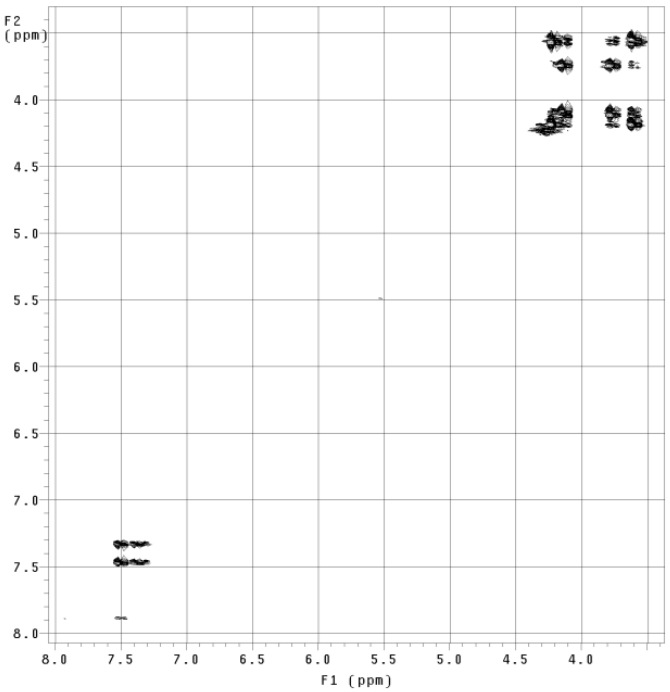

STANDARD 13C
74867
2180-BGE
Berecz Gabor
2008.06.24. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 90.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
2019 repetitions
OBSERVE C13, 125.6055303 MHz
DECOUPLE H1, 499.5269647 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 84 minutes
INDEX FREQUENCY PPM HEIGHT
1 18178.230 144.714 7.8
2 18111.335 144.181 26.0
3 18092.781 144.033 28.9
4 17126.960 136.345 28.1
5 16871.589 134.312 10.6
6 16715.339 133.068 68.9
7 16639.656 132.465 126.4
8 16510.261 131.435 6.0
9 16384.285 130.432 7.7
10 16070.808 127.937 120.6
11 15036.628 119.704 142.6
12 14732.429 117.282 155.8
13 10448.250 83.177 128.3
14 9704.109 77.253 43.3
15 9672.371 77.000 45.6
16 9640.144 76.743 44.0
17 8075.203 64.285 149.9
18 8061.042 64.173 154.2
19 7772.468 61.875 157.0
20 6609.382 52.616 101.6
Cl
S
N
O
27
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

GMQFCOPS_DA
74867
2180-BGE
Berecz Gabor
2008.07.02. (DA)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
SEQUENCE: gmqfcops_da
Relax. delay 1.500 sec
Acq. time 0.197 sec
Width 5204.6 Hz
2D Width 5204.6 Hz
Single scan
2 x 256 increments
OBSERVE H1, 499.5244693 MHz
DATA PROCESSING
Sq. sine bell 0.197 sec
Shifted by -0.197 sec
F1 DATA PROCESSING
Sine bell 0.049 sec
Shifted by -0.049 sec
FT size 4096 x 512
Total time 14 minutes

27

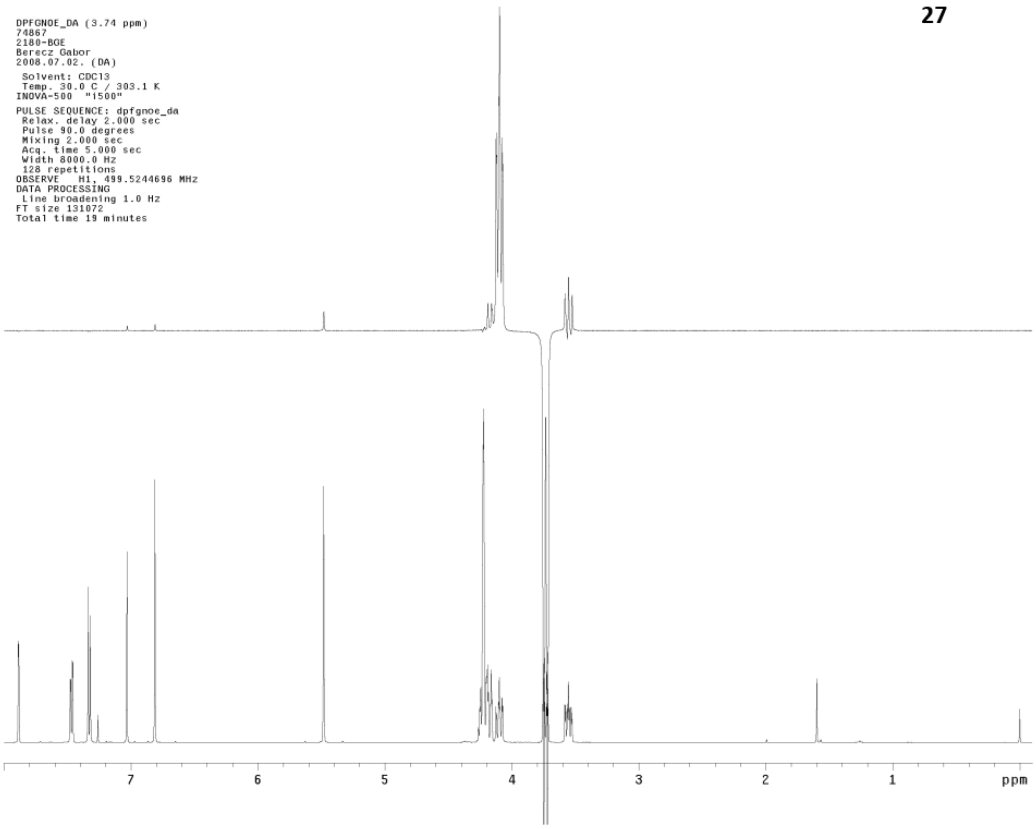


27



DPFGNOE_DA (3.74 ppm)
74867
2180-BGE
Berecz Gabor
2008.07.02. (DA)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE: dpfgnoe_da
Relax. delay 2.000 sec
Pulse 90.0 degrees
Mixing 2.000 sec
Acq. time 5.000 sec
Width 8000.0 Hz
128 repetitions
OBSERVE H1, 499.5244696 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 19 minutes

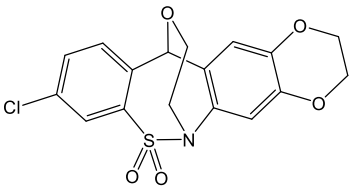
27



GHSQC_DA (140 Hz)
74867
2180-BGE
Berecz Gabor
2008.07.02. (DA)

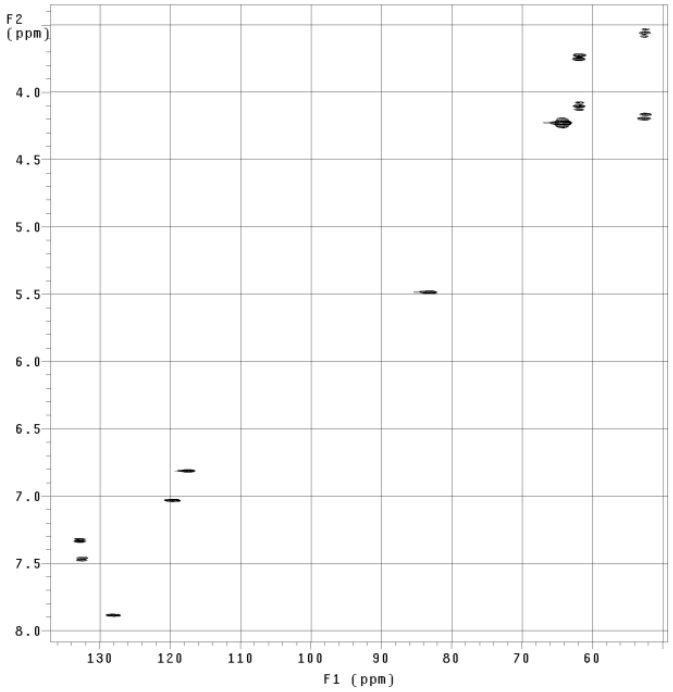
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"

PULSE SEQUENCE: ghsqc_da
Relax. delay 1.500 sec
Acq. time 0.197 sec
Width 5204.6 Hz
2D Width 20576.1 Hz
2 repetitions
2 x 256 increments
OBSERVE H1, 499.5244709 MHz
DECOUPLE C13, 125.6148077 MHz
Power 44 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sq. sine bell 0.203 sec
Shifted by -0.203 sec
F1 DATA PROCESSING
Sq. sine bell 0.006 sec
Shifted by -0.006 sec
FT size 4096 x 512
Total time 29 minutes



27

27

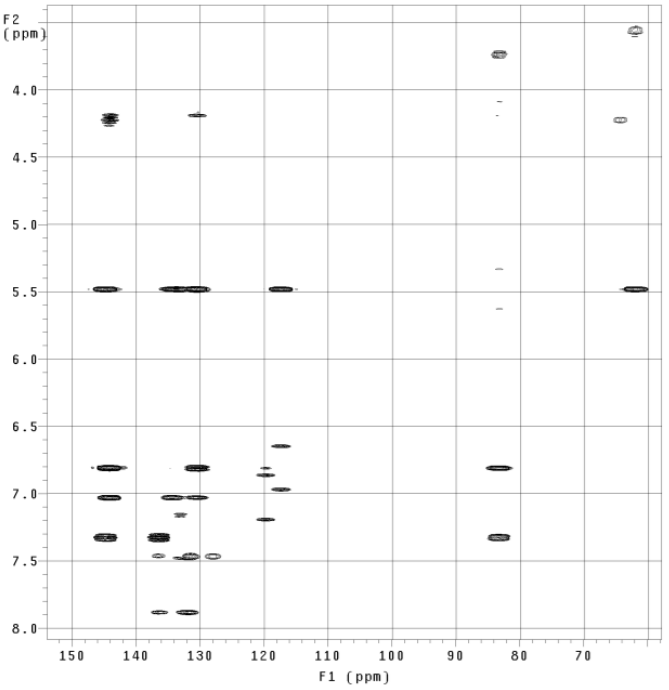


GHMQC_DA (140 Hz, 8 Hz)
74867
2180-BGE
Berecz Gabor
2008.07.02. (DA)

Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"

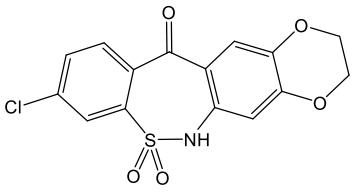
PULSE SEQUENCE: ghmqc_da
Relax. delay 1.500 sec
Acq. time 0.197 sec
Width 5204.6 Hz
2D Width 20576.1 Hz
4 repetitions
256 increments
OBSERVE H1, 499.5244711 MHz
DATA PROCESSING
Sine bell 0.098 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 4096 x 512
Total time 29 minutes

27

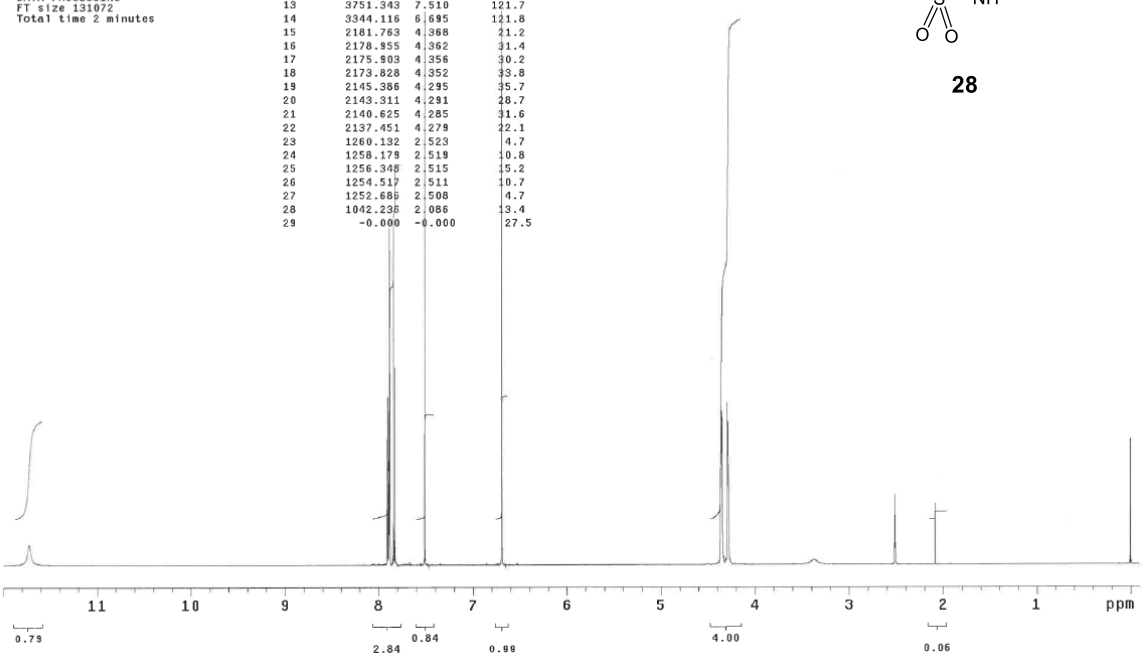


```
STANDARD 1H
64576
1986-BGE
Berecz Gabor
2006.07.25. (BT)
 Solvent: DMSO
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 6.4 usec
 Acq. time 5.000 sec
 Width 8000.0 Hz
 16 repetitions
OBSERVE   H1, 499.5268278 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
```

INDEX	FREQUENCY	PPM	HEIGHT
1	5856.567	11.724	4.5
2	3950.317	7.908	27.7
3	3948.242	7.904	36.9
4	3942.139	7.892	33.7
5	3940.063	7.888	73.9
6	3937.500	7.882	63.4
7	3937.134	7.882	69.1
8	3935.425	7.878	42.0
9	3917.114	7.842	67.1
10	3916.626	7.841	58.7
11	3908.936	7.825	43.3
12	3908.447	7.824	38.0
13	3751.343	7.510	121.7
14	3344.116	6.695	121.8
15	2181.763	4.368	21.2
16	2178.955	4.362	31.4
17	2175.903	4.356	30.2
18	2173.828	4.352	33.8
19	2145.386	4.295	35.7
20	2143.311	4.291	28.7
21	2140.625	4.285	31.6
22	2137.451	4.279	22.1
23	1260.132	2.523	4.7
24	1258.179	2.519	10.8
25	1256.345	2.515	15.2
26	1254.517	2.511	10.7
27	1252.686	2.508	4.7
28	1042.236	2.086	13.4
29	-0.000	-0.000	27.5



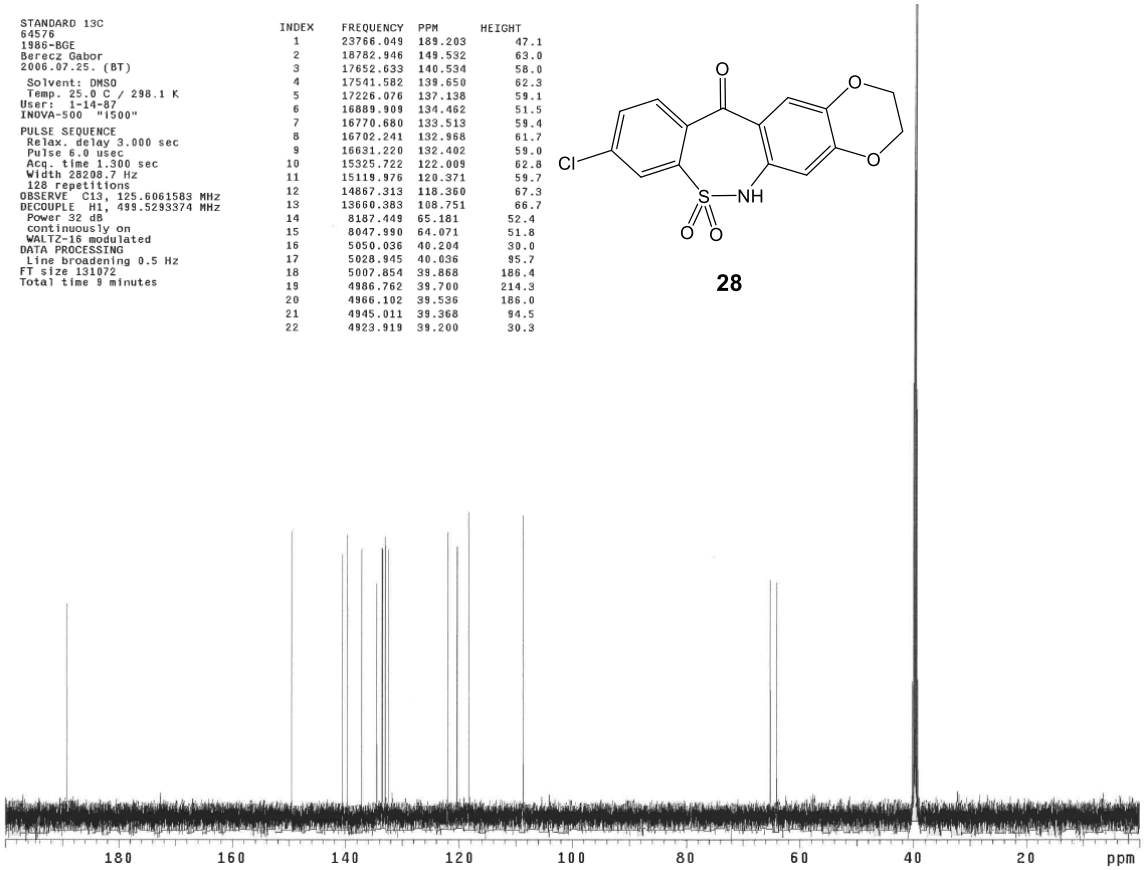
28

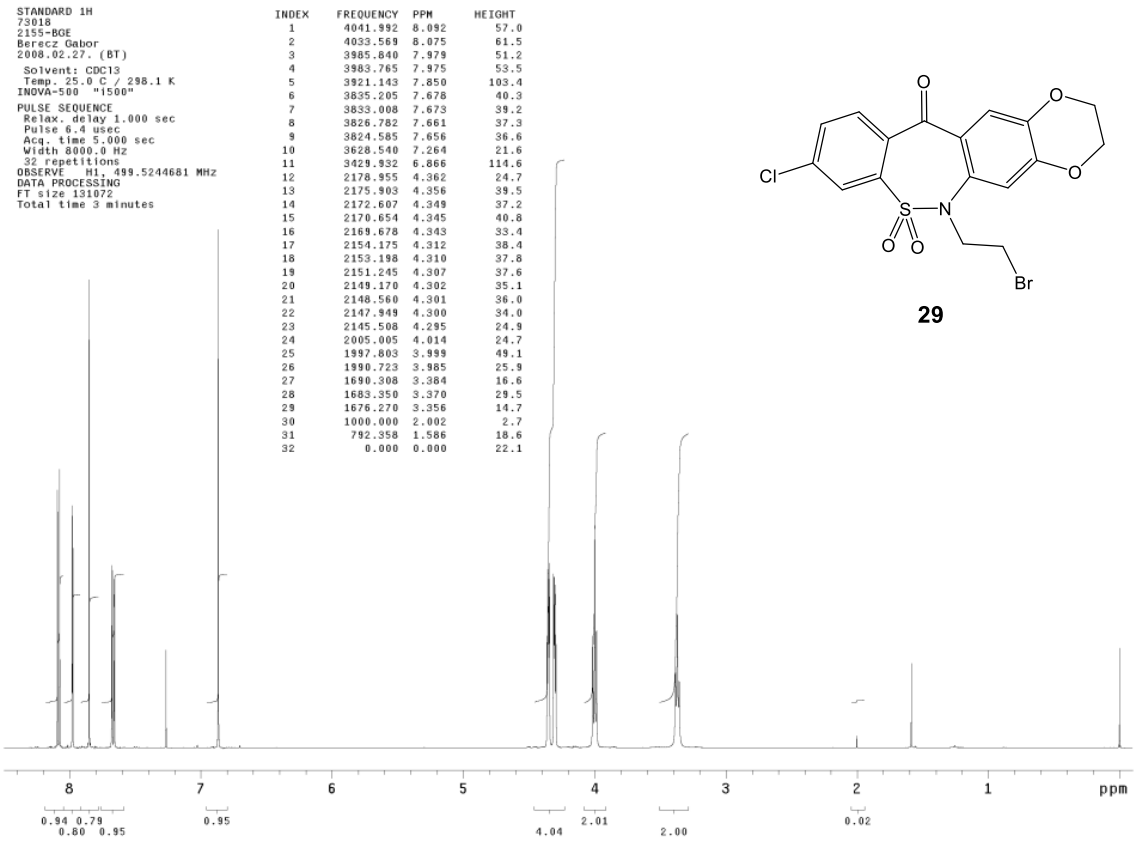



```
STANDARD 13C
64576
1986-BGE
Berecz Gabor
2006.07.25. (BT)
 Solvent: DMSO
 Temp. 25.0 C / 298.1 K
User:  1-14-87
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 6.0 usec
 Acq. time 1.300 sec
 Width 28208.7 Hz
 128 repetitions
OBSERVE   C13, 125.6061583 MHz
DECOUPLE  H1, 499.5293374 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 0.5 Hz
FT size 131072
Total time 9 minutes
```

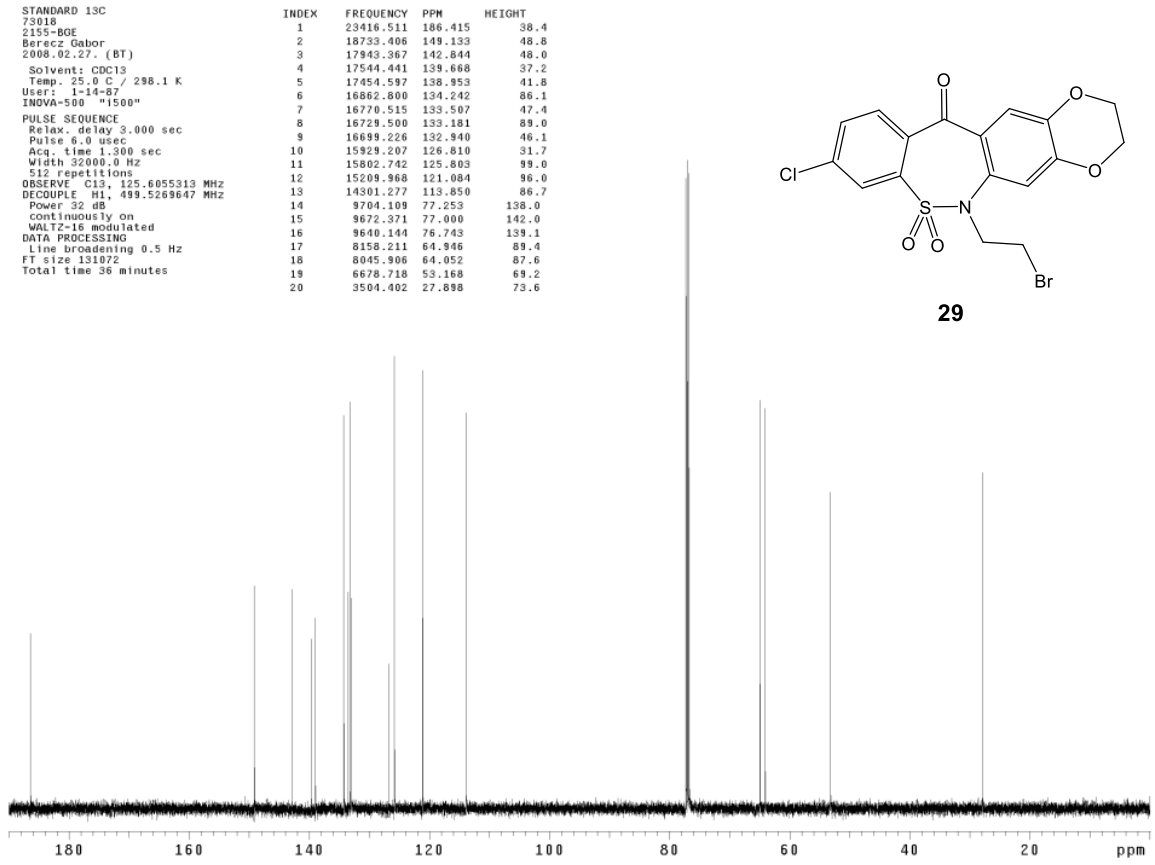
INDEX	FREQUENCY	PPM	HEIGHT
1	23766.049	189.203	47.1
2	18782.946	149.532	63.0
3	17652.633	140.534	58.0
4	17541.582	139.650	62.3
5	17226.076	137.138	59.1
6	16889.909	134.462	51.5
7	16770.680	133.513	59.4
8	16702.241	132.968	61.7
9	16631.220	132.402	59.0
10	15325.722	122.009	62.8
11	15119.976	120.371	59.7
12	14867.313	118.360	67.3
13	13660.383	108.751	66.7
14	8187.449	65.181	52.4
15	8047.990	64.071	51.8
16	5050.036	40.204	30.0
17	5028.945	40.036	95.7
18	5007.854	39.868	186.4
19	4986.762	39.700	214.3
20	4966.102	39.536	186.0
21	4945.011	39.368	94.5
22	4923.919	39.200	30.3

28

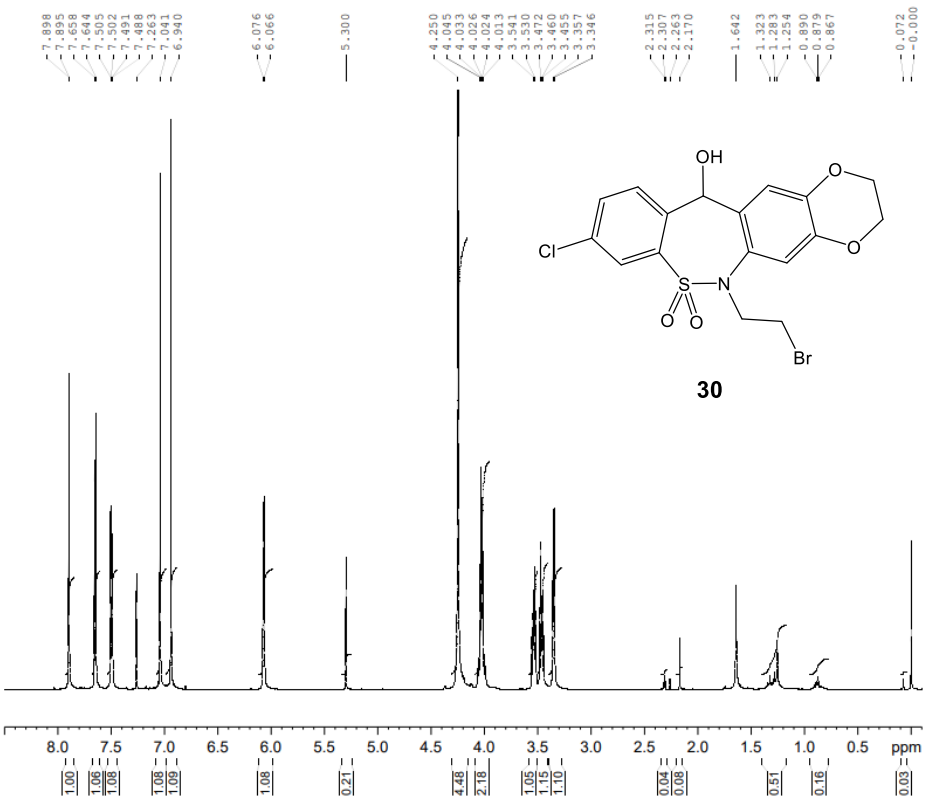



STANDARD 1H
73018
2155-BGE
Berecz Gabor
2008.02.27. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.5244681 MHz
DATA PROCESSING
FT size 131072
Total time 3 minutes
INDEX FREQUENCY PPM HEIGHT
1 4041.992 8.092 57.0
2 4033.569 8.075 61.5
3 3985.840 7.979 51.2
4 3983.765 7.975 53.5
5 3921.143 7.850 103.4
6 3835.205 7.678 40.3
7 3833.008 7.673 39.2
8 3826.782 7.661 37.3
9 3824.585 7.656 36.6
10 3628.540 7.264 21.6
11 3429.932 6.866 114.6
12 2178.955 4.362 24.7
13 2175.903 4.356 39.5
14 2172.607 4.349 37.2
15 2170.654 4.345 40.8
16 2169.678 4.343 33.4
17 2154.175 4.312 38.4
18 2153.198 4.310 37.8
19 2151.245 4.307 37.6
20 2149.170 4.302 35.1
21 2148.560 4.301 36.0
22 2147.949 4.300 34.0
23 2145.508 4.295 24.9
24 2005.005 4.014 24.7
25 1997.803 3.999 49.1
26 1990.723 3.985 25.9
27 1690.308 3.384 16.6
28 1683.350 3.370 29.5
29 1676.270 3.356 14.7
30 1000.000 2.002 2.7
31 792.358 1.586 18.6
32 0.000 0.000 22.1
Cl
O
O
O
S
N
O
O
Br
8
7
6
5
4
3
2
1
ppm
0.94 0.79
0.80 0.95
0.95
4.04
2.01
2.00
0.02

29


STANDARD 13C
73018
2155-BGE
Berecz Gabor
2008.02.27. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
512 repetitions
OBSERVE C13, 125.6055313 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 36 minutes
INDEX FREQUENCY PPM HEIGHT
1 23416.511 186.415 38.4
2 18733.406 149.133 48.8
3 17943.367 142.844 48.0
4 17544.441 139.668 37.2
5 17454.597 138.953 41.8
6 16862.800 134.242 86.1
7 16770.515 133.507 47.4
8 16729.500 133.181 89.0
9 16699.226 132.940 46.1
10 15929.207 126.810 31.7
11 15802.742 125.803 99.0
12 15209.968 121.084 96.0
13 14301.277 113.850 86.7
14 9704.109 77.253 138.0
15 9672.371 77.000 142.0
16 9640.144 76.743 139.1
17 8158.211 64.946 89.4
18 8045.906 64.052 87.6
19 6678.718 53.168 69.2
20 3504.402 27.898 73.6
Cl
O
O
O
S
N
O
O
Br
180
160
140
120
100
80
60
40
20
ppm

29

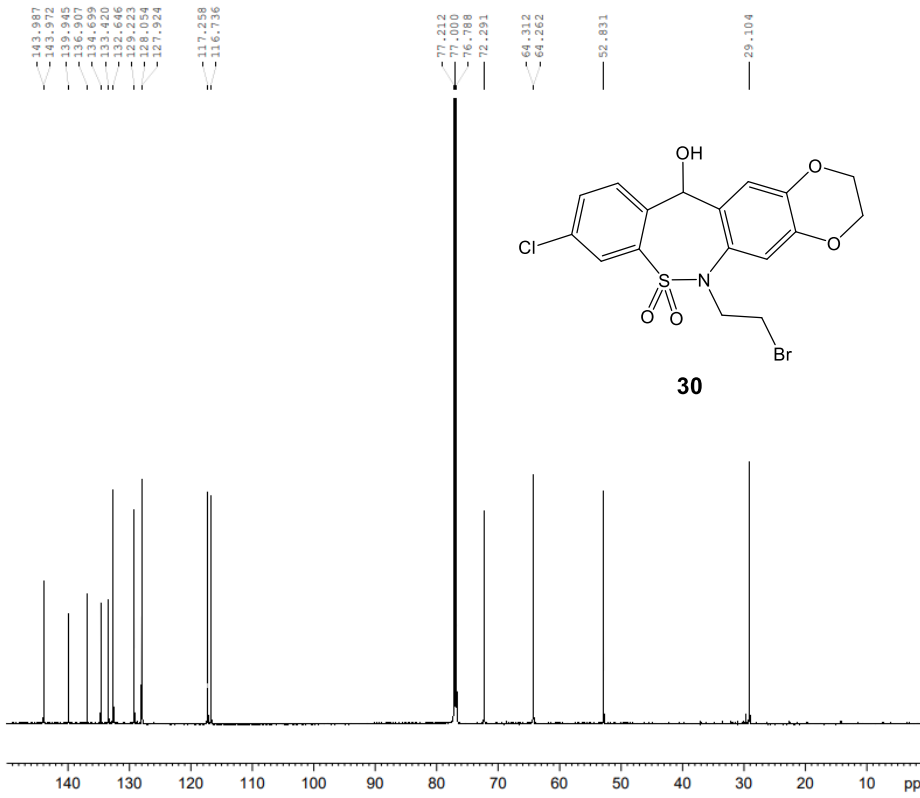



```
Standard 1H
144447
bge2363-2363-BGE_1
Berecz Gabor
2025.03.28. (KP)

Current Data Parameters
NAME                144447
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20250328
Time                 10.34 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                       16
DS                        2
SWH               12019.230 Hz
FIDRES                0.366798 Hz
AQ                    2.7262976 sec
RG                      196.07
DW                     41.600 usec
DE                     25.00 usec
TE                     295.0 K
D1                1.00000000 sec
TD0                       1
SFO1              600.0037050 MHz
NUC1                     1H
P1                     11.50 usec
PLW1              28.00000000 W

F2 - Processing parameters
SI                    65536
SF                600.0000120 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

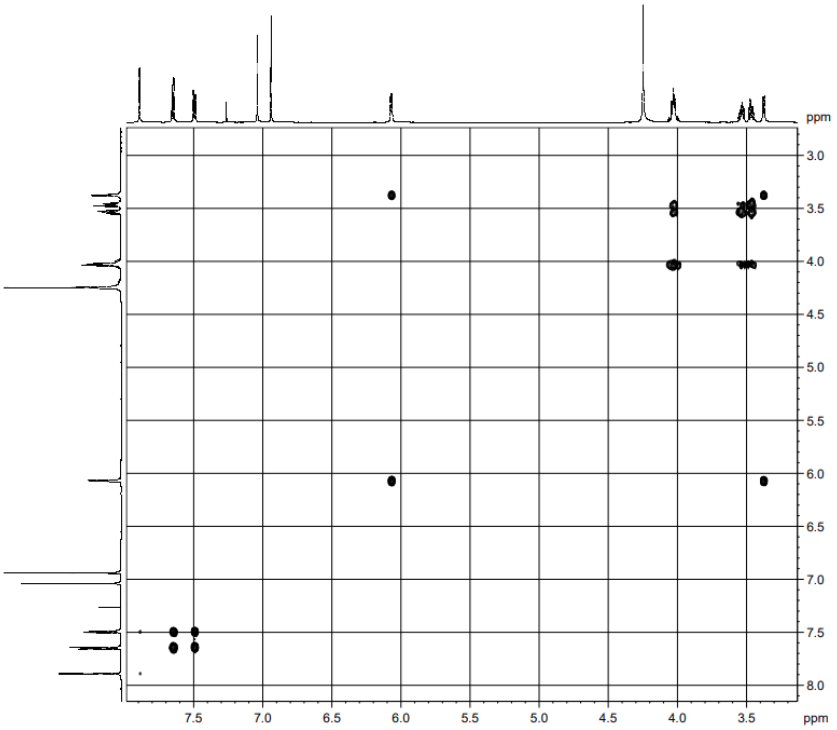



```
Standard 13C
144447
bge2363-2363-BGE_1
Berecz Gabor
2025.03.28. (KP)

Current Data Parameters
NAME                144447
EXPNO                   21
PROCNO                   1

F2 - Acquisition Parameters
Date_              20250329
Time                 12.15 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDC13
NS                     2048
DS                        4
SWH               36231.883 Hz
FIDRES                1.105709 Hz
AQ                    0.9043968 sec
RG                      196.07
DW                     13.800 usec
DE                     18.00 usec
TE                     295.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1              150.8852070 MHz
NUC1                     13C
P1                      9.80 usec
PLW1              72.69999695 W
SFO2              600.0024000 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2              32.50000000 W
PLW12              0.70708001 W
PLW13              0.35508999 W

F2 - Processing parameters
SI                   131072
SF                150.8701299 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



COSY **30**
144447
bge2363-2363-BGE_1
Berecz Gabor
2025.03.28. (KP)

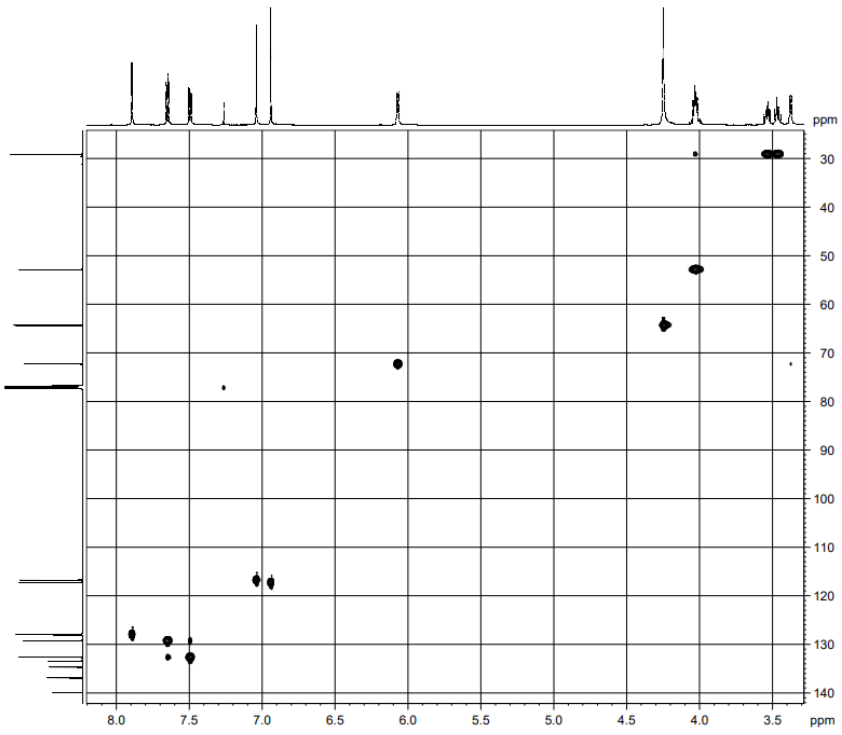
Current Data Parameters
NAME 144447
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250329
Time 12.16 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
ING 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0136 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000119 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000119 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



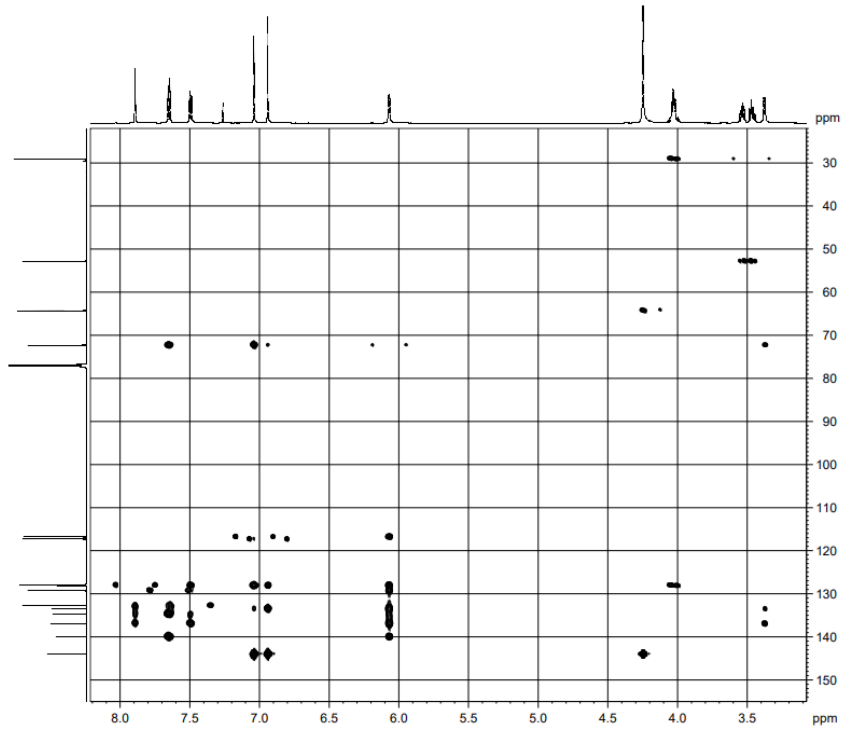
HSQC (140Hz) **30**
144447
bge2363-2363-BGE_1
Berecz Gabor
2025.03.28. (KP)

Current Data Parameters
NAME 144447
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250329
Time 12.37 h
INSTRUM spect
PROBHD 2145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
ING 0.00001745 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 ha_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P83 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Cgp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW31 5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW51 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000120 MHz
WDW QSINE



HMBC (8Hz, 140Hz) **30**
144447
bge2363-2363-BGE_1
Berecz Gabor
2025.03.28. (KP)

Current Data Parameters
NAME 144447
EXPNO 24
PROCNO 1

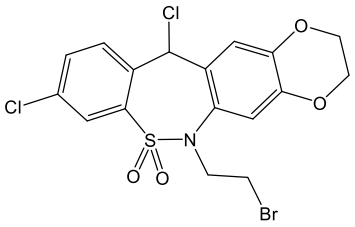
F2 - Acquisition Parameters
Date_ 20250329
Time 13.07 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000119 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

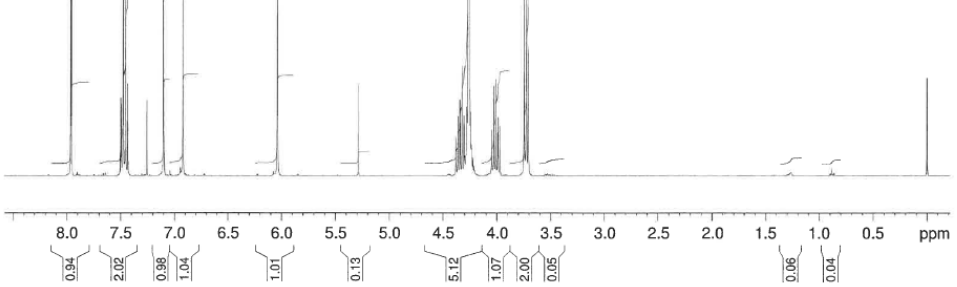
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701299 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

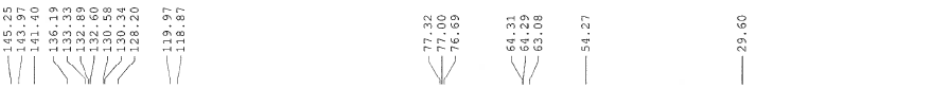
Standard 1H
85354
2364-BGE
Berecz Gabor
2010.03.18. (BB)



