Regio and Stereospecific Synthesis of *β*-Sulfonamidodisulfides and *β*-Sulfonamidosulfides from Aziridines Using Tetrathiomolybdate as a Sulfur Transfer Reagent

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Supporting Information

Contents

Page No

Experimental

General Procedures. All reactions were carried out in oven-dried apparatus using dry solvents under anhydrous conditions, unless otherwise noted. Reaction mixtures were stirred magnetically unless otherwise stated. Commercial grade solvents were distilled and dried according to literature procedures ("Purification of laboratory chemicals", 3rd Ed., D. D. Perrin, W. L. F. Armarego, Pergamon Press, Oxford, 1988). Analytical TLC was performed on commercial plates coated with silica gel GF_{254} (0.25 mm). Silica gel (230 - 400 mesh) was used for column chromatography. Melting points determined are uncorrected. Yields refer to chromatographically and spectroscopically (^{1}H NMR) homogeneous materials, unless otherwise stated. NMR spectra were recorded on 300 or 400 MHz instruments and calibrated using residual undeuterated solvent as an internal reference. The following abbreviations explain the multiplicity s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. IR spectra were recorded on a FT-IR spectrometer. High-resolution mass spectra (HR-MS) were recorded on a Q-TOF mass spectrometer.

Preparation of ammonium tetrathiomolybdate[1] $[NH_4]_2MoS_4$: Ammonium molybdate (10 g) was dissolved in a mixture of ammonium hydroxide (60 mL) water (20 mL), and the solution was filtered. Hydrogen sulfide was bubbled rapidly at ambient temperature into the solution mixture until it was saturated and then the temperature was raised to 60 °C while maintaining a slow stream of hydrogen sulfide. After 60 min, the mixture was cooled to 0 °C for 30 min and the product was isolated by filtration. The crystalline solid was washed with isopropyl alcohol (25 mL) and ether (25 mL) and dried under vacuum to obtain brick red crystals of ammonium molybdate (13.4 – 14.2 g, 92%).

UV – Vis (H_2O): λ_{max} (nm), (ε): 472 (11,850); 326 (16,750); 241 (24,700). IR (KBr): 750, 700, 525, 450.

Preparation of Benzyltriethylammonium tetrathiomolybdate[2] **$[BnEt_3N]_2MoS_4$:** A solution of benzyltriethylammonium chloride (23.3 g, 102.5 mmol) in distilled water (60 mL) was added to a well stirred solution of ammonium tetrathiomolybdate (13 g, 50 mmol) in distilled water (60 mL). Vigorous stirring was continued for 2 h at room temperature and the solid was filtered and washed with isopropyl alcohol (40 mL) and diethyl ether (40 mL). After drying at high vacuum, brick red powder of benzyltriethylammonium tetrathiomolybdate **1** was stored in a desiccator (24 g, 80%).

mp: 150 °C (decomp). UV – Vis (DMF): λ_{max} (nm), (ε): 472 (11, 850); 320 (16,750); 274 (24,700); Anal. Calcd for ($C_{26}H_{44}N_2S_4Mo$) C, 51.29; H, 7.28; N, 4.60. Found C, 50.93; H, 7.31; N, 4.31.

***β*-Sulfonamidodisulfide 4b:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.101 g, 88%; IR (neat) V_{max}: 3246, 1353, 1182, 836, 671 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.21 (t, *J* = 5.7 Hz, 1H), 3.24 (dd, *J* = 12.9, 6.0 Hz, 2H), 2.70 (t, *J* = 6.6 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.7, 136.8, 129.8, 127.1, 41.6, 37.9, 21.5; HR - MS m/z: calcd for $C_{18}H_{24}N_2O_4S_4H^+$[M+H$^+$]: 461.0697; found: 461.0678.

***β*-Sulfonamidodisulfide 4c:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.098 g, 80%; $[\alpha]^{27}_D$ = + 36 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3226, 1345, 1167, 878, 664 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.11 (d, *J* = 7.8 Hz, 1H), 3.62-3.53 (m, 1H), 2.88 (dd, *J* = 13.8, 5.4 Hz, 1H), 2.66 (dd, *J* = 13.8, 6.6 Hz, 1H), 2.43 (s, 3H), 1.12 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.5, 137.7, 129.7, 127.1, 49.1, 45.8, 21.5, 20.2; HR - MS m/z: calcd for $C_{20}H_{28}N_2O_4S_4Na^+$[M+Na$^+$]: 511.0830; found: 511.0843.

Compound 4d and 5d: R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.111 g, 86%; $[\alpha]^{27}_D$ = +54.164 (c = 6.0, CH_2Cl_2); IR (neat) V_{max}: 3279, 1323, 1159, 1092, 814, 666 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 9 : 1 mixture): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 5.18 (d, *J* = 7.8 Hz, 1H), 5.01 (d, *J* = 6.6 Hz, 0.12H), 3.45-3.35 (m, 1H), 2.93 (dd, *J* = 14.1, 4.8 Hz, 1H), 2.82 (dd, *J* = 13.5, 5.5 Hz, 0.13H), 2.69 (dd, *J* = 14.1, 6.0 Hz, 1H), 2.43 (s, 3H), 1.67-1.58 (m, 1.13H), 1.46-1.37 (m, 1.16H), 0.73 (t, *J* = 7.5 Hz, 3.38 H); ^{13}C NMR (75 MHz, $CDCl_3$, 9 : 1 mixture): δ 143.4, 137.7, 129.7, 127.1, 127.0, 54.6, 54.4, 43.8, 26.5, 26.4, 21.5, 9.8; HR - MS m/z: calcd for $C_{22}H_{32}N_2O_4S_4Na^+$[M+Na$^+$]: 539.1143; found: 539.1147.

***β*-Sulfonamidodisulfide 4e:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.120 g, 88%; $[\alpha]^{27}_D$ = - 45.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3281, 1324, 1159, 1093, 814, 665 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 5.14 (d, *J* = 8.4 Hz, 1H), 3.36-3.28 (m, 1H), 2.86 (dd, *J* = 13.8, 5.4 Hz, 1H), 2.73 (dd, *J* = 13.8, 6.3 Hz, 1H), 2.42 (s, 3H), 2.01-1.89 (m, 1H), 0.77 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.3, 137.8, 129.6, 127.1, 58.5, 41.3, 29.8, 21.5, 18.9, 17.3; HR - MS m/z: calcd for $C_{24}H_{36}N_2O_4S_4Na^+$[M+Na$^+$]: 567.1456; found: 567.1477.

***β*-Sulfonamidodisulfide 4f:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.119 g, 83%; $[\alpha]^{27}_D$ = -159.00 (c = 1.0, CH_2Cl_2); IR (neat) V_{max}: 3275, 1328, 1162, 818, 648 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.13 (d, *J* = 8.1

Hz, 1H), 3.57-3.48 (m, 1H), 2.95 (dd, *J* = 13.5, 3.9 Hz, 1H), 2.66 (dd, *J* = 13.5, 6.6 Hz, 1H), 2.43 (s, 3H), 1.47-1.24 (m, 3H), 0.79 (d, *J* = 6.3 Hz, 3H), 0.61 (d, *J* = 5.7 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.4, 137.7, 129.6, 127.1, 51.4, 44.7, 42.8, 24.3, 22.9, 21.5; HR - MS m/z: calcd for $C_{26}H_{40}N_2O_4S_4K^+$[M+K$^+$]: 611.1508; found: 611.1507. Anal. Calcd for $C_{26}H_{40}N_2O_4S_4$: C, 54.51; H, 7.04; N, 4.89; S, 22.39; Found: C, 54.85; H, 7.20; N, 4.98; S, 22.46.

***β*-Sulfonamidodisulfide 4g:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.122 g, 85%; $[\alpha]^{27}_D$ = +19.05 (c = 7.4, CH_2Cl_2); IR (neat) V_{max}: 3280, 1329, 1159, 1093, 813, 667 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.77 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 5.13 (d, *J* = 8.1 Hz, 1H), 3.43-3.35 (m, 1H), 2.82-2.68 (m, 2H), 2.43 (s, 3H), 1.38-1.27 (m, 1H), 1.01-0.89 (m, 1H), 0.81 (t, *J* = 6.9 Hz, 3H), 0.75 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.3, 137.8, 129.6, 127.1, 57.5, 40.6, 37.2, 27.7, 21.5, 14.9, 11.5; HR - MS m/z: calcd for $C_{26}H_{40}N_2O_4S_4K^+$[M+K$^+$]: 611.1508; found: 611.1539.

***β*-Sulfonamidodisulfide 4h:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.115 g, 80%; $[\alpha]^{27}_D$ = -137.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3286, 1320, 1155, 812, 732, 666 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 5.39 (d, *J* = 9.3 Hz, 1H), 3.41-3.34 (m, 1H), 3.00-2.86 (m, 2H), 2.42 (s, 3H), 0.81 (m, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.0, 138.8, 129.5, 126.9, 63.1, 41.9, 35.5, 26.9, 21.5; HR - MS m/z: calcd for $C_{26}H_{40}N_2O_4S_4K^+$[M+K$^+$]: 611.1508; found: 611.1524.

***β*-Sulfonamidodisulfide 4i:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.119 g, 78%; $[\alpha]^{27}_D$ = -145.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3243, 1348, 1164, 823, 748, 667 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.29 (d, *J* = 8.1 Hz, 1H), 3.77-3.63 (m, 1H), 3.03 (dd, *J* = 14.1, 4.5 Hz, 1H), 2.75 (dd, *J* = 14.1, 6.9

Hz, 1H) 2.44 (s, 3H), 2.37-2.19 (m, 2H), 1.97 (s, 3H), 1.91-1.86 (m, 1H), 1.75-1.67 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.6, 137.6, 129.8, 127.2, 52.4, 44.3, 32.1, 30.1, 21.6, 15.2; HR - MS m/z: calcd for $C_{24}H_{36}N_2O_4S_6Na^+$[M+Na$^+$]: 631.0897; found: 631.0891.

***β*-Sulfonamidodisulfide 4j:** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.181 g, 74%; $[\alpha]^{27}_D$ = -87.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3268, 1356, 1179, 863, 765, 666 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 5.08 (d, *J* = 7.8 Hz, 1H), 3.73-3.61 (m, 1H), 3.04 (dd, *J* = 13.8, 4.5 Hz, 1H), 2.87 (dd, *J* = 13.8, 5.7 Hz, 1H), 2.75 (dd, *J* = 14.1, 6.6 Hz, 1H), 2.65 (dd, *J* = 14.1, 7.8 Hz, 1H), 2.45 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.4, 145.5, 143.6, 136.9, 135.5, 132.3, 130.9, 130.4, 129.8, 129.6, 128.4, 126.8, 122.4, 54.3, 43.7, 38.6, 21.7, 21.5; HR - MS m/z: calcd for $C_{46}H_{48}N_2O_{10}S_6Na^+$[M+Na$^+$]: 1003.1531; found: 1003.1565.