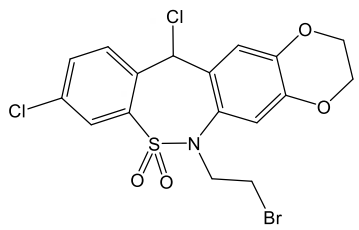
31

NAME	85354
EXPNO	1
PROCNO	1
Date_	20100318
Time	14.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	71.8
DW	60.800 usec
DE	6.50 usec
TE	303.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	1.00 dB
PL1W	11.97157383 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300114 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



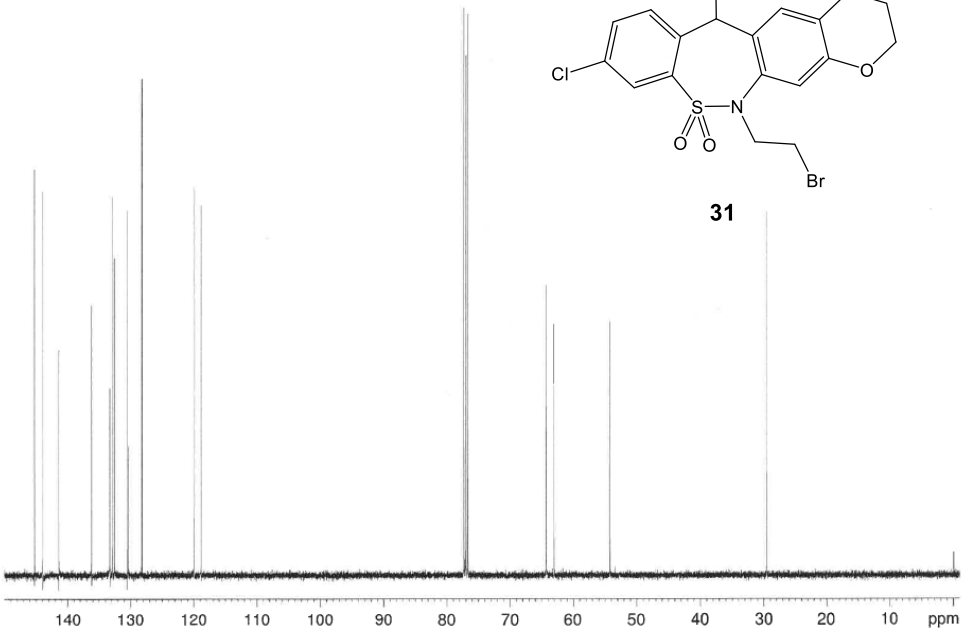


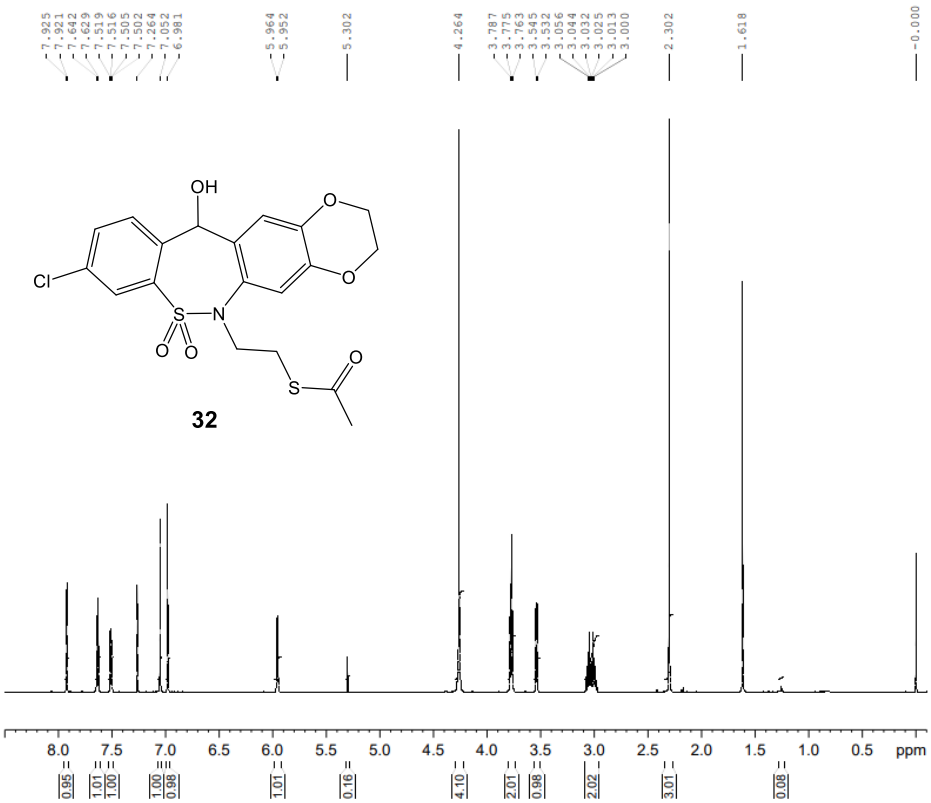
Standard 13C
85354
2364-BGE
Berecz Gabor
2010.03.18. (BB)



31

NAME	85354
EXPNO	2
PROCNO	1
Date_	20100318
Time	15.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.80 dB
PL1W	40.49391937 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	2.00 dB
PL12	20.00 dB
PL13	20.00 dB
PL2W	9.50935936 W
PL12W	0.15071319 W
PL13W	0.15071319 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127744 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



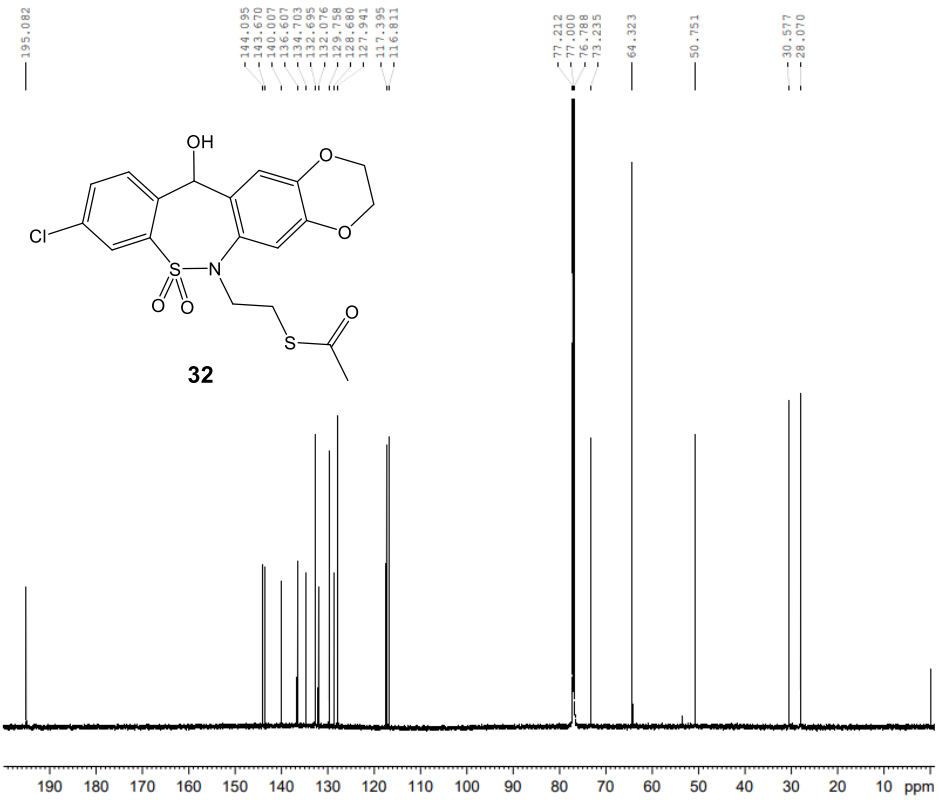


Standard 1H
143408
BEG0700_1A
Berecz Gabor
2024.09.02. (KP)

Current Data Parameters
NAME 143408
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240902
Time 17.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

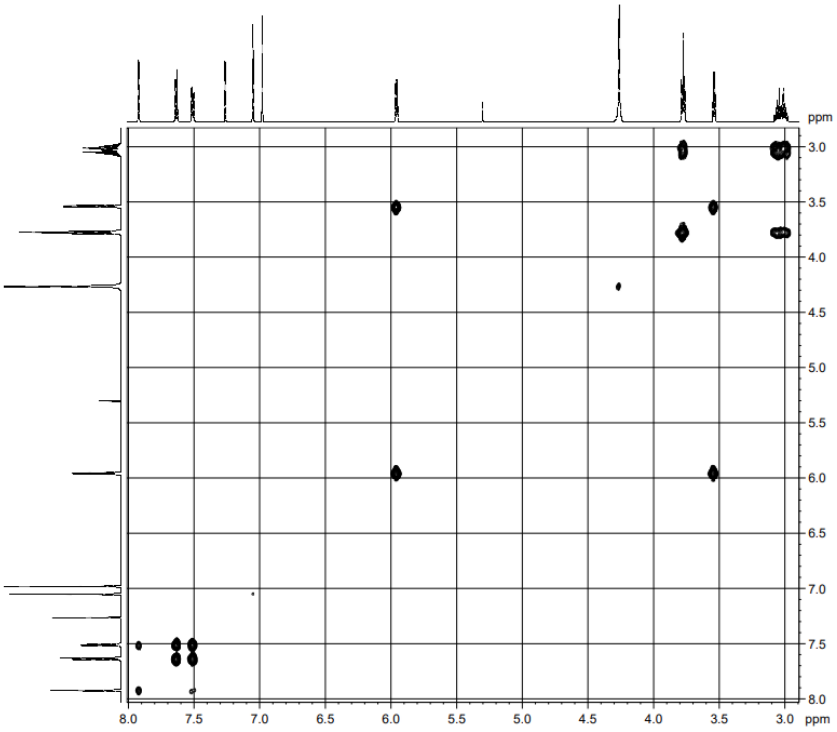


Standard 13C
143408
BEG0700_1A
Berecz Gabor
2024.09.02. (KP)

Current Data Parameters
NAME 143408
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240902
Time 18.57 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701271 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



COSY
143408
BEG0700_1A
Berecz Gábor
2024.09.02. (KP)

32

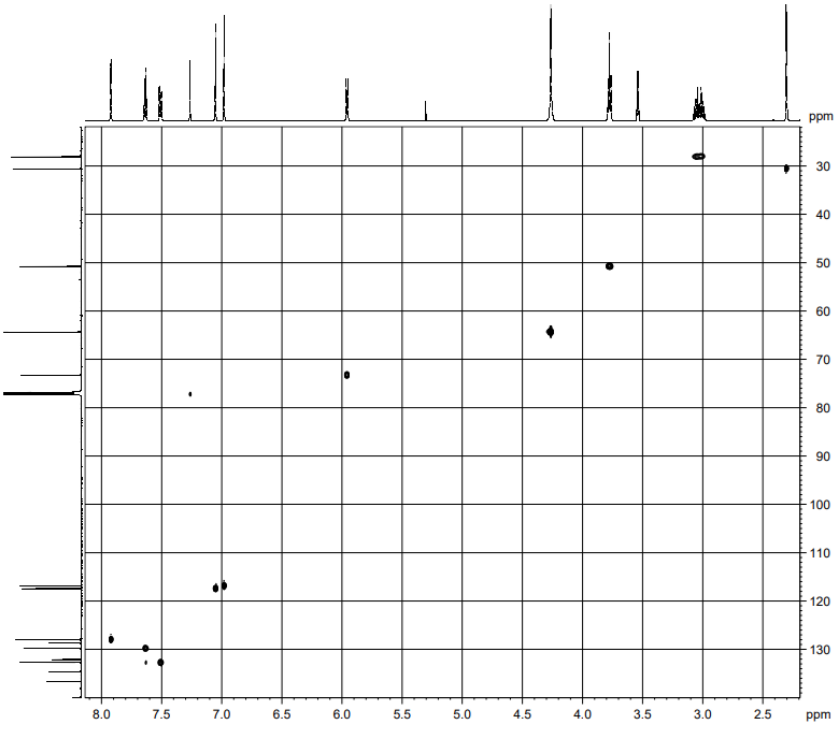
Current Data Parameters
NAME 143408
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240902
Time 18.58 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000128 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000128 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



HSQC (140Hz)
143408
BEG0700_1A
Berecz Gábor
2024.09.02. (KP)

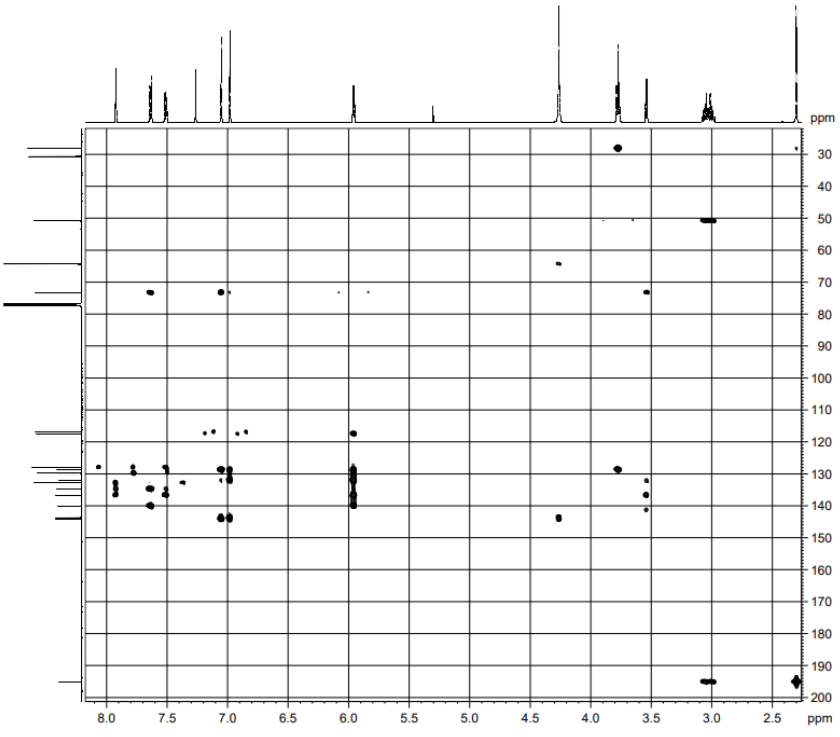
32

Current Data Parameters
NAME 143408
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240902
Time 19.19 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 19.41
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
INO 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P3 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.90 usec
P14 500.00 usec
P24 2000.00 usec
P43 1500.00 usec
PLW0 0 W
PLW2 71.00000000 W
PLW12 2.30040002 W
SPNAM[3] Crp40,0.7,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.63199997 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.63199997 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.95400000 W
SPNAM[32 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.48850000 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000128 MHz
WDW QSINE



HMBC (8Hz, 140Hz) **32**
143408
BEG0700_1A
Berecz Gabor
2024.09.02. (KP)

Current Data Parameters
NAME 143408
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240902
Time 19.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.90 usec
PLW2 71.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

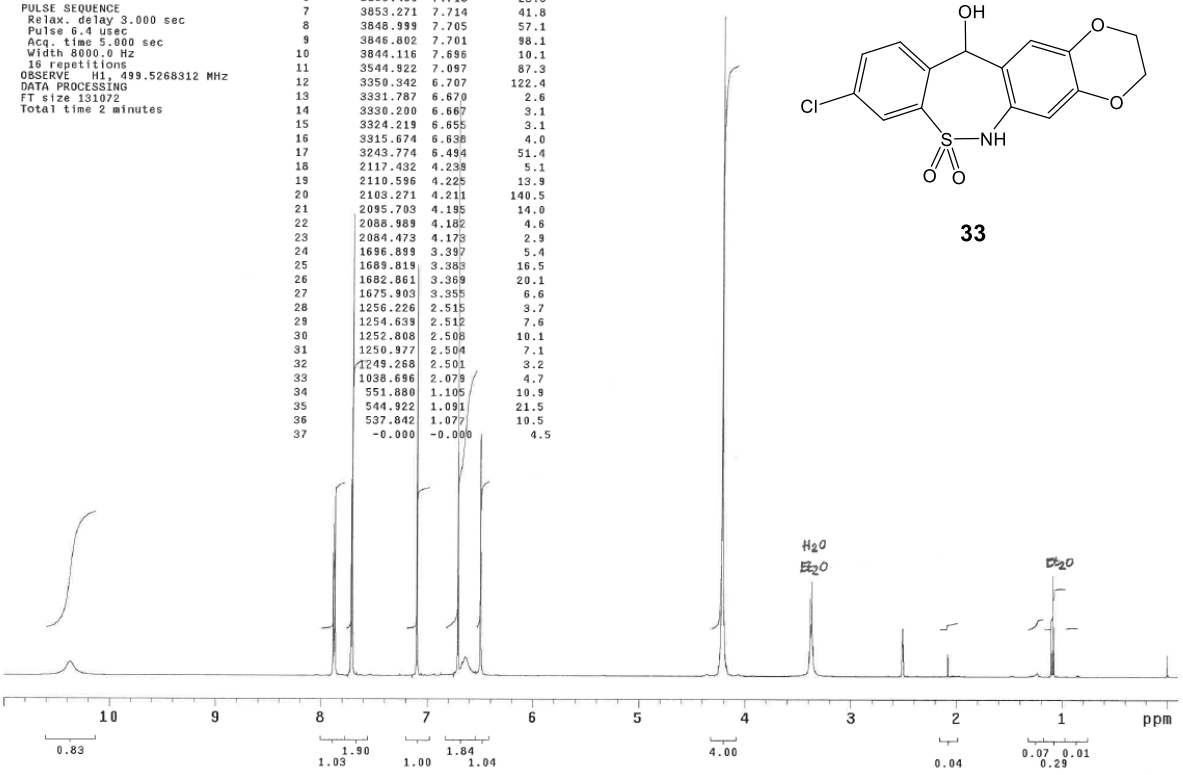
F2 - Processing parameters
SI 2048
SF 600.0000128 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701271 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

STANDARD 1H
65409
2007-BGE
Berecz Gabor
2006.09.20. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268312 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

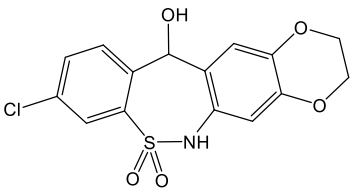
INDEX	FREQUENCY	PPM	HEIGHT
1	5182.129	10.374	2.9
2	3937.378	7.882	32.4
3	3934.448	7.876	9.5
4	3931.152	7.870	8.6
5	3928.223	7.864	40.0
6	3855.469	7.718	23.5
7	3853.271	7.714	41.8
8	3848.999	7.705	57.1
9	3846.802	7.701	98.1
10	3844.116	7.696	10.1
11	3544.922	7.097	87.3
12	3350.342	6.707	122.4
13	3331.787	6.670	2.6
14	3330.200	6.667	3.1
15	3324.219	6.655	3.1
16	3315.674	6.638	4.0
17	3243.774	6.494	51.4
18	2117.432	4.238	5.1
19	2110.596	4.225	13.9
20	2103.271	4.211	140.5
21	2095.703	4.195	14.0
22	2088.989	4.182	4.6
23	2084.473	4.173	2.9
24	1696.899	3.397	5.4
25	1689.819	3.383	16.5
26	1682.861	3.369	20.1
27	1675.903	3.355	6.6
28	1256.226	2.515	3.7
29	1254.639	2.512	7.6
30	1252.808	2.508	10.1
31	1250.977	2.504	7.1
32	1249.268	2.501	3.2
33	1038.696	2.079	4.7
34	551.880	1.105	10.9
35	544.922	1.091	21.5
36	537.842	1.077	10.5
37	-0.000	-0.000	4.5

33

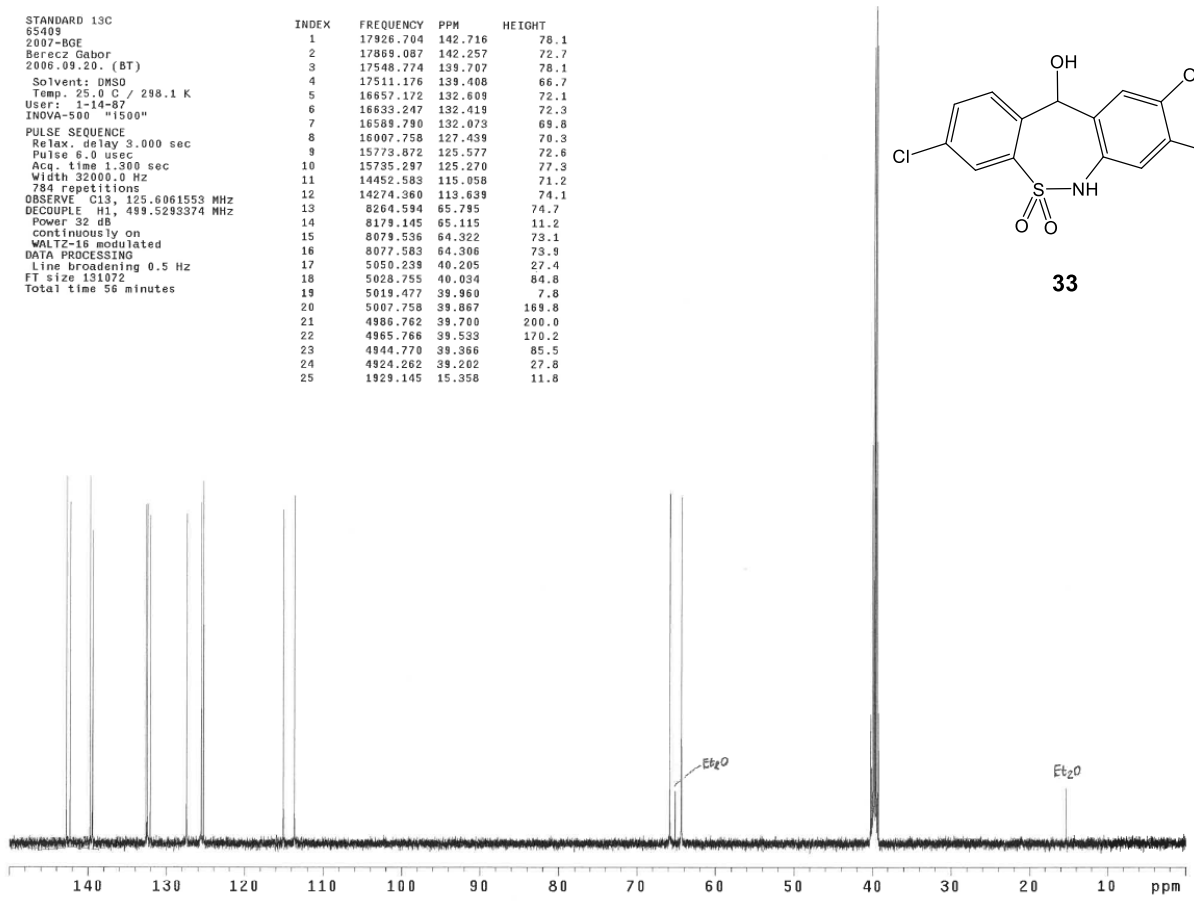


STANDARD 13C
65409
2007-BGE
Berecz Gabor
2006.09.20. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
784 repetitions
OBSERVE C13, 125.6061553 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 56 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	17926.704	142.716	78.1
2	17869.087	142.257	72.7
3	17548.774	139.707	78.1
4	17511.176	139.408	66.7
5	16657.172	132.609	72.1
6	16633.247	132.419	72.3
7	16589.790	132.073	69.8
8	16007.758	127.439	70.3
9	15773.872	125.577	72.6
10	15735.297	125.270	77.3
11	14452.583	115.058	71.2
12	14274.360	113.639	74.1
13	8264.594	65.795	74.7
14	8179.145	65.115	11.2
15	8079.536	64.322	73.1
16	8077.583	64.306	73.9
17	5050.239	40.205	27.4
18	5028.755	40.034	84.8
19	5019.477	39.960	7.8
20	5007.758	39.867	169.8
21	4986.762	39.700	200.0
22	4965.766	39.533	170.2
23	4944.770	39.366	85.5
24	4924.262	39.202	27.8
25	1929.145	15.358	11.8

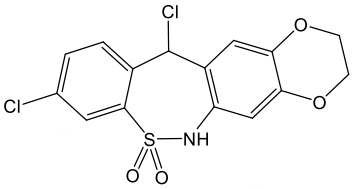


33

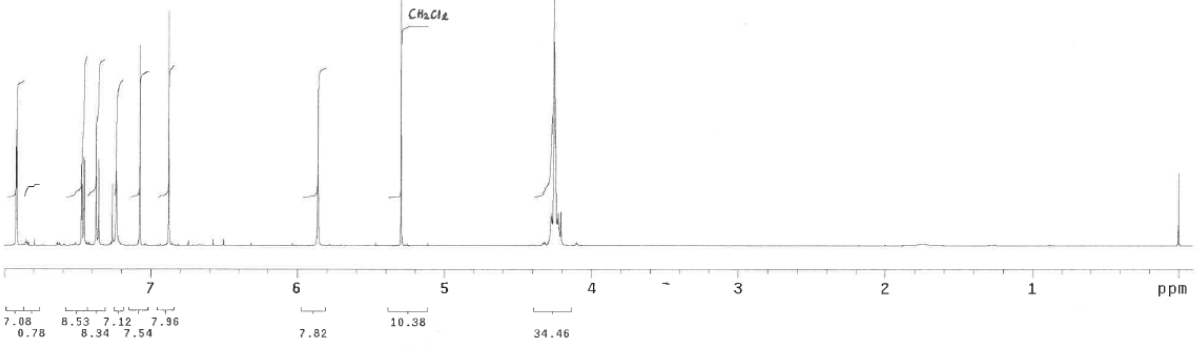


```
STANDARD 1H
67203
2039-BGE
Berecz Gabor
2007.01.16. (BB)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 6.4 usec
 Acq. time 5.000 sec
 Width 8000.0 Hz
 16 repetitions
OBSERVE    H1, 499.5244692 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
```

INDEX	FREQUENCY	PPM	HEIGHT
1	3954.712	7.917	24.4
2	3952.515	7.913	24.8
3	3731.934	7.471	13.1
4	3729.736	7.467	12.7
5	3723.633	7.454	18.4
6	3721.436	7.450	17.8
7	3682.251	7.372	25.1
8	3673.828	7.355	18.0
9	3626.831	7.261	12.8
10	3612.793	7.232	15.6
11	3534.058	7.075	42.1
12	3435.791	6.878	49.3
13	2927.246	5.860	32.8
14	2645.386	5.296	111.9
15	2126.587	4.257	27.1
16	2123.535	4.251	42.7
17	2119.751	4.244	24.2
18	2102.173	4.208	7.0
19	-0.000	-0.000	15.2



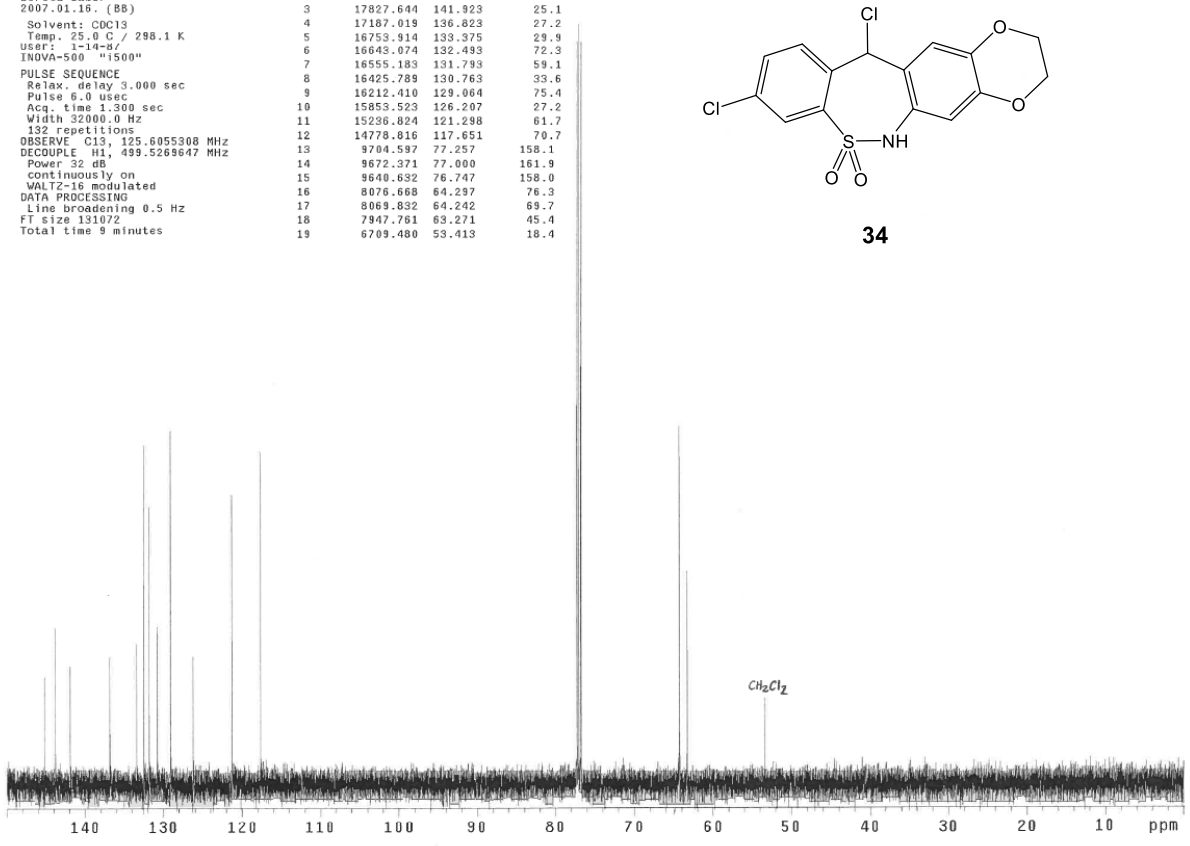
34




```
STANDARD 13C
67203
2039-BGE
Berecz Gabor
2007.01.16. (BB)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
user:  1-14-a/
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 6.0 usec
 Acq. time 1.300 sec
 Width 32000.0 Hz
 132 repetitions
OBSERVE  C13, 125.6055308 MHz
DECOUPLE  H1, 499.5269647 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 0.5 Hz
FT size 131072
Total time 9 minutes
```

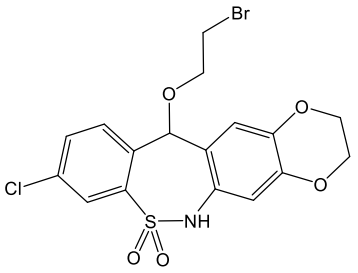
INDEX	FREQUENCY	PPM	HEIGHT
1	18230.964	145.133	22.9
2	18063.484	143.800	33.4
3	17827.644	141.923	25.1
4	17187.019	136.823	27.2
5	16753.914	133.375	29.9
6	16643.074	132.493	72.3
7	16555.183	131.793	59.1
8	16425.789	130.763	33.6
9	16212.410	129.064	75.4
10	15853.523	126.207	27.2
11	15236.824	121.298	61.7
12	14778.816	117.651	70.7
13	9704.597	77.257	158.1
14	9672.371	77.000	161.9
15	9640.632	76.747	158.0
16	8076.668	64.297	76.3
17	8069.832	64.242	69.7
18	7947.761	63.271	45.4
19	6709.480	53.413	18.4

34

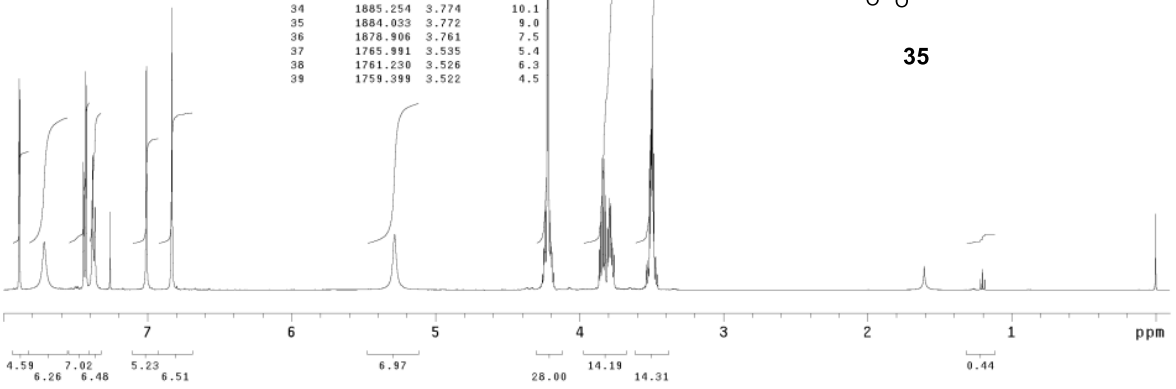


STANDARD 1H
74813
2177-BGE
Berecz Gabor
2008.06.19. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244712 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3942.139	7.892	45.2	40	1755.127	3.514	29.8
2	3939.941	7.887	42.9	41	1750.732	3.505	47.4
3	3854.736	7.717	10.2	42	1748.657	3.501	34.6
4	3719.238	7.446	27.4	43	1745.850	3.495	45.1
5	3717.041	7.441	25.2	44	1744.019	3.491	30.1
6	3710.938	7.429	46.7	45	1740.356	3.484	29.2
7	3708.862	7.425	43.8	46	1734.619	3.473	7.1
8	3687.500	7.382	28.9	47	1729.614	3.463	3.4
9	3679.199	7.365	17.7	48	802.612	1.607	5.1
10	3626.343	7.260	16.7	49	600.342	1.202	4.4
11	3500.610	7.008	47.8	50	0.000	0.000	16.3
12	3412.354	6.831	60.4				
13	2640.015	5.285	11.9				
14	2127.197	4.258	3.5				
15	2121.826	4.248	9.1				
16	2119.019	4.242	8.3				
17	2116.333	4.237	16.9				
18	2108.887	4.222	156.5				
19	2107.056	4.218	149.5				
20	2099.609	4.203	17.0				
21	2096.680	4.197	9.2				
22	2093.506	4.191	8.0				
23	2088.745	4.181	3.8				
24	1929.810	3.863	8.7				
25	1924.927	3.854	14.4				
26	1919.312	3.842	28.2				
27	1914.307	3.832	28.0				
28	1913.696	3.831	27.3				
29	1908.813	3.821	20.3				
30	1901.001	3.806	13.2				
31	1895.996	3.796	19.7				
32	1894.531	3.793	17.2				
33	1889.648	3.783	18.6				
34	1885.254	3.774	10.1				
35	1884.033	3.772	9.0				
36	1878.906	3.761	7.5				
37	1765.991	3.535	5.4				
38	1761.230	3.526	6.3				
39	1759.399	3.522	4.5				

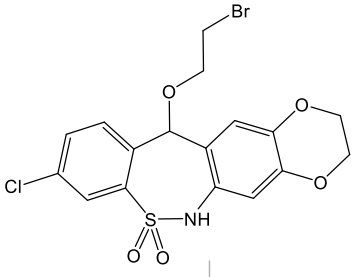


35

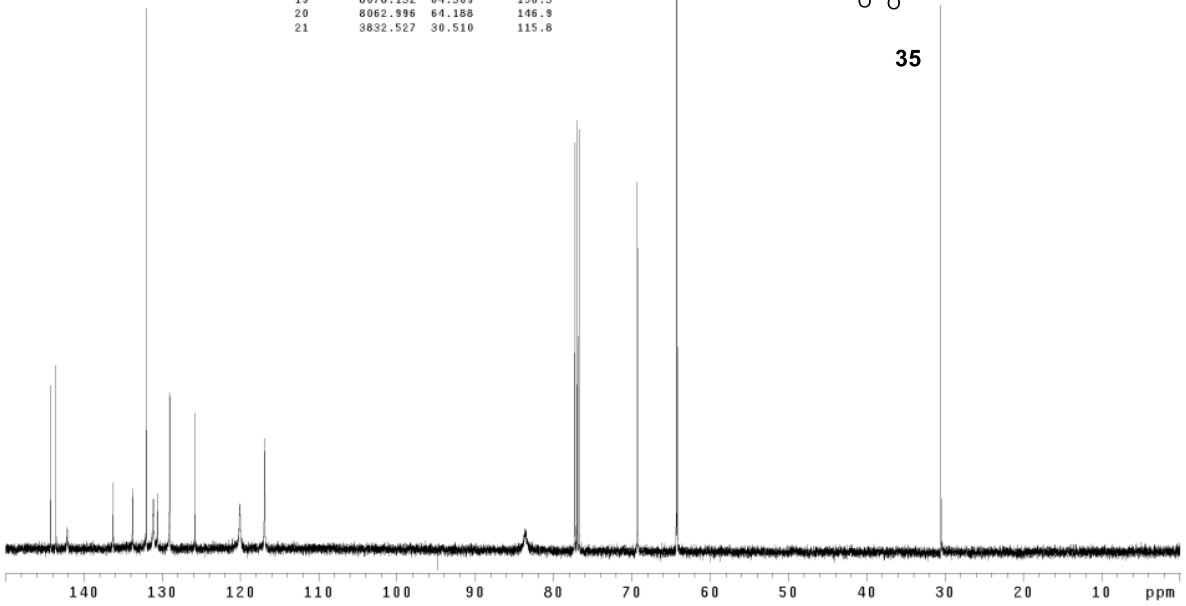


STANDARD 13C
74813
2177-BGE
Berecz Gabor
2008.06.19. (BB)
Solvent: CDCl3
Temp. 30.0 C / 303.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
1658 repetitions
OBSERVE C13, 125.6055303 MHz
DECOUPLE H1, 499.5269647 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 118 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18119.148	144.243	34.9
2	18031.746	143.547	39.2
3	17853.523	142.129	4.7
4	17114.265	136.244	14.3
5	16803.718	133.771	12.9
6	16583.503	132.018	115.2
7	16470.710	131.120	10.8
8	16404.304	130.592	12.0
9	16208.503	129.033	33.3
10	15807.136	125.838	29.1
11	15080.574	120.054	9.8
12	14684.578	116.901	23.6
13	11900.886	94.741	-4.3
14	10510.261	83.670	4.5
15	9704.597	77.257	86.6
16	9672.371	77.000	91.2
17	9640.632	76.747	89.4
18	8701.667	69.272	78.2
19	8078.132	64.309	156.3
20	8062.996	64.188	146.9
21	3832.527	30.510	115.8

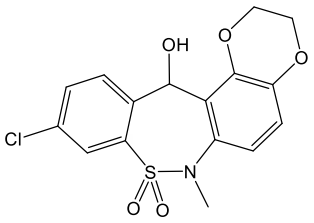


35

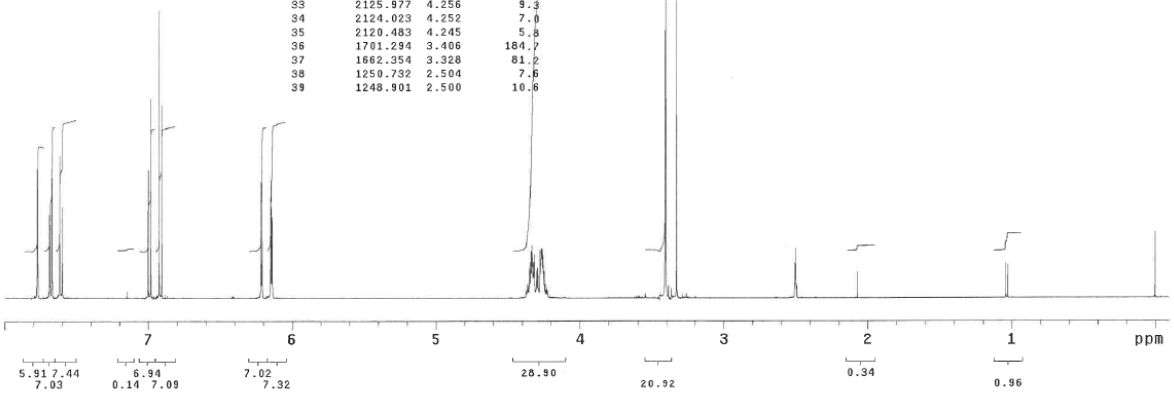


```
STANDARD 1H
65227
2000-BGE
Berecz Gabor
2006.09.06. (SzA)
 Solvent: DMSO
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 6.4 usec
 Acq. time 5.000 sec
 Width 8000.0 Hz
 16 repetitions
OBSERVE    H1, 499.5268346 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
```

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3883.667	7.775	27.7	40	1247.070	2.497	7.3
2	3881.470	7.770	30.4	41	1035.278	2.073	5.6
3	3841.187	7.690	17.8	42	519.653	1.040	7.4
4	3838.867	7.685	15.7	43	513.672	1.028	7.1
5	3832.886	7.673	27.7	44	0.000	0.000	14.2
6	3830.566	7.668	25.9				
7	3804.688	7.617	30.6				
8	3796.265	7.600	19.4				
9	3496.460	7.000	27.5				
10	3487.793	6.982	42.8				
11	3458.862	6.924	62.0				
12	3450.195	6.907	41.5				
13	3106.201	6.218	25.0				
14	3101.929	6.210	30.2				
15	3071.655	6.149	21.6				
16	3067.383	6.141	17.4				
17	2171.387	4.347	6.5				
18	2168.579	4.341	7.6				
19	2166.870	4.338	10.2				
20	2164.063	4.332	11.4				
21	2161.377	4.327	8.6				
22	2159.302	4.323	5.5				
23	2158.203	4.320	7.6				
24	2155.884	4.316	9.3				
25	2147.461	4.299	6.0				
26	2144.043	4.292	6.4				
27	2135.498	4.275	10.3				
28	2133.667	4.271	6.3				
29	2132.568	4.269	8.4				
30	2130.859	4.266	10.5				
31	2129.395	4.263	10.5				
32	2128.540	4.261	10.3				
33	2125.977	4.256	9.3				
34	2124.023	4.252	7.0				
35	2120.483	4.245	5.8				
36	1701.294	3.406	184.7				
37	1662.354	3.328	81.2				
38	1250.732	2.504	7.6				
39	1248.901	2.500	10.6				