***β*-Sulfonamidodisulfide 4k:** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.117 g, 65%; $[\alpha]^{27}_D$ = -52.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 3238, 1362, 1156, 864, 788, 663 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.00 (bs, 1H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.33-7.26 (m, 2H), 7.19-7.14 (m, 1H), 7.09-6.95 (m, 4H), 4.96 (d, *J* = 6.6 Hz, 1H), 3.80-3.74 (m, 1H), 3.08-3.02 (m, 2H), 2.90 (dd, *J* = 14.7, 7.2 Hz, 1H), 2.78 (d, *J* = 14.7, 6.9 Hz, 1H), 2.30(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.1, 136.7, 136.3, 129.4, 127.1, 126.8, 123.3, 122.2, 119.7, 118.6, 111.2, 110.3, 52.9, 43.4, 28.9, 21.5; HR - MS m/z: calcd for $C_{36}H_{38}N_4O_4S_4Na^+$[M+Na$^+$]: 741.1674; found: 741.1691.

***β*-Sulfonamidodisulfide 3p:** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.120 g, 60%; $[\alpha]^{27}_D$ = -18.00 (c = 1.0, $CHCl_3$); IR (neat) V_{max}: 1532, 1460, 1312, 1160, 1045, 678 cm^{-1};

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 4.14 (dd, *J* = 8.4, 6.3 Hz, 1H), 4.04-3.98 (m, 1H), 3.94 (dd, *J* = 7.5, 4.5 Hz, 1H), 3.87 (dd, *J* = 8.5, 4.8 Hz, 1H), 3.73 (t, *J* = 7.5 Hz, 1H), 3.03-2.98 (m, 1H), 2.59 (d, *J* = 7.2 Hz, 1H), 2.45 (s, 3H), 2.37 (d, *J* = 4.5 Hz, 1H), 1.46 (s, 3H), 1.33 (s, 3H), 1.31 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 144.5, 134.8, 129.5, 128.0, 110.3, 109.7, 79.9, 77.9, 76.8, 67.7, 40.3, 30.9, 27.1, 26.5, 26.4, 25.1, 21.6; HR - MS m/z: calcd for $C_{19}H_{27}NO_6SNa^+$[M+Na^+]: 420.1457; found: 420.1468.

***β*-Sulfonamidodisulfide 7a:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.114 g, 75%; m. p: 162 ºC; IR (neat) V_{max}: 3266, 1349, 1132, 866, 796, 623 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 5.18 (s, 1H), 3.06 (s, 2H), 2.42 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.1, 140.1, 129.5, 126.9, 57.2, 47.9, 27.0, 21.5; HR - MS m/z: calcd for $C_{22}H_{32}N_2O_4S_4Na^+$[M+$Na^+$]: 539.1143; found: 539.1132. Anal. Calcd for $C_{22}H_{32}N_2O_4S_4$: C, 51.13; H, 6.24; N, 5.42; S, 24.82; Found: C, 51.29; H, 6.54; N, 5.61; S, 24.99.

***β*-Sulfonamidodisulfides 7b and 7b':** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.117 g, 82%; IR (neat) V_{max}: 3243, 1363, 1175, 816, 738, 645 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomeric): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.01 (s, 1H), 3.07 (s, 1H), 2.83 (s, 1H), 2.42 (s, 3H), 1.54-1.48 (m, 2H), 1.26-1.16 (m, 4H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.0, 140.2, 129.5, 127.0, 59.9, 59.7, 51.6, 51.4, 42.2, 42.1, 23.5, 21.5, 16.8, 14.1, 14.0; HR - MS m/z: calcd for $C_{26}H_{40}N_2O_4S_4Na^+$[M+$Na^+$]: 595.1769; found: 595.1778.

***β*-Sulfonamidodisulfides 7d and 7d':** R_f = 0.30 (EtOAc/hexane, 1 : 1); Yield: 0.101 g, 70%; IR (neat) V_{max}: 3500, 3273, 1321, 1154, 1091, 816, 664 cm^{-1}; ^{1}H NMR (300 MHz,

$CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.78 (d, *J* = 8.1 Hz, 4H), 7.28 (d, *J* = 8.1 Hz, 4H), 6.26 (s, 1H), 6.19 (s, 1H), 3.86-3.76 (m, 4H), 3.29-3.22 (m, 4H), 2.42 (s, 6H), 1.91-1.82 (m, 4H), 1.22 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.1, 140.3, 129.6, 126.8, 59.6, 58.9, 51.5, 41.0, 23.7, 21.5; HR - MS m/z: calcd for $C_{24}H_{36}N_2O_6S_4Na^+$[M+Na$^+$]: 599.1354; found: 599.1361

***anti-β*-Sulfonamidodisulfides 9a and 9a':** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.113 g, 79%; m. p: 132 ºC; IR (neat) V_{max}: 3278, 1325, 1161, 1098, 817, 668 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 6.14-6.09 (m, 1H), 3.44-3.35 (m, 1H), 2.89-2.84 (m, 1H), 2.50-2.45 (, 1H), 2.41 (s, 3H), 1.78-1.59 (m, 2H), 1.46-1.25 (m, 2H), 1.05-0.91 (m, 3H), 069-0.57 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 142.6, 138.3, 129.2, 126.7, 58.2, 58.1, 23.3, 23.2, 22.2, 21.3, 12.2, 12.1, 10.6, 10.5; HR - MS m/z: calcd for $C_{26}H_{40}$ $N_2O_4S_4Na^+$[M+Na$^+$]: 595.1769; found: 595.1775. Anal. Calcd for $C_{26}H_{40}N_2O_4S_4$: C, 54.51; H, 7.04; N, 4.89; S, 22.39; Found: C, 54.83; H, 7.27; N, 5.10; S, 22.51.

***anti-β*-Sulfonamidodisulfides 9b and 9b':** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.117 g, 82%; m. p: 166 ºC; IR (neat) V_{max}: 3276, 1321, 1160, 1093, 1010, 815, 667 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 4H), 5.22 (d, *J* = 9.3 Hz, 2H), 4.98 (d, *J* = 9.0 Hz, 2H), 3.41-3.31 (m, 2), 2.99-2.93 (m, 1H), 2.73-2.67 (m, 1H), 2.42 (s, 6H), 1.59-1.38 (m, 8H), 1.01 (t, *J* = 7.5 Hz, 3H), 0.93 (t, *J* = 7.5 Hz, 3H), 0.74 (t, *J* = 7.5 Hz, 3H), 0.67 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.1, 138.1, 129.5, 127.2, 63.4, 61.1, 58.6, 58.4, 25.9, 24.9, 23.5, 22.8, 21.5, 12.3, 12.2, 10.7, 10.6; HR - MS m/z: calcd for $C_{26}H_{40}$ $N_2O_4S_4K^+$[M+K$^+$]: 611.1508; found:

611.1520. Anal. Calcd for $C_{26}H_{40}N_2O_4S_4$: C, 54.51; H, 7.04; N, 4.89; S, 22.39; Found: C, 54.79; H, 7.31; N, 5.15; S, 22.43.

***β*-Sulfonamidodisulfides 11b and 11b':** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.097 g, 68%; m. p: 160 ºC; IR (neat) V_{max}: 3289, 1323, 1157, 811, 664 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.78 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 5.36 (d, *J* = 6.9 Hz, 1H), 3.49-3.47 (m, 1H), 2.73-2.68 (m, 1H), 2.43 (s, 3H), 2.13-2.09 (m, 1H), 1.69-1.68 (m, 1H), 1.66-1.56 (m, 2H), 1.40-1.19 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.3, 138.3, 129.7, 127.0, 56.8, 55.7, 33.3, 32.3, 25.0, 23.9, 21.6; HR - MS m/z: calcd for $C_{26}H_{36}N_2O_4S_4Na^+$[M+Na$^+$]: 591.1456; found: 591.1462. Anal. Calcd for $C_{26}H_{36}N_2O_4S_4$: C, 54.90; H, 6.38; N, 4.92; S, 22.55; Found: C, 55.12; H, 6.42; N, 5.14; S, 22.63.

***β*-Sulfonamidodisulfides 11c and 11c':** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.075 g, 50%; IR (neat) V_{max}: 3276, 1329, 1162, 803, 670 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.82-7.76 (m, 4H), 7.31-7.26 (m, 4H), 5.28 (d, *J* = 7.5 Hz, 1H), 5.19 (d, *J* = 6.9 Hz, 1H), 3.58-3.54 (m, 2H), 3.43-3.39 (m, 2H), 2.96-2.87 (m, 4H), 2.43 (s, 6H), 1.99-1.92 (m, 4H), 1.68-1.61 (m, 6H), 1.50-1.46 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.3, 143.2, 137.9, 137.8, 129.6, 127.6, 127.1, 59.4, 58.7, 57.4, 55.5, 32.4, 31.7, 31.5, 29.7, 28.6, 28.3, 25.5, 24.9, 22.8, 22.6, 21.6; HR - MS m/z: calcd for $C_{28}H_{40}N_2O_4S_4Na^+$[M+Na$^+$]: 619.1769; found: 619.1781.

***β*-Sulfonamidodisulfides 11f and 11f':** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.116 g, 78%; IR (neat) V_{max}: 3268, 1433, 1324, 1158, 1091, 814, 734, 669 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.78 (d, *J* = 8.4 Hz, 4H), 7.32 (d, *J* = 8.4 Hz, 4H), 5.71 (d, *J* = 8.4 Hz, 1H), 5.38 (d, *J* = 6.9 Hz, 1H), 3.38-3.30 (m, 2H), 3.11 (bs, 3H), 3.07 (bs, 1H), 2.98-2.88 (m, 1H), 2.81-2.72 (m, 1H), 2.68-2.49 (m, 3H), 2.44 (s, 6H), 2.21 (dd, *J* = 14.7, 3.0 Hz, 1H), 2.09-1.97 (m, 2H), 1.69-1.65 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.7, 143.6, 138.1, 137.3, 128.9, 127.3, 126.9, 52.6, 52.1, 51.4, 51.0, 50.8, 50.2, 49.9, 32.1, 31.8, 30.8, 30.4, 21.6; HR - MS m/z: calcd for $C_{26}H_{32}N_2O_6S_4Na^+$[M+Na$^+$]: 619.1041; found: 619.1030.

***β*-Sulfonamidodisulfides 11g and 11g':** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.134 g, 76%; IR (neat) V_{max}: 3265, 1435, 1324, 1158, 1092, 813, 662 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.77 (d, *J* = 8.1 Hz, 4H), 7.32 (d, *J* = 8.1 Hz, 4H), 5.46 (d, *J* = 7.5 Hz, 1H), 5.15 (d, *J* = 6.3 Hz, 1H), 3.34-3.25 (m, 2H), 2.98-2.89 (m, 1H), 2.79-2.69 (m, 1H), 2.44 (s, 6H), 2.37-1.87 (m, 8H), 1.37-1.25 (m, 16H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.6, 138.0, 129.8, 127.3, 127.0, 62.5, 61.5, 61.2, 60.4, 52.5, 51.1, 38.2, 37.0, 30.5, 29.3, 29.0, 21.6, 20.1, 19.7; HR - MS m/z: calcd for $C_{34}H_{44}N_2O_6S_4Na^+$[M+Na$^+$]: 727.1980; found: 727.1948.