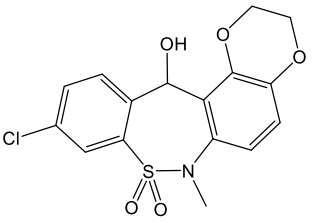


36




```
STANDARD 13C
65227
2000-BGE
Berecz Gabor
2006.09.06. (SzA)
 Solvent: DMSO
 Temp. 25.0 C / 298.1 K
User:  1-14-87
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 1.200 sec
 Pulse 6.0 usec
 Acq. time 1.300 sec
 Width 32000.0 Hz
 368 repetitions
OBSERVE    C13, 125.6061592 MHz
DECOUPLE   H1, 499.5293374 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 131072
Total time 15 minutes
```

INDEX	FREQUENCY	PPM	HEIGHT
1	18025.337	143.501	27.6
2	17947.212	142.879	23.0
3	17682.563	140.772	28.2
4	17168.891	136.683	30.9
5	16875.923	134.351	33.5
6	16818.794	133.896	26.1
7	16600.532	132.158	40.1
8	16518.012	131.501	28.8
9	16351.997	130.180	22.9
10	15943.305	126.926	41.5
11	15401.313	122.611	41.1
12	14773.872	117.616	41.1
13	8389.106	66.786	45.3
14	8103.462	64.512	36.9
15	8025.337	63.890	34.2
16	5115.180	40.722	44.9
17	5050.239	40.205	23.5
18	5029.243	40.038	68.9
19	5007.759	39.867	137.5
20	4986.762	39.700	162.0
21	4965.766	39.533	137.6
22	4944.770	39.366	69.2
23	4923.774	39.199	23.1



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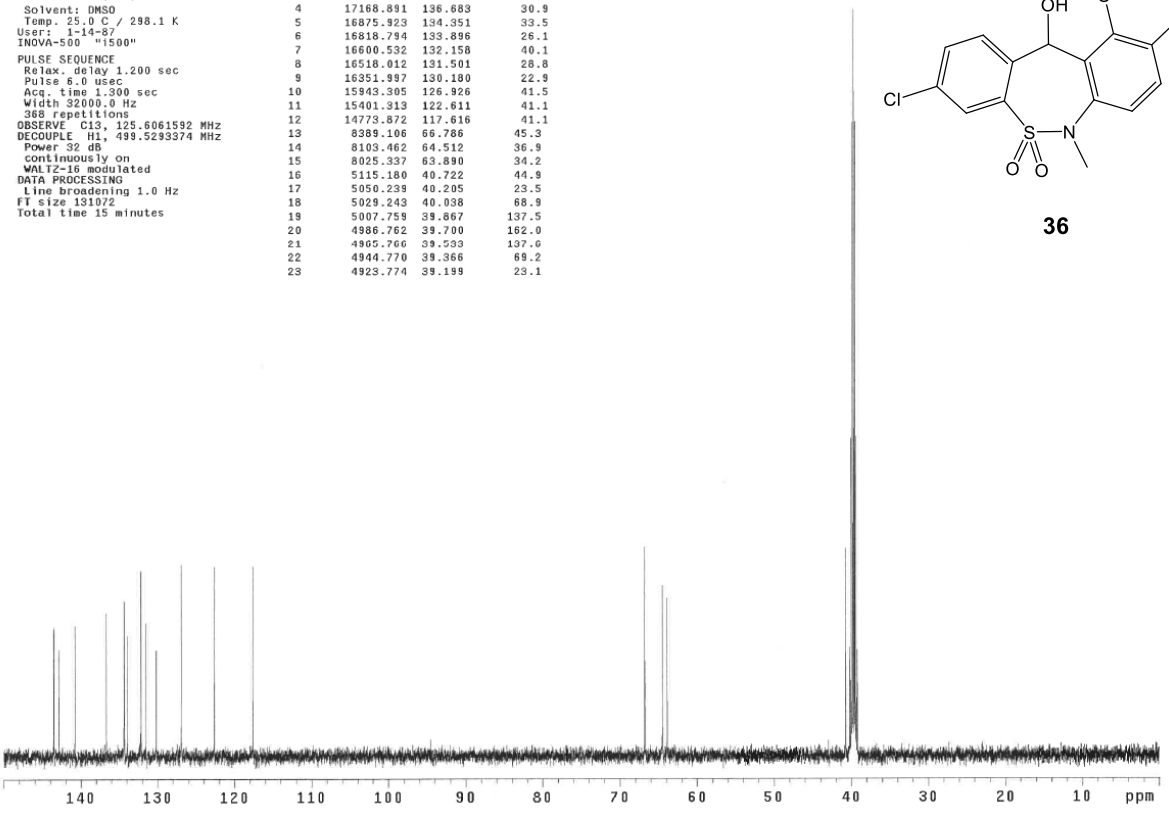
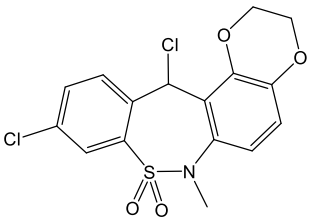


STANDARD 1H
62897
1951-BGE
Berecz Gabor
2006.04.06. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244718 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	3981.079	7.970	13.3
2	3980.835	7.969	14.5
3	3979.980	7.968	23.8
4	3978.638	7.965	13.7
5	3734.131	7.475	77.8
6	3732.788	7.473	62.0
7	3625.122	7.257	12.0
8	3503.296	7.013	18.6
9	3494.629	6.996	41.9
10	3481.812	6.970	61.4
11	3473.145	6.953	28.2
12	3354.980	6.716	46.9
13	2642.212	5.289	73.4
14	2186.035	4.376	5.9
15	2183.105	4.370	8.0
16	2180.664	4.365	9.1
17	2177.368	4.359	13.0
18	2172.607	4.349	6.8
19	2168.335	4.341	6.7
20	2165.894	4.336	8.7
21	2162.964	4.330	10.6
22	2160.645	4.325	12.4
23	2152.222	4.309	23.2
24	2143.677	4.291	12.3
25	2141.235	4.287	9.9
26	2138.550	4.281	8.5
27	2135.986	4.276	6.1
28	2126.953	4.258	6.2
29	2122.314	4.249	13.3
30	2118.896	4.242	8.6
31	2116.455	4.237	7.5
32	2113.403	4.231	6.2
33	2107.422	4.219	4.7
34	1769.287	3.542	151.2
35	-0.000	-0.000	13.5



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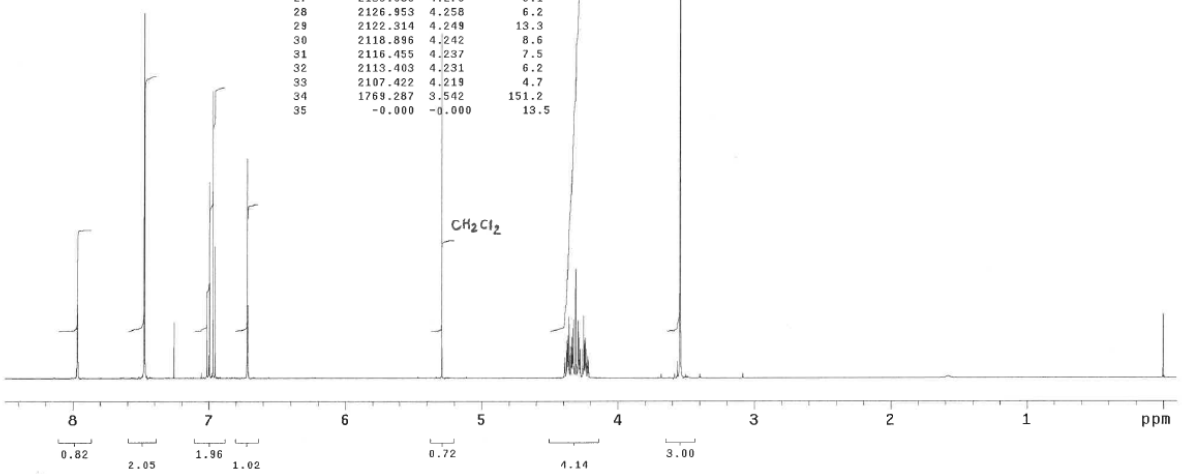
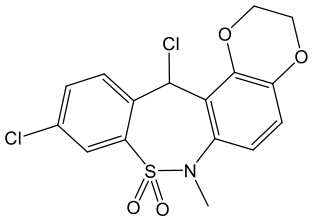


STANDARD 13C
62897
1951-BGE
Berecz Gabor
2006.04.06. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
272 repetitions
OBSERVE C13, 125.6055332 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 19 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18020.027	143.454	35.5
2	17863.289	142.206	25.8
3	17649.422	140.504	26.9
4	17099.617	136.127	38.9
5	16760.750	133.429	78.3
6	16731.453	133.196	37.3
7	16672.371	132.726	29.7
8	16612.312	132.248	81.8
9	16062.019	127.867	80.5
10	15843.758	126.129	15.4
11	15264.656	121.519	85.7
12	14991.218	119.342	89.0
13	9704.109	77.253	104.8
14	9672.371	77.000	109.1
15	9640.144	76.743	105.2
16	8119.636	64.639	81.5
17	8013.191	63.792	82.8
18	6731.941	53.592	59.8
19	6708.504	53.405	9.6 - DCM
20	4954.109	39.439	61.8



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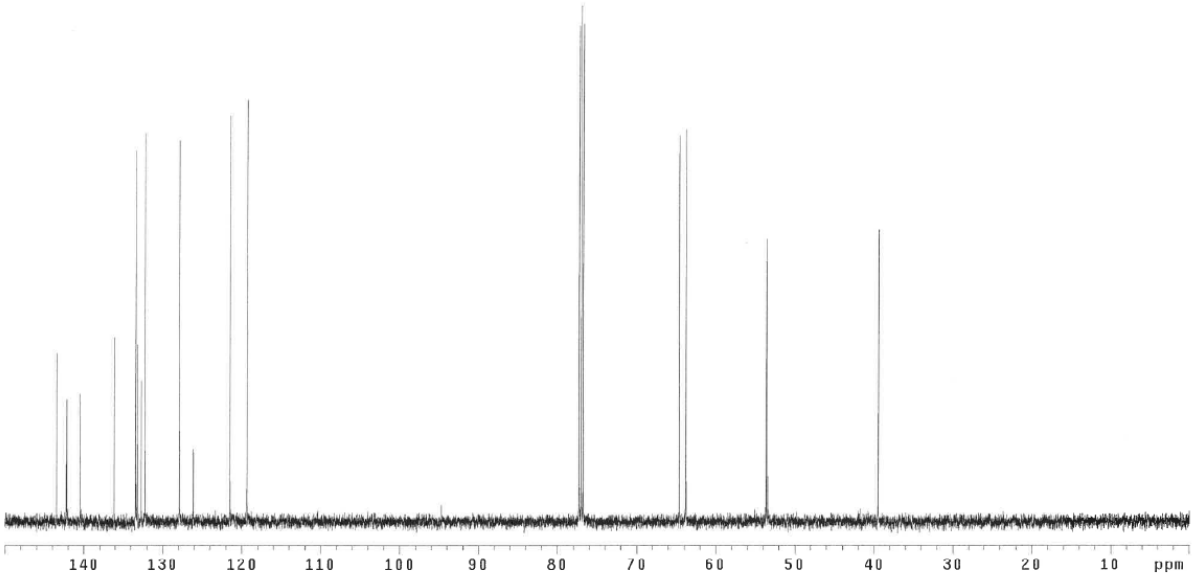

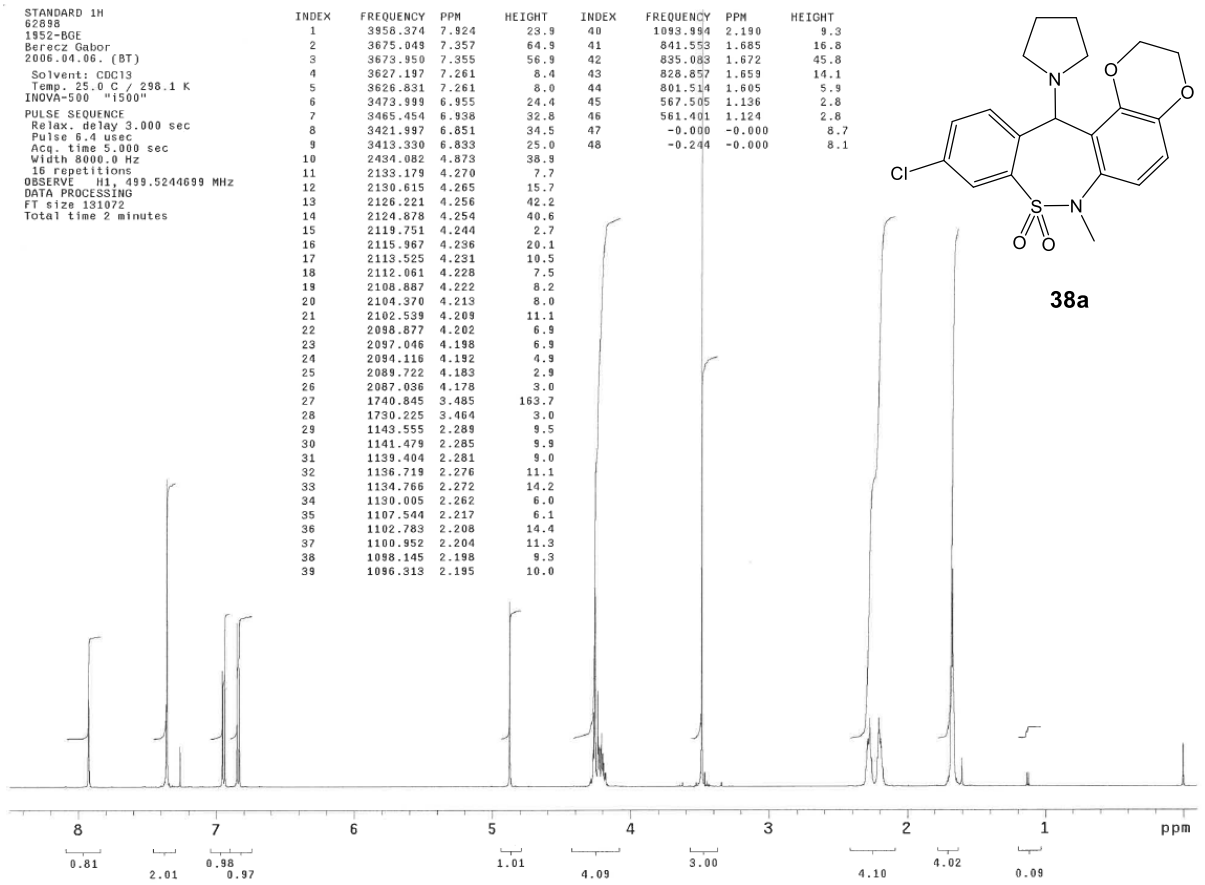
STANDARD 1H
62898
1952-BGE
Berecz Gabor
2006.04.06. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244699 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3958.374 7.924 23.9 40 1093.994 2.190 9.3
2 3675.049 7.357 64.9 41 841.553 1.685 16.8
3 3673.950 7.355 56.9 42 835.083 1.672 45.8
4 3627.197 7.261 8.4 43 828.857 1.659 14.1
5 3626.831 7.261 8.0 44 801.514 1.605 5.9
6 3473.999 6.955 24.4 45 567.505 1.136 2.8
7 3465.454 6.938 32.8 46 561.401 1.124 2.8
8 3421.997 6.851 34.5 47 -0.000 -0.000 8.7
9 3413.330 6.833 25.0 48 -0.244 -0.000 8.1
10 2434.082 4.873 38.9
11 2133.179 4.270 7.7
12 2130.615 4.265 15.7
13 2126.221 4.256 42.2
14 2124.878 4.254 40.6
15 2119.751 4.244 2.7
16 2115.967 4.236 20.1
17 2113.525 4.231 10.5
18 2112.061 4.228 7.5
19 2108.887 4.222 8.2
20 2104.370 4.213 8.0
21 2102.539 4.209 11.1
22 2098.877 4.202 6.9
23 2097.046 4.198 6.9
24 2094.116 4.192 4.9
25 2089.722 4.183 2.9
26 2087.036 4.178 3.0
27 1740.845 3.485 163.7
28 1730.225 3.464 3.0
29 1143.555 2.289 9.5
30 1141.479 2.285 9.9
31 1139.404 2.281 9.0
32 1136.719 2.276 11.1
33 1134.766 2.272 14.2
34 1130.005 2.262 6.0
35 1107.544 2.217 6.1
36 1102.783 2.208 14.4
37 1100.952 2.204 11.3
38 1098.145 2.198 9.3
39 1096.313 2.195 10.0
Cl
N
O
O
S
N
O
O
38a
8
7
6
5
4
3
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ppm
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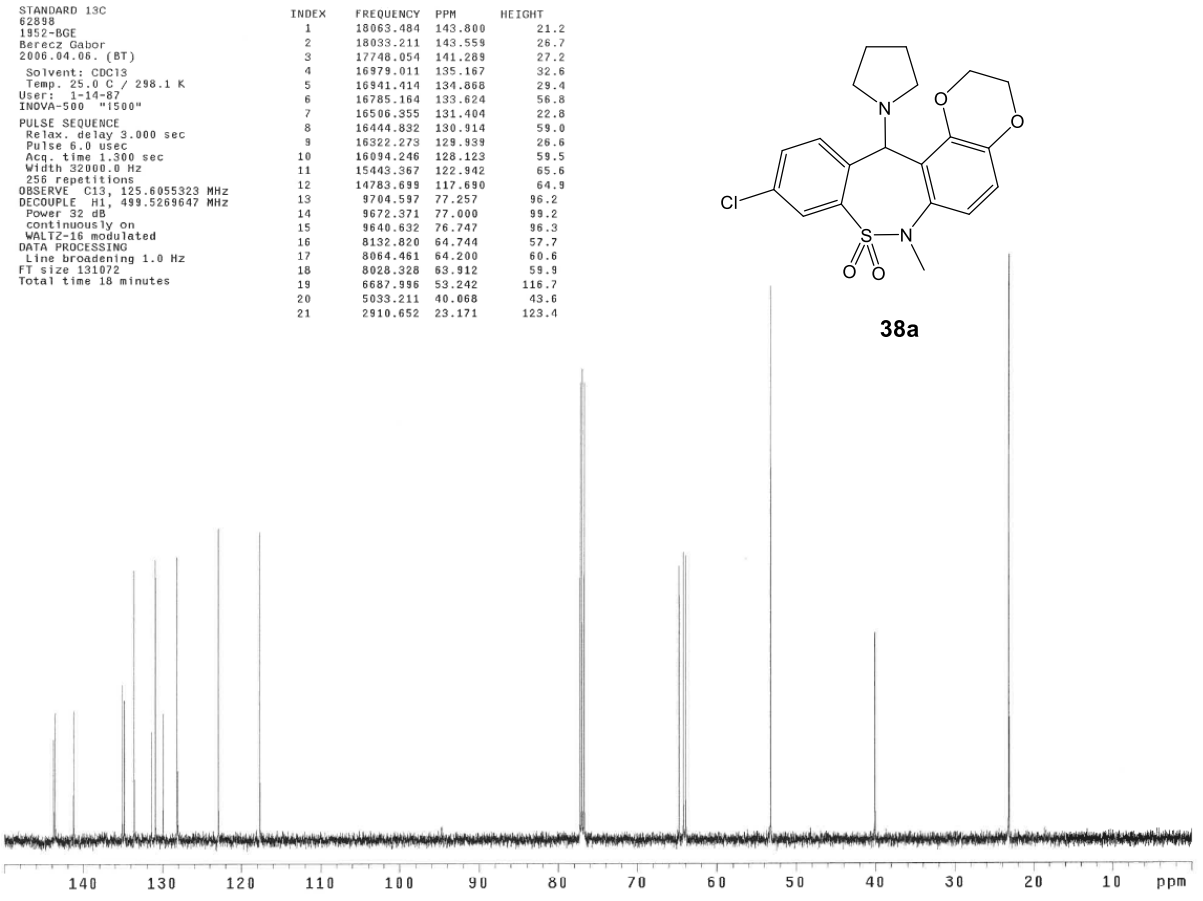
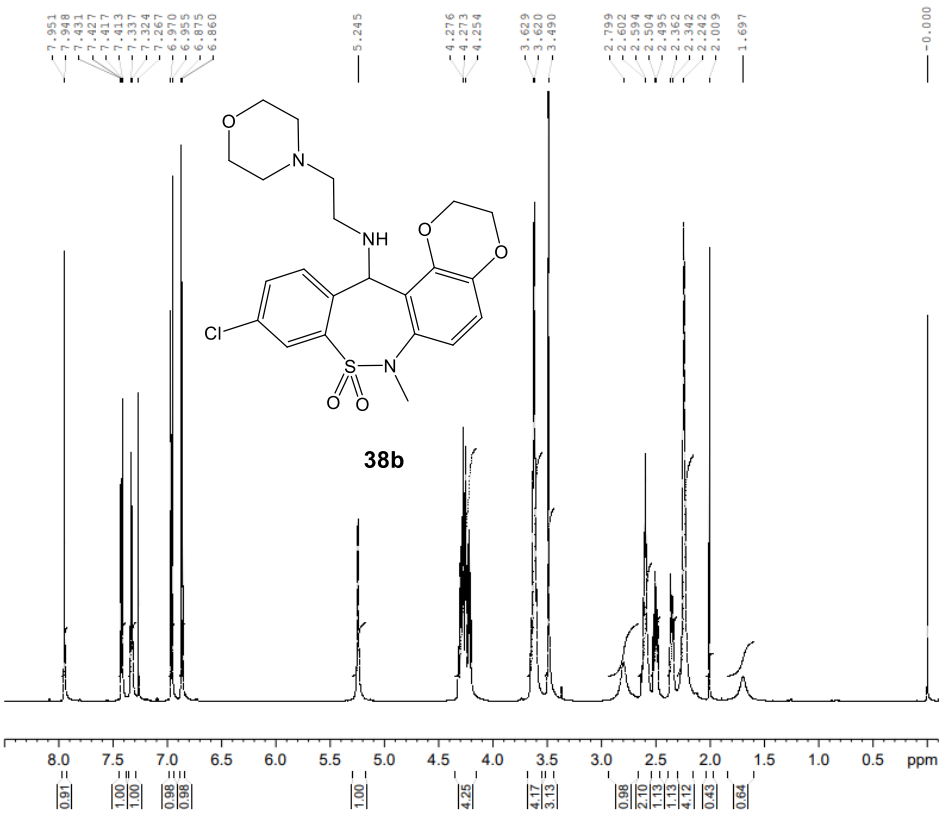
2.01
0.98
0.97
1.01
4.09
3.00
4.10
4.02
0.09


STANDARD 13C
62898
1952-BGE
Berecz Gabor
2006.04.06. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
256 repetitions
OBSERVE C13, 125.6055323 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 18 minutes
INDEX FREQUENCY PPM HEIGHT
1 18063.484 143.800 21.2
2 18033.211 143.559 26.7
3 17748.054 141.289 27.2
4 16979.011 135.167 32.6
5 16941.414 134.868 29.4
6 16785.164 133.624 56.8
7 16506.355 131.404 22.8
8 16444.832 130.914 59.0
9 16322.273 129.939 26.6
10 16094.246 128.123 59.5
11 15443.367 122.942 65.6
12 14783.699 117.690 64.9
13 9704.597 77.257 96.2
14 9672.371 77.000 99.2
15 9640.632 76.747 98.3
16 8132.820 64.744 57.7
17 8064.461 64.200 60.6
18 8028.328 63.912 59.9
19 6687.996 53.242 116.7
20 5033.211 40.068 43.6
21 2910.652 23.171 123.4
Cl
N
O
O
S
N
O
O
38a
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

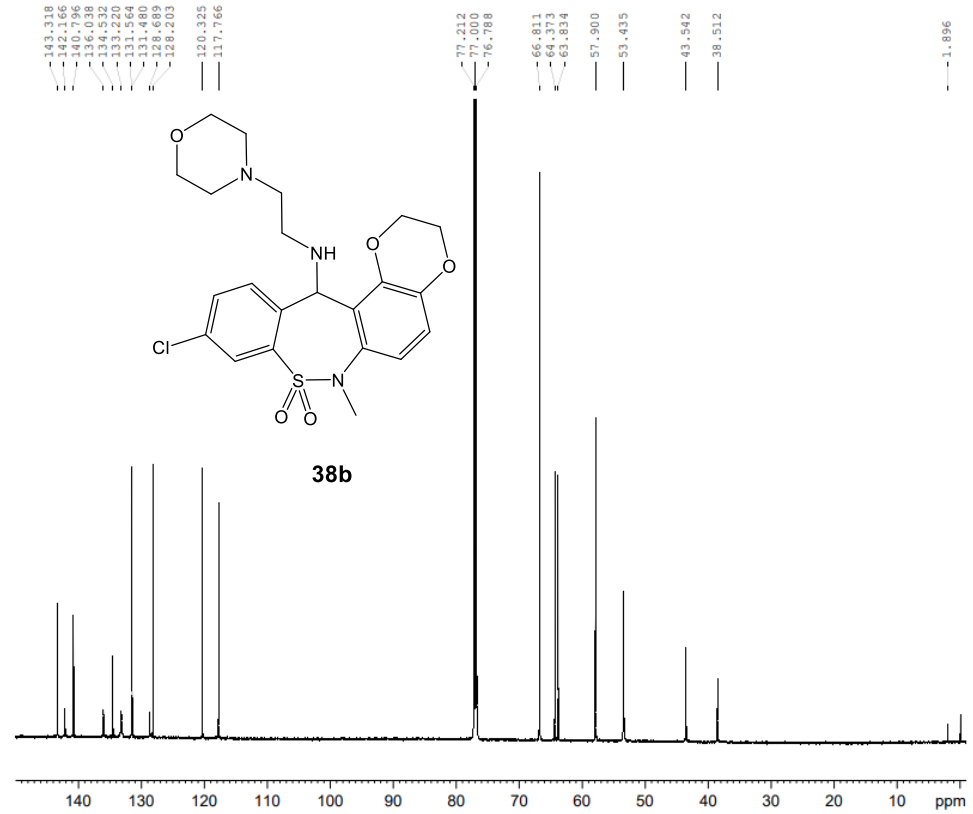


Standard 1H
144464
bge1953-1953-BGE_1
Berecz Gabor
2025.04.02. (KP)

Current Data Parameters
NAME 144464
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250402
Time 21.38 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

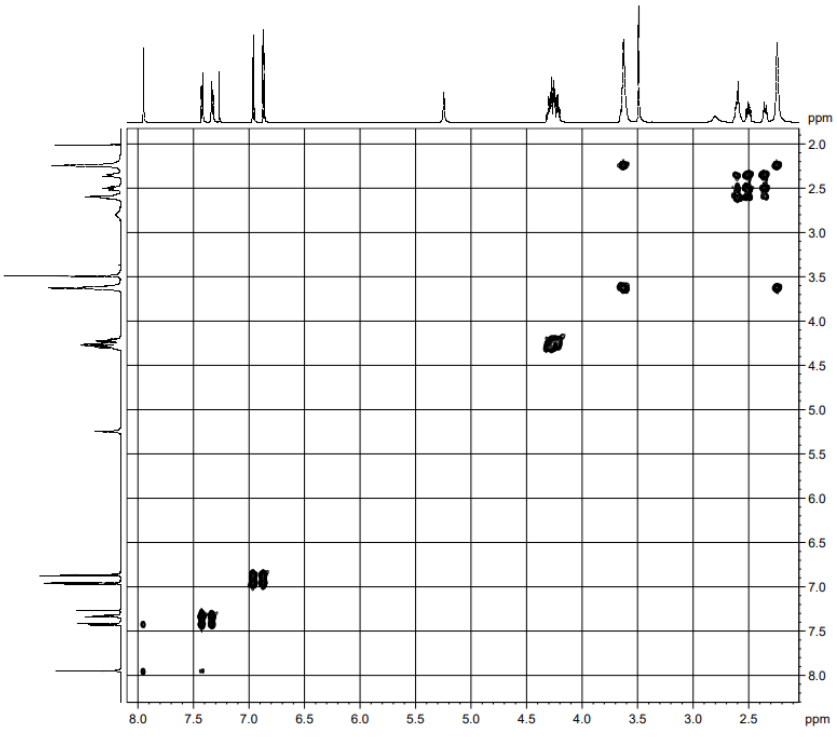


Standard 13C
144464
bge1953-1953-BGE_1
Berecz Gabor
2025.04.02. (KP)

Current Data Parameters
NAME 144464
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250402
Time 22.46 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.80 usec
PLW1 72.69999695 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.50000000 W
PLW12 0.70708001 W
PLW13 0.35508999 W

F2 - Processing parameters
SI 131072
SF 150.8701289 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



38b

COSY
144464
bge1953-1953-BGE_1
Berecz Gabor
2025.04.02. (KP)

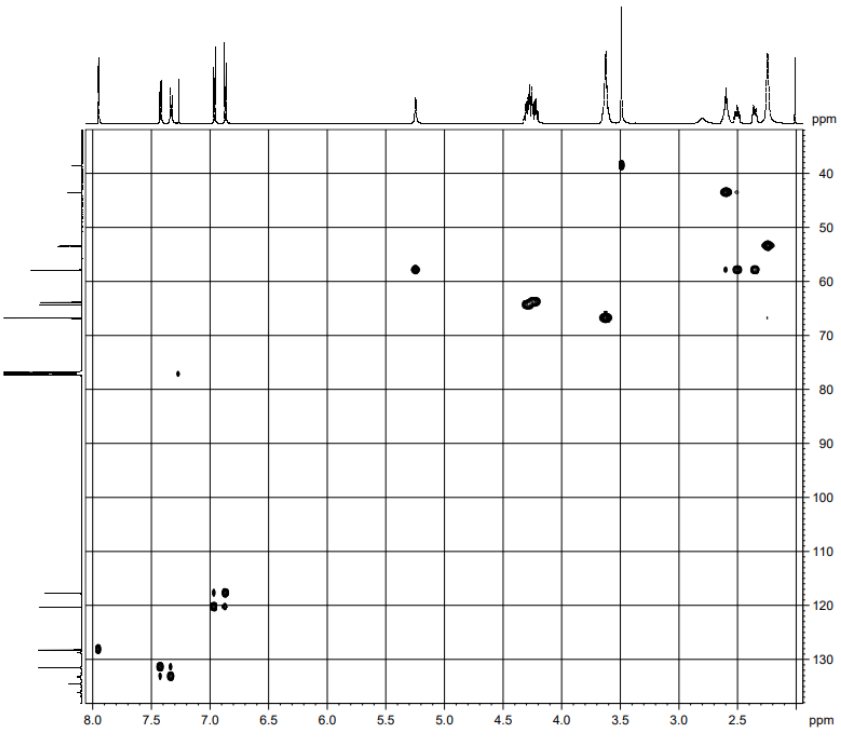
Current Data Parameters
NAME 144464
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250402
Time 22.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 41.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



38b

HSQC (140Hz)
144464
bge1953-1953-BGE_1
Berecz Gabor
2025.04.02. (KP)

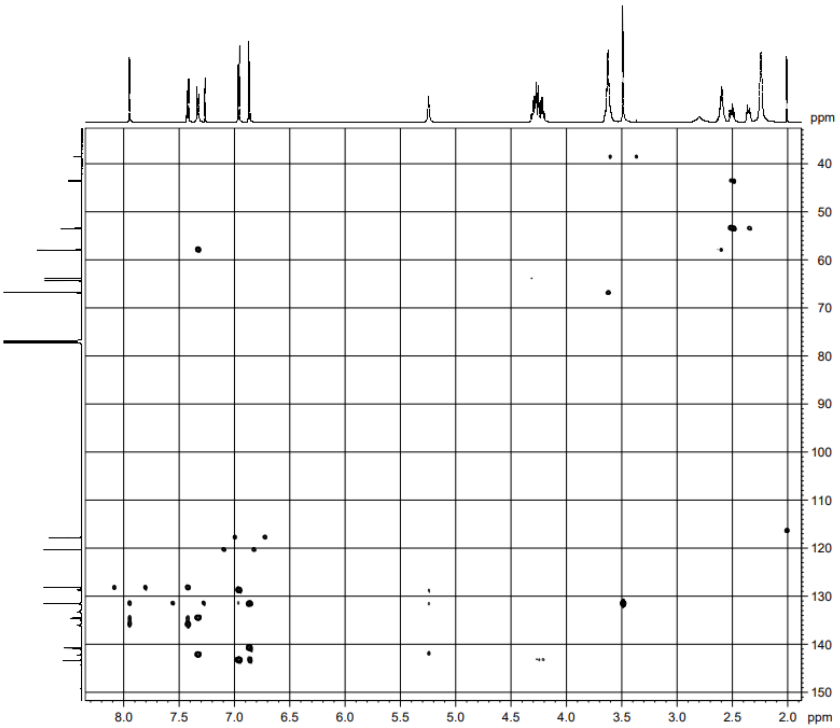
Current Data Parameters
NAME 144464
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250402
Time 23.09 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1311721 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001916 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Cwp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000099 MHz
WDW QSINE

38b



HMBC (8Hz, 140Hz)
144464
bge1953-1953-BGE_1
Berecz Gabor
2025.04.02. (KP)

Current Data Parameters
NAME 144464
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250402
Time 23.38 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

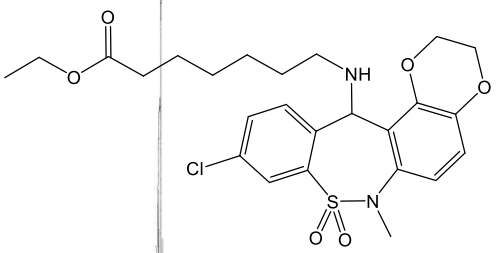
F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.662047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

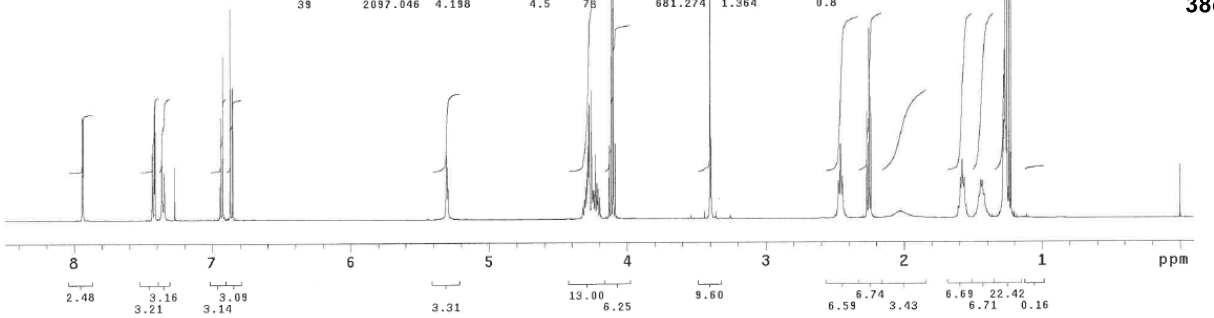
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701289 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

STANDARD 1H
63034
1954-BGE
Berecz Gabor
2006.04.13. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244656 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3966.797	7.941	21.6	40	2095.459	4.195	2.5	79	645.874	1.293	2.9
2	3964.600	7.937	21.5	41	2090.454	4.185	0.6	80	640.991	1.283	16.9
3	3714.478	7.436	14.1	42	2074.707	4.153	0.6	81	638.672	1.279	17.5
4	3712.280	7.432	13.4	43	2067.627	4.139	0.6	82	637.085	1.275	20.8
5	3706.177	7.419	22.2	44	2061.768	4.127	15.4	83	633.911	1.269	35.7
6	3703.979	7.415	22.1	45	2054.565	4.113	47.6	84	630.493	1.262	19.3
7	3683.960	7.375	0.9	46	2047.485	4.099	48.2	85	625.854	1.253	66.6
8	3678.345	7.364	15.4	47	2040.283	4.084	15.8	86	618.652	1.238	114.8
9	3670.044	7.347	10.0	48	2034.546	4.073	0.6	87	611.572	1.224	56.4
10	3631.226	7.269	11.1	49	1767.456	3.538	0.7	88	608.276	1.218	1.3
11	3467.041	6.941	21.5	50	1718.018	3.439	1.6	89	605.835	1.213	1.1
12	3463.379	6.933	0.6	51	1697.876	3.399	151.7	90	602.051	1.205	0.9
13	3458.374	6.923	34.4	52	1677.856	3.359	1.4	91	598.633	1.198	1.4
14	3451.782	6.910	0.7	53	1625.854	3.255	0.8	92	591.553	1.184	0.7
15	3431.641	6.870	44.4	54	1247.437	2.497	0.7	93	554.443	1.110	0.7
16	3428.223	6.863	0.8	55	1235.962	2.474	7.9	94	0.000	0.000	11.1
17	3426.392	6.859	0.7	56	1228.882	2.460	15.6				
18	3422.974	6.852	27.6	57	1221.680	2.446	8.9				
19	2648.804	5.303	13.3	58	1209.106	2.421	0.8				
20	2645.264	5.296	4.6	59	1133.301	2.269	22.5				
21	2644.287	5.294	6.5	60	1125.977	2.254	40.1				
22	2157.349	4.319	2.9	61	1118.286	2.239	25.5				
23	2154.785	4.314	0.9	62	1013.062	2.028	1.4				
24	2151.733	4.308	4.0	63	803.467	1.608	2.4				
25	2148.682	4.301	6.7	64	796.021	1.594	8.6				
26	2143.311	4.291	9.9	65	793.701	1.589	6.3				
27	2139.038	4.282	15.4	66	788.696	1.579	12.3				
28	2134.644	4.273	24.0	67	783.691	1.569	6.9				
29	2130.737	4.266	2.1	68	781.372	1.564	8.6				
30	2129.395	4.263	1.9	69	773.926	1.549	2.7				
31	2125.732	4.256	27.0	70	741.699	1.485	0.8				
32	2121.094	4.246	6.1	71	728.516	1.458	4.6				
33	2119.751	4.244	5.9	72	721.924	1.445	7.9				
34	2115.723	4.235	6.1	73	715.942	1.433	8.0				
35	2111.084	4.226	13.7	74	709.717	1.421	5.0				
36	2106.323	4.217	7.6	75	703.247	1.408	2.4				
37	2105.469	4.215	7.4	76	696.289	1.394	1.1				
38	2102.295	4.209	6.3	77	688.477	1.378	0.7				
39	2097.046	4.198	4.5	78	681.274	1.364	0.8				

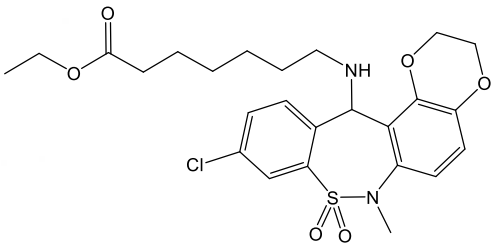


38c

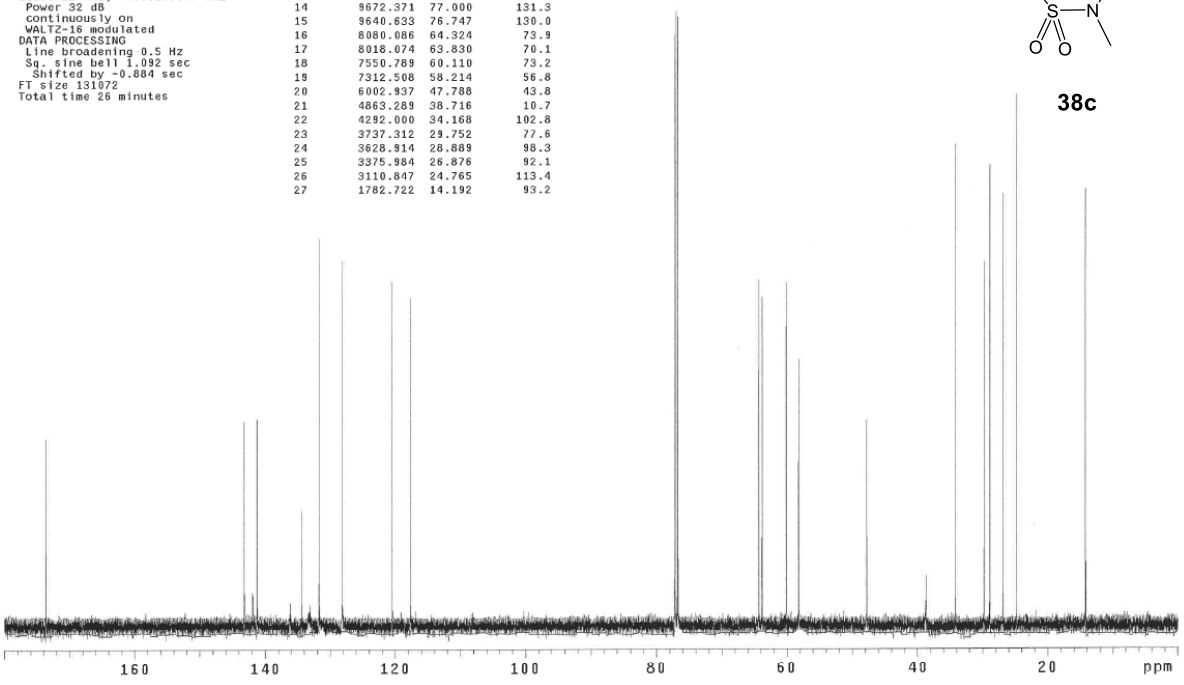


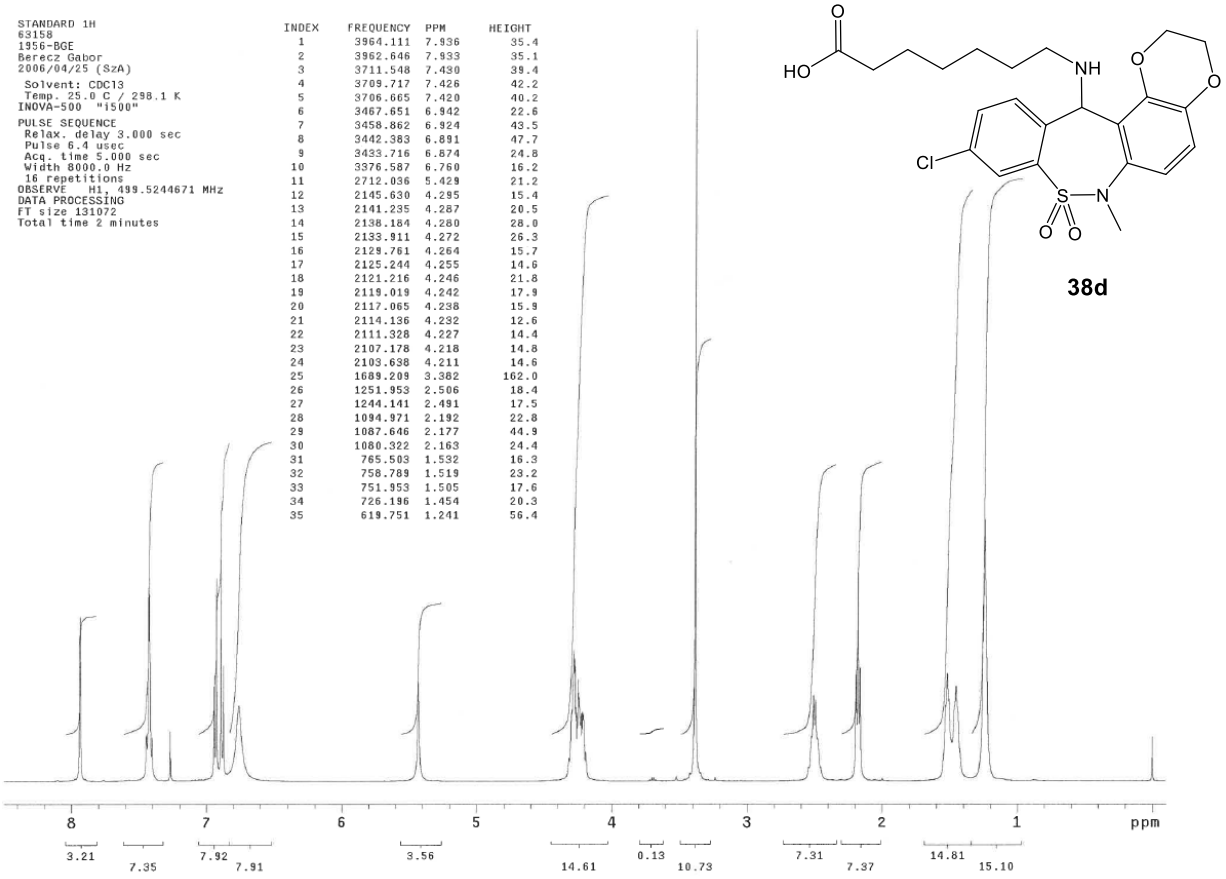
STANDARD 13C
63034
1954-BGE
Berecz Gabor
2006.04.13. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
368 repetitions
OBSERVE C13, 125.6055337 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
Sq. sine bell 1.092 sec
Shifted by -0.884 sec
FT size 131072
Total time 26 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	21812.508	173.645	40.0
2	17985.847	143.182	43.7
3	17825.691	141.907	7.2
4	17741.219	141.235	44.2
5	17100.105	136.131	4.9
6	16883.308	134.405	24.6
7	16728.035	133.169	4.6
8	16553.719	131.781	9.1
9	16539.558	131.668	82.6
10	16094.734	128.127	77.8
11	15128.426	120.435	73.5
12	14781.258	117.671	70.0
13	9704.597	77.257	125.9
14	9672.371	77.000	131.3
15	9640.633	76.747	130.0
16	8080.086	64.324	73.9
17	8018.074	63.830	70.1
18	7550.789	60.110	73.2
19	7312.508	58.214	56.8
20	6002.937	47.788	43.8
21	4863.289	38.716	10.7
22	4292.000	34.168	102.8
23	3737.312	29.752	77.6
24	3628.914	28.889	98.3
25	3375.984	26.876	92.1
26	3110.847	24.765	113.4
27	1782.722	14.192	93.2

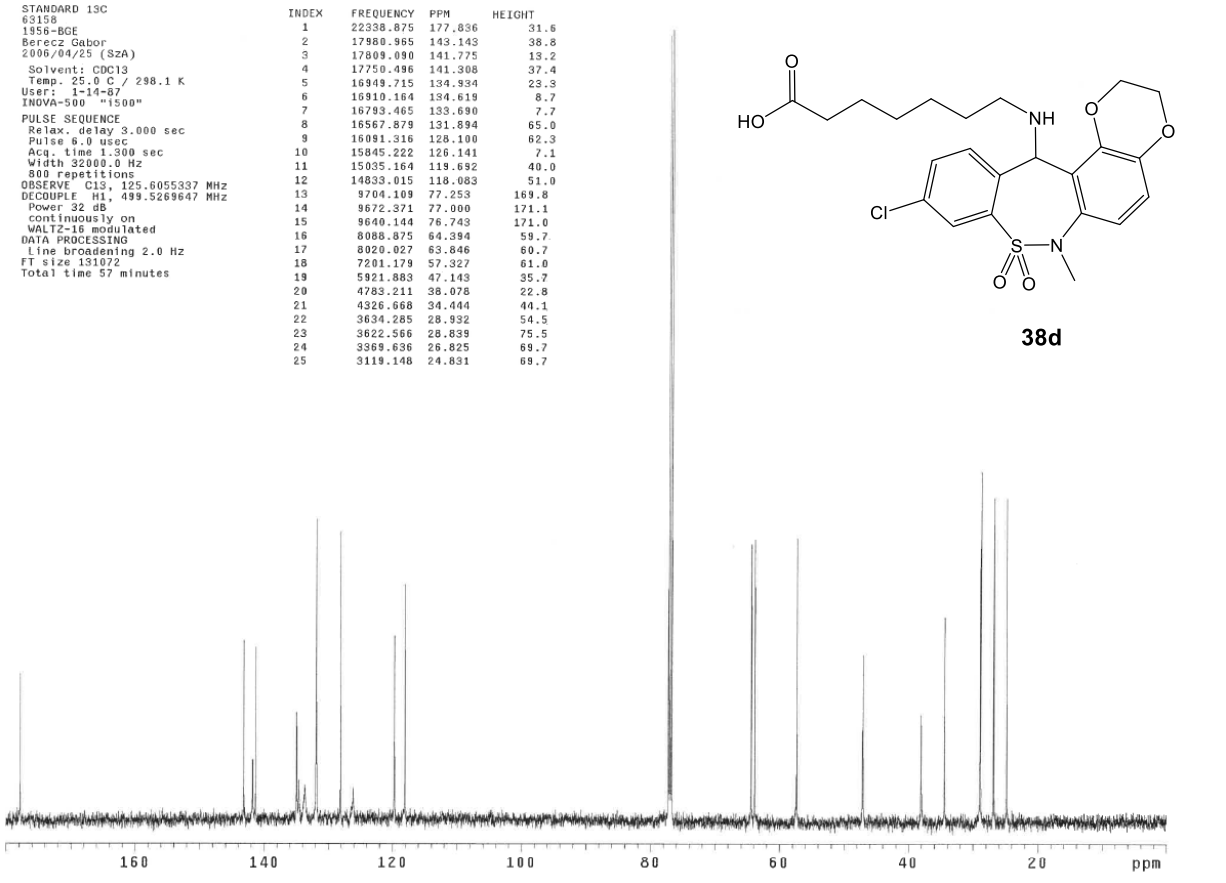


38c




STANDARD 1H
63158
1956-BGE
Berecz Gabor
2006/04/25 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244671 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 3964.111 7.936 35.4
2 3962.646 7.933 35.1
3 3711.548 7.430 38.4
4 3709.717 7.426 42.2
5 3706.665 7.420 40.2
6 3467.651 6.942 22.6
7 3458.862 6.924 43.5
8 3442.383 6.891 47.7
9 3433.716 6.874 24.8
10 3376.587 6.760 16.2
11 2712.036 5.429 21.2
12 2145.630 4.295 15.4
13 2141.235 4.287 20.5
14 2138.184 4.280 28.0
15 2133.911 4.272 26.3
16 2129.761 4.264 15.7
17 2125.244 4.255 14.6
18 2121.216 4.246 21.8
19 2119.019 4.242 17.9
20 2117.065 4.238 15.9
21 2114.136 4.232 12.6
22 2111.328 4.227 14.4
23 2107.178 4.218 14.8
24 2103.638 4.211 14.6
25 1689.209 3.382 162.0
26 1251.953 2.506 18.4
27 1244.141 2.491 17.5
28 1094.971 2.192 22.8
29 1087.646 2.177 44.9
30 1080.322 2.163 24.4
31 765.503 1.532 16.3
32 758.789 1.519 23.2
33 751.953 1.505 17.6
34 726.196 1.454 20.3
35 619.751 1.241 56.4
HO
O
NH
O
O
Cl
S
N
O
O
8
7
6
5
4
3
2
1
ppm
3.21
7.35
7.92
7.91
3.56
14.61
0.13
10.73
7.31
7.37
14.81
15.10

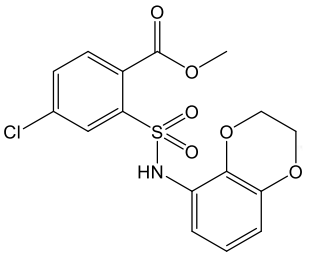
38d


STANDARD 13C
63158
1956-BGE
Berecz Gabor
2006/04/25 (SzA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 8.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
800 repetitions
OBSERVE C13, 125.6055337 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 57 minutes
INDEX FREQUENCY PPM HEIGHT
1 22338.875 177.836 31.6
2 17980.965 143.143 38.8
3 17809.090 141.775 13.2
4 17750.496 141.308 37.4
5 16949.715 134.934 23.3
6 16910.164 134.619 8.7
7 16793.465 133.690 7.7
8 16567.879 131.894 65.0
9 16091.316 128.100 62.3
10 15845.222 126.141 7.1
11 15035.164 119.692 40.0
12 14833.015 118.083 51.0
13 9704.109 77.253 169.8
14 9672.371 77.000 171.1
15 9640.144 76.743 171.0
16 8088.875 64.394 59.7
17 8020.027 63.846 60.7
18 7201.179 57.327 61.0
19 5921.883 47.143 35.7
20 4783.211 38.078 22.8
21 4326.668 34.444 44.1
22 3634.285 28.932 54.5
23 3622.566 28.839 75.5
24 3369.636 26.825 69.7
25 3119.148 24.831 69.7
HO
O
NH
O
O
Cl
S
N
O
O
160
140
120
100
80
60
40
20
ppm

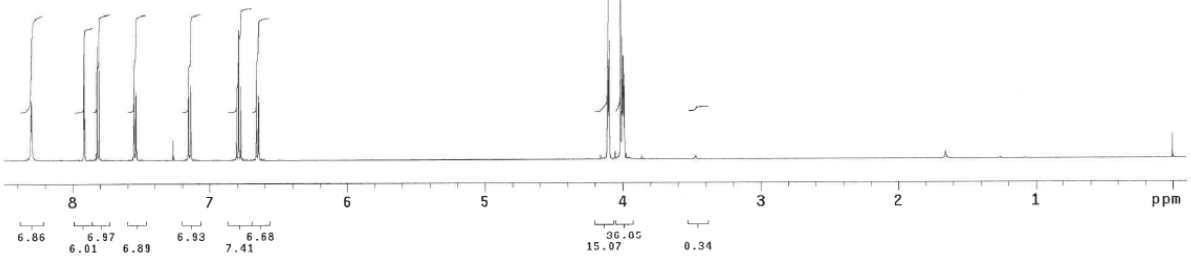
38d

STANDARD 1H
63992
1975-BGE
Berecz Gabor
2006.06.20. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244685 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	4145.752	8.299	12.5
2	3954.224	7.916	22.4
3	3952.026	7.912	22.3
4	3907.715	7.823	24.1
5	3899.414	7.806	27.4
6	3773.315	7.554	15.9
7	3771.118	7.549	15.4
8	3765.015	7.537	14.3
9	3762.939	7.533	13.5
10	3628.784	7.264	4.2
11	3574.097	7.155	13.9
12	3572.632	7.152	13.3
13	3565.918	7.139	15.6
14	3564.453	7.136	14.2
15	3400.146	6.807	13.4
16	3391.846	6.790	27.4
17	3383.667	6.774	15.5
18	3328.491	6.663	16.7
19	3327.026	6.660	15.9
20	3320.190	6.647	13.5
21	3318.726	6.644	12.0
22	2053.955	4.112	18.2
23	2051.392	4.107	16.6
24	2049.927	4.104	21.0
25	2047.852	4.100	16.7
26	2045.654	4.095	25.0
27	2025.635	4.055	1.7
28	2025.146	4.054	1.6
29	2005.127	4.014	159.1
30	2000.000	4.004	25.9
31	1997.803	3.999	16.9
32	1995.850	3.995	21.8
33	1994.263	3.992	15.4
34	1991.821	3.987	18.0
35	1985.107	3.974	1.4
36	827.637	1.657	1.5
37	0.000	0.000	5.1

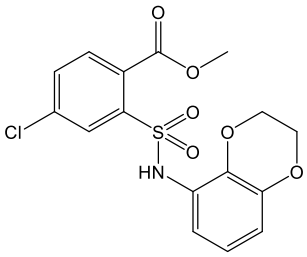


39

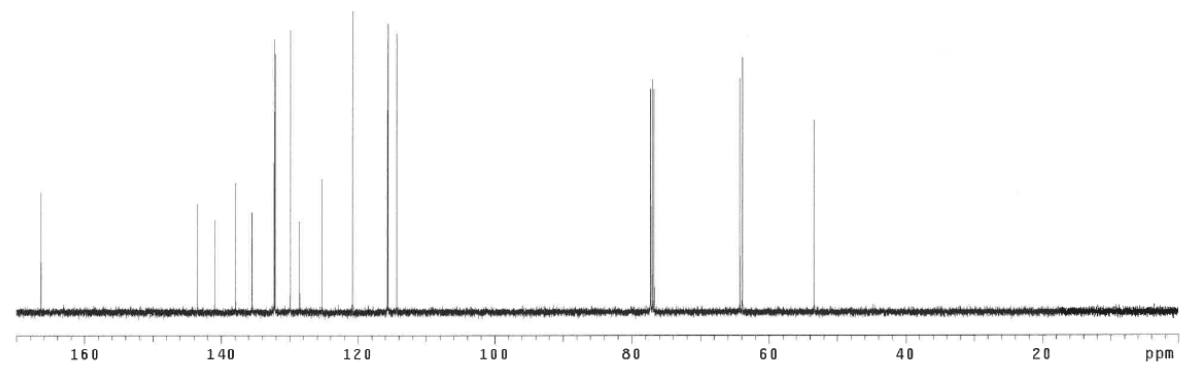


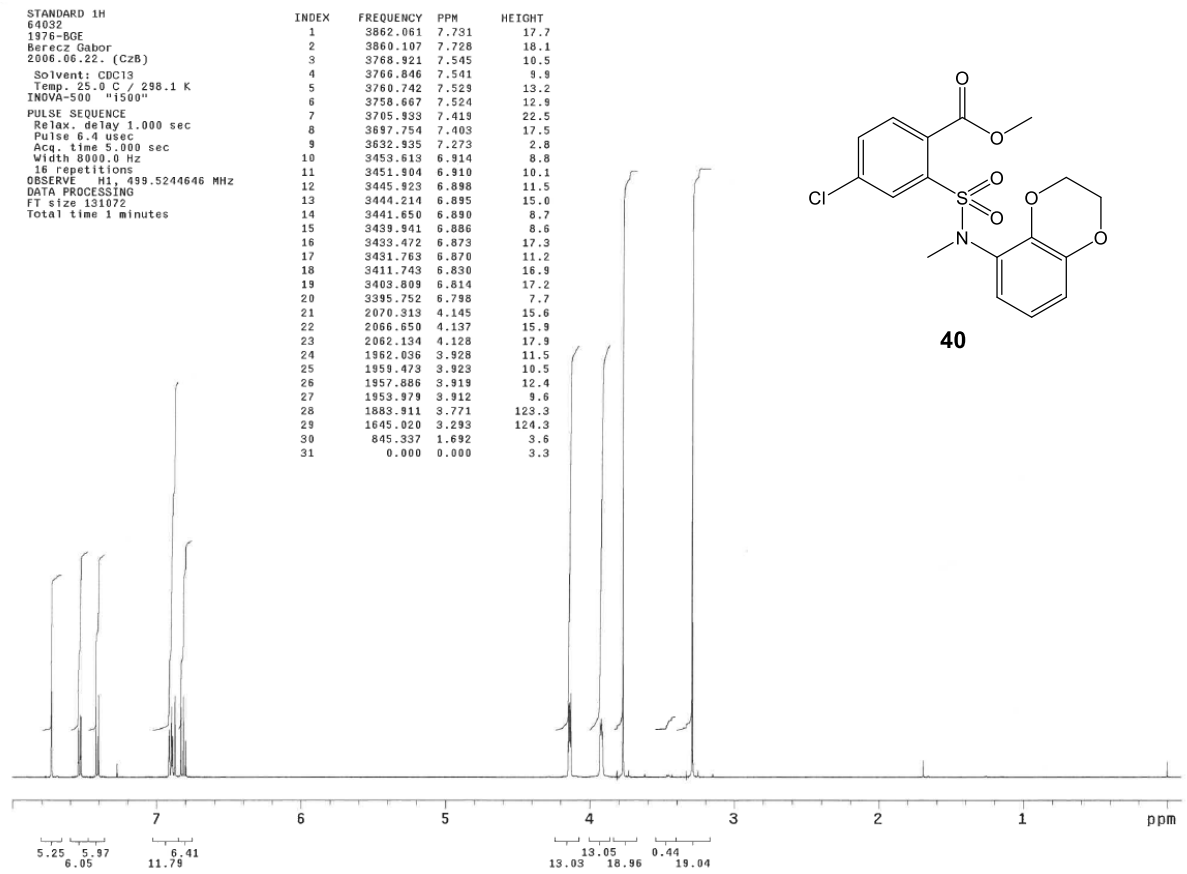
STANDARD 13C
63992
1975-BGE
Berecz Gabor
2006.06.20. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
user: 1-14-8/
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
183 repetitions
OBSERVE C13, 125.6055357 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 13 minutes

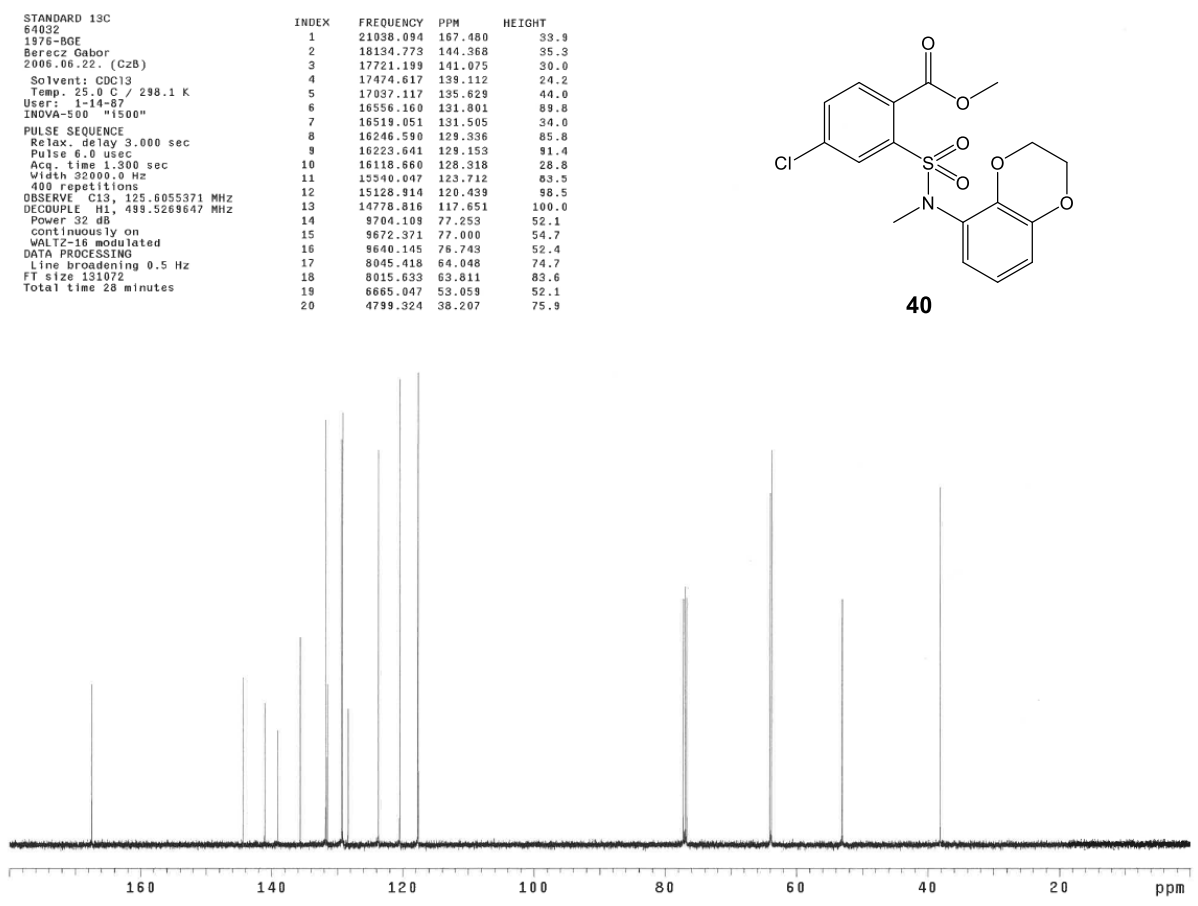
INDEX	FREQUENCY	PPM	HEIGHT
1	20898.445	166.369	25.7
2	18025.398	143.497	23.3
3	17708.016	140.970	19.8
4	17319.344	137.876	27.7
5	17022.957	135.517	21.4
6	16615.730	132.275	58.8
7	16593.758	132.100	55.5
8	16315.926	129.888	60.8
9	16145.516	128.532	19.4
10	15734.383	125.259	28.6
11	15176.766	120.819	64.8
12	14521.492	115.603	62.1
13	14357.918	114.301	60.0
14	9704.109	77.253	48.0
15	9672.371	77.000	50.1
16	9640.144	76.743	47.9
17	8074.226	64.277	50.4
18	8026.375	63.897	54.8
19	6707.039	53.394	41.3



39



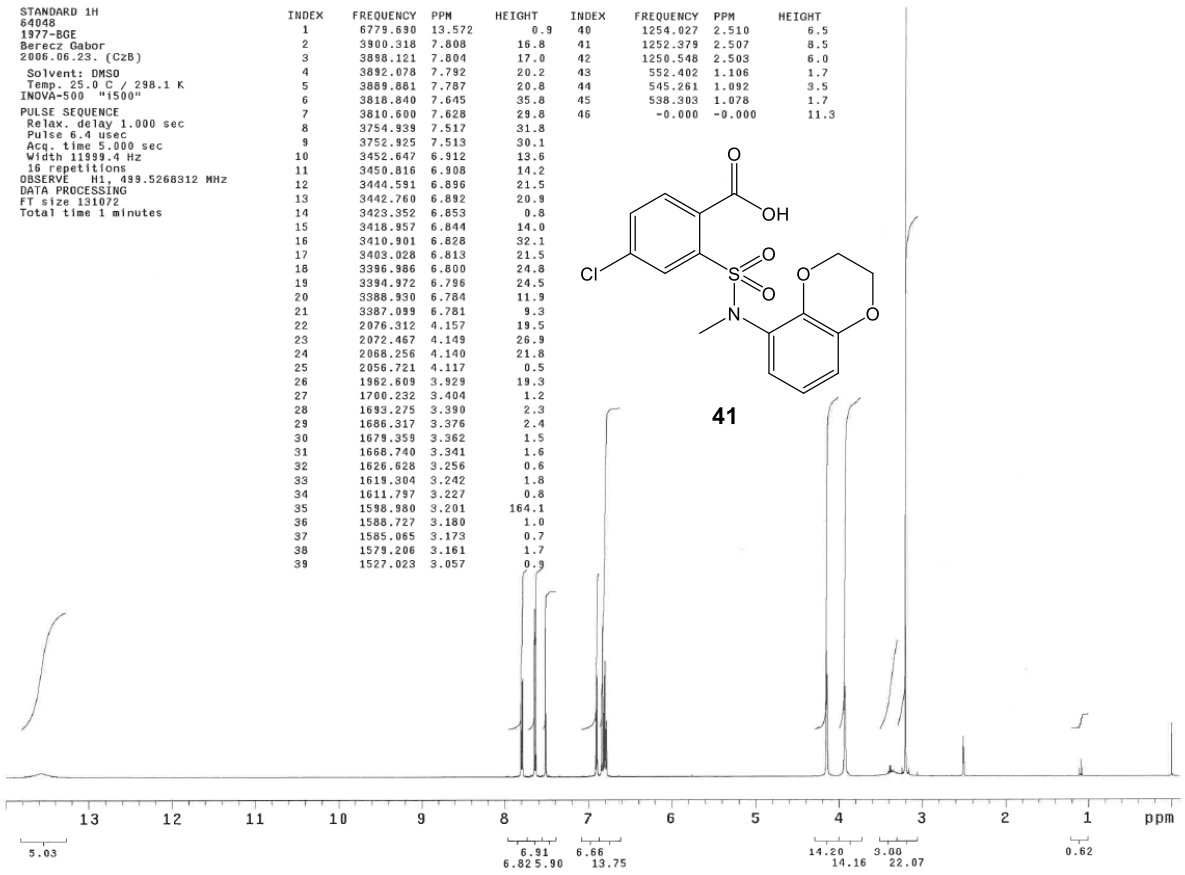

STANDARD 1H
64032
1976-BGE
Berecz Gabor
2006.06.22. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244646 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3862.061 7.731 17.7
2 3860.107 7.728 18.1
3 3768.921 7.545 10.5
4 3766.846 7.541 9.9
5 3760.742 7.529 13.2
6 3758.667 7.524 12.9
7 3705.933 7.419 22.5
8 3697.754 7.403 17.5
9 3632.935 7.273 2.8
10 3453.613 6.914 8.8
11 3451.904 6.910 10.1
12 3445.923 6.898 11.5
13 3444.214 6.895 15.0
14 3441.650 6.890 8.7
15 3439.941 6.886 8.6
16 3433.472 6.873 17.3
17 3431.763 6.870 11.2
18 3411.743 6.830 16.9
19 3403.809 6.814 17.2
20 3395.752 6.798 7.7
21 2070.313 4.145 15.6
22 2066.650 4.137 15.9
23 2062.134 4.128 17.9
24 1962.036 3.928 11.5
25 1959.473 3.923 10.5
26 1957.886 3.919 12.4
27 1953.979 3.912 9.6
28 1883.911 3.771 123.3
29 1645.020 3.293 124.3
30 845.337 1.692 3.6
31 0.000 0.000 3.3
O
O
Cl
S
O
O
O
O
N
40
7
6
5
4
3
2
1
ppm
5.25
5.97
6.05
6.41
11.79
13.03
13.05
18.96
0.44
19.04


STANDARD 13C
64032
1976-BGE
Berecz Gabor
2006.06.22. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
400 repetitions
OBSERVE C13, 125.6055371 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 28 minutes
INDEX FREQUENCY PPM HEIGHT
1 21038.094 167.480 33.9
2 18134.773 144.368 35.3
3 17721.199 141.075 30.0
4 17474.617 139.112 24.2
5 17037.117 135.629 44.0
6 16556.160 131.801 89.8
7 16519.051 131.505 34.0
8 16246.590 129.336 85.8
9 16223.641 129.153 91.4
10 16118.660 128.318 28.8
11 15540.047 123.712 83.5
12 15128.914 120.439 98.5
13 14778.816 117.651 100.0
14 9704.109 77.253 52.1
15 9672.371 77.000 54.7
16 9640.145 76.743 52.4
17 8045.418 64.048 74.7
18 8015.633 63.811 83.6
19 6665.047 53.059 52.1
20 4799.324 38.207 75.9
O
O
Cl
S
O
O
O
O
N
40
160
140
120
100
80
60
40
20
ppm

STANDARD 1H
64048
1977-BGE
Berecz Gabor
2006.06.23. (CzB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 11999.4 Hz
16 repetitions
OBSERVE H1, 499.5268312 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	6779.690	13.572	0.9	40	1254.027	2.510	6.5
2	3900.318	7.808	16.8	41	1252.379	2.507	8.5
3	3898.121	7.804	17.0	42	1250.548	2.503	6.0
4	3892.078	7.792	20.2	43	552.402	1.106	1.7
5	3889.881	7.787	20.8	44	545.261	1.092	3.5
6	3818.840	7.645	35.8	45	538.303	1.078	1.7
7	3810.600	7.628	29.8	46	-0.000	-0.000	11.3
8	3754.939	7.517	31.8				
9	3752.925	7.513	30.1				
10	3452.647	6.912	13.6				
11	3450.816	6.908	14.2				
12	3444.591	6.896	21.5				
13	3442.760	6.892	20.9				
14	3423.352	6.853	0.8				
15	3418.957	6.844	14.0				
16	3410.901	6.828	32.1				
17	3403.028	6.813	21.5				
18	3396.986	6.800	24.8				
19	3394.972	6.796	24.5				
20	3388.930	6.784	11.9				
21	3387.099	6.781	9.3				
22	2076.312	4.157	19.5				
23	2072.467	4.149	26.9				
24	2068.256	4.140	21.8				
25	2056.721	4.117	0.5				
26	1962.609	3.929	19.3				
27	1700.232	3.404	1.2				
28	1693.275	3.390	2.3				
29	1686.317	3.376	2.4				
30	1679.359	3.362	1.5				
31	1668.740	3.341	1.6				
32	1626.628	3.256	0.6				
33	1619.304	3.242	1.8				
34	1611.797	3.227	0.8				
35	1598.980	3.201	164.1				
36	1588.727	3.180	1.0				
37	1585.065	3.173	0.7				
38	1579.206	3.161	1.7				
39	1527.023	3.057	0.9				

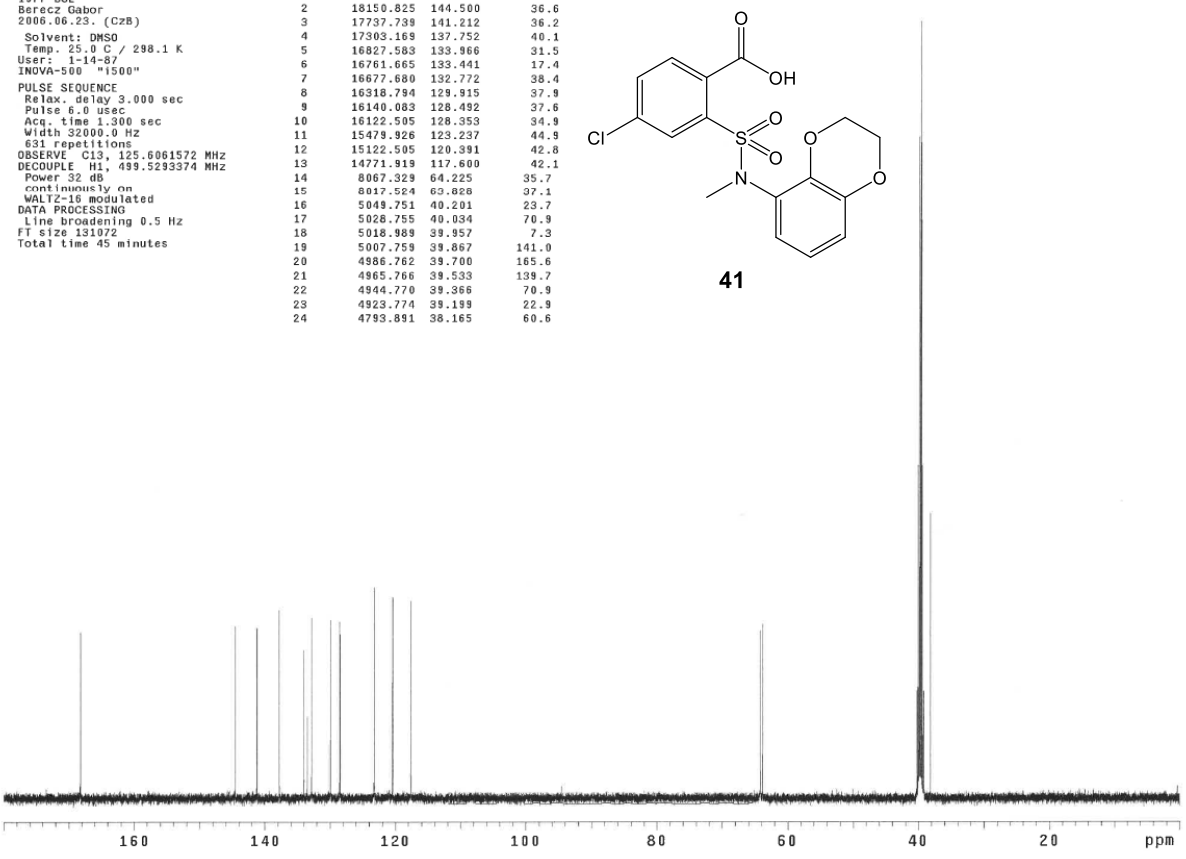
41



STANDARD 13C
64048
1977-BGE
Berecz Gabor
2006.06.23. (CzB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
631 repetitions
OBSERVE C13, 125.6061572 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 45 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	21128.364	168.205	35.2
2	18150.825	144.500	36.6
3	17737.739	141.212	36.2
4	17303.169	137.752	40.1
5	16827.583	133.966	31.5
6	16761.665	133.441	17.4
7	16677.680	132.772	38.4
8	16318.794	129.915	37.9
9	16140.083	128.492	37.6
10	16122.505	128.353	34.9
11	15479.926	123.237	44.9
12	15122.505	120.391	42.8
13	14771.919	117.600	42.1
14	8067.329	64.225	35.7
15	8017.524	63.828	37.1
16	5049.751	40.201	23.7
17	5028.755	40.034	70.9
18	5018.989	39.957	7.3
19	5007.759	39.867	141.0
20	4986.762	39.700	165.6
21	4965.766	39.533	139.7
22	4944.770	39.366	70.9
23	4923.774	39.199	22.9
24	4793.891	38.165	60.6

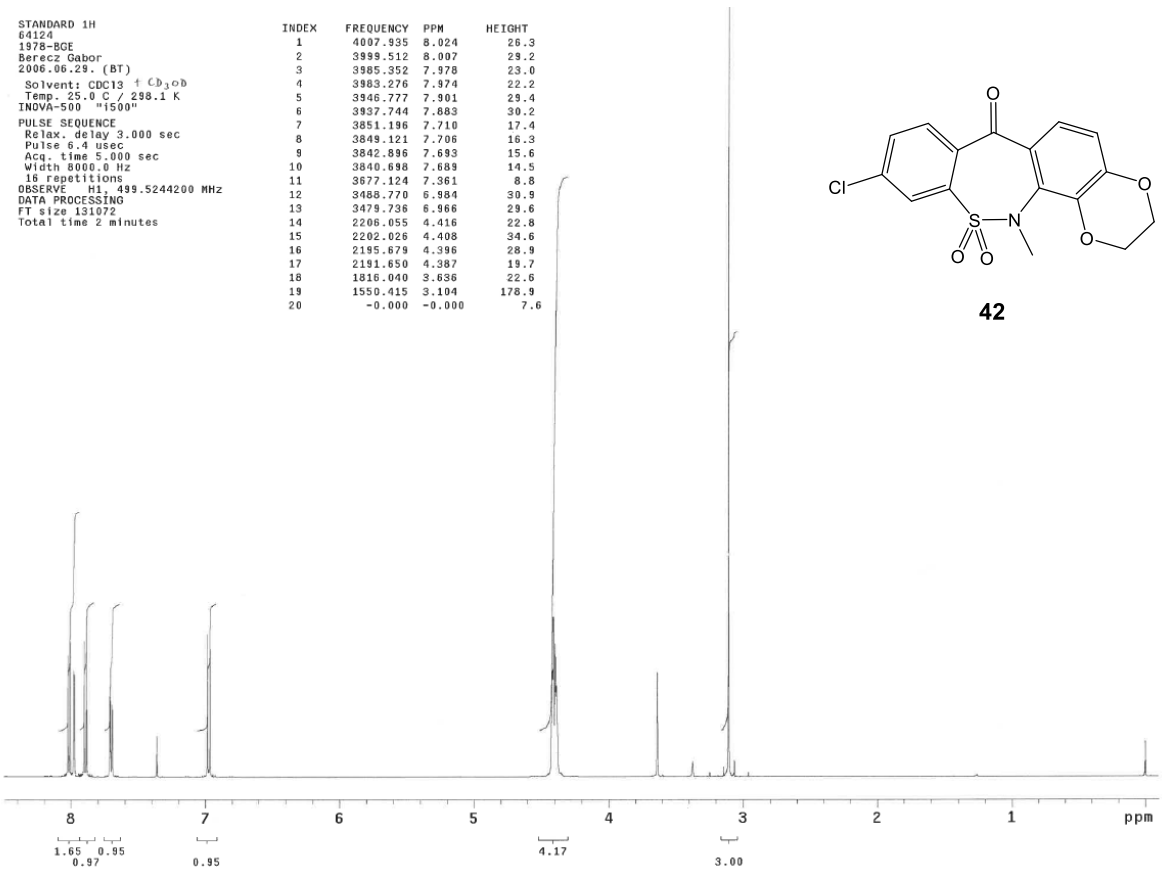
41



STANDARD 1H
64124
1978-BGE
Berecz Gabor
2006.06.29. (BT)
Solvent: CDCl3 + CD_3OD
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244200 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

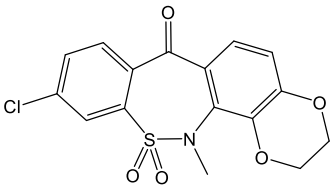
INDEX	FREQUENCY	PPM	HEIGHT
1	4007.935	8.024	26.3
2	3999.512	8.007	29.2
3	3985.352	7.978	23.0
4	3983.276	7.974	22.2
5	3946.777	7.901	29.4
6	3937.744	7.883	30.2
7	3851.196	7.710	17.4
8	3849.121	7.706	16.3
9	3842.896	7.693	15.6
10	3840.698	7.689	14.5
11	3677.124	7.361	8.8
12	3488.770	6.984	30.9
13	3479.736	6.966	29.6
14	2206.055	4.416	22.8
15	2202.026	4.408	34.6
16	2195.679	4.396	28.9
17	2191.650	4.387	19.7
18	1816.040	3.636	22.6
19	1550.415	3.104	178.9
20	-0.000	-0.000	7.6

42



STANDARD 13C
64124
1978-BGE
Berecz Gabor
2006.06.29. (BT)
Solvent: CDCl3 + CD_3OD
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
288 repetitions
OBSERVE C13, 125.6055381 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	23565.926	187.604	23.9
2	18758.797	149.335	35.0
3	17411.141	138.607	24.5
4	17397.469	138.498	33.7
5	17279.793	137.561	23.7
6	16842.781	134.082	32.5
7	16812.996	133.845	98.7
8	16720.223	133.107	85.4
9	16393.074	130.502	17.0
10	15881.844	126.432	100.0
11	15820.320	125.943	24.2
12	15622.078	124.365	87.6
13	14605.477	116.272	85.7
14	9704.598	77.257	81.4
15	9672.371	77.000	90.2
16	9640.145	76.743	87.6
17	8080.574	64.328	85.4
18	8051.766	64.099	90.5
19	6175.301	49.160	21.0
20	6153.817	48.989	45.5
21	6132.332	48.818	58.1
22	6110.848	48.647	52.3
23	6089.363	48.476	25.0
24	4740.242	37.736	71.2



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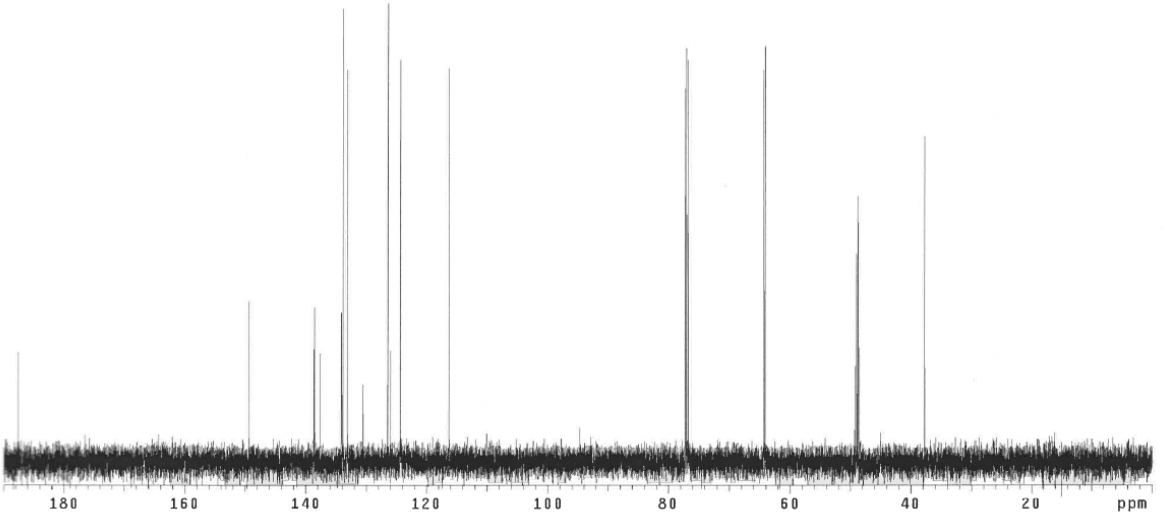
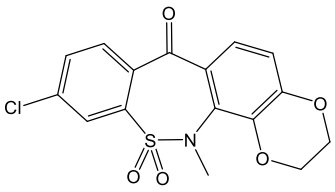


GHSQC_DA (140 Hz)
64124
1978-BGE
Berecz Gabor
2006.06.29. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE: ghsqc_da
Relax. delay 1.500 sec
Acq. time 0.205 sec
Width 5002.2 Hz
2D Width 32000.0 Hz
2 repetitions
2 x 256 increments
OBSERVE H1, 499.5244235 MHz
DECOUPLE C13, 125.6174312 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Gauss apodization 0.095 sec
F1 DATA PROCESSING
Gauss apodization 0.015 sec
FT size 2048 x 2048
Total time 30 minutes