***β*-Sulfonamidodisulfides 11h and 11h':** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.118 g, 70%; IR (neat) V_{max}: 3272, 1438, 1328, 1162, 1098, 816, 741, 663 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.77 (d, *J* = 8.1 Hz, 4H), 7.32 (d, *J* = 8.1 Hz, 4H), 5.53 (d, *J* = 8.4 Hz, 1H), 5.37 (d, *J* = 6.6 Hz, 1H), 3.43-3.35 (m, 2H), 3.11-3.02 (m, 2H), 2.84-2.76 (m, 2H), 2.56-2.40 (m, 4H), 2.44 (s, 6H), 2.21-2.04 (m, 4H), 1.97-1.83 (m, 4H), 1.77-1.28 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.7, 143.6, 138.0, 137.1, 129.9, 127.3, 126.9, 67.7, 66.9, 66.6, 66.1, 52.5, 52.2, 51.3, 50.9, 33.7, 33.4, 32.9, 31.9, 31.3, 31.2, 31.0, 30.8, 21.6, 19.9, 19.8; HR - MS m/z: calcd for $C_{32}H_{40}N_2O_6S_4Na^+$[M+Na$^+$]: 699.1667; found: 699.1632.

Synthesis of aziridino-epoxide 16a: R_f = 0.60 (EtOAc/hexane, 2 : 8); Yield: 0.466 g, 55%; IR (neat) V_{max}: 1596, 1322, 1161, 1093, 923, 714, 694, 660 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.84 (d, *J* = 7.8 Hz, 2H), 7.35 (d, *J* = 7.8 Hz, 2H), 3.73-3.62 (m, 2H), 3.49-3.38 (m, 1H), 3.44-3.25 (m, 1H), 3.04-3.97 (m, 2H), 2.76-2.71 (m, 1H), 2.65 (d, *J* = 6.9 Hz, 1H), 2.53-2.48 (m, 1H), 2.45 (s, 3H), 2.12 (t, *J* = 5.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 144.6, 134.6, 129.6, 127.9, 71.6, 71.2, 70.1, 69.9, 50.5, 50.4, 43.8, 38.5, 38.4, 30.6, 21.5; HR - MS m/z: calcd for $C_{13}H_{17}NO_4SNa^+$[M+Na^+]: 306.0776; found: 306.0785.

Synthesis of *β*-sulfonamidodisulfide 16b: To a well-stirred solution of aziridine **16a** (0.50 mmol) in CH_3CN (6 mL) was added **1** (0.335 g, 0.55 mmol) at once and stirred at room temperature (28 °C) for 2 h. The solvent was evaporated under reduced pressure and the black residue was extracted with CH_2Cl_2 : Et_2O (1:5, 3 x 10 mL) and was filtered through a Celite pad. The filtrate was concentrated and the residue was purified by flash column chromatography on silica gel to give diastereomeric mixture of *β*-sulfonamidodisulfide **16b** in good yield. R_f = 0.30 (EtOAc/hexane, 2 : 8); Yield: 0.125 g, 79%; IR (neat) V_{max}: 3271, 1331, 1159, 1092, 815, 660 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.77 (d, *J* = 7.5 Hz, 4H), 7.31 (d, *J* = 7.5 Hz, 4H), 5.37-5.20 (m, 2H), 3.71-3.51 (m, 4H), 3.42-3.17 (m, 6H), 3.06 (bs, 2H), 2.82-2.78 (m, 3H), 2.61-2.55 (m, 3H), 2.43 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.6, 137.6, 129.7, 127.1, 127.0, 71.9, 71.7, 70.8, 70.5, 70.3, 52.9, 52.6, 50.6, 50.5, 44.1, 43.9, 34.7, 34.5, 21.5; HR - MS m/z: calcd for $C_{26}H_{36}N_2O_8S_4Na^+$[M+$Na^+$]: 655.1252; found: 655.1270.

***β*-Sulfonamidodisulfide 19a:** R_f = 0.30 (EtOAc/hexane, 1 : 1); Yield: 0.107 g, 74%; IR (neat) V_{max}: 3483, 3291, 1326, 1157, 1090, 814, 741, 666 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 7.77 (d, *J* = 8.1 Hz, 4H), 7.31 (d, *J* = 8.1 Hz, 4H), 5.51 (d, *J* = 8.4 Hz, 1H), 5.27 (d, *J* = 8.7 Hz, 1H), 3.93 (d, *J* = 11.4 Hz, 1H), 3.74 (dd, *J* = 11.4, 7.8 Hz, 1H), 3.62-3.54 (m, 2H), 3.24-3.22 (m, 1H), 3.03 (d, *J* = 8.1 Hz, 1H), 2.43 (s, 6H), 1.29 (s, 3H), 1.26 (s, 3H), 1.19 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, 1 : 1 mixture of diastereomers): δ 143.6, 137.6, 129.7, 127.2, 127.0, 73.7, 63.0, 60.5, 27.4, 27.3, 25.6, 21.5; HR - MS m/z: calcd for $C_{24}H_{36}N_2O_6S_4Na^+$[M+Na$^+$]: 599.1354; found: 599.1368.

***β*-Sulfonamidosulfide 31:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.164 g, 76%; $[\alpha]^{27}_D$ = - 62.00 (c = 1, CH_2Cl_2); IR (neat) V_{max}: 3279, 1477, 1329, 1158, 1094, 812, 665 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.23-7.09 (m, 9H), 6.95-6.92 (m, 2H), 4.77 (d, *J* = 6.6 Hz, 1H), 3.48-3.73 (m, 1H), 3.15 (dd, *J* = 14.1, 1.5 Hz, 1H), 2.98 (dd, *J* = 13.8, 6.3 Hz, 1H), 2.85 (dd, *J* = 14.1, 7.5 Hz, 1H), 2.76 (dd, *J* = 13.8, 6.9 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.3, 136.4, 136.2, 133.4, 132.4, 130.8, 129.5, 129.2, 129.1, 128.7, 126.9, 126.8, 53.8, 39.4, 38.2, 21.5; HR - MS m/z: calcd for $C_{22}H_{22}ClNO_2S_2Na^+$[M+Na$^+$]: 454.0678; found: 454.0685.

***β*-Sulfonamidosulfide 32:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.124 g, 65%; IR (neat) V_{max}: 3265, 1486, 1339, 1161, 1084, 1012, 816, 665 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.28-7.18 (m, 6H), 5.29 (d, *J* = 5.7 Hz, 1H), 3.40-3.29 (m, 2H), 2.43 (s, 3H), 2.18-1.99 (m, 2H), 1.75-1.64 (m, 2H), 1.59-1.46 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.5, 136.8, 133.1, 132.7, 129.7, 128.9, 127.2, 59.5, 52.6, 31.5, 30.2, 21.6, 21.5; HR - MS m/z: calcd for $C_{18}H_{20}ClNO_2S_2Na^+$[M+Na$^+$]: 404.0522;

found: 404.0536. Anal. Calcd for $C_{18}H_{20}ClNO_2S_2$: C, 56.60; H, 5.28; N, 3.67; S, 16.74; Found: C, 56.72; H, 5.31; N, 3.78; S, 16.63.

***β*-Sulfonamidosulfide 33:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.140 g, 71%; IR (neat) V_{max}: 3275, 2935, 1475, 1326, 1156, 1093, 1012, 814, 666 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.1 Hz, 2H), 7.31-7.20 (m, 6H), 5.30 (d, *J* = 4.5 Hz, 1H), 3.00-2.80 (m, 2H), 2.44 (s, 3H), 2.22-2.16 (m, 1H), 2.05-1.98 (m, 1H), 1.59-1.57 (m, 2H), 1.27-1.26 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.4, 137.3, 134.3, 133.7, 131.4, 129.6, 129.0, 127.2, 54.9, 51.3, 31.9, 31.3, 24.3, 23.1, 21.5; HR - MS m/z: calcd for $C_{19}H_{22}ClNO_2S_2Na^+$[M+Na$^+$]: 418.0678; found: 418.0688.

***β*-Sulfonamidosulfide 35:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.135 g, 68%; IR (neat) V_{max}: 3264, 1328, 1162, 1094, 816, 665 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.35-7.22 (m, 6H), 4.86 (d, *J* = 7.8 Hz, 1H), 3.21-3.11 (m, 2H), 2.41 (s, 3H), 1.81-1.68 (m, 2H), 1.38-1.09 (m, 2H), 1.04 (t, *J* = 7.2 Hz, 3H), 0.54 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.4, 137.3, 133.3, 132.9, 132.7, 129.5, 129.1, 127.0, 58.5, 55.6, 23.4, 22.8, 21.5, 12.5, 10.7; HR - MS m/z: calcd for $C_{19}H_{24}ClNO_2S_2Na^+$[M+Na$^+$]: 420.0835; found: 420.0849.

***β*-Sulfonamidosulfide 36:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.139 g, 70%; m. p: 135 ºC; IR (neat) V_{max}: 3236, 1443, 1332, 1152, 813, 745, 666 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.25-7.07 (m, 6H), 4.94 (d, *J* = 9.6 Hz, 1H), 3.48-3.40 (m, 1H), 2.90-2.85 (m, 1H), 2.43 (s, 3H), 1.69-1.48 (m, 2H), 1.41-1.26 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.3, 138.3, 134.3, 132.9, 132.5, 129.6, 129.1, 126.9, 58.9, 57.8, 27.2, 22.9, 21.5, 12.3, 10.7; HR - MS m/z: calcd for $C_{19}H_{24}ClNO_2S_2Na^+$[M+Na$^+$]: 420.0835; found: 420.0821.

***β*-Sulfonamidosulfide 39:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.135 g, 68%; IR (neat) V_{max}: 3288, 2965, 1471, 1326, 1158, 1093, 817, 667 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.33-7.24 (m, 6H), 4.65 (d, *J* = 9.3 Hz, 1H), 3.49-3.41 (m, 1H), 3.20-3.13 (m, 1H), 2.41 (s, 3H), 1.98-1.87 (m, 1H), 1.16 (d, *J* = 6.9 Hz, 3H), 0.80 (d, *J* = 6.9 Hz, 3H), 0.77 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.2, 138.5, 133.9, 133.6, 132.8, 129.5, 129.1, 126.9, 63.8, 47.7, 30.3, 21.5, 20.8, 19.4, 19.2; HR - MS m/z: calcd for $C_{19}H_{24}ClNO_2S_2Na^+$[M+Na$^+$]: 420.0835; found: 420.0849.

***β*-Sulfonamidosulfide 40:** R_f = 0.60 (EtOAc/hexane, 3 : 7); Yield: 0.143 g, 72%; IR (neat) V_{max}: 3266, 2958, 1478, 1328, 1156, 812, 666 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.41-7.13 (m, 6H), 4.88 (d, *J* = 9.9 Hz, 1H), 3.44-3.34 (m, 1H), 3.13-3.05 (m, 1H), 2.41 (s, 3H), 2.06-1.91 (m, 1H), 1.24 (d, *J* = 6.9 Hz, 3H), 0.85 (t, *J* = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.1, 138.6, 133.1, 129.5, 129.2, 129.0, 127.0, 126.9, 62.4, 49.1, 29.3, 21.5, 20.9, 19.1, 17.6; HR - MS m/z: calcd for $C_{19}H_{24}ClNO_2S_2Na^+$[M+Na$^+$]: 420.0835; found: 420.0848.