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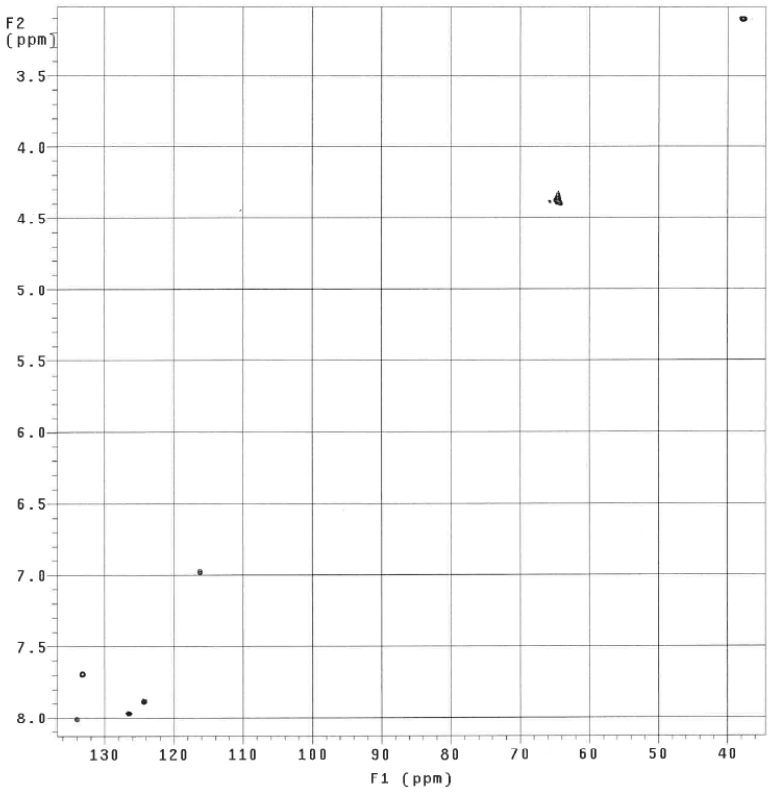
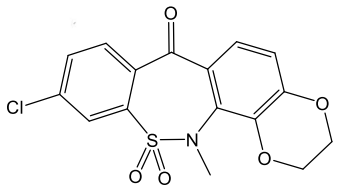


GHMQC_DA (140Hz, 8Hz)
64124
1978-BGE
Berecz Gabor
2006.06.29. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE: ghmqc_da
Relax. delay 1.500 sec
Acq. time 0.205 sec
Width 5002.2 Hz
2D Width 32000.0 Hz
4 repetitions
256 increments
OBSERVE H1, 499.5244235 MHz
DATA PROCESSING
Sine bell 0.102 sec
F1 DATA PROCESSING
Sine bell 0.002 sec
FT size 4096 x 512
Total time 29 minutes



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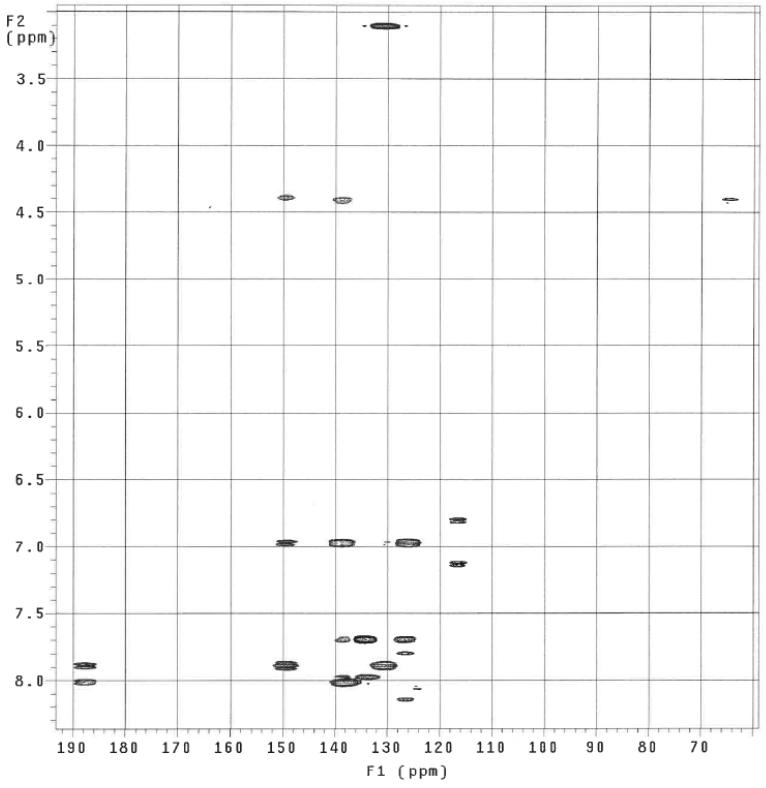

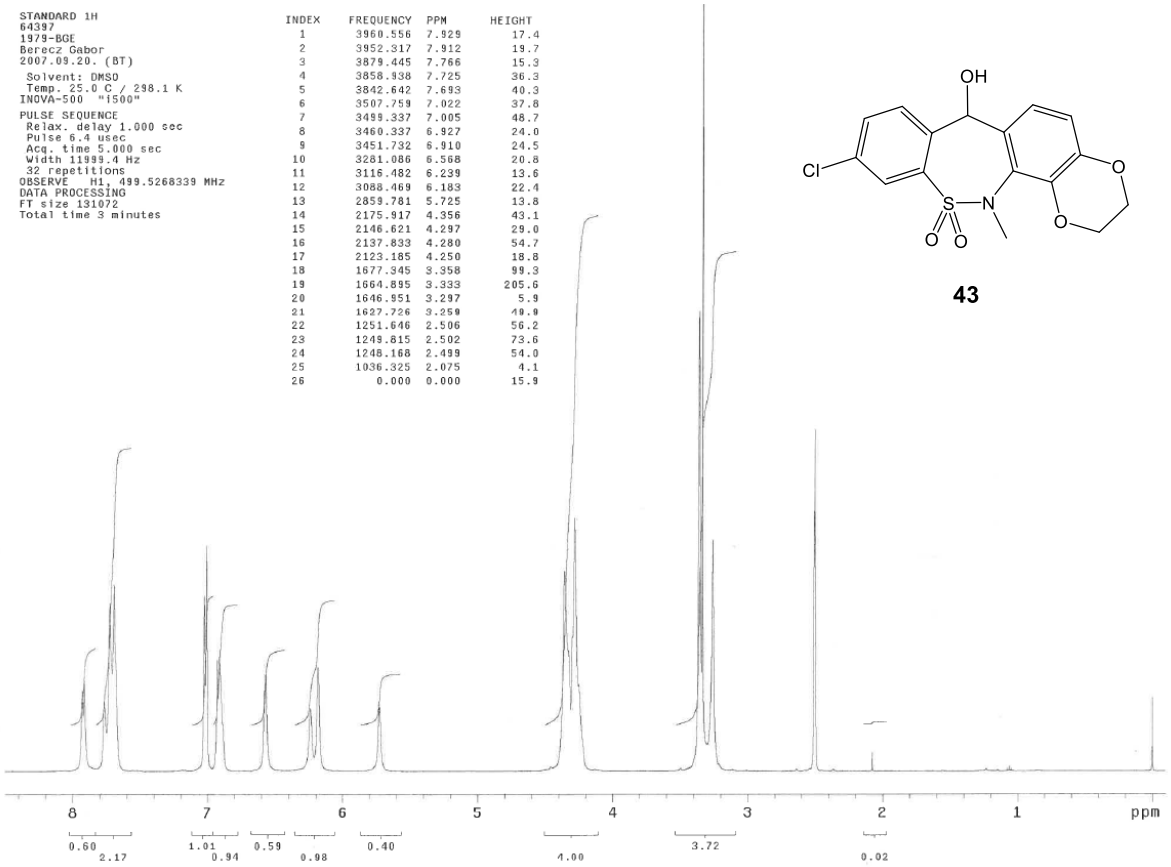
STANDARD 1H
64397
1979-BGE
Berecz Gabor
2007.09.20. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 11989.4 Hz
32 repetitions
OBSERVE H1, 499.5268339 MHz
DATA PROCESSING
FT size 131072
Total time 3 minutes
INDEX FREQUENCY PPM HEIGHT
1 3960.556 7.929 17.4
2 3952.317 7.912 19.7
3 3879.445 7.766 15.3
4 3858.938 7.725 36.3
5 3842.642 7.693 40.3
6 3507.759 7.022 37.8
7 3499.337 7.005 48.7
8 3460.337 6.927 24.0
9 3451.732 6.910 24.5
10 3281.086 6.568 20.8
11 3116.482 6.239 13.6
12 3088.469 6.183 22.4
13 2859.781 5.725 13.8
14 2175.917 4.356 43.1
15 2146.621 4.297 29.0
16 2137.833 4.280 54.7
17 2123.185 4.250 18.8
18 1677.345 3.358 99.3
19 1664.895 3.333 205.6
20 1646.951 3.297 5.9
21 1627.726 3.259 49.9
22 1251.646 2.506 56.2
23 1249.815 2.502 73.6
24 1248.168 2.499 54.0
25 1036.325 2.075 4.1
26 0.000 0.000 15.9
OH
Cl
S
N
O
O
O
O
43
8
7
6
5
4
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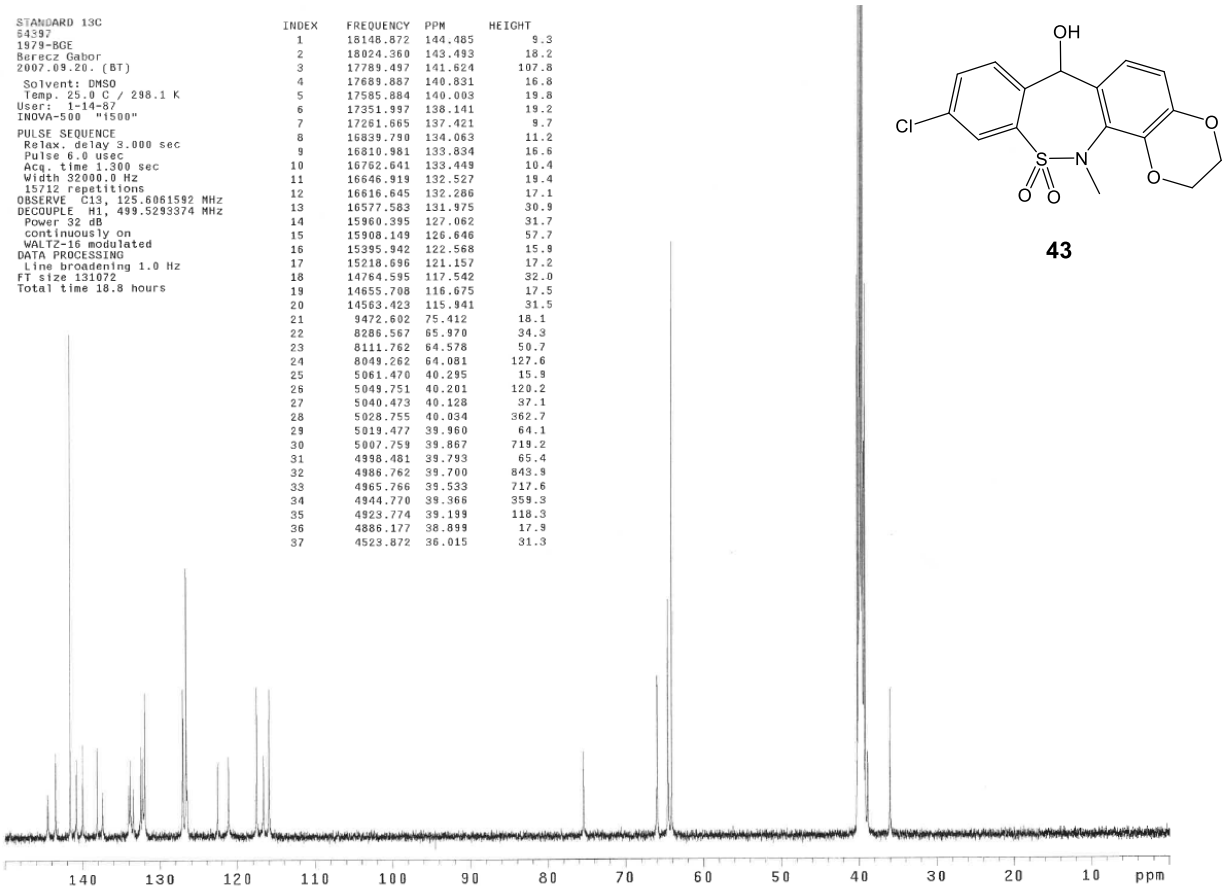
STANDARD 13C
54397
1979-BGE
Berecz Gabor
2007.09.20. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
15712 repetitions
OBSERVE C13, 125.6061592 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 18.8 hours
INDEX FREQUENCY PPM HEIGHT
1 18148.872 144.485 9.3
2 18024.360 143.493 18.2
3 17789.497 141.624 107.8
4 17689.887 140.831 16.8
5 17585.884 140.003 19.8
6 17351.997 138.141 19.2
7 17261.665 137.421 9.7
8 16839.790 134.063 11.2
9 16810.981 133.834 16.6
10 16762.641 133.449 10.4
11 16646.919 132.527 19.4
12 16616.645 132.286 17.1
13 16577.583 131.975 30.9
14 15960.395 127.062 31.7
15 15908.149 126.646 57.7
16 15395.942 122.568 15.9
17 15218.696 121.157 17.2
18 14764.595 117.542 32.0
19 14655.708 116.675 17.5
20 14563.423 115.941 31.5
21 9472.602 75.412 18.1
22 8286.567 65.970 34.3
23 8111.762 64.578 50.7
24 8049.262 64.081 127.6
25 5061.470 40.295 15.9
26 5049.751 40.201 120.2
27 5040.473 40.128 37.1
28 5028.755 40.034 362.7
29 5019.477 39.960 64.1
30 5007.759 39.867 719.2
31 4998.481 39.793 65.4
32 4986.762 39.700 843.9
33 4965.766 39.533 717.6
34 4944.770 39.366 359.3
35 4923.774 39.199 118.3
36 4886.177 38.899 17.9
37 4523.872 36.015 31.3
OH
Cl
S
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20
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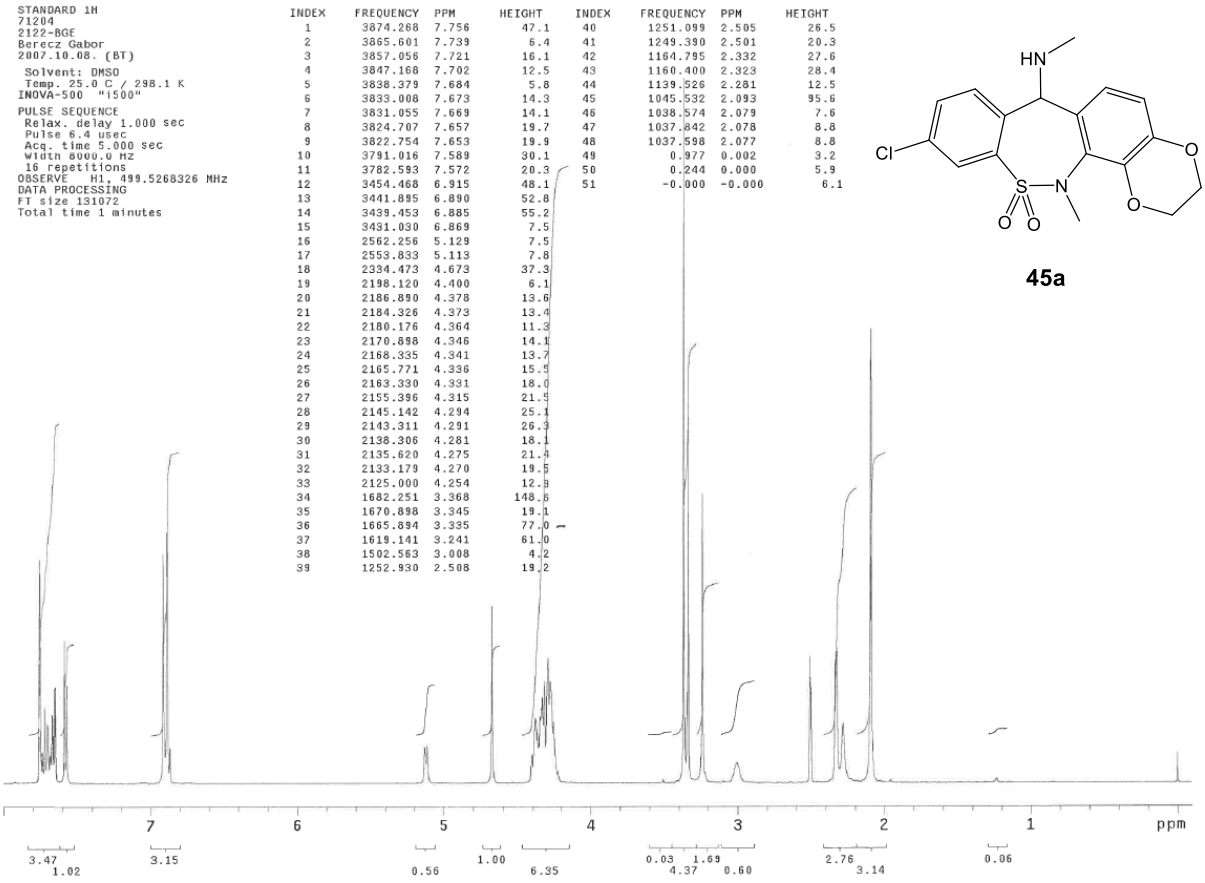
ppm


STANDARD 1H
71204
2122-BGE
Berecz Gabor
2007.10.08. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268326 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes
INDEX FREQUENCY PPM HEIGHT
1 3874.268 7.756 47.1
2 3865.601 7.739 6.4
3 3857.056 7.721 16.1
4 3847.168 7.702 12.5
5 3838.379 7.684 5.8
6 3833.008 7.673 14.3
7 3831.055 7.669 14.1
8 3824.707 7.657 19.7
9 3822.754 7.653 19.9
10 3791.016 7.589 30.1
11 3782.593 7.572 20.3
12 3454.468 6.915 48.1
13 3441.895 6.890 52.8
14 3439.453 6.885 55.2
15 3431.030 6.869 7.5
16 2562.256 5.129 7.5
17 2553.833 5.113 7.8
18 2334.473 4.673 37.3
19 2198.120 4.400 6.1
20 2186.890 4.378 13.6
21 2184.326 4.373 13.4
22 2180.176 4.364 11.3
23 2170.898 4.346 14.1
24 2168.335 4.341 13.7
25 2165.771 4.336 15.5
26 2163.330 4.331 18.0
27 2155.396 4.315 21.5
28 2145.142 4.294 25.1
29 2143.311 4.291 26.3
30 2138.306 4.281 18.1
31 2135.620 4.275 21.4
32 2133.179 4.270 19.5
33 2125.000 4.254 12.8
34 1682.251 3.368 148.8
35 1670.898 3.345 19.1
36 1665.894 3.335 77.0
37 1619.141 3.241 61.0
38 1502.563 3.008 4.2
39 1252.930 2.508 19.2
INDEX FREQUENCY PPM HEIGHT
40 1251.099 2.505 26.5
41 1249.390 2.501 20.3
42 1164.795 2.332 27.6
43 1160.400 2.323 28.4
44 1139.526 2.281 12.5
45 1045.532 2.093 95.6
46 1038.574 2.079 7.6
47 1037.842 2.078 8.8
48 1037.598 2.077 8.8
49 0.977 0.002 3.2
50 0.244 0.000 5.9
51 -0.000 -0.000 6.1
HN
Cl
S
N
O
O
O
O
45a
7
6
5
4
3
2
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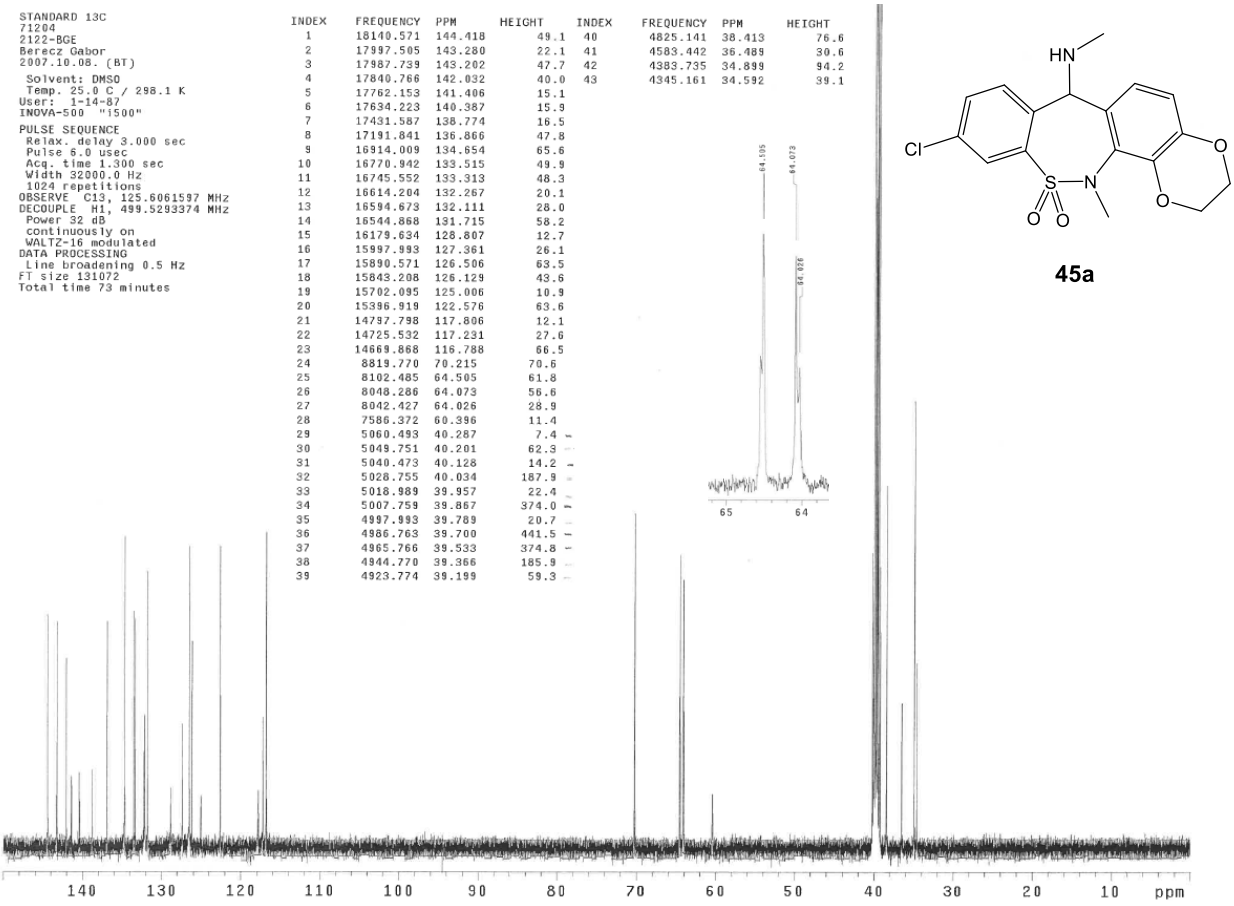
STANDARD 13C
71204
2122-BGE
Berecz Gabor
2007.10.08. (BT)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
1024 repetitions
OBSERVE C13, 125.6061597 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 73 minutes
INDEX FREQUENCY PPM HEIGHT
1 18140.571 144.418 49.1
2 17997.505 143.280 22.1
3 17987.739 143.202 47.7
4 17840.766 142.032 40.0
5 17762.153 141.406 15.1
6 17634.223 140.387 15.9
7 17431.587 138.774 16.5
8 17191.841 136.866 47.8
9 16914.009 134.654 65.6
10 16770.942 133.515 49.9
11 16745.552 133.313 48.3
12 16614.204 132.267 20.1
13 16594.673 132.111 28.0
14 16544.868 131.715 58.2
15 16179.634 128.807 12.7
16 15997.993 127.361 26.1
17 15890.571 126.506 63.5
18 15843.208 126.129 43.6
19 15702.095 125.006 10.9
20 15396.919 122.576 63.6
21 14797.798 117.806 12.1
22 14725.532 117.231 27.6
23 14669.868 116.788 66.5
24 8819.770 70.215 70.6
25 8102.485 64.505 61.8
26 8048.286 64.073 56.6
27 8042.427 64.026 28.9
28 7586.372 60.396 11.4
29 5060.493 40.287 7.4
30 5049.751 40.201 62.3
31 5040.473 40.128 14.2
32 5028.755 40.034 187.9
33 5018.989 39.957 22.4
34 5007.759 39.867 374.0
35 4997.993 39.789 20.7
36 4986.763 39.700 441.5
37 4965.766 39.533 374.8
38 4944.770 39.366 185.9
39 4923.774 39.199 59.3
INDEX FREQUENCY PPM HEIGHT
40 4825.141 38.413 76.6
41 4583.442 36.489 30.6
42 4383.735 34.899 94.2
43 4345.161 34.592 39.1
64.195
64.073
64.026
65
64
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Cl
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O
O
O
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120
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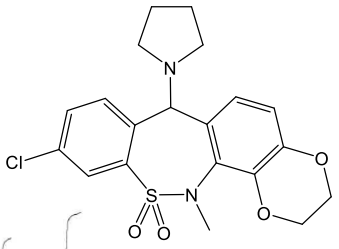
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
64558
1982-BGE
Berecz Gabor
2006.07.24. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244689 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3966.309	7.940	19.0	40	1110.962	2.224	8.2
2	3964.111	7.936	18.8	41	1108.765	2.220	7.6
3	3676.514	7.360	11.1	42	1106.567	2.215	9.1
4	3674.316	7.356	10.5	43	1104.248	2.211	12.3
5	3668.213	7.343	18.7	44	1099.976	2.202	5.1
6	3666.016	7.339	18.4	45	1077.393	2.157	4.7
7	3644.043	7.295	26.4	46	1075.928	2.154	5.0
8	3635.742	7.278	16.0	47	1071.045	2.144	12.4
9	3629.395	7.266	2.1	48	1069.092	2.140	9.3
10	3628.418	7.264	7.1	49	1064.697	2.131	8.2
11	3395.508	6.797	20.7	50	1062.134	2.126	8.2
12	3387.085	6.781	37.2	51	1057.617	2.117	3.5
13	3367.676	6.742	30.8	52	848.633	1.699	1.7
14	3359.131	6.725	17.0	53	844.116	1.690	2.9
15	2199.219	4.403	2.3	54	840.576	1.683	14.2
16	2195.435	4.395	3.8	55	836.792	1.675	20.8
17	2194.458	4.393	3.9	56	834.106	1.670	41.1
18	2190.796	4.386	3.4	57	831.543	1.665	19.7
19	2187.622	4.379	6.9	58	827.759	1.657	12.0
20	2184.204	4.373	9.2	59	819.946	1.641	1.6
21	2182.739	4.370	10.9	60	814.331	1.630	6.4
22	2179.565	4.363	9.0	61	0.977	0.002	2.3
23	2176.636	4.357	6.5	62	-0.000	-0.000	8.1
24	2172.852	4.350	14.1				
25	2168.579	4.341	9.9				
26	2165.039	4.334	2.2				
27	2161.133	4.326	5.3				
28	2157.227	4.319	4.4				
29	2151.001	4.306	1.9				
30	2149.414	4.303	1.9				
31	2142.822	4.290	20.7				
32	2138.794	4.282	27.2				
33	2135.132	4.274	11.6				
34	2017.700	4.039	32.0				
35	1730.591	3.464	1.6				
36	1717.773	3.439	1.6				
37	1710.327	3.424	163.4				
38	1119.263	2.241	3.2				
39	1113.281	2.229	8.2				



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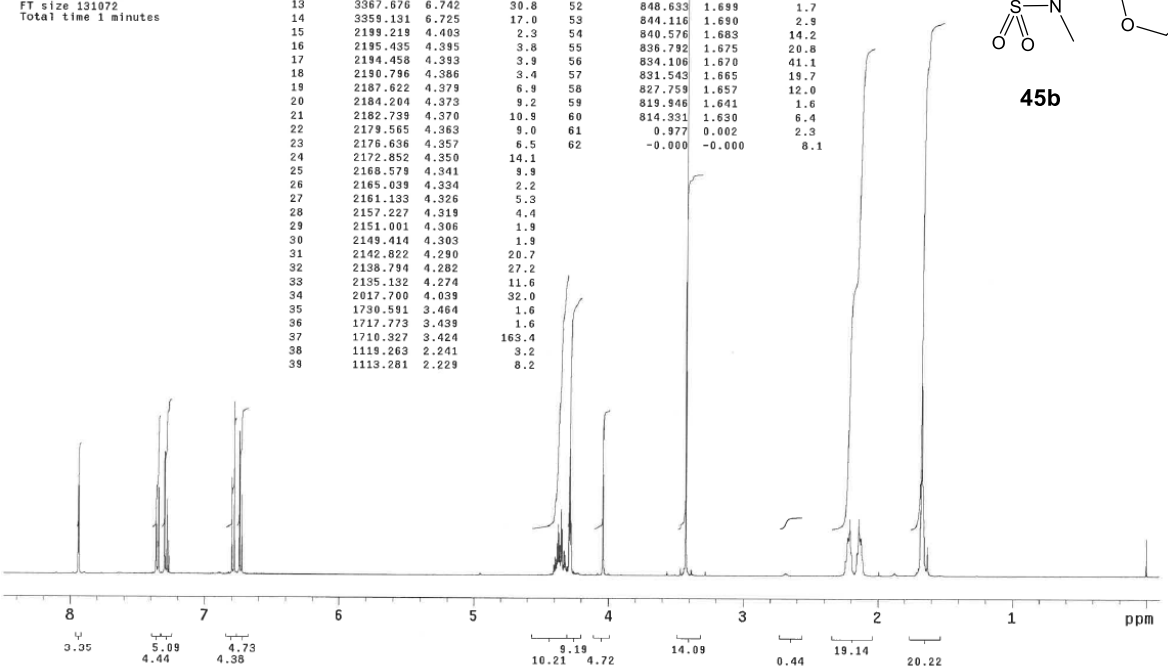
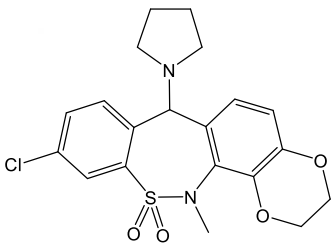


STANDARD 13C
64558
1982-BGE
Berecz Gabor
2006.07.24. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 27220.1 Hz
102 repetitions
OBSERVE C13, 125.6055333 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 7 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18160.806	144.575	19.1
2	18019.588	143.451	17.6
3	17881.277	142.350	15.2
4	17038.955	135.644	23.0
5	16935.118	134.817	24.6
6	16928.473	134.765	22.0
7	16713.323	133.052	46.4
8	16440.441	130.879	43.5
9	16090.304	128.092	46.4
10	15785.024	125.662	15.5
11	15235.521	121.287	45.0
12	14712.600	117.124	46.6
13	9704.353	77.255	64.8
14	9672.371	77.000	66.0
15	9640.389	76.745	65.0
16	9613.807	76.534	43.2
17	8099.039	64.475	44.2
18	8053.350	64.111	43.0
19	6739.194	53.650	86.2
20	4787.482	38.112	33.9
21	2909.700	23.164	89.6



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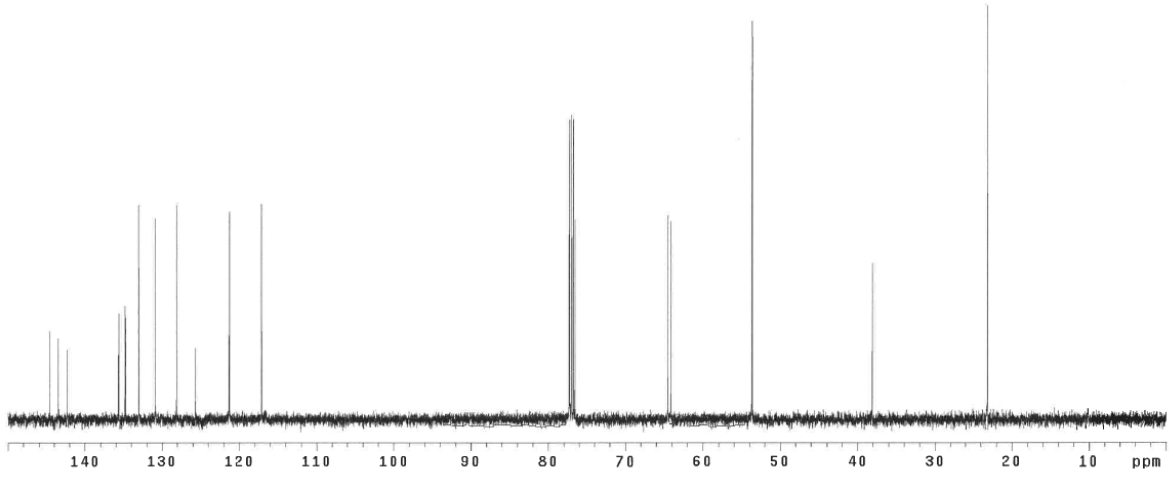
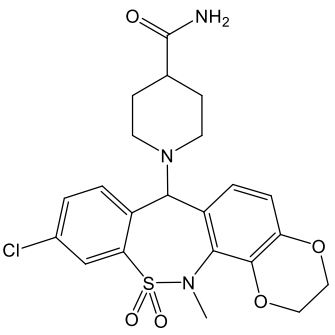
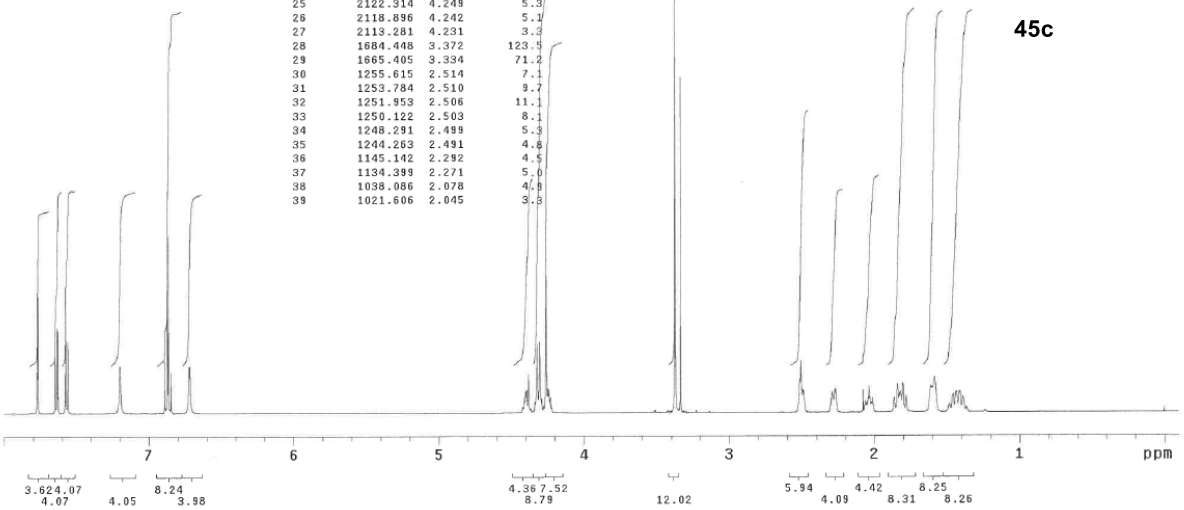


STANDARD 1H
66309
2025-BGE
Berecz Gabor
2006.11.14. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268317 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3881.470	7.770	24.0	40	1017.822	2.038	5.6
2	3879.272	7.766	24.7	41	1014.160	2.030	3.4
3	3820.923	7.649	11.8	42	1006.226	2.014	3.1
4	3818.726	7.645	10.5	43	929.932	1.862	3.3
5	3812.622	7.632	18.1	44	920.166	1.842	6.1
6	3810.303	7.628	17.5	45	918.457	1.839	6.0
7	3783.813	7.575	23.6	46	913.696	1.829	3.6
8	3775.391	7.558	15.1	47	911.011	1.824	4.4
9	3596.191	7.199	10.1	48	909.180	1.820	4.5
10	3441.284	6.889	11.0	49	901.855	1.805	6.3
11	3432.861	6.872	47.2	50	899.658	1.801	6.1
12	3428.589	6.864	37.6	51	890.137	1.782	3.6
13	3420.166	6.847	8.6	52	804.565	1.611	5.8
14	3357.300	6.721	10.0	53	800.659	1.603	5.4
15	2203.369	4.411	3.4	54	793.845	1.589	7.0
16	2198.853	4.402	4.4	55	791.260	1.584	7.6
17	2197.510	4.399	4.9	56	730.835	1.463	3.6
18	2194.214	4.393	4.8	57	727.539	1.456	4.0
19	2188.354	4.381	8.3	58	717.529	1.436	4.5
20	2158.569	4.321	14.6	59	704.712	1.411	4.6
21	2150.757	4.306	15.2	60	695.190	1.392	3.5
22	2149.414	4.303	11.9	61	692.261	1.386	3.1
23	2142.578	4.289	3.1				
24	2127.808	4.260	34.8				
25	2122.314	4.249	5.3				
26	2118.896	4.242	5.1				
27	2113.281	4.231	3.3				
28	1684.448	3.372	123.5				
29	1665.405	3.334	71.2				
30	1255.615	2.514	7.1				
31	1253.784	2.510	9.7				
32	1251.953	2.506	11.1				
33	1250.122	2.503	8.1				
34	1248.291	2.499	5.3				
35	1244.263	2.491	4.8				
36	1145.142	2.292	4.5				
37	1134.399	2.271	5.0				
38	1038.086	2.078	4.9				
39	1021.606	2.045	3.3				



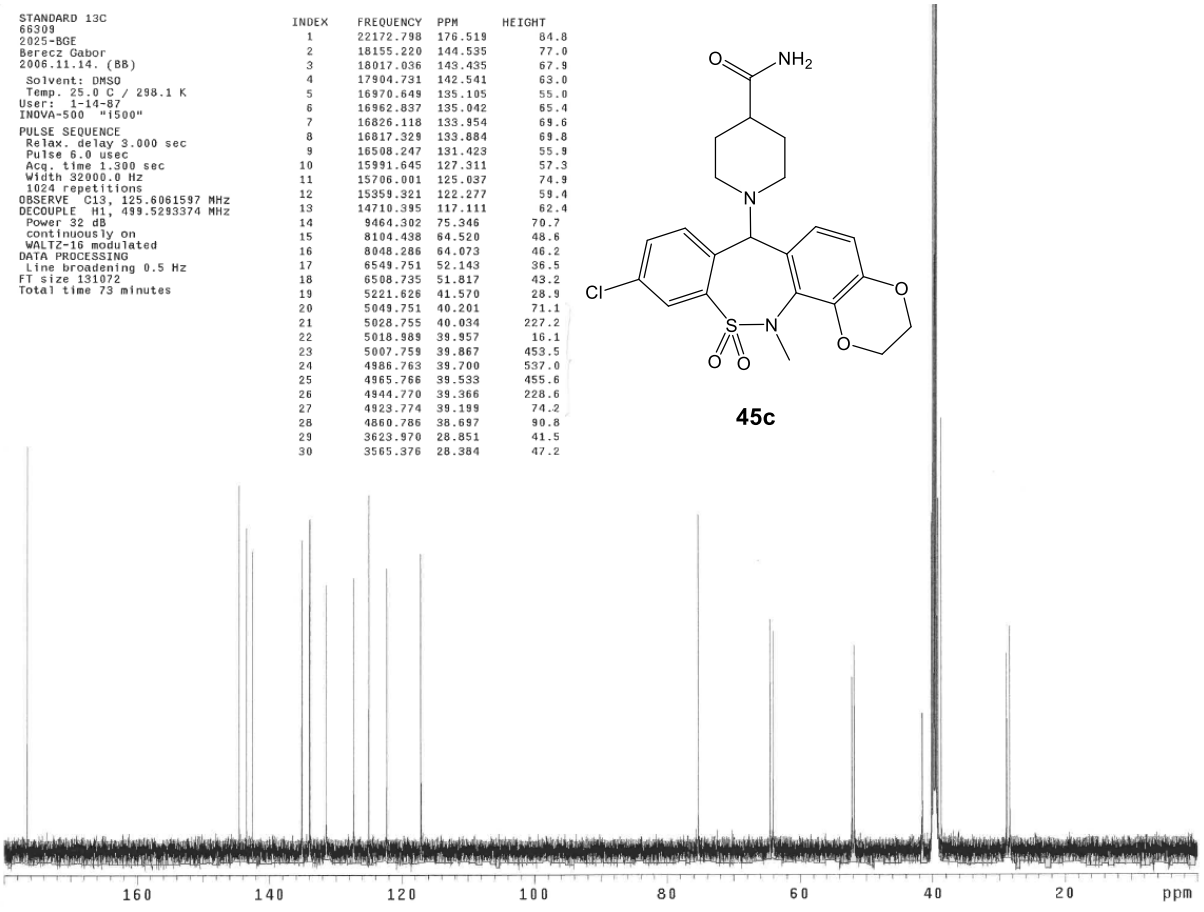
45c



STANDARD 13C
66309
2025-BGE
Berecz Gabor
2006.11.14. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
1024 repetitions
OBSERVE C13, 125.6061597 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 73 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	22172.798	176.519	84.8
2	18155.220	144.535	77.0
3	18017.036	143.435	67.8
4	17904.731	142.541	63.0
5	16970.649	135.105	55.0
6	16962.837	135.042	65.4
7	16826.118	133.954	69.6
8	16817.329	133.884	69.8
9	16508.247	131.423	55.9
10	15991.645	127.311	57.3
11	15706.001	125.037	74.9
12	15359.321	122.277	59.4
13	14710.395	117.111	62.4
14	9464.302	75.346	70.7
15	8104.438	64.520	48.6
16	8048.286	64.073	46.2
17	6549.751	52.143	36.5
18	6508.735	51.817	43.2
19	5221.626	41.570	28.9
20	5049.751	40.201	71.1
21	5028.755	40.034	227.2
22	5018.989	39.957	16.1
23	5007.759	39.867	453.5
24	4986.763	39.700	537.0
25	4965.766	39.533	455.6
26	4944.770	39.366	228.6
27	4923.774	39.199	74.2
28	4860.786	38.697	90.8
29	3623.970	28.851	41.5
30	3565.376	28.384	47.2

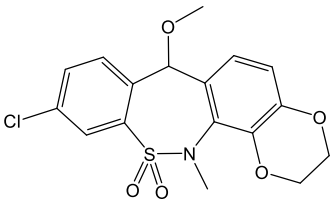
45c



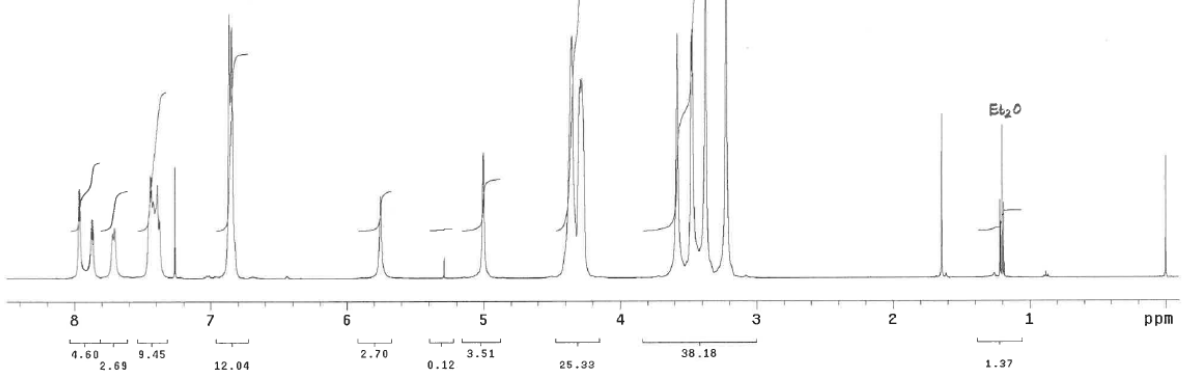
STANDARD 1H
64557
1981-BGE
Berecz Gabor
2006.07.24. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244693 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

2 konferencia

INDEX	FREQUENCY	PPM	HEIGHT
1	3978.760	7.965	18.8
2	3931.763	7.871	12.5
3	3932.007	7.871	12.5
4	3857.300	7.722	9.6
5	3849.365	7.706	10.7
6	3723.389	7.454	13.3
7	3716.553	7.440	22.0
8	3707.031	7.421	16.4
9	3692.383	7.392	19.9
10	3684.082	7.375	12.5
11	3627.319	7.262	23.6
12	3429.443	6.865	56.3
13	3421.021	6.849	53.6
14	2873.901	5.753	17.4
15	2641.846	5.289	4.4
16	2498.657	5.002	26.8
17	2174.927	4.354	51.7
18	2143.677	4.291	42.3
19	2137.329	4.279	42.6
20	1790.039	3.583	52.1
21	1746.460	3.496	11.8
22	1739.380	3.482	50.2
23	1736.572	3.476	53.0
24	1732.422	3.468	43.6
25	1725.464	3.454	15.2
26	1685.547	3.374	81.7
27	1610.474	3.224	81.7
28	821.899	1.645	35.0
29	608.521	1.218	16.5
30	601.562	1.204	32.5
31	594.482	1.190	16.0
32	-0.000	-0.000	25.9



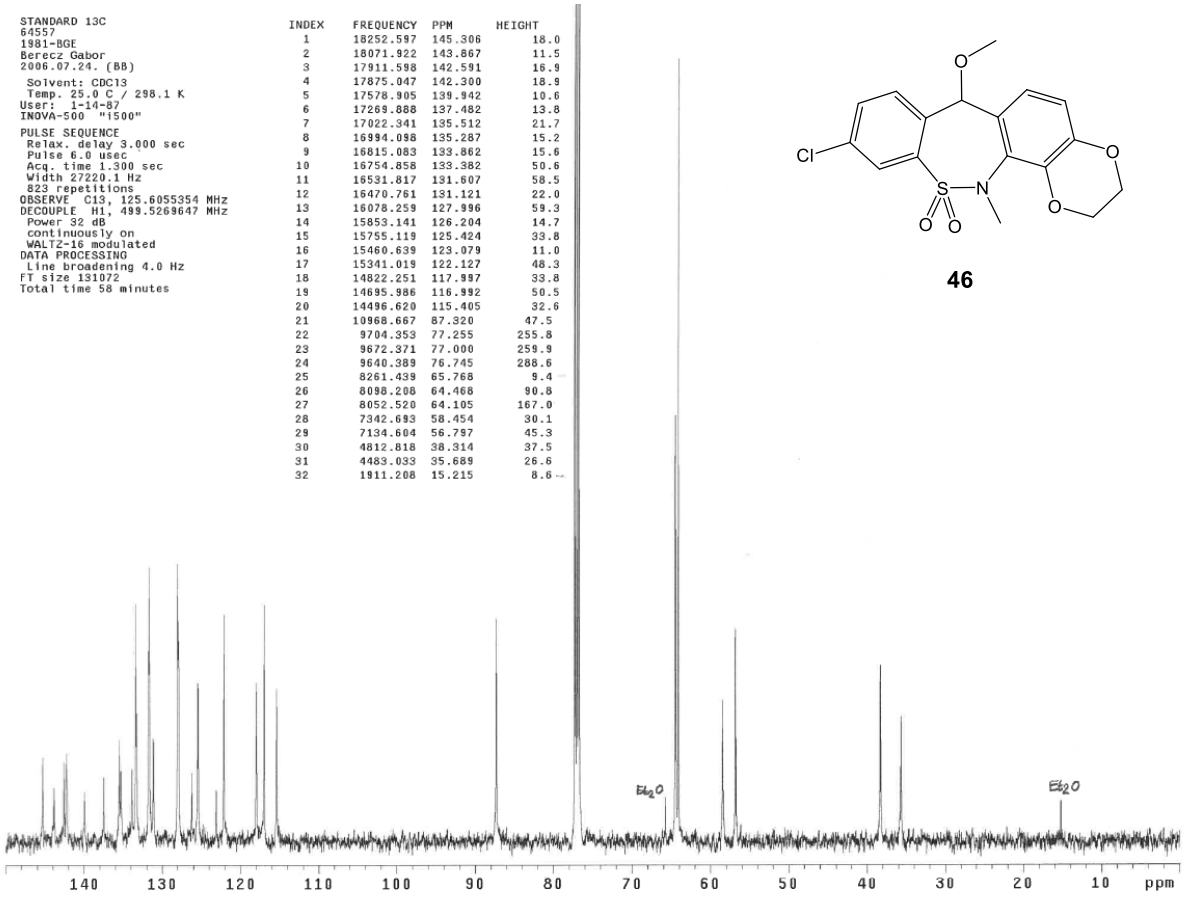
46

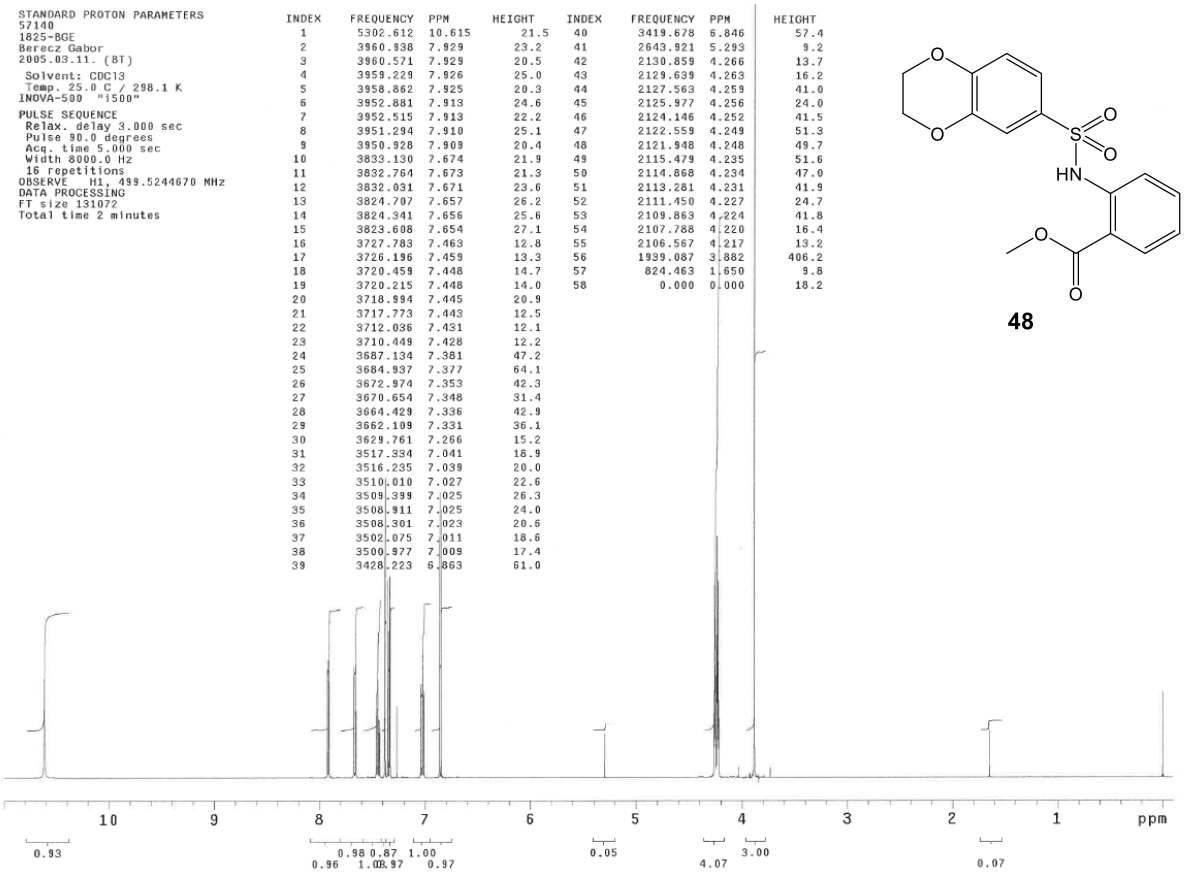


STANDARD 13C
64557
1981-BGE
Berecz Gabor
2006.07.24. (BB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 27220.1 Hz
823 repetitions
OBSERVE C13, 125.6055354 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 131072
Total time 58 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18252.597	145.306	18.0
2	18071.922	143.867	11.5
3	17911.598	142.591	16.9
4	17875.047	142.300	18.9
5	17578.905	139.942	10.6
6	17269.888	137.482	13.8
7	17022.341	135.512	21.7
8	16994.098	135.287	15.2
9	16815.083	133.862	15.6
10	16754.858	133.382	50.6
11	16531.817	131.607	58.5
12	16470.761	131.121	22.0
13	16078.259	127.996	59.3
14	15853.141	126.204	14.7
15	15755.119	125.424	33.8
16	15460.639	123.079	11.0
17	15341.019	122.127	48.3
18	14822.251	117.997	33.8
19	14695.986	116.992	50.5
20	14496.620	115.405	32.6
21	10968.667	87.320	47.5
22	9704.353	77.255	255.8
23	9672.371	77.000	259.9
24	9640.389	76.745	288.6
25	8261.439	65.768	9.4
26	8098.208	64.468	90.8
27	8052.520	64.105	167.0
28	7342.693	58.454	30.1
29	7134.604	56.797	45.3
30	4812.818	38.314	37.5
31	4483.033	35.689	26.6
32	1911.208	15.215	8.6

46




STANDARD PROTON PARAMETERS
57140
1825-BGE
Berecz Gabor
2005.03.11. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244670 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT
1 5302.612 10.615 21.5
2 3960.938 7.929 23.2
3 3960.571 7.929 20.5
4 3959.229 7.926 25.0
5 3958.862 7.925 20.3
6 3952.881 7.913 24.6
7 3952.515 7.913 22.2
8 3951.294 7.910 25.1
9 3950.928 7.909 20.4
10 3833.130 7.674 21.9
11 3832.764 7.673 21.3
12 3832.031 7.671 23.6
13 3824.707 7.657 26.2
14 3824.341 7.656 25.6
15 3823.608 7.654 27.1
16 3727.783 7.463 12.8
17 3726.196 7.459 13.3
18 3720.459 7.448 14.7
19 3720.215 7.448 14.0
20 3718.994 7.445 20.9
21 3717.773 7.443 12.5
22 3712.036 7.431 12.1
23 3710.449 7.428 12.2
24 3687.134 7.381 47.2
25 3684.937 7.377 64.1
26 3672.974 7.353 42.3
27 3670.654 7.348 31.4
28 3664.429 7.336 42.9
29 3662.109 7.331 36.1
30 3629.761 7.266 15.2
31 3517.334 7.041 18.9
32 3516.235 7.039 20.0
33 3510.010 7.027 22.6
34 3509.399 7.025 26.3
35 3508.911 7.025 24.0
36 3508.301 7.023 20.6
37 3502.075 7.011 18.6
38 3500.977 7.009 17.4
39 3428.223 6.863 61.0
INDEX FREQUENCY PPM HEIGHT
40 3419.678 6.846 57.4
41 2643.921 5.293 9.2
42 2130.859 4.266 13.7
43 2129.639 4.263 16.2
44 2127.563 4.259 41.0
45 2125.977 4.256 24.0
46 2124.146 4.252 41.5
47 2122.559 4.249 51.3
48 2121.948 4.248 49.7
49 2115.479 4.235 51.6
50 2114.868 4.234 47.0
51 2113.281 4.231 41.9
52 2111.450 4.227 24.7
53 2109.863 4.224 41.8
54 2107.788 4.220 16.4
55 2106.567 4.217 13.2
56 1939.087 3.882 406.2
57 824.463 1.650 9.8
58 0.000 0.000 18.2
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0.05
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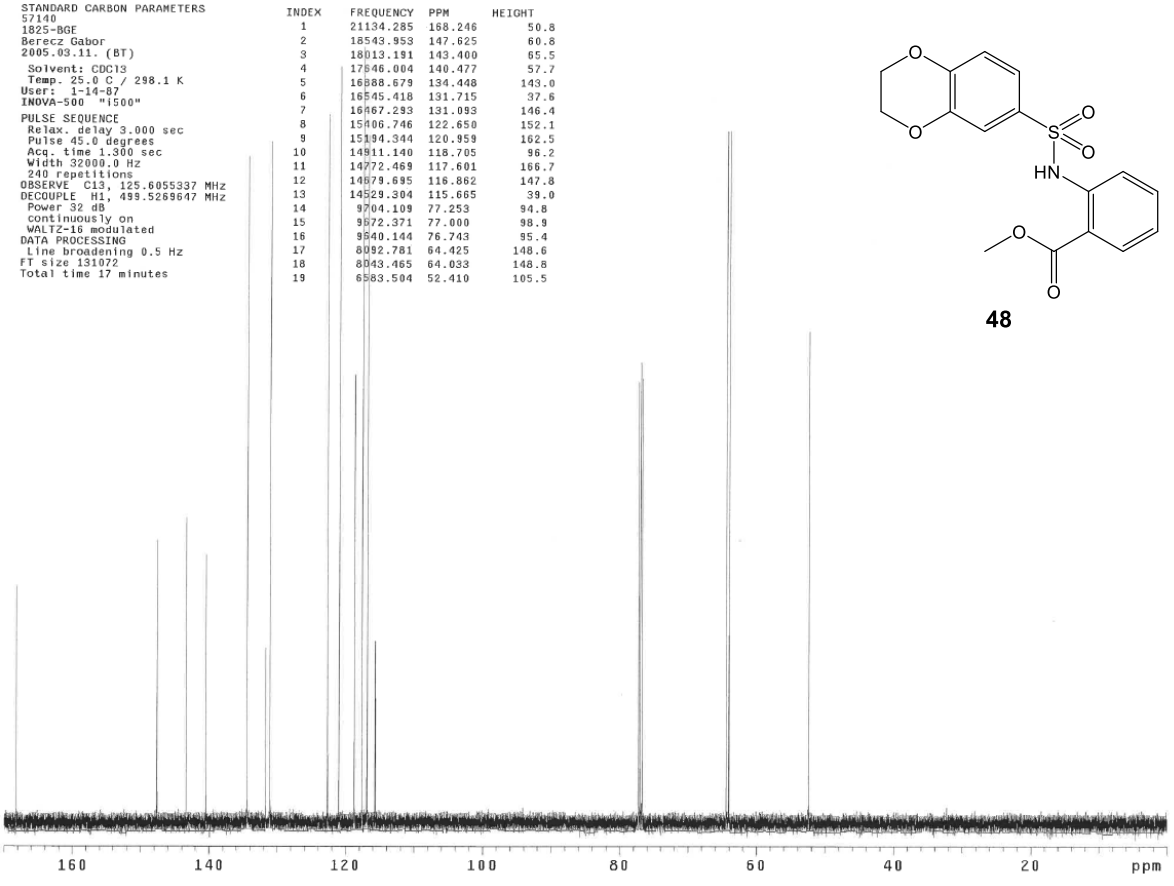
STANDARD CARBON PARAMETERS
57140
182S-BGE
Berecz Gabor
2005.03.11. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
240 repetitions
OBSERVE C13, 125.6055337 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 0.5 Hz
FT size 131072
Total time 17 minutes
INDEX FREQUENCY PPM HEIGHT
1 21134.285 168.246 50.8
2 18543.953 147.625 60.8
3 18013.191 143.400 65.5
4 17846.004 140.477 57.7
5 16888.679 134.448 143.0
6 16545.418 131.715 37.6
7 16467.293 131.093 146.4
8 15406.746 122.650 152.1
9 15194.344 120.959 162.5
10 14911.140 118.705 96.2
11 14772.469 117.601 166.7
12 14679.695 116.862 147.8
13 14529.304 115.665 39.0
14 9704.109 77.253 94.8
15 9672.371 77.000 98.9
16 9640.144 76.743 95.4
17 8092.781 64.425 148.6
18 8043.465 64.033 148.8
19 6583.504 52.410 105.5
O
O
S
O
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HN
O
O
48
160
140
120
100
80
60
40
20
ppm

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STANDARD PROTON PARAMETERS
57243
1830-BGE
Berecz Gabor
2005.03.23. (CzB)
 Solvent: CDCl3
 Temp. 25.0 C / 298.1 K
INOVA-500  "i500"
PULSE SEQUENCE
 Relax. delay 3.000 sec
 Pulse 90.0 degrees
 Acq. time 5.000 sec
 Width 8000.0 Hz
 16 repetitions
OBSERVE    H1, 499.5244681 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
```
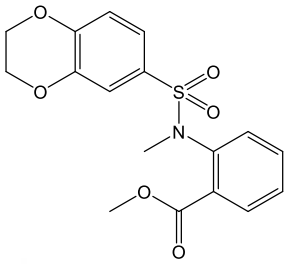
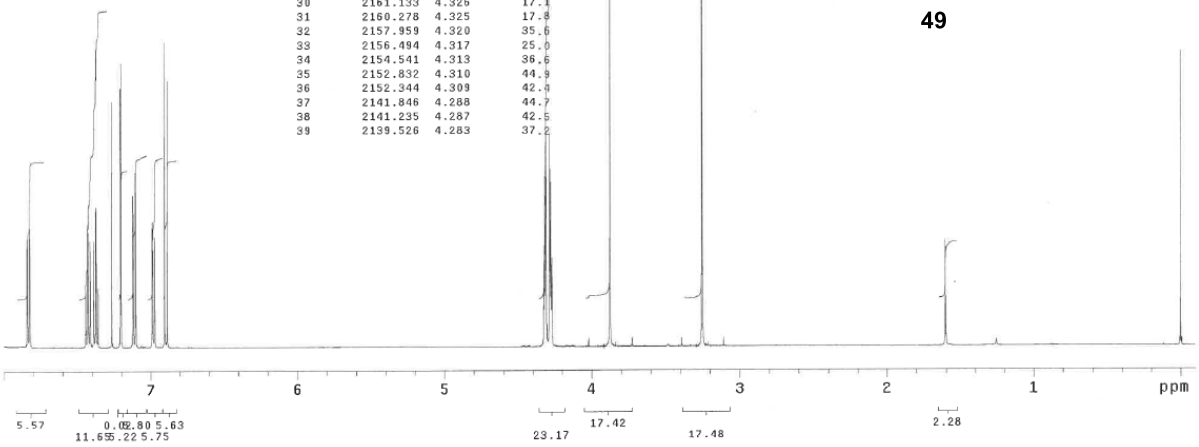
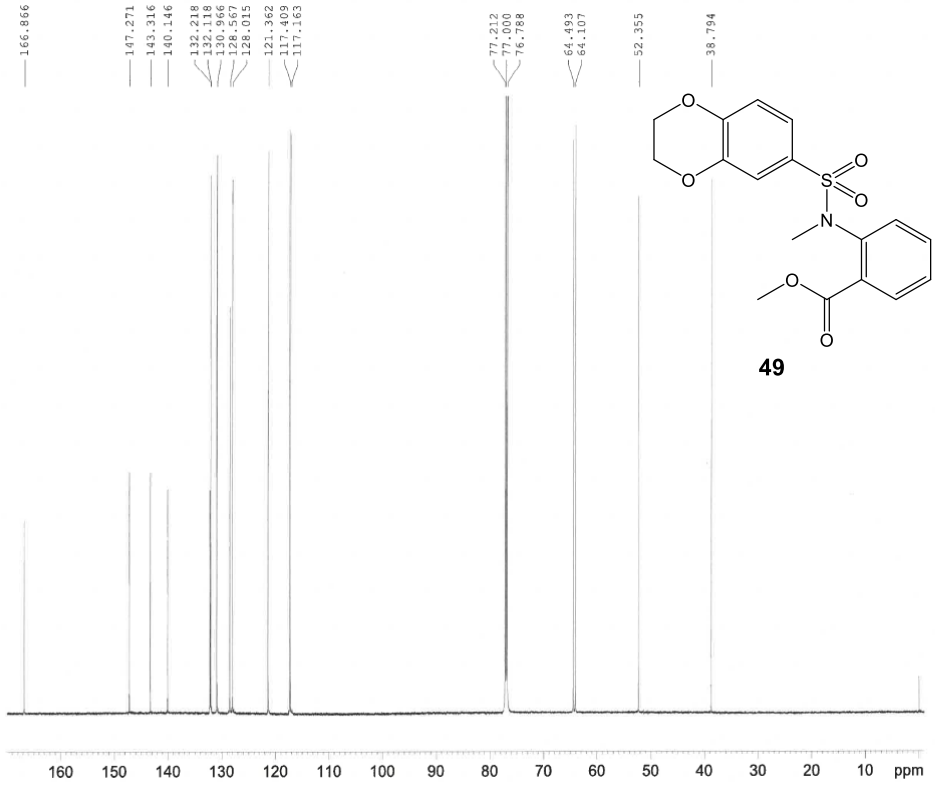

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3916.504	7.840	22.7	40	2137.573	4.279	26.3
2	3914.673	7.837	22.4	41	2136.108	4.276	34.5
3	3908.813	7.825	26.4	42	2133.789	4.272	18.5
4	3906.982	7.821	24.8	43	2132.935	4.270	16.1
5	3718.384	7.444	11.1	44	1936.768	3.877	371.8
6	3716.553	7.440	11.7	45	1625.000	3.253	371.1
7	3710.815	7.429	25.7	46	801.147	1.604	22.1
8	3709.106	7.425	23.9	47	-0.122	-0.000	61.7
9	3703.125	7.413	22.2				
10	3701.294	7.410	20.1				
11	3691.040	7.389	20.4				
12	3689.697	7.386	22.2				
13	3683.472	7.374	28.4				
14	3682.129	7.371	29.4				
15	3675.903	7.359	12.3				
16	3674.683	7.356	11.2				
17	3628.418	7.264	51.4				
18	3599.731	7.206	54.2				
19	3597.534	7.202	59.6				
20	3557.373	7.122	31.7				
21	3555.176	7.117	28.2				
22	3548.828	7.104	36.6				
23	3546.631	7.100	33.8				
24	3491.333	6.989	25.0				
25	3490.112	6.987	26.3				
26	3483.643	6.974	22.2				
27	3482.300	6.971	23.0				
28	3448.486	6.904	64.0				
29	3439.941	6.886	55.8				
30	2161.133	4.326	17.1				
31	2160.278	4.325	17.8				
32	2157.959	4.320	35.6				
33	2156.494	4.317	25.0				
34	2154.541	4.313	36.6				
35	2152.832	4.310	44.9				
36	2152.344	4.309	42.0				
37	2141.846	4.288	44.7				
38	2141.235	4.287	42.5				
39	2139.526	4.283	37.2				



49





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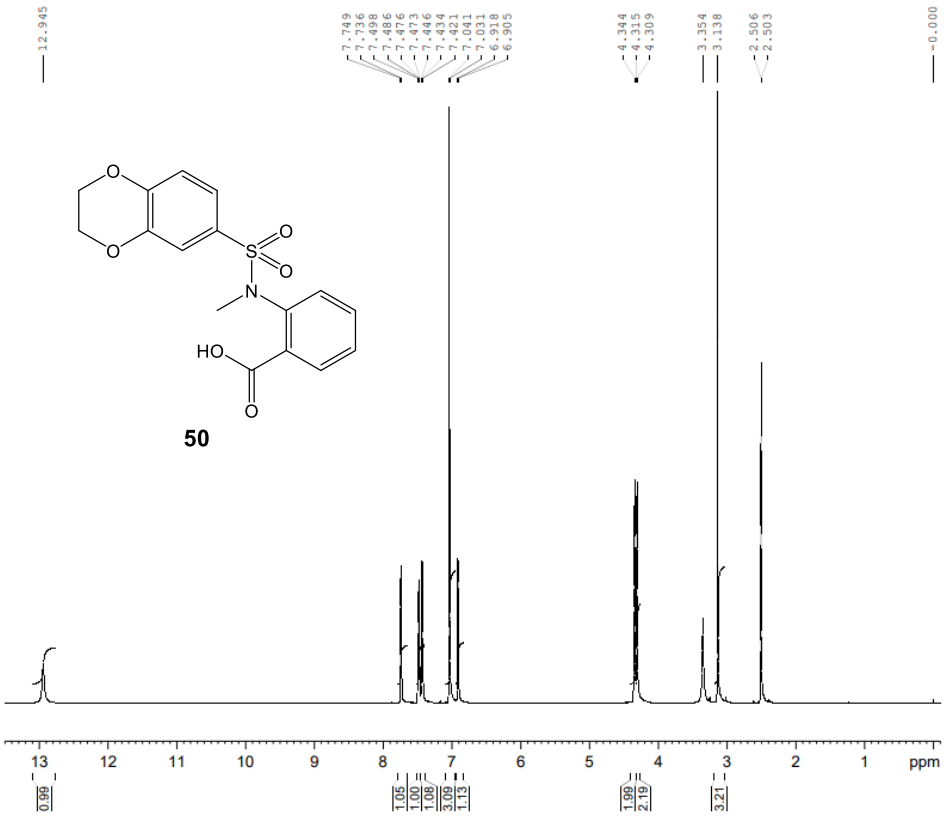
```
Standard 13C
143708
bge1830-1830-BGE_1
Berecz Gabor
2024.10.11. (KP)

Current Data Parameters
NAME                143708
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_             20241012
Time                  4.08 h
INSTRUM              spect
PROBHD    Z145856_0002 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   2048
DS                      4
SWH           36231.883 Hz
FIDRES         1.105709 Hz
AQ            0.9043968 sec
RG                 196.07
DW                 13.800 usec
DE                 18.00 usec
TE                 295.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         150.8852070 MHz
NUC1                 13C
P1                  9.90 usec
PLW1         71.00000000 W
SFO2         600.0024000 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         32.90000153 W
PLW12         0.70370001 W
PLW13         0.35339001 W

F2 - Processing parameters
SI                 131072
SF           150.8701291 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

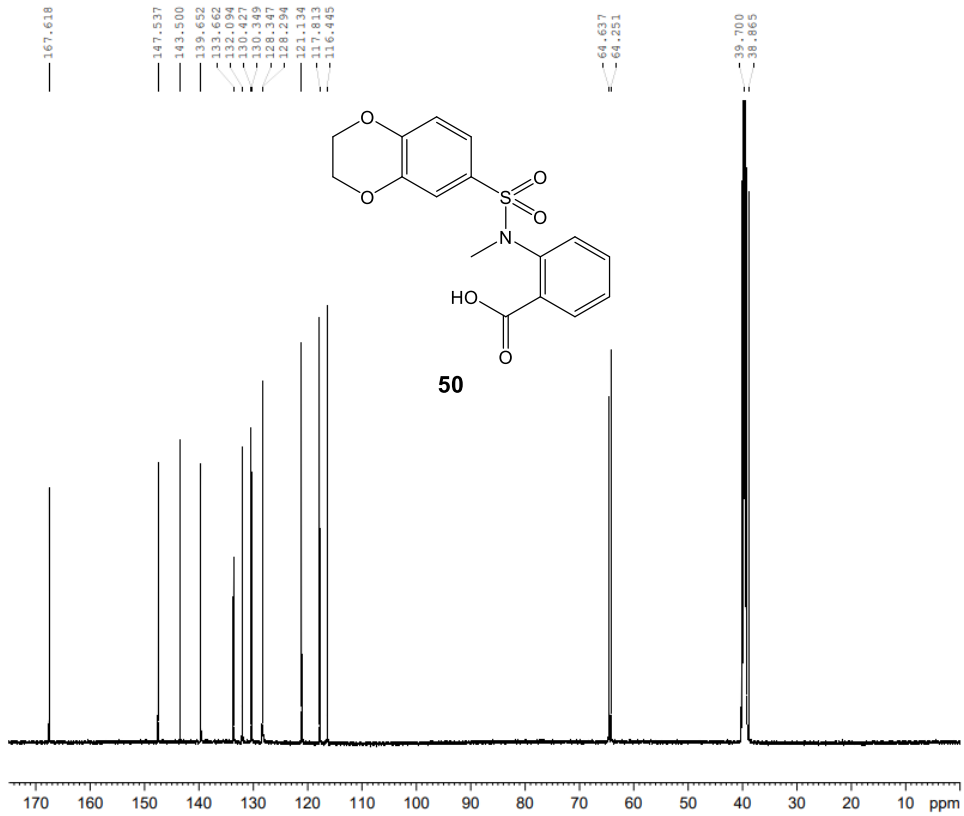



```
Standard 1H
144479
bge1827-1827-BGE_1
Berecz Gabor
2025.04.04. (KP)

Current Data Parameters
NAME                144479
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_            20250404
Time                19.11 h
INSTRUM              spect
PROBHD    Z145856_0002 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH             12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                 196.07
DW                41.600 usec
DE                25.00 usec
TE                295.0 K
D1             1.00000000 sec
TD0                     1
SFO1          600.0037050 MHz
NUC1                   1H
P1                 11.50 usec
PLW1          28.00000000 W

F2 - Processing parameters
SI                  65536
SF            600.0000004 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

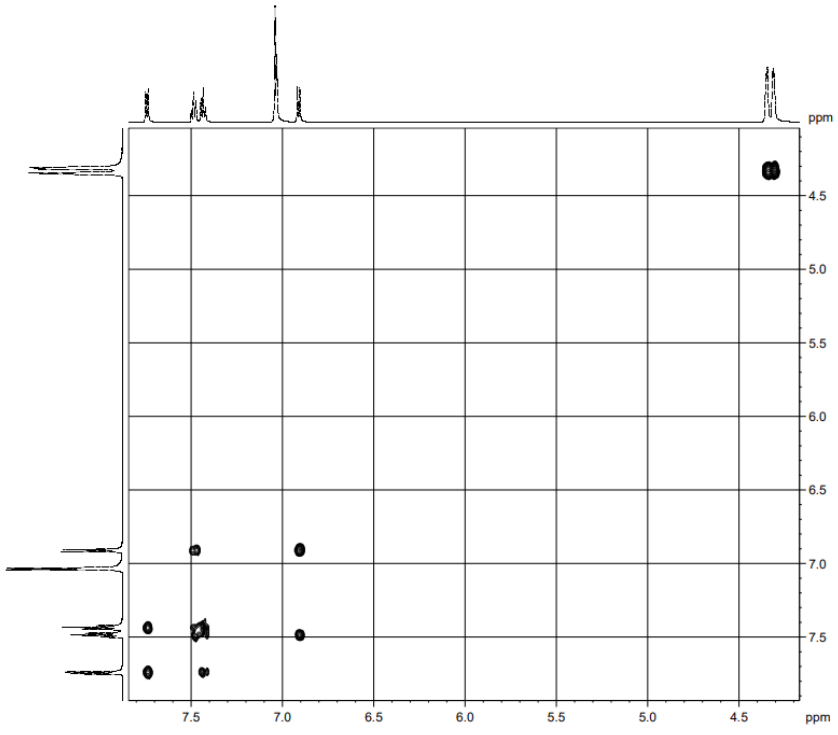



```
Standard 13C
144479
bge1827-1827-BGE_1
Berecz Gabor
2025.04.04. (KP)

Current Data Parameters
NAME                144479
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_            20250404
Time                20.19 h
INSTRUM              spect
PROBHD    Z145856_0002 (
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                   2048
DS                      4
SWH             36231.883 Hz
FIDRES          1.105709 Hz
AQ              0.9043968 sec
RG                 196.07
DW                13.800 usec
DE                18.00 usec
TE                295.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          150.8852070 MHz
NUC1                   13C
P1                  9.80 usec
PLW1          72.69999695 W
SFO2          600.0024000 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          32.50000000 W
PLW12          0.70708001 W
PLW13          0.35508999 W

F2 - Processing parameters
SI                 131072
SF            150.8701581 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



COSY
144479
bge1827-1827-BGE_1
Berecz Gabor
2025.04.04. (KP)

50

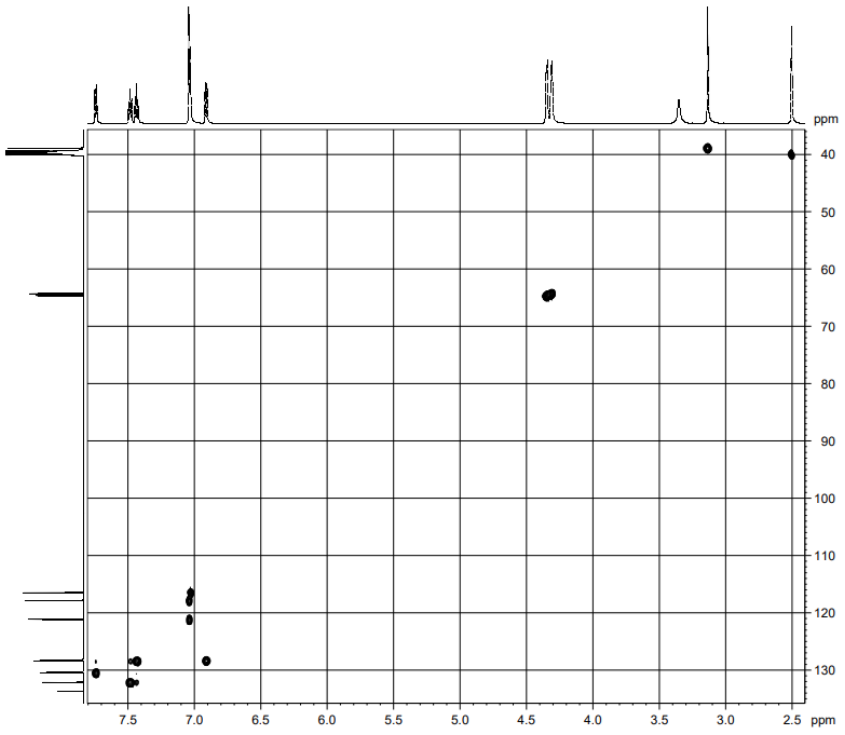
Current Data Parameters
NAME 144479
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250404
Time 20.24 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT DMSO
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000004 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000004 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



HSQC (140Hz)
144479
bge1827-1827-BGE_1
Berecz Gabor
2025.04.04. (KP)

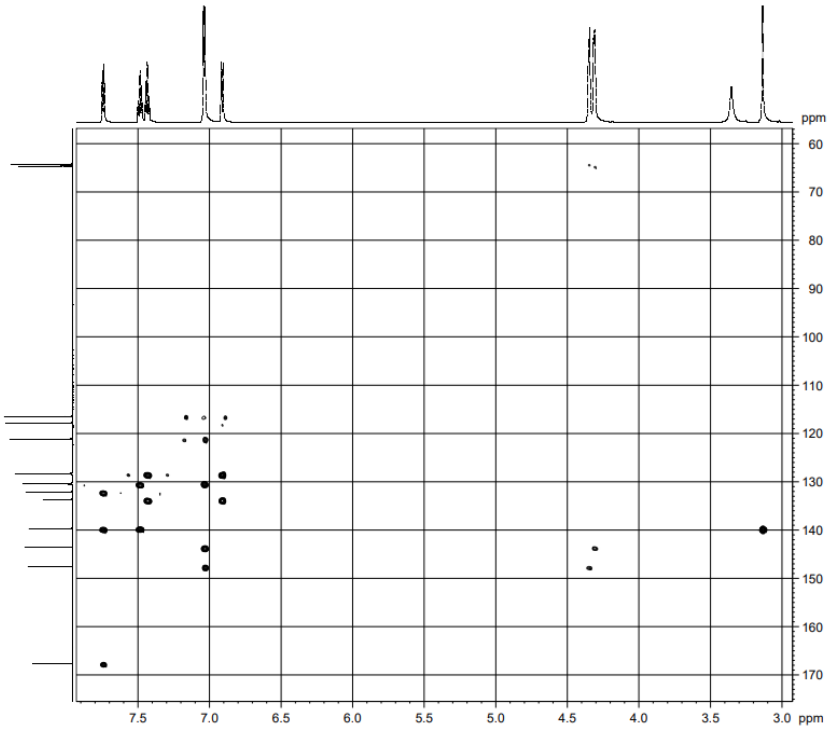
50

Current Data Parameters
NAME 144479
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250404
Time 20.41 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT DMSO
NS 4
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00001536 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p5m4sp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[31 Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000004 MHz
WDW QSINE



HMBC (8Hz, 140Hz)
144479
bge1827-1827-BGE_1
Berecz Gabor
2025.04.04. (KP)

50

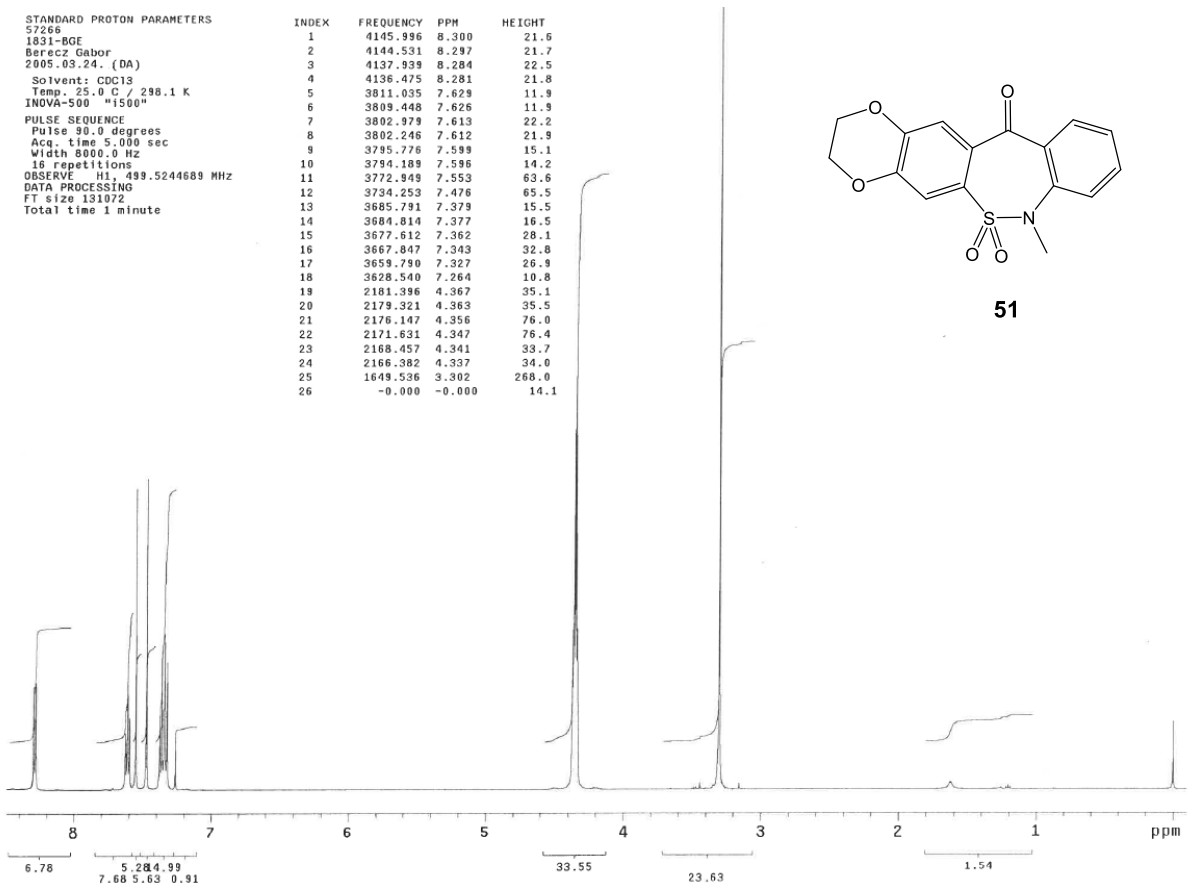
Current Data Parameters
NAME 144479
EXPNO 15
PROCNO 1