***β*-Sulfonamidosulfide 41:** R_f = 0.70 (EtOAc/hexane, 3 : 7); Yield: 0.139 g, 68%; IR (neat) V_{max}: 3267, 1324, 1160, 1082, 824, 668 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.30-7.11 (m, 6H), 5.63 (d, *J* = 5.7 Hz, 1H), 3.30-3.22 (m, 1H), 3.03 (dd, *J* = 14.1, 6.9 Hz, 1H), 2.72 (dd, *J* = 15.3, 5.1 Hz, 1H), 2.45 (s, 3H), 2.37 (dd, *J* = 15.3, 6.6 Hz, 1H) 2.16 (dd, *J* = 15.0, 7.2 Hz, 1H), 1.93-1.87 (m, 2H), 1.76 (dd, *J* = 15.0, 6.9 Hz, 1H), 1.52-1.26 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 143.8, 138.7, 133.5, 133.3, 132.6, 129.8, 129.1, 127.1, 66.4, 65.9, 50.6, 47.0, 32.8, 31.5, 31.3, 31.0, 21.6, 19.6; HR - MS m/z: calcd for $C_{22}H_{24}ClNO_3S_2Na^+$[M+Na$^+$]: 472.0784; found: 472.0795.

***β*-Sulfonamidosulfide 42:** R_f = 0.50 (EtOAc/hexane, 3 : 7); Yield: 0.181 g, 71%; IR (neat) V_{max}: 3282, 1753, 1256, 1042, 667 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.33-7.13 (m, 6H), 5.46 (d, *J* = 5.4 Hz, 1H), 5.18-5.15 (m, 1H), 4.97 (bs, 1H), 3.27 (bs, 1H), 3.09 (bs, 3H), 2.46 (s, 3H) 2.39-2.34 (m, 1H), 2.29-2.21 (m, 1H), 2.05 (s, 3H), 2.04 (s, 3H), 1.82-1.62 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.9, 169.6, 143.9, 136.7, 134.8, 134.6, 129.8, 129.3, 127.2, 76.6, 68.8, 67.6, 21.6, 20.9, 20.8; HR - MS m/z: calcd for $C_{23}H_{26}ClNO_6S_2Na^+$[M+$Na^+$]: 534.0788; found: 534.0797.

***β*-Sulfonamidosulfide 44:** R_f = 0.50 (EtOAc/hexane, 2 : 8); Yield: 0.137 g, 62%; m. p: 142 ºC; $[\alpha]^{27}_D$ = - 56.00 (c = 1, CH_2Cl_2); IR (neat) V_{max}: 3282, 1753, 1256, 1042, 667 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 8.08 (d, *J* = 9.0 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.28-7.10 (m, 7H), 6.98-6.95 (m, 2H), 4.88 (d, *J* = 7.2 Hz, 1H), 3.59-3.48 (m, 1H), 3.32 (dd, *J* = 14.1, 5.4 Hz, 1H), 3.05 (dd, *J* = 14.1, 7.5 Hz, 1H), 2.98 (dd, *J* = 13.5, 6.3 Hz, 1H), 2.78 (dd, *J* = 13.5, 6.9 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 145.6, 145.3, 143.5, 136.3, 135.9, 129.6, 129.2, 128.8, 127.0, 126.9, 126.6, 123.9, 53.7, 39.6, 36.3, 21.5; HR - MS m/z: calcd for $C_{22}H_{22}N_2O_4S_2$[M+Na^+]: 465.0919; found: 465.0913.

X-Ray Structures:

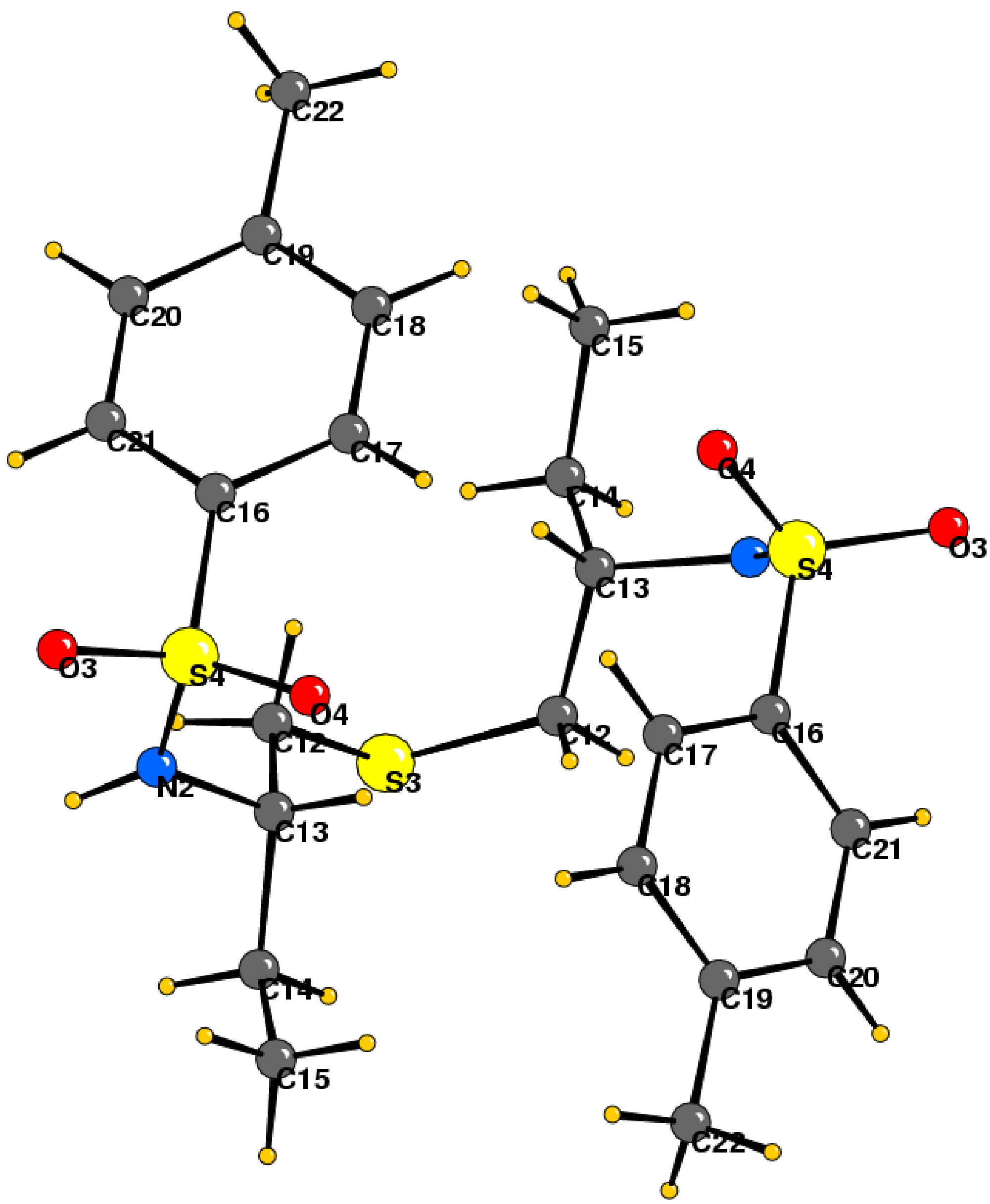


Figure 1. X-ray CAMERON diagram of *β*-sulfonamidosulfide **5d**

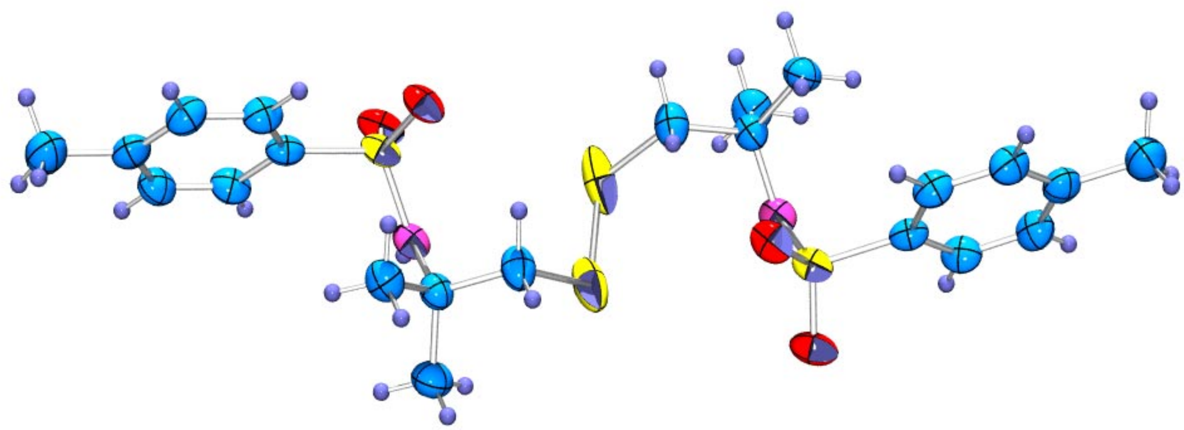


Figure 2. ORTEP diagram of β-sulfonamidodisulfide **7a**

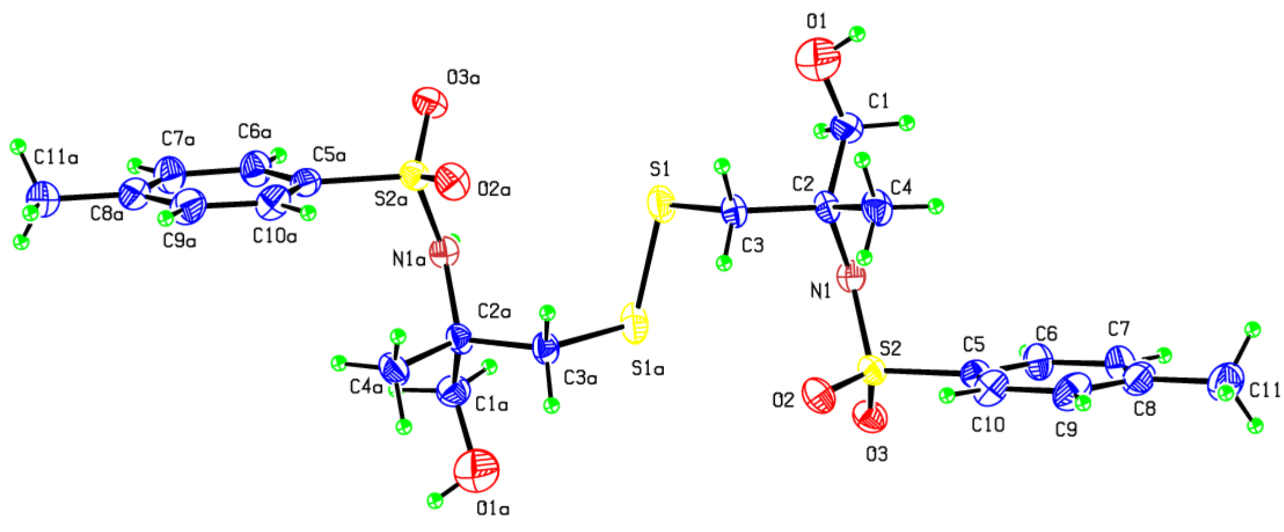


Figure 3. ORTEP diagram of β-sulfonamidodisulfide **7c**

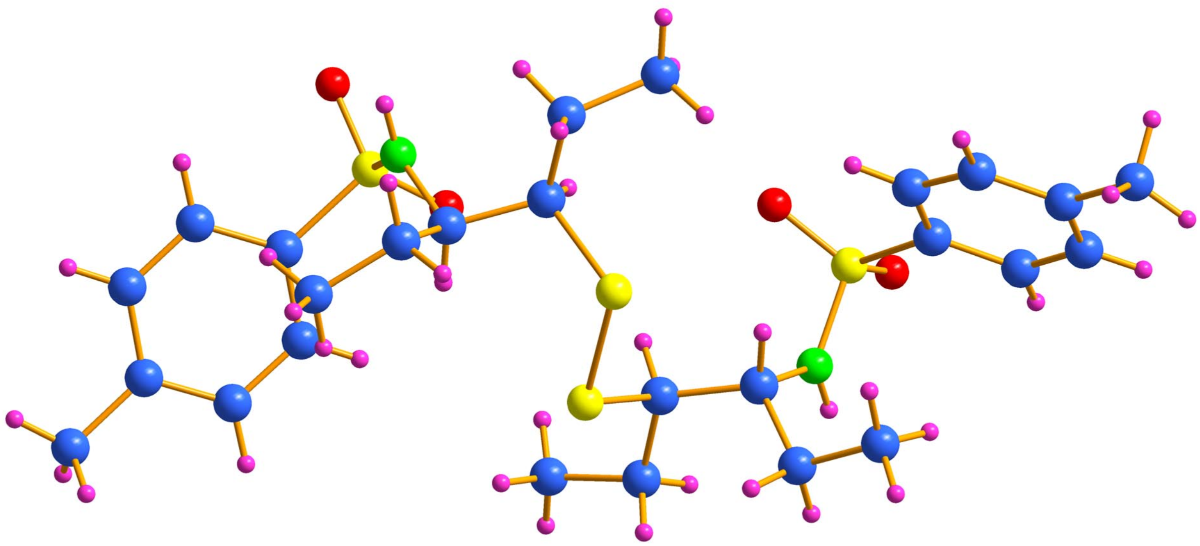


Figure 4. X-ray structure of *β*-sulfonamidodisulfide **9a**

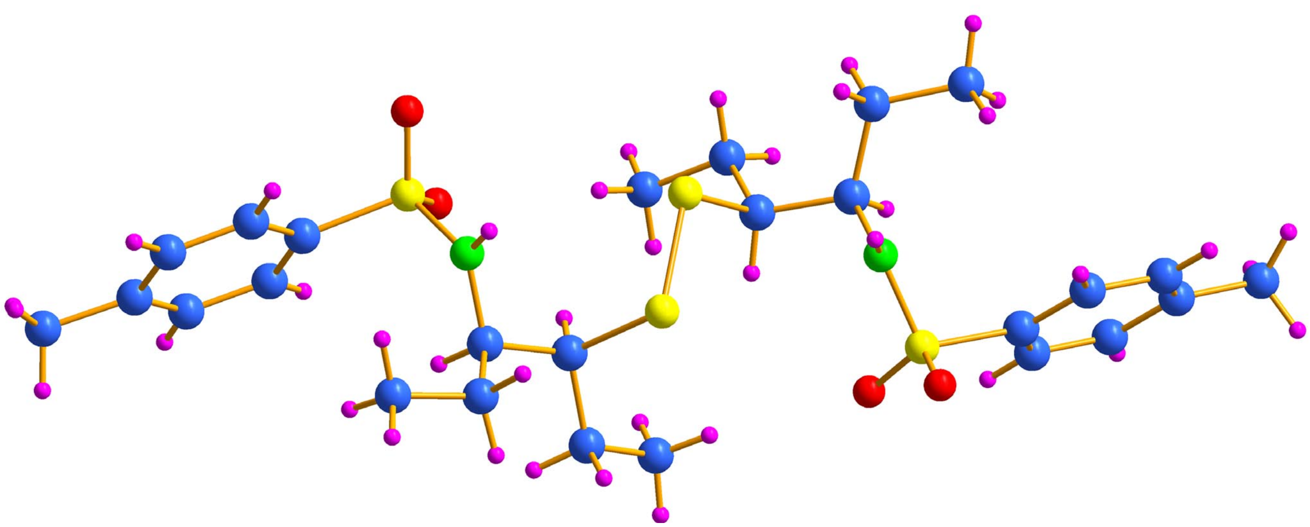


Figure 5. X-ray structure of *β*-sulfonamidodisulfide **9b**

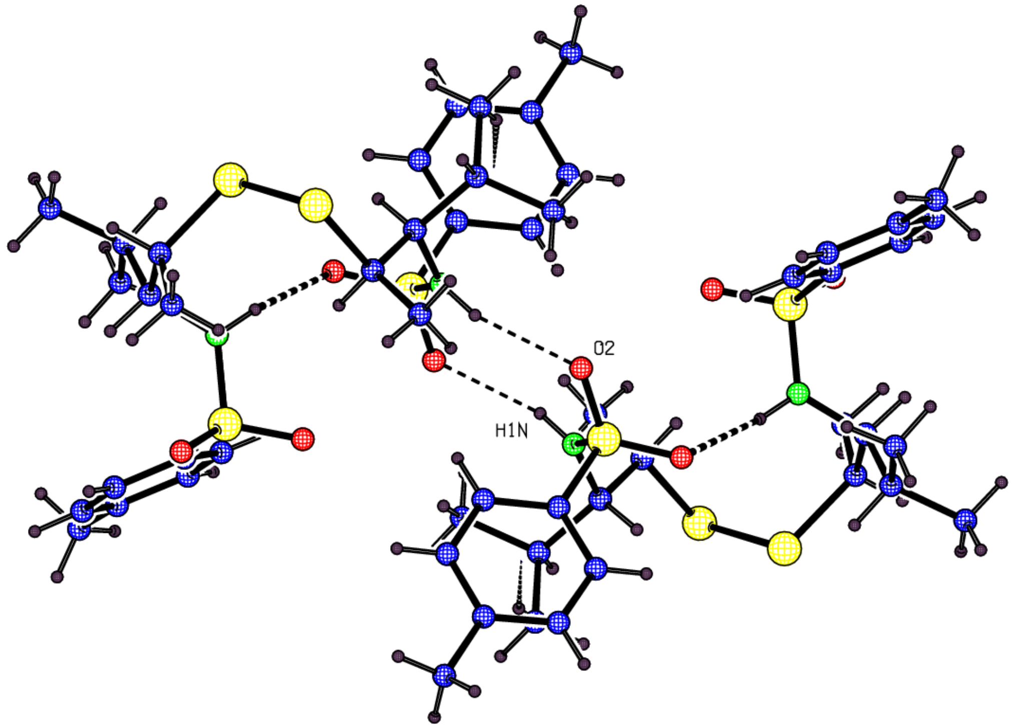


Figure 6. X-ray PLATON diagram of *β*-sulfonamidodisulfide **9c** forms centro-symmetric dimer via intermolecular N-H…O hydrogen bonding

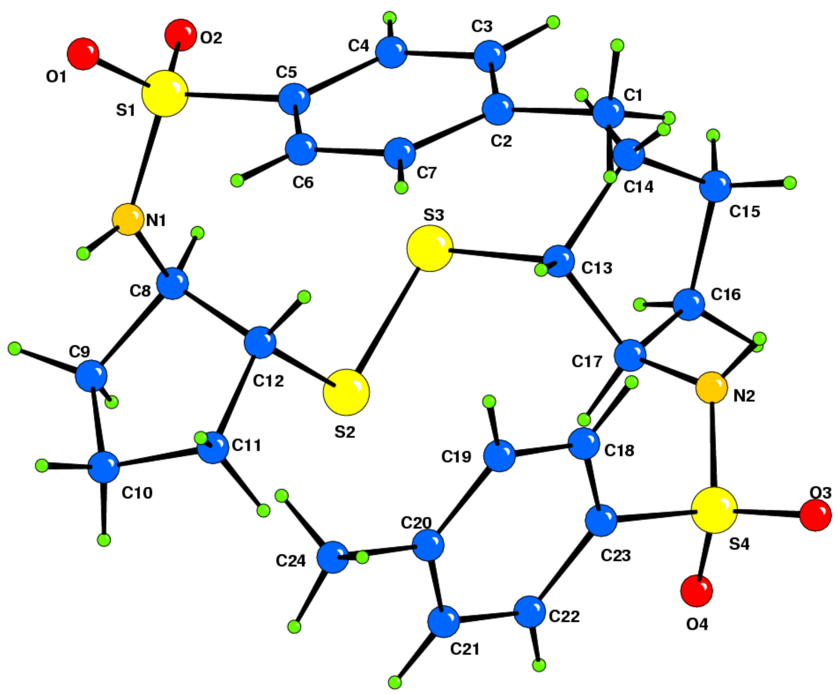


Figure 7. X-ray CAMERON diagram of *β*-sulfonamidodisulfide **11a**

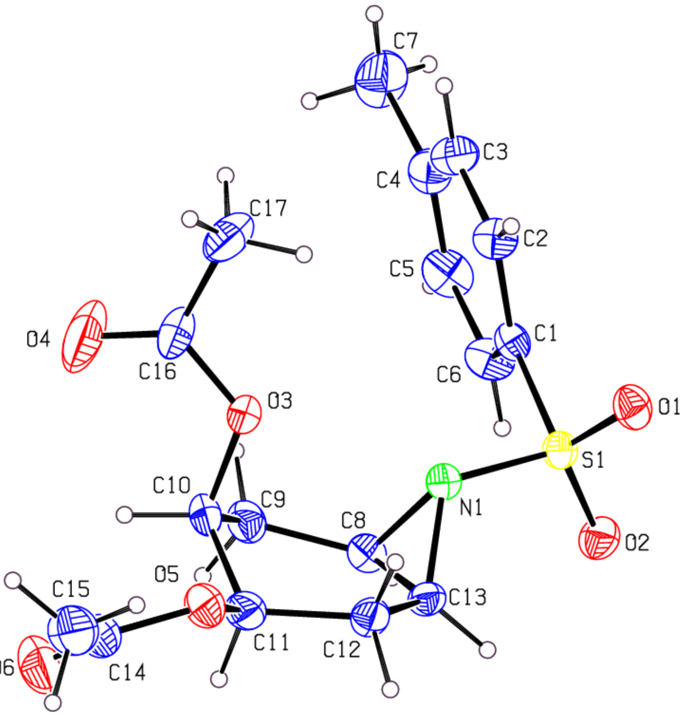
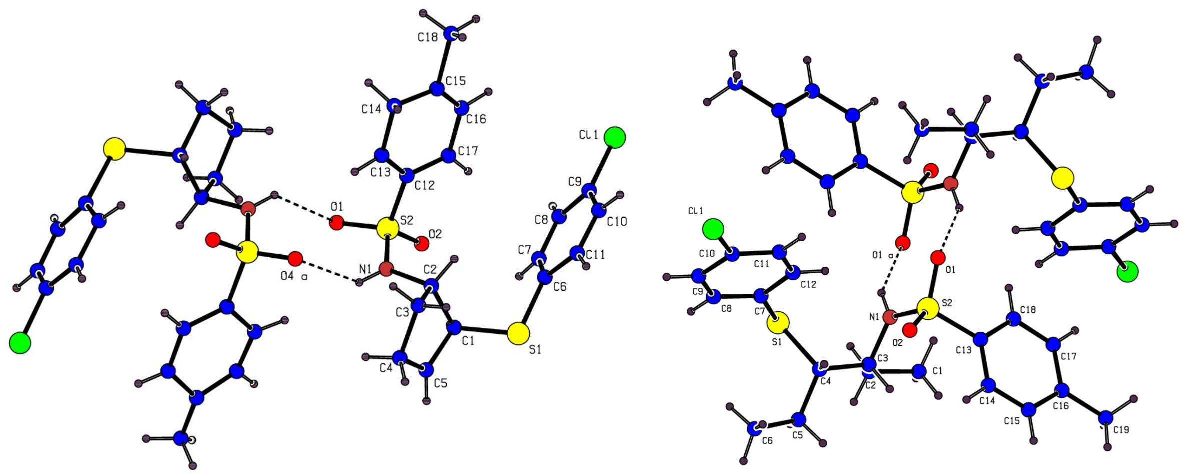