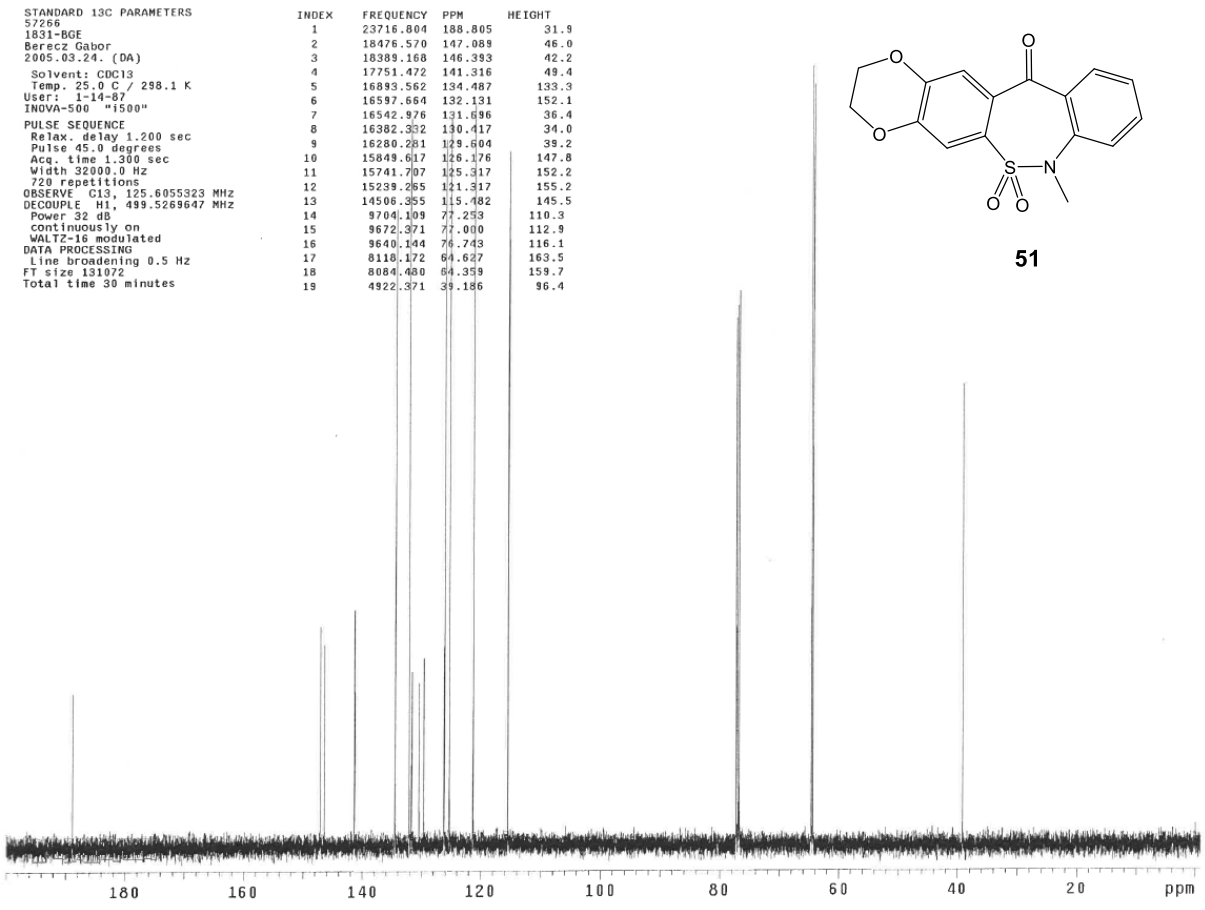
F2 - Acquisition Parameters
Date_ 20250404
Time 21.15 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT DMSO
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

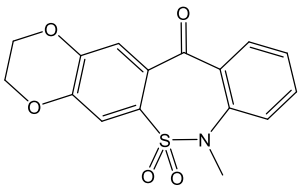
F2 - Processing parameters
SI 2048
SF 600.0000000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701200 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0


STANDARD PROTON PARAMETERS
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Pulse 90.0 degrees
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244689 MHz
DATA PROCESSING
FT size 131072
Total time 1 minute
INDEX FREQUENCY PPM HEIGHT
1 4145.996 8.300 21.6
2 4144.531 8.297 21.7
3 4137.939 8.284 22.5
4 4136.475 8.281 21.8
5 3811.035 7.629 11.9
6 3809.448 7.626 11.9
7 3802.979 7.613 22.2
8 3802.246 7.612 21.9
9 3795.776 7.599 15.1
10 3794.189 7.596 14.2
11 3772.949 7.553 63.6
12 3734.253 7.476 65.5
13 3685.791 7.379 15.5
14 3684.814 7.377 16.5
15 3677.612 7.362 28.1
16 3667.847 7.343 32.8
17 3659.790 7.327 26.9
18 3628.540 7.264 10.8
19 2181.396 4.367 35.1
20 2179.321 4.363 35.5
21 2176.147 4.356 76.0
22 2171.631 4.347 76.4
23 2168.457 4.341 33.7
24 2166.382 4.337 34.0
25 1649.536 3.302 268.0
26 -0.000 -0.000 14.1
O
O
O
S
N
O
O
51
8
7
6
5
4
3
2
1
ppm
6.78
7.68
5.28
5.63
4.99
0.91
33.55
23.63
1.54


STANDARD 13C PARAMETERS
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 32000.0 Hz
720 repetitions
OBSERVE C13, 125.6055323 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 30 minutes
INDEX FREQUENCY PPM HEIGHT
1 23716.804 188.805 31.9
2 18476.570 147.089 46.0
3 18389.168 146.393 42.2
4 17751.472 141.316 49.4
5 16893.562 134.487 133.3
6 16597.664 132.131 152.1
7 16542.976 131.696 36.4
8 16382.332 130.417 34.0
9 16280.281 129.604 39.2
10 15849.617 126.176 147.8
11 15741.707 125.317 152.2
12 15239.265 121.317 155.2
13 14506.355 115.482 145.5
14 9704.109 77.253 110.3
15 9672.371 77.000 112.9
16 9640.144 76.743 116.1
17 8118.172 64.627 163.5
18 8084.480 64.359 159.7
19 4922.371 39.186 96.4
O
O
O
S
N
O
O
51
180
160
140
120
100
80
60
40
20
ppm

GMQFCOPS_DA
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
SEQUENCE: gmqfcops_da
Relax. delay 1.500 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
Single scan
2 x 256 increments
OBSERVE H1, 499.5244665 MHz
DATA PROCESSING
Sq. sine bell 0.128 sec
Shifted by -0.128 sec
F1 DATA PROCESSING
Sine bell 0.042 sec
Shifted by -0.042 sec
FT size 4096 x 512
Total time 14 minutes



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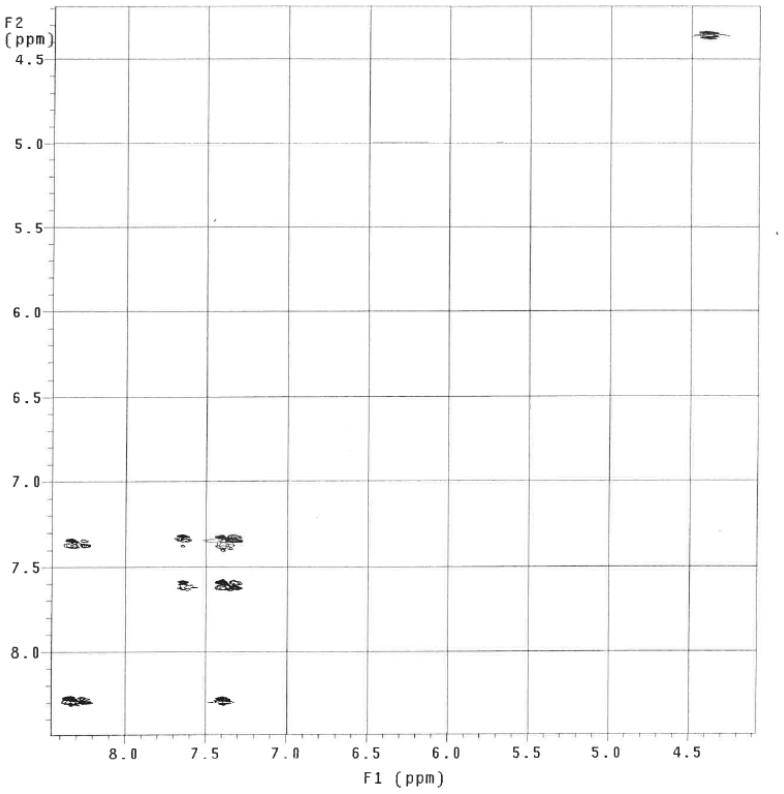
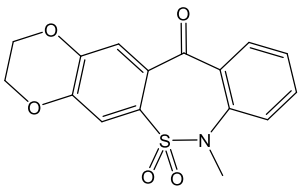


GHSQC_DA (140 Hz)
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE: ghsqc_da
Relax. delay 1.500 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 26507.6 Hz
2 repetitions
2 x 256 increments
OBSERVE H1, 499.5244687 MHz
DECOUPLE C13, 125.6176221 MHz
Power 42 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sq. sine bell 0.200 sec
Shifted by -0.200 sec
F1 DATA PROCESSING
Sq. sine bell 0.005 sec
Shifted by -0.005 sec
FT size 4096 x 512
Total time 28 minutes



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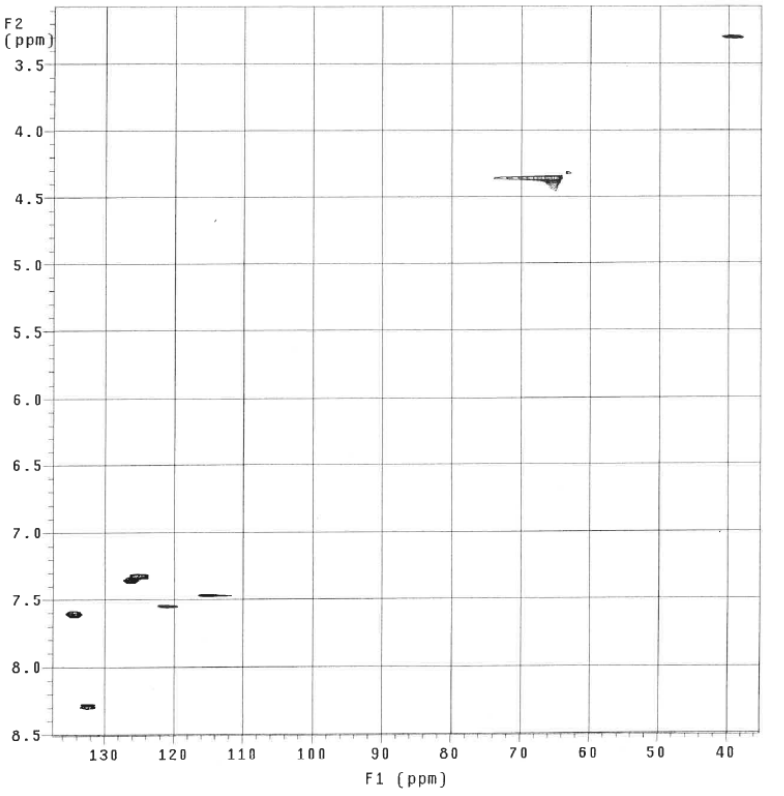
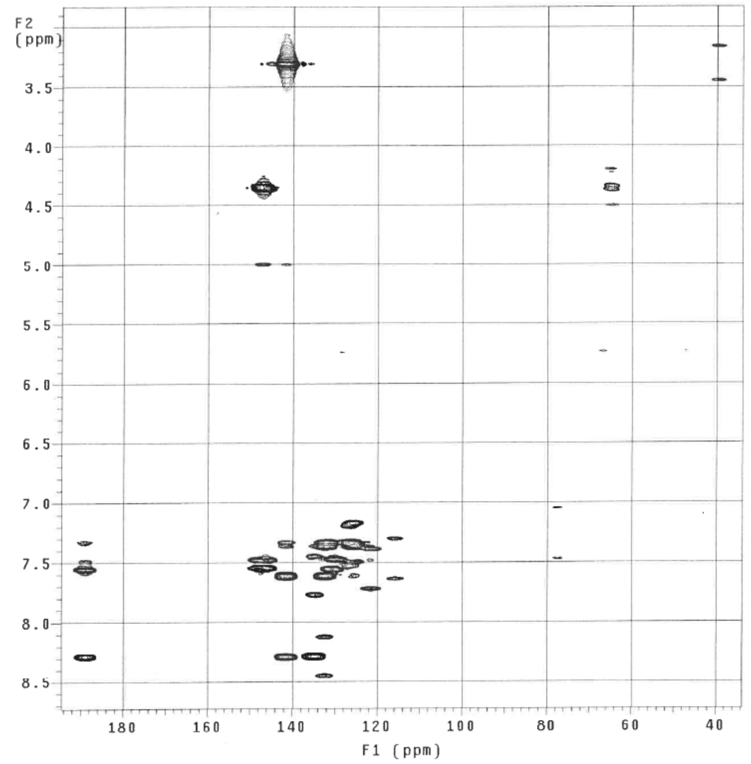
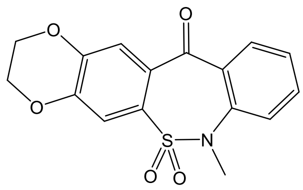



GHMQC_DA (140 Hz, 8 Hz)
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE: ghmqc_da
Relax. delay 1.500 sec
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 26507.6 Hz
4 repetitions
256 increments
OBSERVE H1, 499.5244689 MHz
DATA PROCESSING
Sine bell 0.128 sec
F1 DATA PROCESSING
Sine bell 0.002 sec
FT size 4096 x 512
Total time 28 minutes
F2 (ppm)
F1 (ppm)



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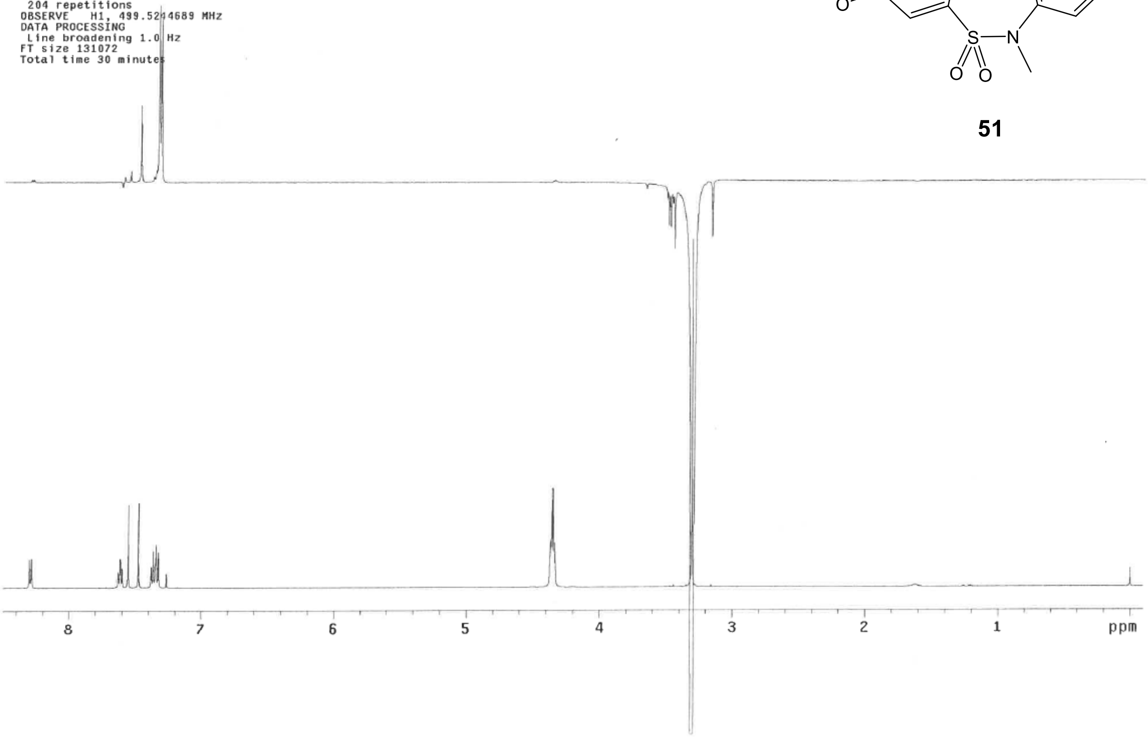
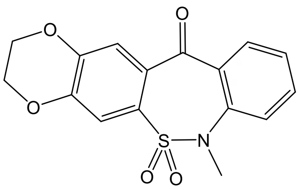

DPFGNOE_DA (3.30 ppm)
57266
1831-BGE
Berecz Gabor
2005.03.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE: dpfgnoe_da
Relax. delay 2.000 sec
Pulse 102.9 degrees
Mixing 2.000 sec
Acq. time 5.000 sec
Width 8000.0 Hz
204 repetitions
OBSERVE H1, 499.5244689 MHz
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 30 minutes
ppm



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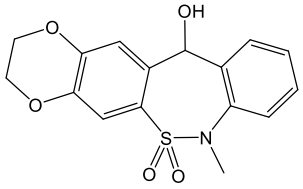
STANDARD 1H
58946
1868-BGE
Berecz Gabor
2005/07/12 (SzA)

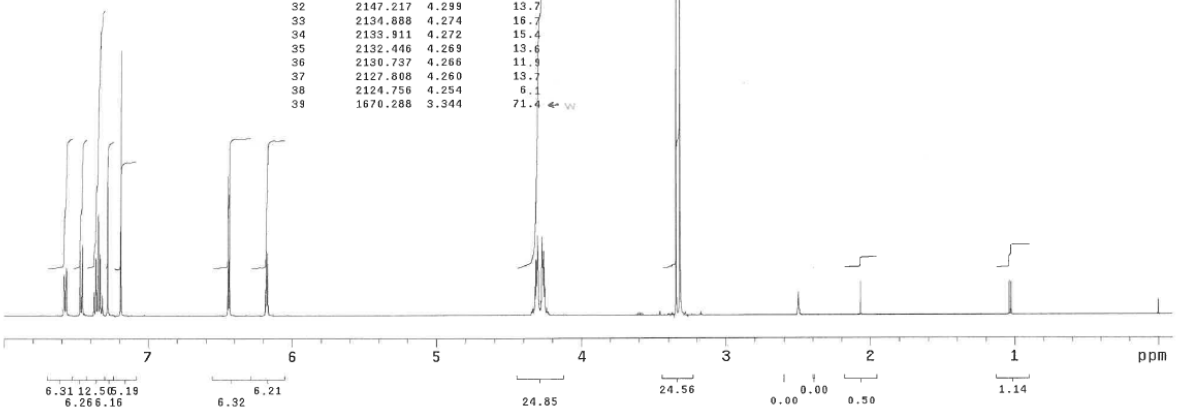
Solvent: DMSO
Temp. 25.0 C / 298.1 K
Sample #1
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268368 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3788.818	7.585	8.3	40	1656.982	3.317	162.0
2	3787.598	7.582	6.7	41	1247.661	2.498	4.9
3	3786.743	7.581	8.8	42	1033.447	2.069	7.1
4	3781.860	7.571	10.0	43	519.165	1.039	7.3
5	3781.250	7.570	10.2	44	513.062	1.027	7.1
6	3779.541	7.566	10.0				
7	3733.643	7.474	10.5				
8	3731.934	7.471	13.8				
9	3726.440	7.460	9.7				
10	3725.830	7.459	11.1				
11	3724.487	7.456	15.1				
12	3684.570	7.376	5.0				
13	3679.077	7.365	12.3				
14	3677.124	7.361	11.8				
15	3671.753	7.350	21.1				
16	3669.556	7.346	21.7				
17	3664.062	7.335	13.2				
18	3662.476	7.332	12.1				
19	3656.738	7.320	4.3				
20	3637.817	7.283	34.1				
21	3636.963	7.281	32.9				
22	3592.163	7.191	56.8				
23	3219.971	6.446	29.9				
24	3214.844	6.436	31.0				
25	3087.891	6.182	13.8				
26	3082.764	6.171	13.3				
27	2157.959	4.320	6.1				
28	2154.419	4.313	12.0				
29	2152.710	4.309	6.8				
30	2150.024	4.304	17.0				
31	2149.170	4.302	14.8				
32	2147.217	4.299	13.7				
33	2134.888	4.274	16.7				
34	2133.911	4.272	15.4				
35	2132.446	4.269	13.6				
36	2130.737	4.266	11.9				
37	2127.808	4.260	13.7				
38	2124.756	4.254	6.1				
39	1670.288	3.344	71.4				



52

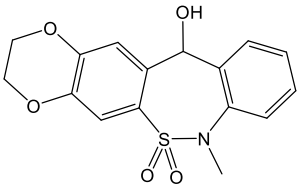


STANDARD 13C
58946
1868-BGE
Berecz Gabor
2005/07/12 (SzA)

Solvent: DMSO
Temp. 25.0 C / 298.1 K
Sample #1, user 1-14-87
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
192 repetitions
OBSERVE C13, 125.6061582 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 13 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18407.173	146.541	60.8
2	17969.204	143.213	51.6
3	17920.356	142.665	58.0
4	17199.165	136.924	55.4
5	16945.259	134.903	60.1
6	16294.868	129.725	49.8
7	16167.427	128.710	68.3
8	16083.442	128.042	68.3
9	16021.430	127.548	70.7
10	15779.731	125.624	66.8
11	14586.860	116.127	72.8
12	14366.645	114.374	75.4
13	8503.852	67.700	78.1
14	8132.759	64.746	67.1
15	8083.930	64.357	65.6
16	5049.751	40.201	33.0
17	5028.755	40.034	100.5
18	5008.247	39.871	199.2
19	4986.762	39.700	238.6
20	4965.766	39.533	200.8
21	4944.770	39.366	101.1
22	4924.262	39.202	33.6
23	4656.196	37.068	96.7



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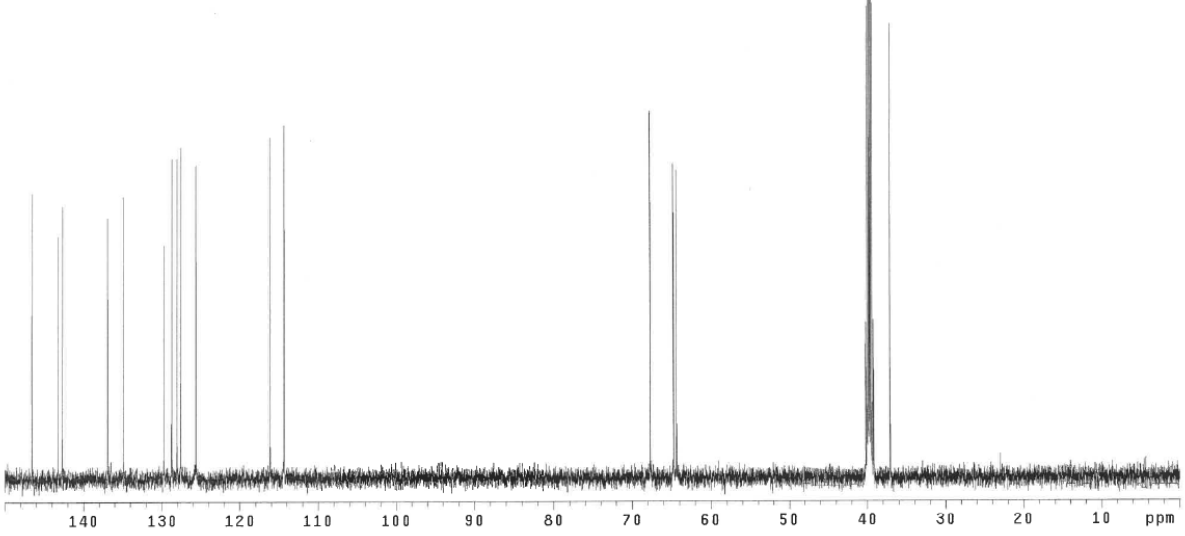
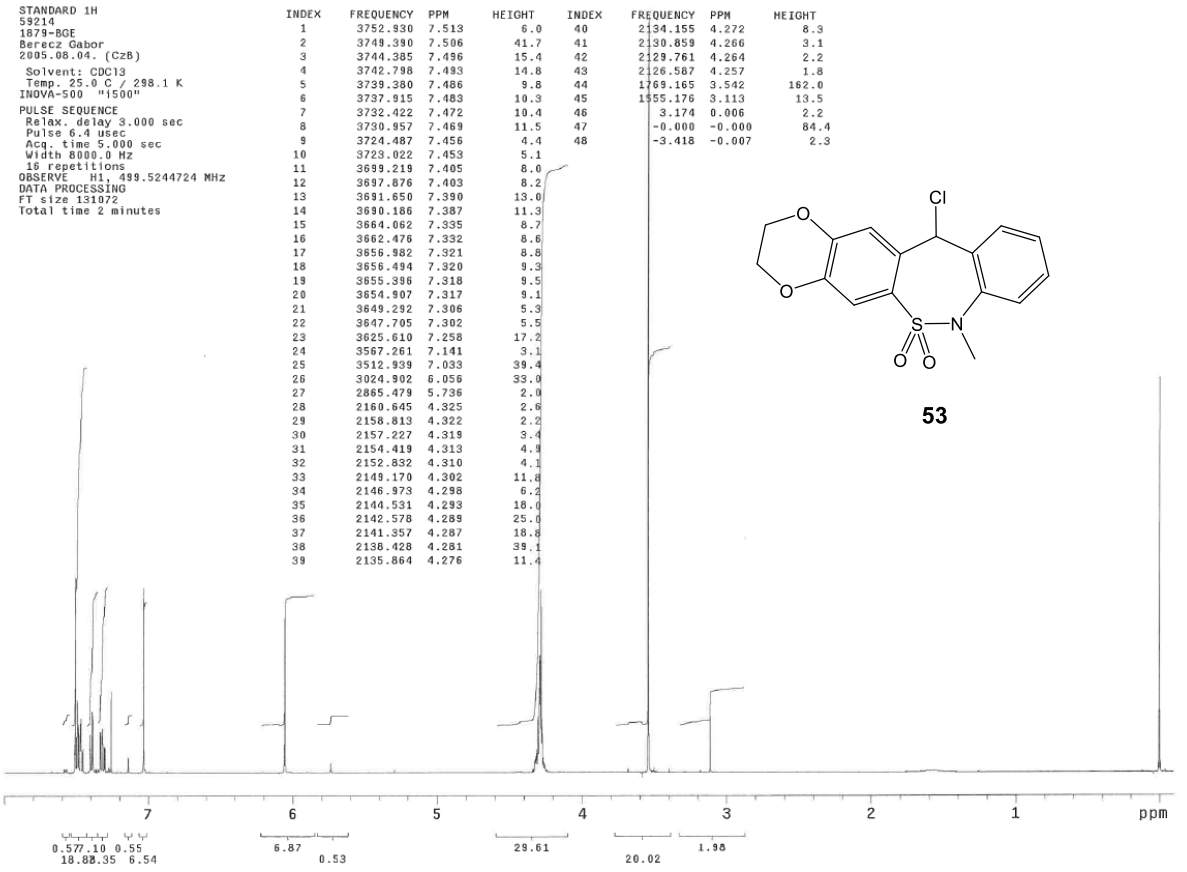
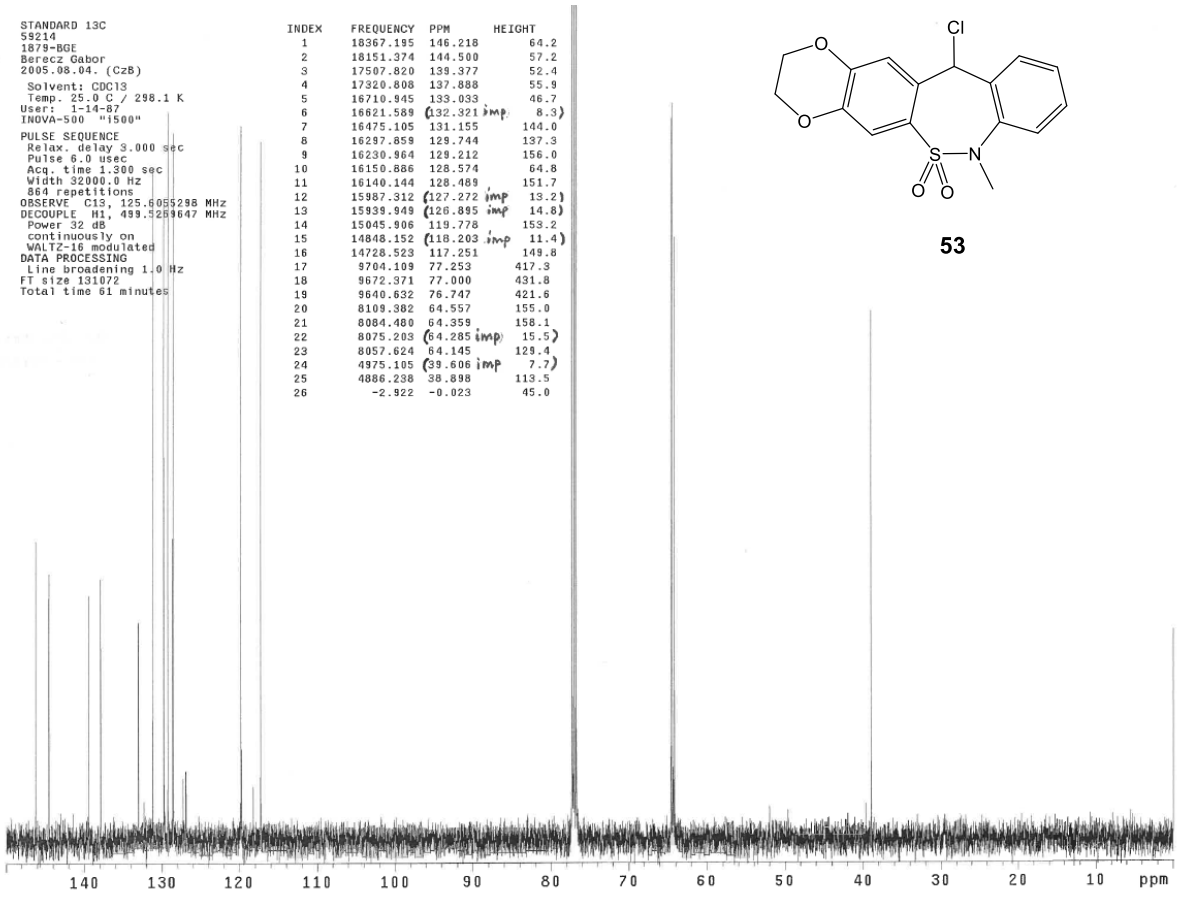
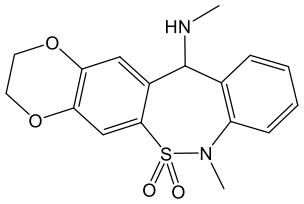



STANDARD 1H
59214
1879-BGE
Berecz Gabor
2005.08.04. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244724 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes
INDEX FREQUENCY PPM HEIGHT INDEX FREQUENCY PPM HEIGHT
1 3752.930 7.513 6.0 40 2134.155 4.272 8.3
2 3749.390 7.506 41.7 41 2130.859 4.266 3.1
3 3744.385 7.496 15.4 42 2129.761 4.264 2.2
4 3742.798 7.493 14.8 43 2126.587 4.257 1.8
5 3739.380 7.486 9.8 44 1769.165 3.542 162.0
6 3737.915 7.483 10.3 45 1555.176 3.113 13.5
7 3732.422 7.472 10.4 46 3.174 0.006 2.2
8 3730.957 7.469 11.5 47 -0.000 -0.000 84.4
9 3724.487 7.456 4.4 48 -3.418 -0.007 2.3
10 3723.022 7.453 5.1
11 3699.219 7.405 8.0
12 3697.876 7.403 8.2
13 3691.650 7.390 13.0
14 3690.186 7.387 11.3
15 3664.062 7.335 8.7
16 3662.476 7.332 8.6
17 3656.982 7.321 8.8
18 3656.494 7.320 9.3
19 3655.396 7.318 9.5
20 3654.907 7.317 9.1
21 3649.292 7.306 5.3
22 3647.705 7.302 5.5
23 3625.610 7.258 17.2
24 3567.261 7.141 3.1
25 3512.939 7.033 39.4
26 3024.902 6.056 33.0
27 2865.479 5.736 2.0
28 2160.645 4.325 2.6
29 2158.813 4.322 2.2
30 2157.227 4.319 3.4
31 2154.419 4.313 4.9
32 2152.832 4.310 4.1
33 2149.170 4.302 11.8
34 2146.973 4.298 6.2
35 2144.531 4.293 18.0
36 2142.578 4.289 25.0
37 2141.357 4.287 18.8
38 2138.428 4.281 39.1
39 2135.864 4.276 11.4
Cl
O
O
S
N
O
O
53
7
6
5
4
3
2
1
ppm
0.57 7.10 0.55
18.88.35 6.54
6.87
0.53
29.61
20.02
1.98

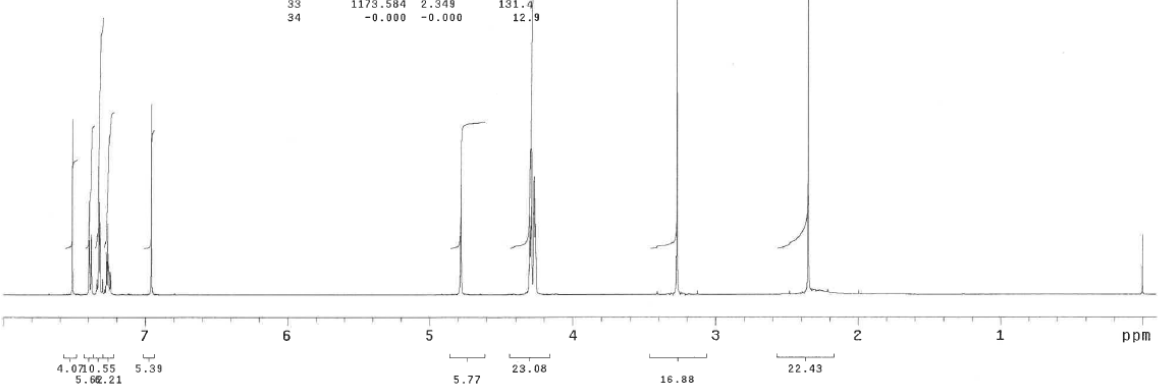

STANDARD 13C
59214
1879-BGE
Berecz Gabor
2005.08.04. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
864 repetitions
OBSERVE C13, 125.6055298 MHz
DECOUPLE H1, 499.5259647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 61 minutes
INDEX FREQUENCY PPM HEIGHT
1 18367.195 146.218 64.2
2 18151.374 144.500 57.2
3 17507.820 139.377 52.4
4 17320.808 137.888 55.9
5 16710.945 133.033 46.7
6 16621.589 (132.321 imp 8.3)
7 16475.105 131.155 144.0
8 16287.859 129.744 137.3
9 16230.964 129.212 156.0
10 16150.886 128.574 64.8
11 16140.144 128.489 151.7
12 15987.312 (127.272 imp 13.2)
13 15939.949 (126.895 imp 14.8)
14 15045.906 119.778 153.2
15 14848.152 (118.203 imp 11.4)
16 14728.523 117.251 149.8
17 9704.109 77.253 417.3
18 9672.371 77.000 431.8
19 9640.632 76.747 421.6
20 8109.382 64.557 155.0
21 8084.480 64.359 158.1
22 8075.203 (64.285 imp 15.5)
23 8057.624 64.145 129.4
24 4975.105 (39.606 imp 7.7)
25 4886.238 38.898 113.5
26 -2.922 -0.023 45.0
Cl
O
O
S
N
O
O
53
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
59373
1883-BGE
Berecz Gabor
2005.08.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244696 MHz
DATA PROCESSING
FT size 131072
Total time 1 minute

INDEX	FREQUENCY	PPM	HEIGHT
1	3752.930	7.513	38.1
2	3694.214	7.395	11.7
3	3687.012	7.381	13.0
4	3686.523	7.380	12.9
5	3661.377	7.330	27.9
6	3660.522	7.328	23.9
7	3658.569	7.324	20.1
8	3655.518	7.318	15.6
9	3654.175	7.315	12.2
10	3633.911	7.275	9.3
11	3631.104	7.269	7.2
12	3628.052	7.263	15.4
13	3626.343	7.260	8.8
14	3625.244	7.257	6.7
15	3623.779	7.254	6.1
16	3620.239	7.247	5.0
17	3617.676	7.242	4.4
18	3475.830	6.958	41.3
19	2388.428	4.781	26.5
20	2150.391	4.305	6.6
21	2146.973	4.298	17.0
22	2144.531	4.293	14.8
23	2143.066	4.290	19.1
24	2141.113	4.286	31.7
25	2134.399	4.273	17.9
26	2133.057	4.270	24.7
27	2132.080	4.268	25.7
28	2129.883	4.264	14.9
29	2128.418	4.261	15.3
30	2126.221	4.256	9.2
31	2125.122	4.254	7.1
32	1634.155	3.271	151.2
33	1173.584	2.349	131.4
34	-0.000	-0.000	12.9

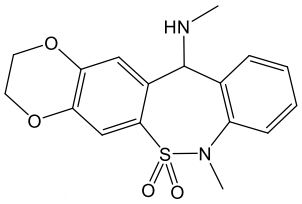


54a

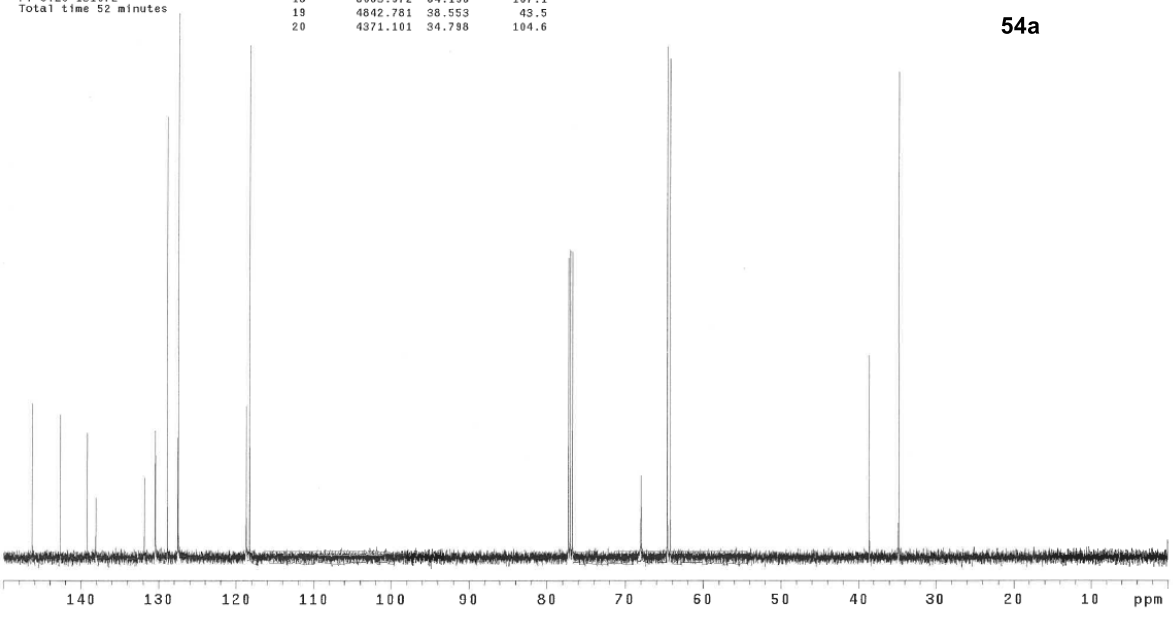


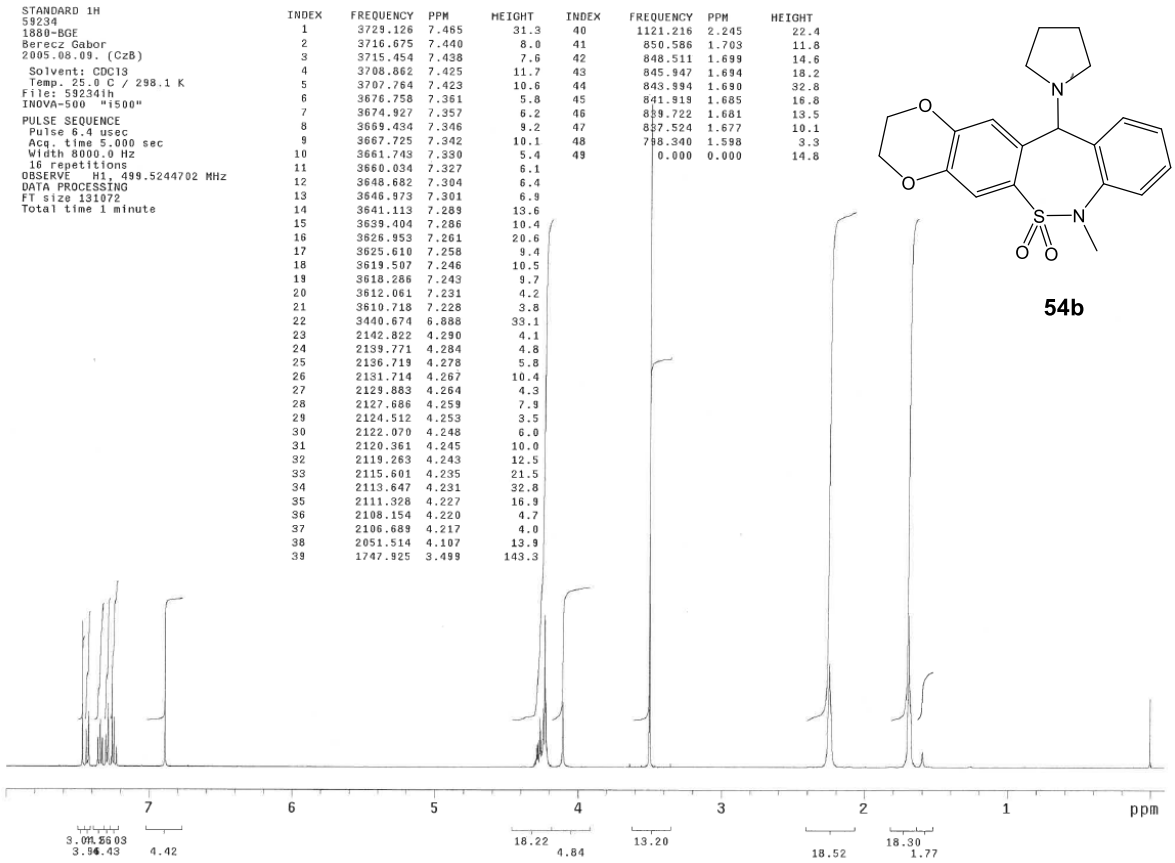
STANDARD 13C
59373
1883-BGE
Berecz Gabor
2005.08.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 12.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
736 repetitions
OBSERVE C13, 125.6055318 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 52 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18377.448	146.300	33.0
2	17918.953	142.650	30.7
3	17484.871	139.194	26.6
4	17344.246	138.074	12.8
5	16558.113	131.816	17.2
6	16389.168	130.471	20.2
7	16381.355	130.409	27.2
8	16190.437	128.889	94.6
9	16015.632	127.498	116.7
10	16013.678	127.482	112.0
11	14913.093	118.720	32.5
12	14859.871	118.297	110.0
13	9704.109	77.253	64.4
14	9672.371	77.000	66.1
15	9640.144	76.743	65.8
16	8537.605	67.966	17.7
17	8115.730	64.608	109.9
18	8063.972	64.196	107.1
19	4842.781	38.553	43.5
20	4371.101	34.798	104.6