Figure 8. ORTEP diagram of Compound **14**



32 **36**

Figure 9. X-ray PLATON diagrams of *β*-sulfonamidosulfide **32** and **36;** form centro-symmetric dimer via intermolecular N-H**…**O hydrogen bonding

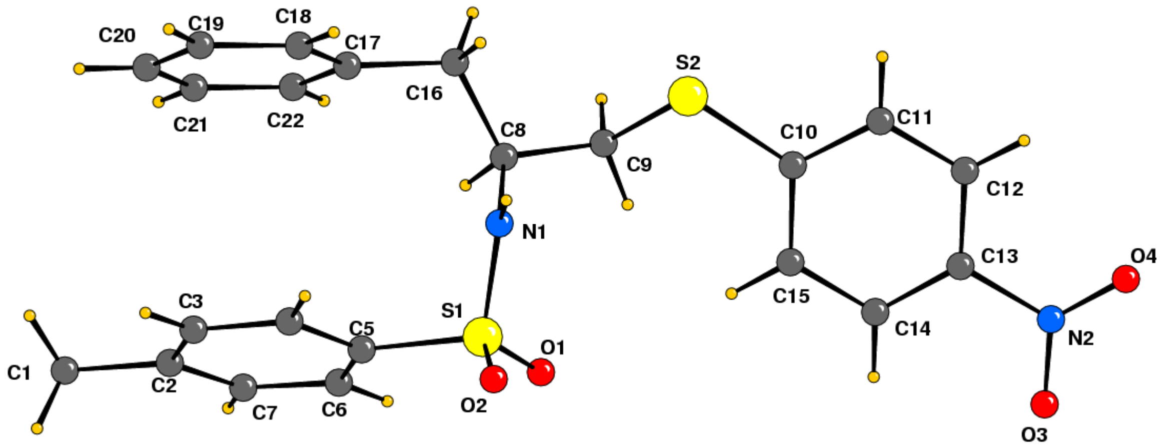


Figure 10. X-ray CAMERON diagram of *β*-sulfonamidosulfide **44**

Details of Theoretical Calculations

All DFT calculations were carried out using a Gaussian 98 program.[S4] Geometry optimization was carried out using B3LYP method. Calculations were done at 6-31G(d) level basis set for intermediates **I** and **II**.

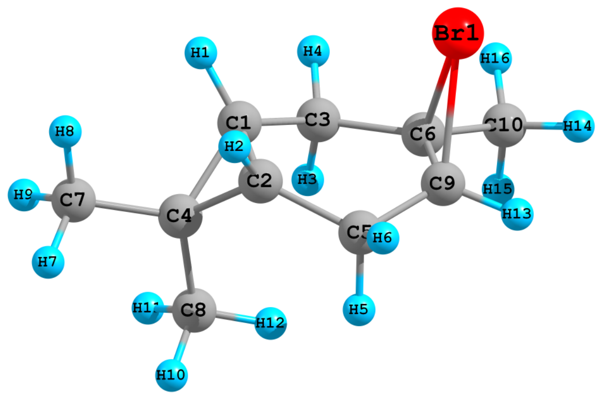


Figure 11. Optimized geometry of Intermediate **I** at B3LYP/6-31G(d) level

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.208075	-.111257	-.910822
2	6	0	1.289200	-.882686	.402226
3	6	0	.280223	1.090529	-1.002156
4	6	0	2.491544	-.101787	-.096907
5	1	0	1.220654	-.711851	-1.816244
6	6	0	.420787	-.423530	1.564004
7	6	0	-.894813	1.101664	-.067035
8	6	0	3.646075	-.923736	-.651761
9	6	0	2.945785	1.159546	.618036
10	1	0	1.352261	-1.963522	.309582
11	1	0	.805963	2.030570	-.756081
12	1	0	-.078658	1.238219	-2.025995
13	6	0	-.847417	.274466	1.146674
14	6	0	-1.890814	2.213663	-.175526
15	35	0	-1.985359	-.834484	-.185281
16	1	0	.936730	.303970	2.211334
17	1	0	.161364	-1.261022	2.218463
18	1	0	4.320818	-1.236215	.153266
19	1	0	3.293266	-1.825771	-1.162807
20	1	0	4.229736	-.337337	-1.370472
21	1	0	3.609962	.905076	1.451792
22	1	0	3.512081	1.802766	-.065384
23	1	0	2.129104	1.762977	1.030377
24	1	0	-1.540189	.549644	1.940776
25	1	0	-2.775232	2.054460	.444962
26	1	0	-1.390371	3.129772	.173391
27	1	0	-2.191779	2.383966	-1.212544

Sum of electronic and zero-point Energies = -2961.872243 hartree

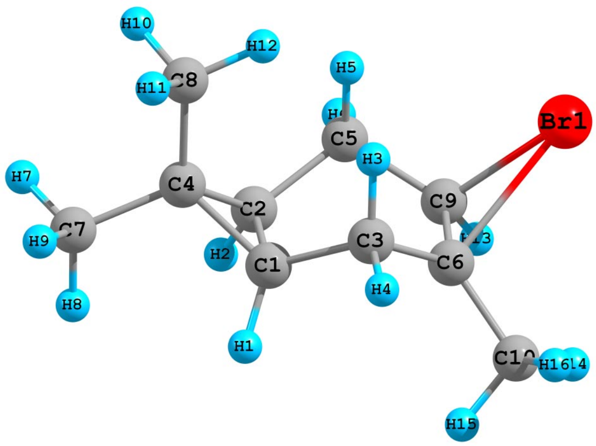


Figure 12. Optimized geometry of Intermediate **II** at B3LYP/6-31G(d) level

Standard orientation:

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1	6	0	-1.636127	.934250	-.181591
2	6	0	-1.632606	-.016688	1.023738
3	6	0	-.385281	.863755	-1.079917
4	6	0	-2.639971	-.215838	-.088777
5	1	0	-2.018285	1.940626	-.031349
6	6	0	-.366214	-.870581	1.160534
7	6	0	.723533	1.056759	-.099714
8	6	0	-4.065456	.217897	.233228
9	6	0	-2.582462	-1.402429	-1.032647
10	1	0	-2.014509	.380476	1.960906
11	1	0	-.314348	-.106358	-1.578522
12	1	0	-.381760	1.639403	-1.848306
13	6	0	.819451	.069725	.987540
14	35	0	2.348890	-.659814	-.151673
15	6	0	1.454164	2.347998	-.034283
16	1	0	-.335769	-1.661718	.408373
17	1	0	-.313224	-1.358956	2.136125
18	1	0	-4.611584	-.602741	.712052
19	1	0	-4.089785	1.077436	.911048
20	1	0	-4.601842	.492037	-.681719
21	1	0	-3.087678	-2.262689	-.579291
22	1	0	-3.105331	-1.166415	-1.965822
23	1	0	-1.571813	-1.727936	-1.297770
24	1	0	1.295438	.429997	1.898557
25	1	0	2.256577	2.358633	.705561
26	1	0	.710773	3.112621	.247217
27	1	0	1.837816	2.639989	-1.017161

Sum of electronic and zero-point Energies = -2961.867281 hartree

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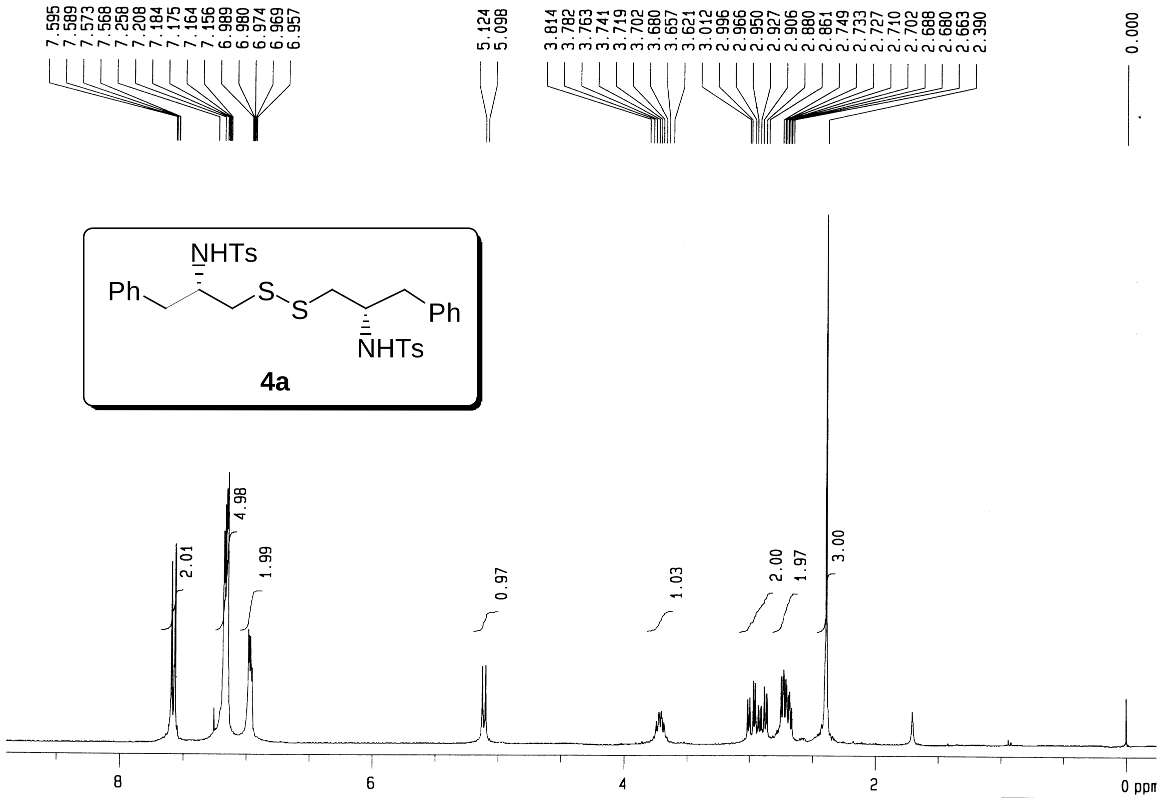
1. Kruss, G. *Justus Liebigs Ann.Chem.* **1884**, *225*, 1.

2. Ramesha, A. R.; Chandrasekaran, S. *Synth. Commun*. **1992**, *22*, 3277 - 3284.

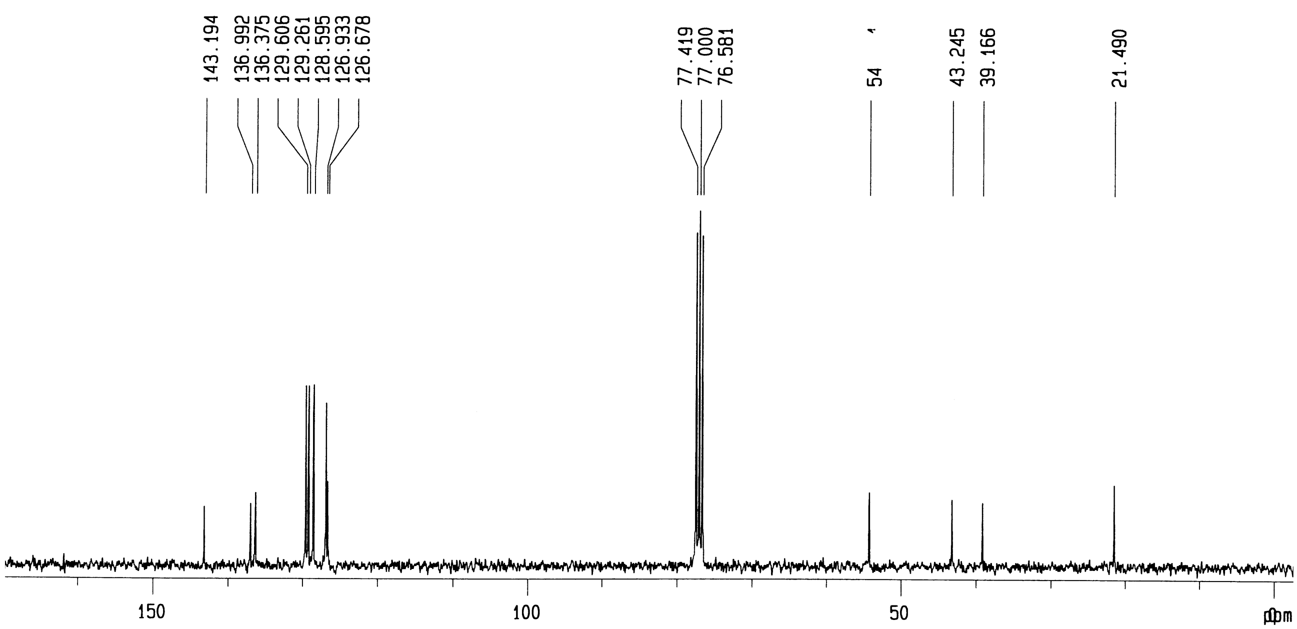
3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al- Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head- Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*; Gaussian, Inc.: Pittsburgh,PA,1998.

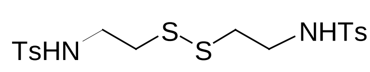
^1H, ^{13}C and DEPT NMR Spectra

^1H NMR – $CDCl_3$ (300 MHz)



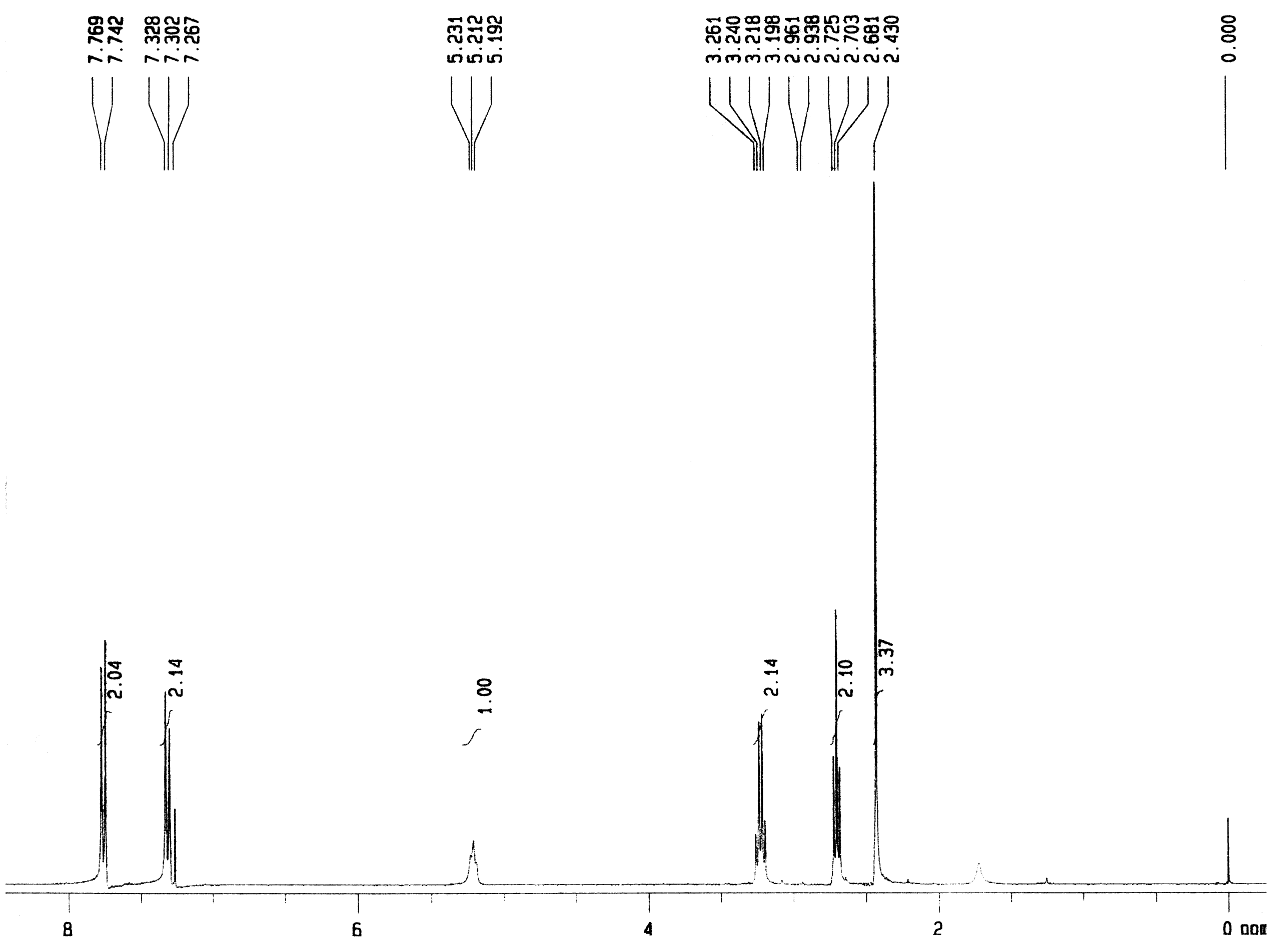
^{13}C NMR – $CDCl_3$ (75 MHz)





4b

^{1}H NMR – $CDCl_3$ (300 MHz)