54a




STANDARD 1H
59234
1880-BGE
Berecz Gabor
2005.08.09. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 59234ih
INOVA-500 "i500"
PULSE SEQUENCE
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244702 MHz
DATA PROCESSING
FT size 131072
Total time 1 minute
INDEX FREQUENCY PPM HEIGHT
1 3729.126 7.465 31.3
2 3716.675 7.440 8.0
3 3715.454 7.438 7.6
4 3708.862 7.425 11.7
5 3707.764 7.423 10.6
6 3676.758 7.361 5.8
7 3674.927 7.357 6.2
8 3669.434 7.346 9.2
9 3667.725 7.342 10.1
10 3661.743 7.330 5.4
11 3660.034 7.327 6.1
12 3648.682 7.304 6.4
13 3646.973 7.301 6.9
14 3641.113 7.289 13.6
15 3639.404 7.286 10.4
16 3626.953 7.261 20.6
17 3625.610 7.258 9.4
18 3619.507 7.246 10.5
19 3618.286 7.243 9.7
20 3612.061 7.231 4.2
21 3610.718 7.228 3.8
22 3440.674 6.888 33.1
23 2142.822 4.290 4.1
24 2139.771 4.284 4.8
25 2136.719 4.278 5.8
26 2131.714 4.267 10.4
27 2129.883 4.264 4.3
28 2127.686 4.259 7.9
29 2124.512 4.253 3.5
30 2122.070 4.248 6.0
31 2120.361 4.245 10.0
32 2119.263 4.243 12.5
33 2115.601 4.235 21.5
34 2113.647 4.231 32.8
35 2111.328 4.227 16.9
36 2108.154 4.220 4.7
37 2106.689 4.217 4.0
38 2051.514 4.107 13.9
39 1747.925 3.499 143.3
INDEX FREQUENCY PPM HEIGHT
40 1121.216 2.245 22.4
41 850.586 1.703 11.8
42 848.511 1.699 14.6
43 845.947 1.694 18.2
44 843.994 1.690 32.8
45 841.918 1.685 16.8
46 839.722 1.681 13.5
47 837.524 1.677 10.1
48 798.340 1.598 3.3
49 0.000 0.000 14.8
O
O
N
S
N
O
O
54b
7
6
5
4
3
2
1
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4.84
13.20
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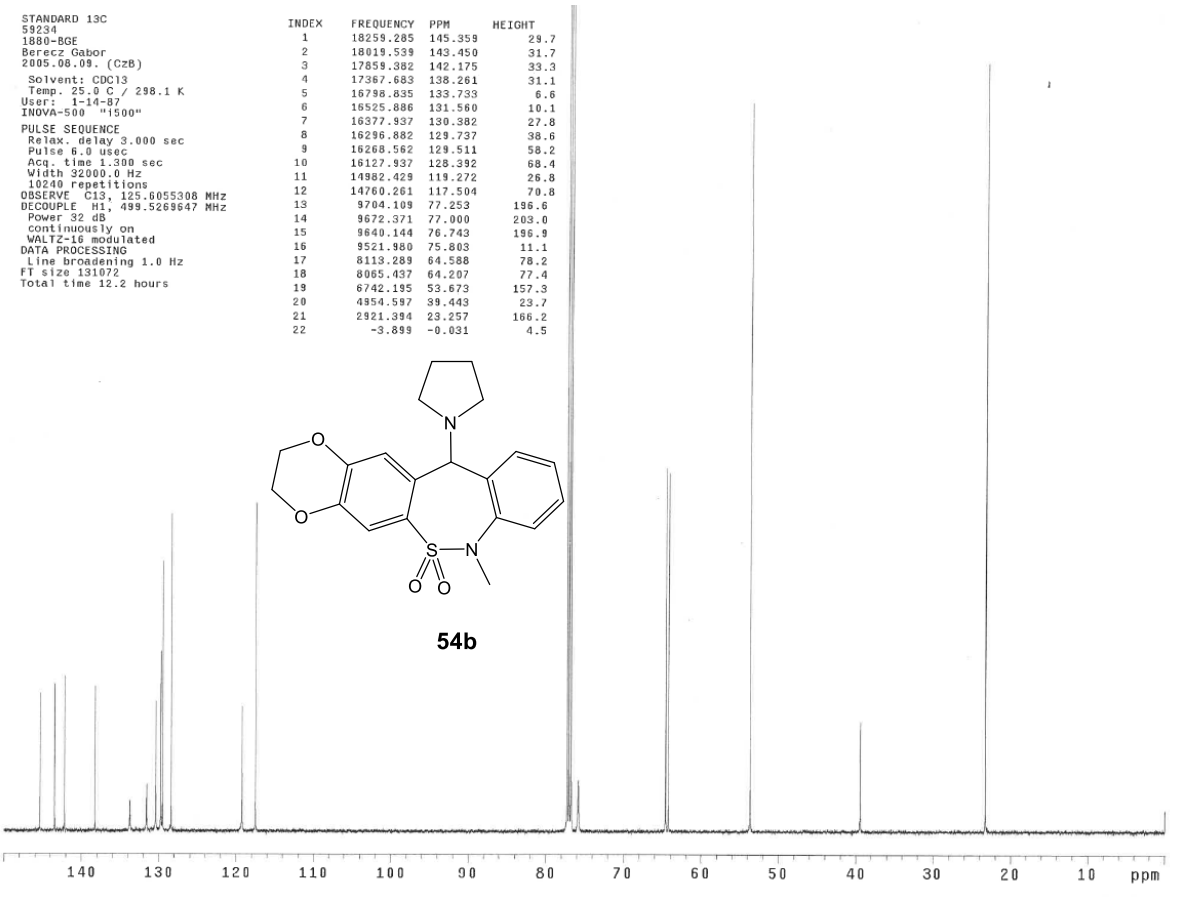
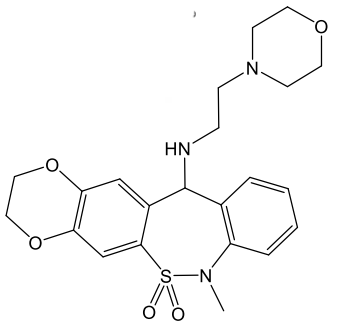
18.30
1.77

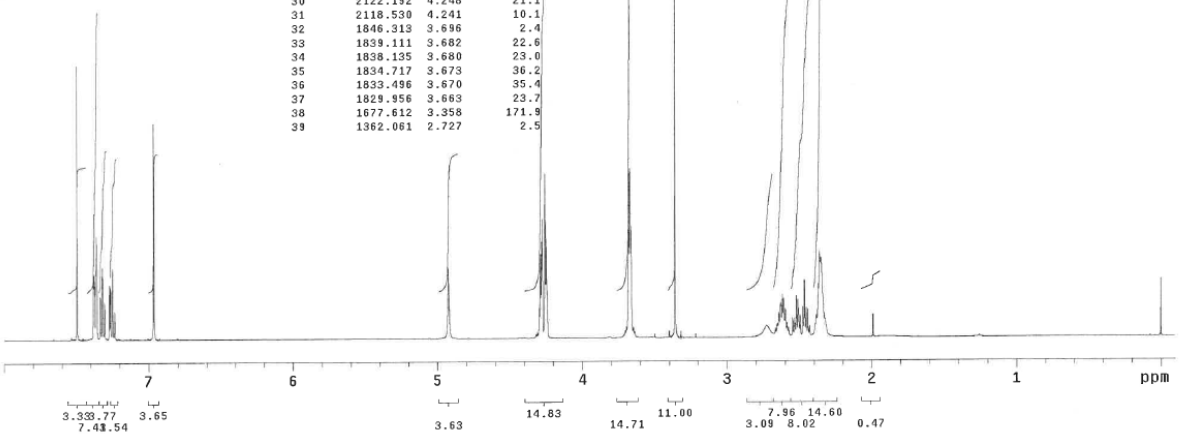

STANDARD 13C
59234
1880-BGE
Berecz Gabor
2005.08.09. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: i-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
10240 repetitions
OBSERVE C13, 125.6055308 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12.2 hours
INDEX FREQUENCY PPM HEIGHT
1 18259.285 145.359 29.7
2 18019.539 143.450 31.7
3 17859.382 142.175 33.3
4 17367.683 138.261 31.1
5 16798.835 133.733 6.6
6 16525.886 131.560 10.1
7 16377.937 130.382 27.8
8 16296.882 129.737 38.6
9 16268.562 129.511 58.2
10 16127.937 128.392 68.4
11 14982.429 119.272 26.8
12 14760.261 117.504 70.8
13 9704.109 77.253 196.6
14 9672.371 77.000 203.0
15 9640.144 76.743 196.9
16 9521.980 75.803 11.1
17 8113.289 64.588 78.2
18 8065.437 64.207 77.4
19 6742.195 53.673 157.3
20 4954.597 39.443 23.7
21 2921.394 23.257 166.2
22 -3.899 -0.031 4.5
O
O
N
S
N
O
O
54b
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

STANDARD 1H
62179
1939-BGE
Berecz Gabor
2006.02.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244668 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3742.798	7.493	58.6	40	1326.172	2.655	2.9
2	3686.035	7.379	11.4	41	1324.341	2.651	3.0
3	3684.448	7.376	13.9	42	1320.068	2.643	5.4
4	3682.007	7.371	11.7	43	1314.575	2.632	7.0
5	3678.467	7.364	14.8	44	1312.866	2.628	7.4
6	3676.880	7.361	17.4	45	1307.495	2.617	9.2
7	3675.537	7.358	22.0	46	1302.979	2.608	8.4
8	3674.194	7.355	20.4	47	1297.485	2.597	6.1
9	3662.964	7.333	9.2	48	1291.504	2.585	3.2
10	3661.377	7.330	9.2	49	1271.484	2.545	4.2
11	3655.640	7.318	15.3	50	1266.857	2.535	4.1
12	3654.175	7.315	13.0	51	1264.038	2.530	3.1
13	3647.705	7.302	7.9	52	1259.155	2.521	8.8
14	3646.240	7.299	6.6	53	1254.028	2.510	8.0
15	3630.981	7.269	11.6	54	1251.831	2.506	6.2
16	3628.540	7.264	11.4	55	1246.582	2.496	4.8
17	3627.075	7.261	11.0	56	1236.816	2.476	6.5
18	3621.094	7.249	15.1	57	1231.323	2.465	12.2
19	3619.629	7.246	14.5	58	1225.708	2.454	6.3
20	3613.770	7.234	6.1	59	1218.994	2.440	6.0
21	3612.305	7.231	5.7	60	1213.623	2.430	2.5
22	3479.248	6.965	46.0	61	1194.580	2.391	2.9
23	2459.229	4.923	15.0	62	1190.308	2.383	4.7
24	2144.897	4.294	7.2	63	1183.350	2.369	11.4
25	2141.479	4.287	17.9	64	1178.711	2.360	18.3
26	2138.550	4.281	17.9	65	1174.072	2.350	17.0
27	2137.329	4.279	20.5	66	1160.645	2.323	4.0
28	2135.132	4.274	25.4	67	993.896	1.990	4.9
29	2125.610	4.255	35.0	68	-0.000	-0.000	12.2
30	2122.192	4.248	21.1				
31	2118.530	4.241	10.1				
32	1846.313	3.696	2.4				
33	1839.111	3.682	22.6				
34	1838.135	3.680	23.0				
35	1834.717	3.673	36.2				
36	1833.496	3.670	35.4				
37	1829.956	3.663	23.7				
38	1677.612	3.358	171.9				
39	1362.061	2.727	2.5				

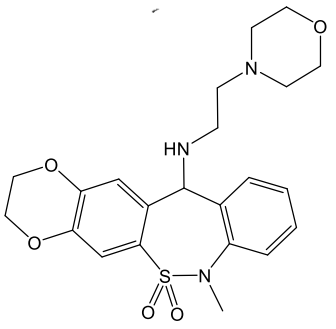


54c

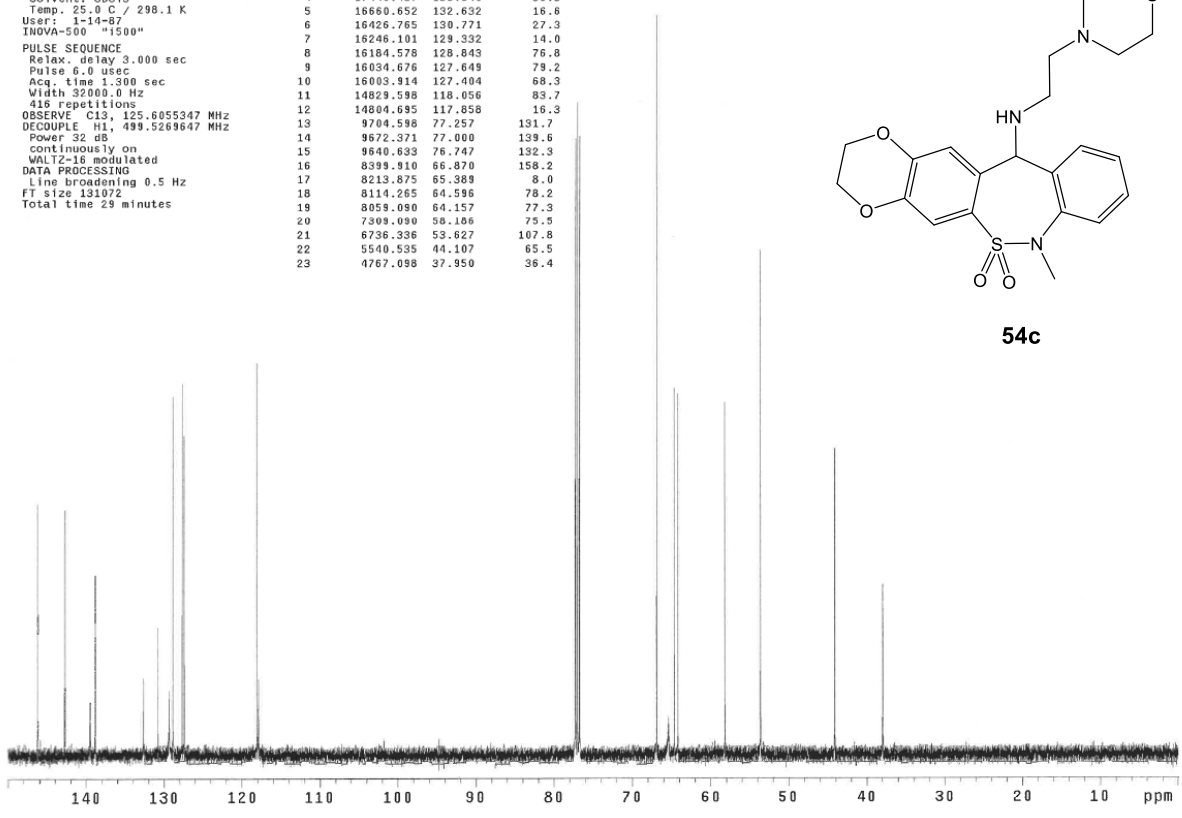


STANDARD 13C
62179
1939-BGE
Berecz Gabor
2006.02.24. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
416 repetitions
OBSERVE C13, 125.6055347 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 29 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	18366.707	146.214	53.6
2	17927.742	142.720	52.4
3	17523.933	139.505	11.4
4	17440.437	138.840	38.3
5	16660.652	132.632	16.6
6	16426.765	130.771	27.3
7	16246.101	129.332	14.0
8	16184.578	128.843	76.8
9	16034.676	127.649	79.2
10	16003.914	127.404	68.3
11	14829.598	118.056	83.7
12	14804.695	117.858	16.3
13	9704.598	77.257	131.7
14	9672.371	77.000	139.6
15	9640.633	76.747	132.3
16	8399.910	66.870	158.2
17	8213.875	65.389	8.0
18	8114.265	64.596	78.2
19	8059.090	64.157	77.3
20	7309.090	58.186	75.5
21	6736.336	53.627	107.8
22	5540.535	44.107	65.5
23	4767.098	37.950	36.4

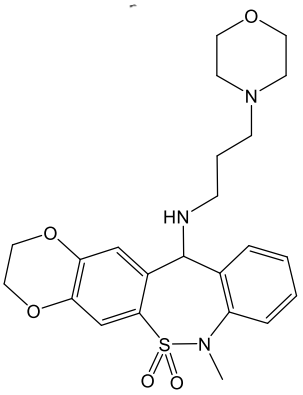


54c

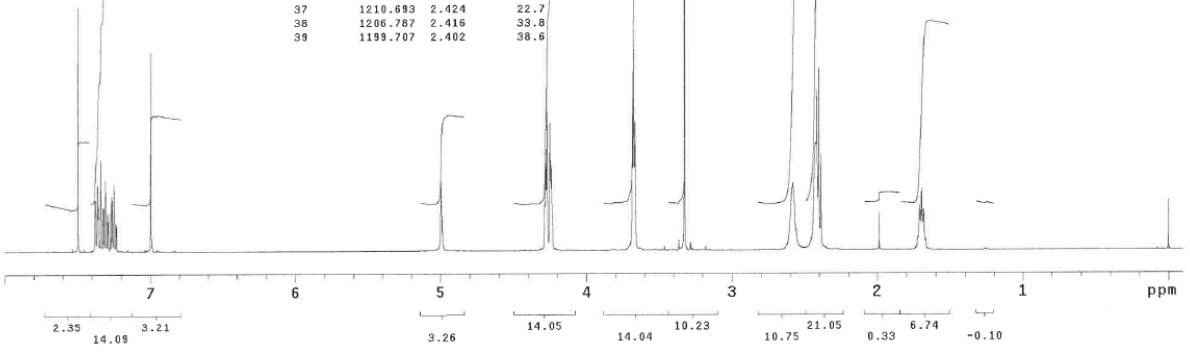


STANDARD 1H
62209
1940-BOE
Berecz Gabor
2006.02.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
File: 62209ih
INOVA-500 "i500"
PULSE SEQUENCE
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244654 MHz
DATA PROCESSING
FT size 131072
Total time 1 minute

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3743.408	7.494	51.7	40	1192.627	2.388	20.1
2	3685.303	7.378	10.6	41	991.943	1.986	7.9
3	3683.838	7.375	10.7	42	854.736	1.711	9.4
4	3677.734	7.362	13.8	43	848.022	1.698	13.0
5	3676.270	7.360	14.1	44	841.309	1.684	8.5
6	3674.194	7.355	9.3	45	-0.000	-0.000	10.4
7	3672.729	7.352	9.6				
8	3666.260	7.339	19.3				
9	3664.917	7.337	18.6				
10	3657.227	7.321	9.3				
11	3655.640	7.318	9.1				
12	3650.024	7.307	15.0				
13	3648.437	7.304	12.4				
14	3642.212	7.291	7.9				
15	3632.812	7.273	8.2				
16	3628.174	7.263	11.6				
17	3626.587	7.260	10.8				
18	3620.728	7.248	14.0				
19	3619.263	7.245	12.9				
20	3494.629	6.996	42.2				
21	2494.385	4.994	14.3				
22	2140.991	4.286	9.8				
23	2140.259	4.285	10.2				
24	2137.329	4.279	18.4				
25	2132.935	4.270	29.4				
26	2122.681	4.249	27.0				
27	2120.972	4.246	16.9				
28	2119.263	4.243	14.5				
29	2117.554	4.239	18.0				
30	2115.845	4.236	9.4				
31	2114.136	4.232	7.2				
32	1839.478	3.682	28.5				
33	1834.839	3.673	42.5				
34	1830.200	3.664	27.1				
35	1660.034	3.323	162.0				
36	1289.551	2.582	14.2				
37	1210.693	2.424	22.7				
38	1206.787	2.416	33.8				
39	1199.707	2.402	38.6				

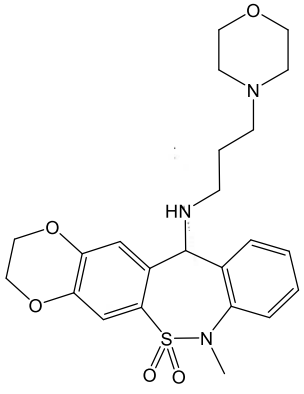


54d

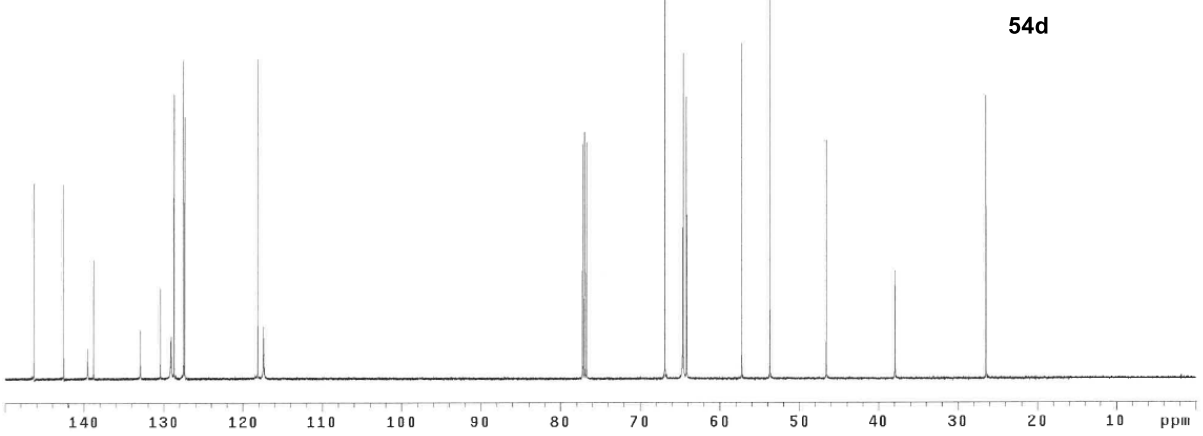


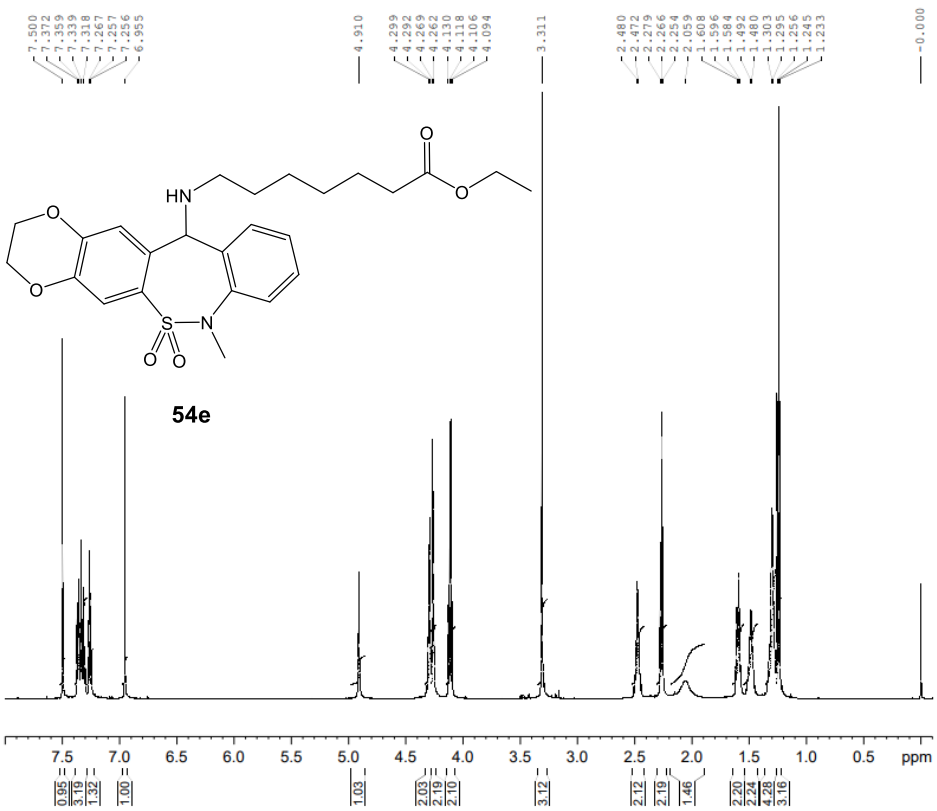
STANDARD 13C
62209
1940-BOE
Berecz Gabor
2006.02.24. (DA)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
Sample #3, user 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
8192 repetitions
OBSERVE C13, 125.6055371 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 5.7 hours

INDEX	FREQUENCY	PPM	HEIGHT
1	18379.891	146.319	41.1
2	17909.676	142.576	40.9
3	17529.305	139.548	6.4
4	17438.484	138.825	25.0
5	16696.785	132.920	10.2
6	16378.914	130.390	19.0
7	16213.387	129.072	9.0
8	16163.094	128.671	58.8
9	16019.539	127.529	66.9
10	15996.590	127.346	54.9
11	14838.387	118.126	67.2
12	14745.613	117.387	11.0
13	9704.598	77.257	49.2
14	9672.371	77.000	51.7
15	9640.633	76.747	49.6
16	8401.375	66.882	146.6
17	8112.801	64.585	68.4
18	8056.160	64.134	59.1
19	7190.438	57.242	70.5
20	6747.078	53.712	154.1
21	5854.500	46.607	50.0
22	4762.703	37.915	22.6
23	3324.715	26.467	59.3



54d



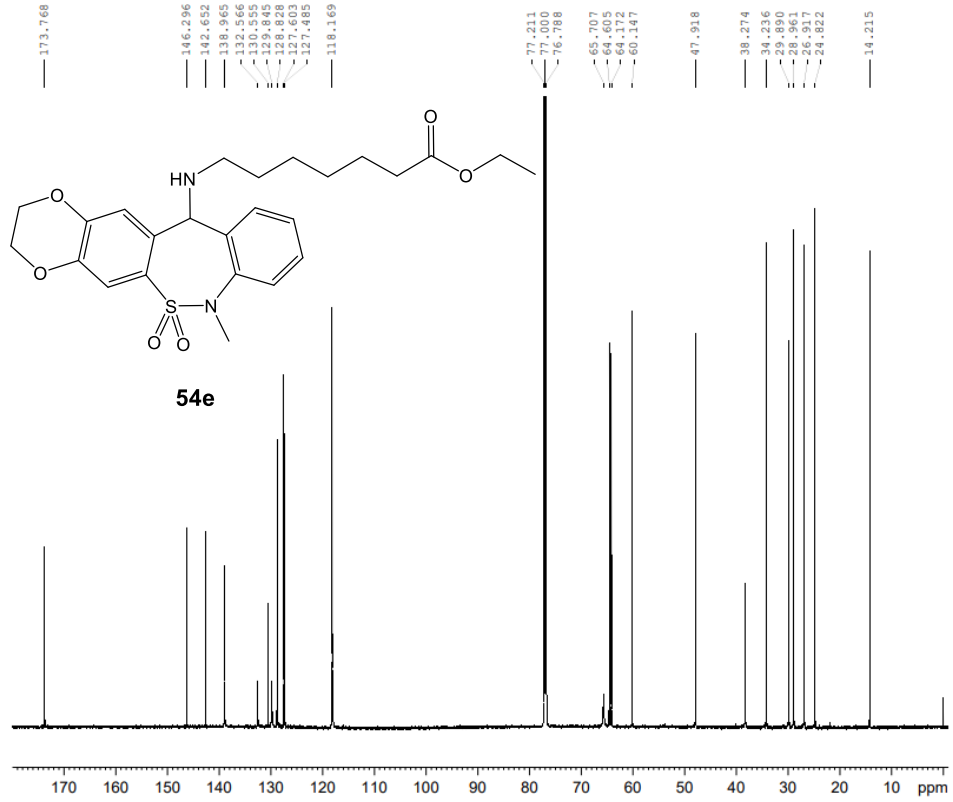


Standard 1H
144500
BGE1941-1941-BGE_1
Berecz Gabor
2025.04.09. (KP)

Current Data Parameters
NAME 144500
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250410
Time 3.01 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 111.4
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

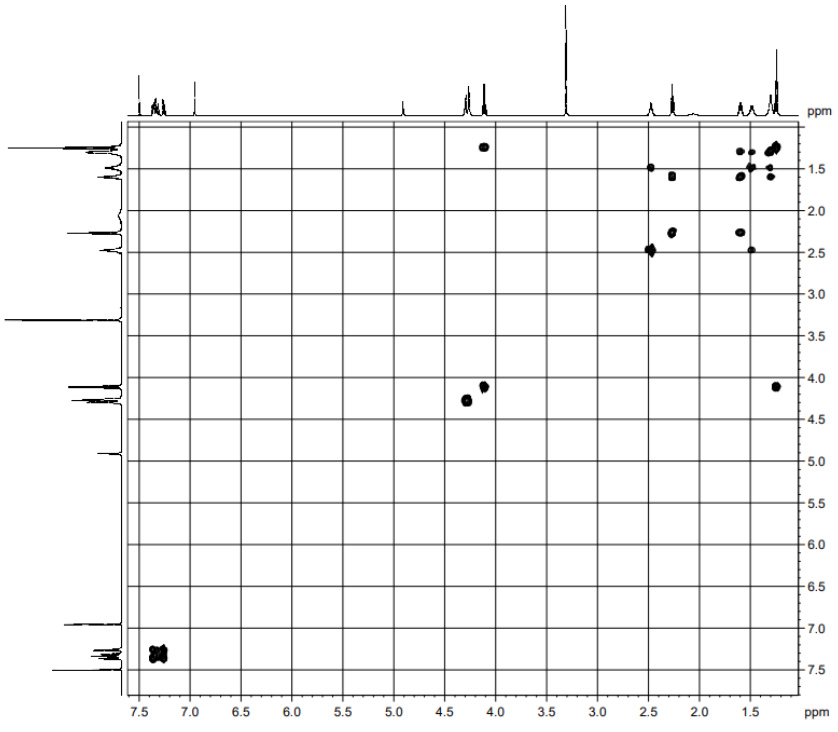


Standard 13C
144500
BGE1941-1941-BGE_1
Berecz Gabor
2025.04.09. (KP)

Current Data Parameters
NAME 144500
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250410
Time 4.10 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.80 usec
PLW1 72.69999695 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 32.50000000 W
PLW12 0.70708001 W
PLW13 0.35508999 W

F2 - Processing parameters
SI 131072
SF 150.8701297 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



54e

COSY
144500
BGE1941-1941-BGE_1
Berecz Gabor
2025.04.09. (KP)

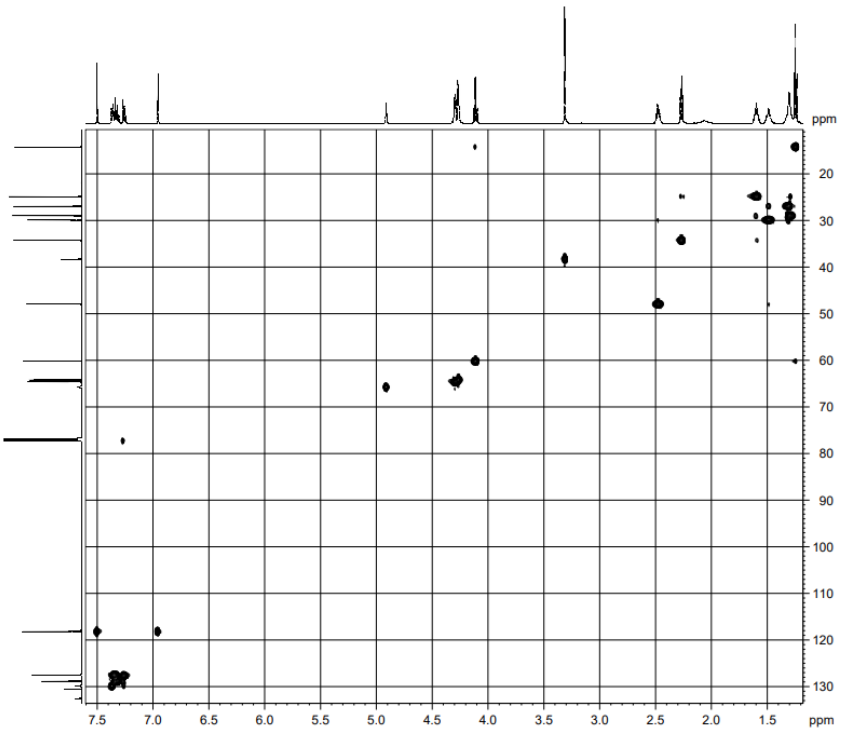
Current Data Parameters
NAME 144500
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250410
Time 4.11 h
INSTRUM spect
PROBHD 3145856_0002 (
PULPROG cosygpmfqf
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
ING 0.00012800 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 16.00 %
GPNAM[2] SMSQ10.100
GPZ2 12.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 600.0036 MHz
FIDRES 61.035156 Hz
SW 13.021 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



54e

HSQC (140Hz)
144500
BGE1941-1941-BGE_1
Berecz Gabor
2025.04.09. (KP)

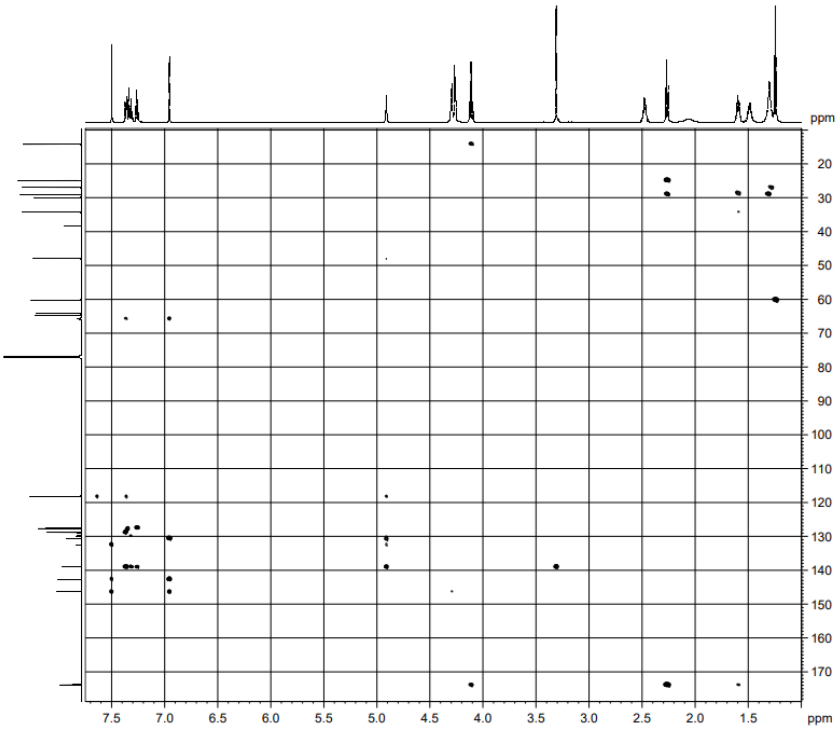
Current Data Parameters
NAME 144500
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250410
Time 4.32 h
INSTRUM spect
PROBHD 3145856_0002 (
PULPROG hsqcetgpsisp2.2
TD 2048
SOLVENT CDCl3
NS 1
DS 32
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST17 -0.5000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00178571 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
ING 0.00001510 sec
TDav 1
SFO1 600.0036000 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P28 0 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
CPDPRG[2 bi_p3mAsp_4sp.2
P3 9.80 usec
P14 500.00 usec
P24 2000.00 usec
P63 1500.00 usec
PLW0 0 W
PLW2 72.69999695 W
PLW12 2.30809999 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 10.66800022 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 10.66800022 W
SPNAM[14 Crp42,1.5,20.2
SPOAL14 0.500
SPOFFS14 0 Hz
SPW14 5.97399998 W
SPNAM[3] Crp42,1.5,20.2
SPOAL31 0.500
SPOFFS31 0 Hz
SPW31 1.49349999 W
GPNAM[1] SMSQ10.100
GPZ1 80.00 %
GPNAM[2] SMSQ10.100
GPZ2 20.10 %
GPNAM[3] SMSQ10.100
GPZ3 11.00 %
GPNAM[4] SMSQ10.100
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 600.0000099 MHz
WDW QSINE

54e



HMBC (8Hz, 140Hz)
144500
BGE1941-1941-BGE_1
Berecz Gabor
2025.04.09. (KP)

Current Data Parameters
NAME 144500
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250410
Time 5.02 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT CDCl3
NS 4
DS 16
SWH 7812.500 Hz
FIDRES 7.629395 Hz
AQ 0.1310720 sec
RG 196.07
DW 64.000 usec
DE 25.00 usec
TE 295.0 K
CNST2 140.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00357143 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.0037800 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
PLW1 28.00000000 W
SFO2 150.8867157 MHz
NUC2 13C
P3 9.80 usec
PLW2 72.69999695 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 30.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

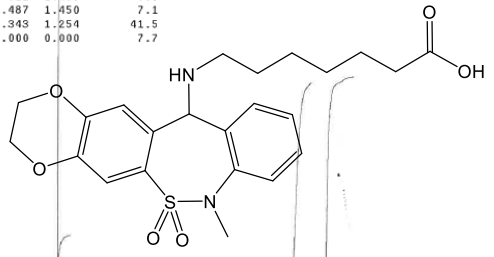
F1 - Acquisition parameters
TD 256
SFO1 150.8867 MHz
FIDRES 258.692047 Hz
SW 219.453 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.0000099 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

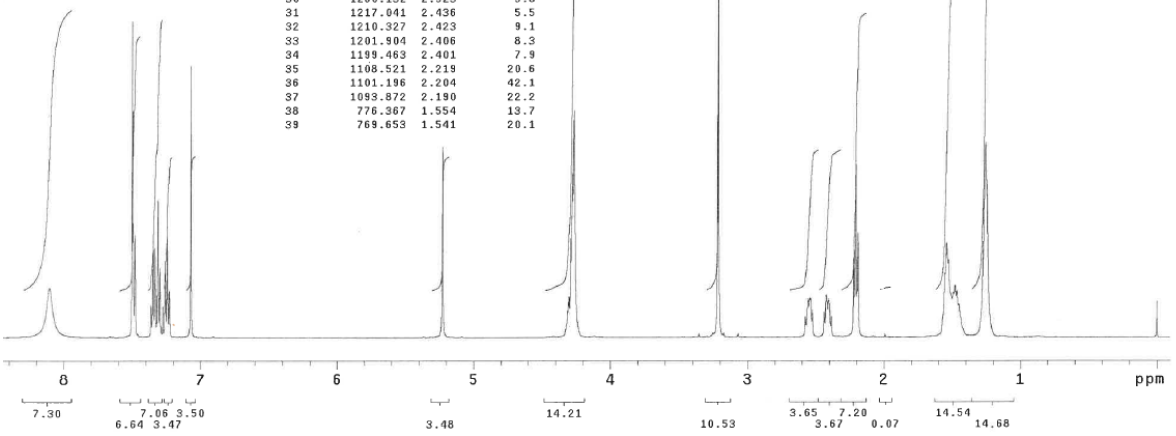
F1 - Processing parameters
SI 1024
MC2 QF
SF 150.8701297 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

STANDARD 1H
62547
1942-BGE
Berecz Gabor
2006.03.16. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244638 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	4047.607	8.103	10.5	40	762.817	1.527	16.5
2	3745.239	7.498	67.1	41	755.005	1.511	9.4
3	3734.985	7.477	21.8	42	744.507	1.490	9.6
4	3677.368	7.362	6.9	43	738.525	1.478	11.1
5	3676.270	7.360	6.4	44	731.812	1.465	9.9
6	3669.434	7.346	19.5	45	724.487	1.450	7.1
7	3662.354	7.332	19.0	46	626.343	1.254	41.5
8	3652.344	7.312	29.2	47	0.000	0.000	7.7
9	3651.489	7.310	29.1				
10	3644.531	7.296	14.8				
11	3633.911	7.275	6.6				
12	3625.244	7.257	13.7				
13	3617.676	7.242	21.0				
14	3610.474	7.228	9.8				
15	3531.128	7.069	57.9				
16	2610.107	5.225	40.6				
17	2154.053	4.312	5.7				
18	2151.001	4.306	7.5				
19	2148.193	4.300	8.7				
20	2142.578	4.289	21.1				
21	2138.550	4.281	25.9				
22	2135.864	4.276	35.0				
23	2130.127	4.264	48.4				
24	1605.713	3.214	160.8				
25	1276.733	2.556	7.7				
26	1274.536	2.551	8.2				
27	1270.752	2.544	8.2				
28	1268.677	2.540	8.4				
29	1265.991	2.534	8.2				
30	1260.132	2.523	5.8				
31	1217.041	2.436	5.5				
32	1210.327	2.423	9.1				
33	1201.904	2.406	8.3				
34	1199.463	2.401	7.9				
35	1108.521	2.219	20.6				
36	1101.196	2.204	42.1				
37	1093.872	2.190	22.2				
38	776.367	1.554	13.7				
39	769.653	1.541	20.1				

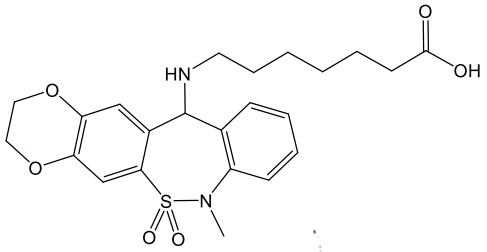


54f



STANDARD 13C
62547
1942-BGE
Berecz Gabor
2006.03.16. (CzB)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
688 repetitions
OBSERVE C13, 125.6055371 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 49 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	22379.891	178.162	61.0
2	18417.000	146.614	79.6
3	17986.824	143.190	76.8
4	17558.602	139.781	50.3
5	16852.547	134.160	7.7
6	16542.000	131.688	13.7
7	16379.402	130.393	49.1
8	16284.676	129.639	54.0
9	16181.160	128.815	11.3
10	16002.938	127.396	62.7
11	15970.711	127.140	64.1
12	15117.684	120.349	15.9
13	14838.875	118.130	70.5
14	9704.109	77.253	151.4
15	9672.371	77.000	162.0
16	9640.145	76.743	154.1
17	8237.313	65.576	15.2
18	8103.523	64.511	60.5
19	8064.949	64.204	58.3
20	5881.356	46.820	52.2
21	4877.938	38.832	47.7
22	4416.512	35.159	56.2
23	3634.285	28.932	93.8
24	3590.340	28.582	63.5
25	3364.754	26.786	86.8
26	3155.770	25.123	85.9



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