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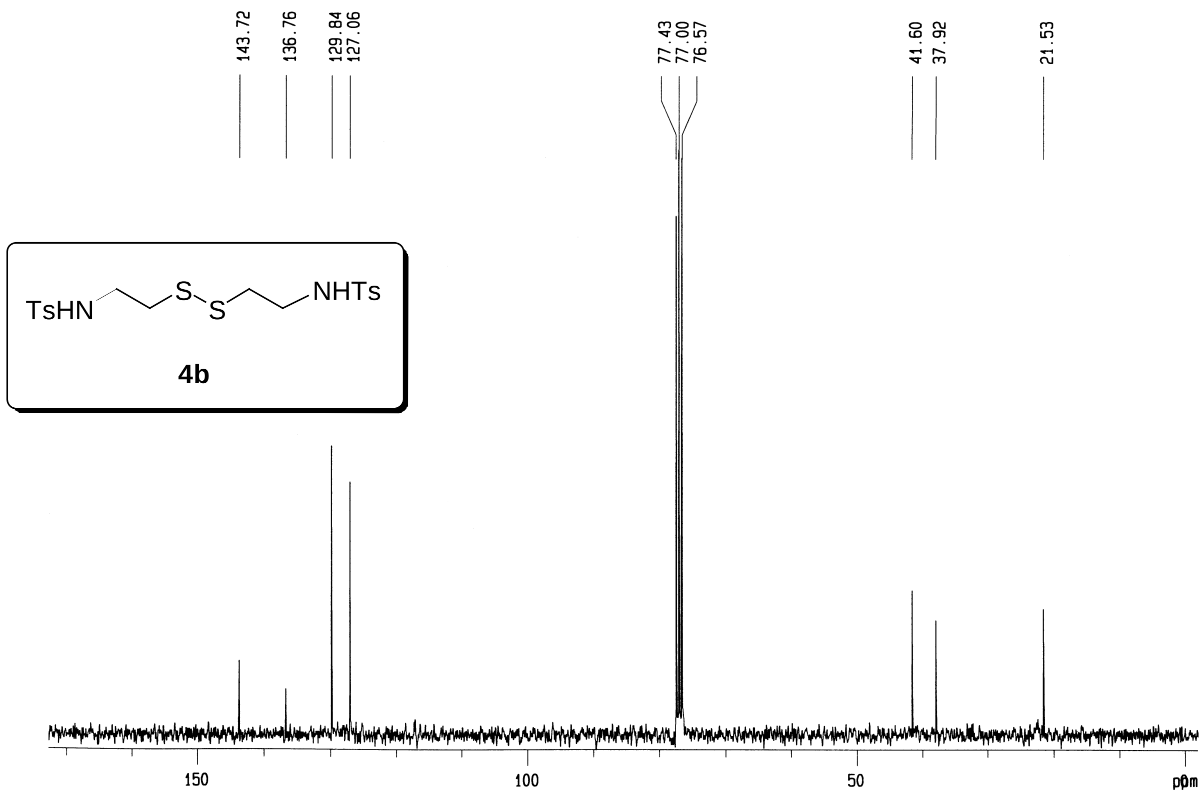
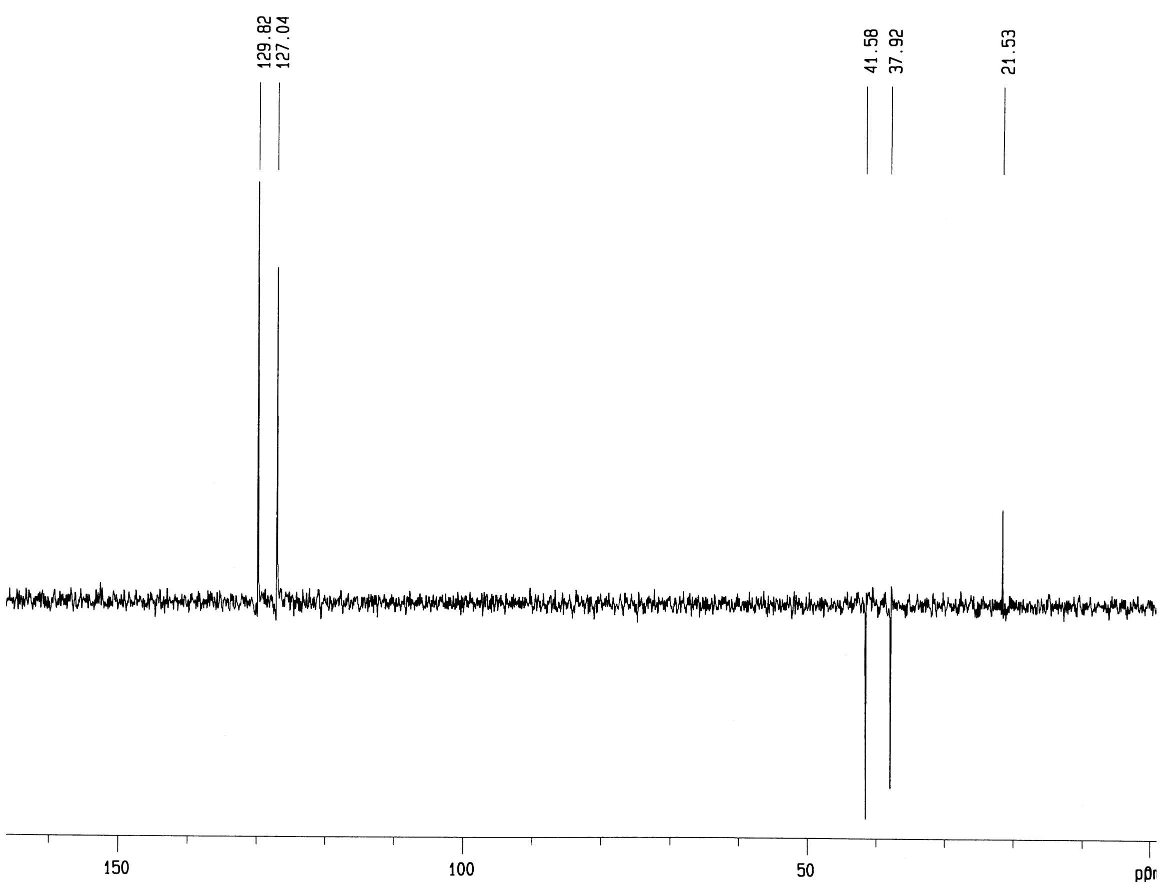
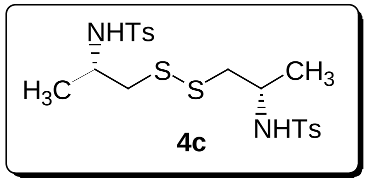
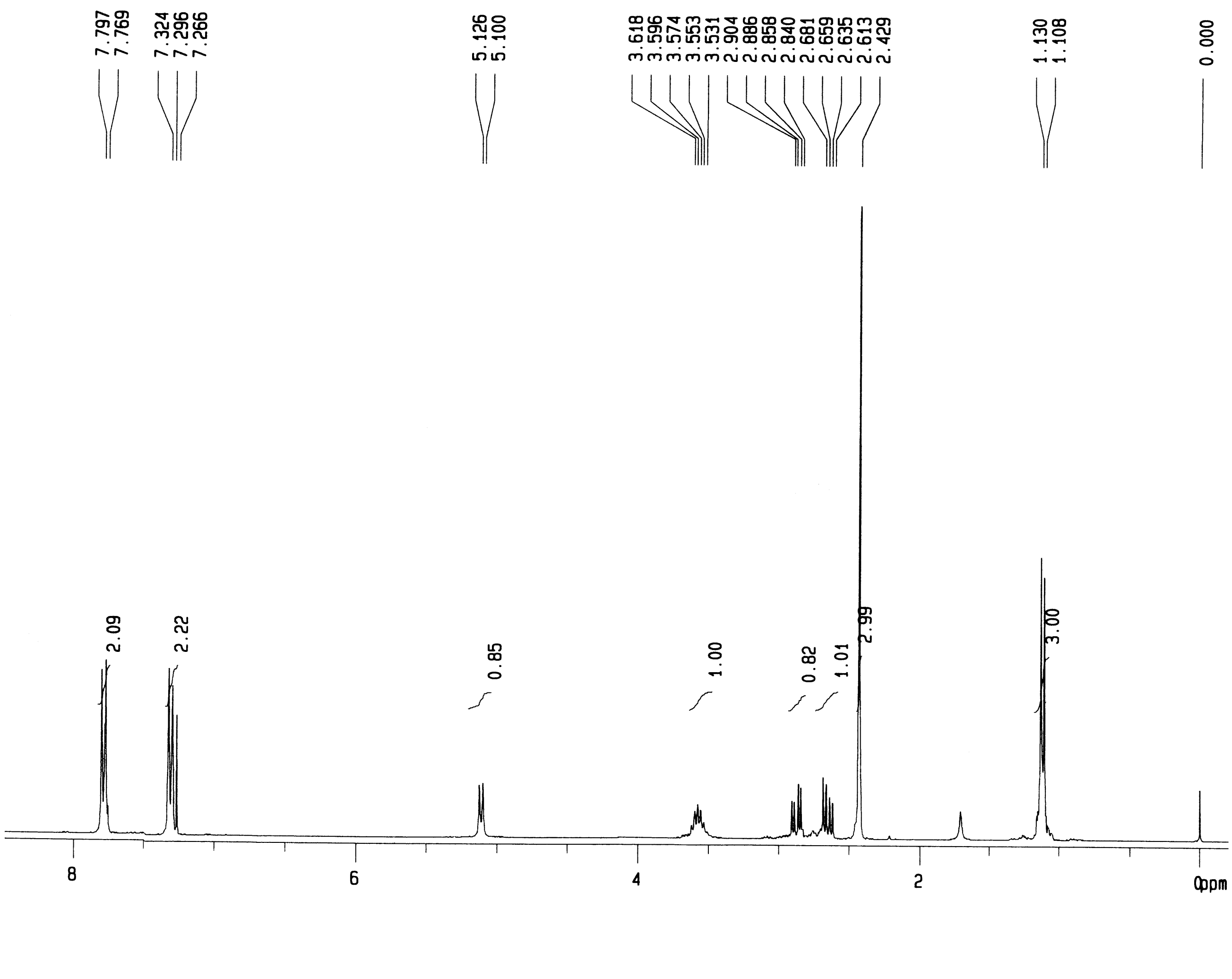


DEPT – $CDCl_3$ (75 MHz)





^{1}H NMR – $CDCl_3$ (300 MHz)



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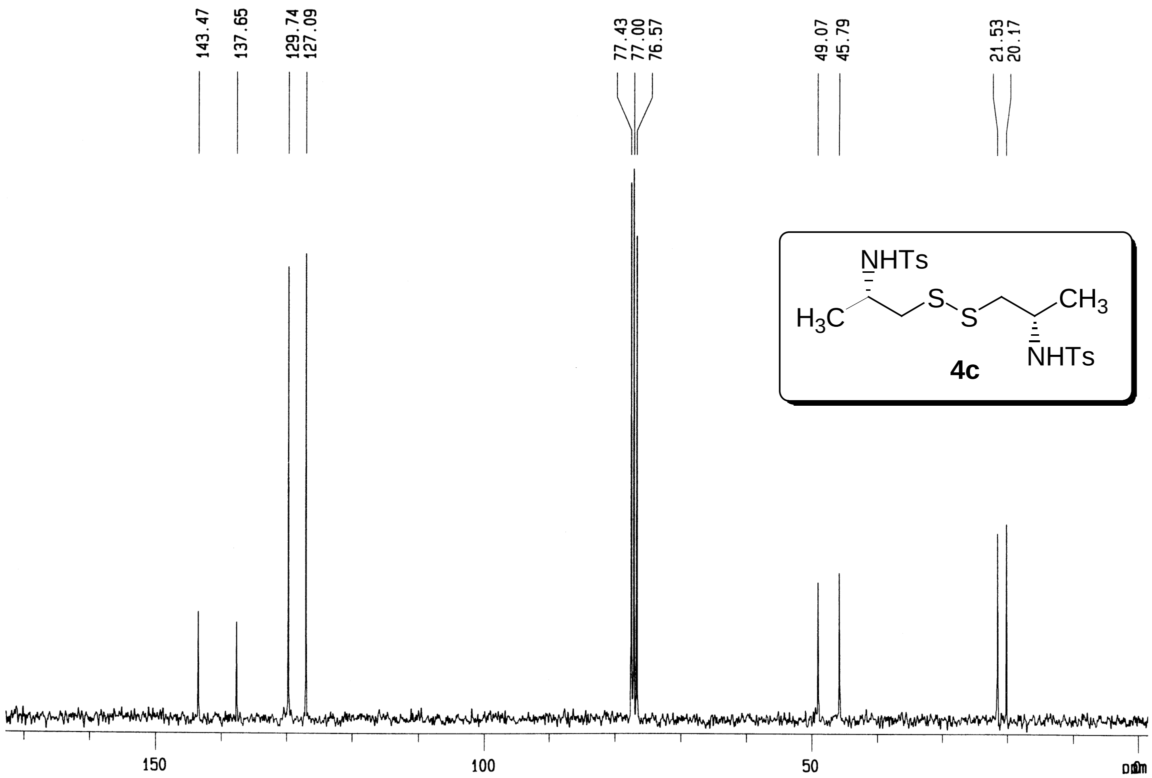

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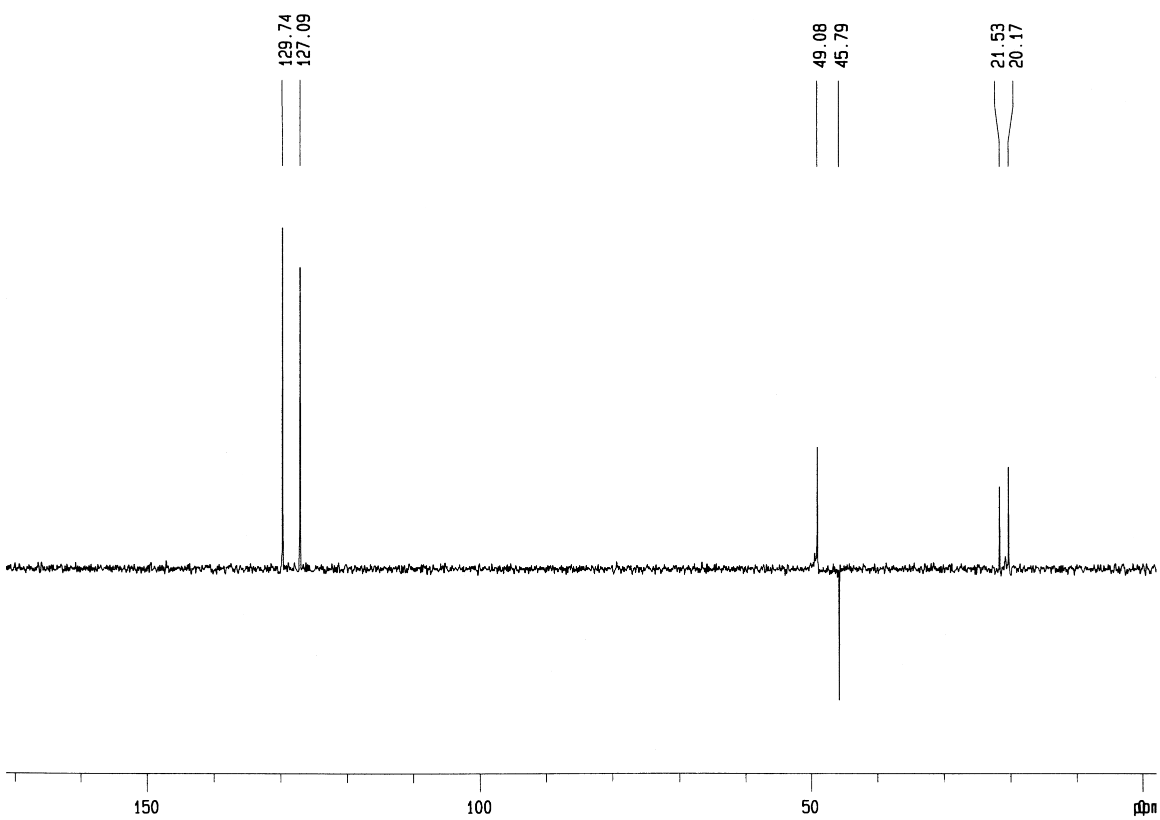

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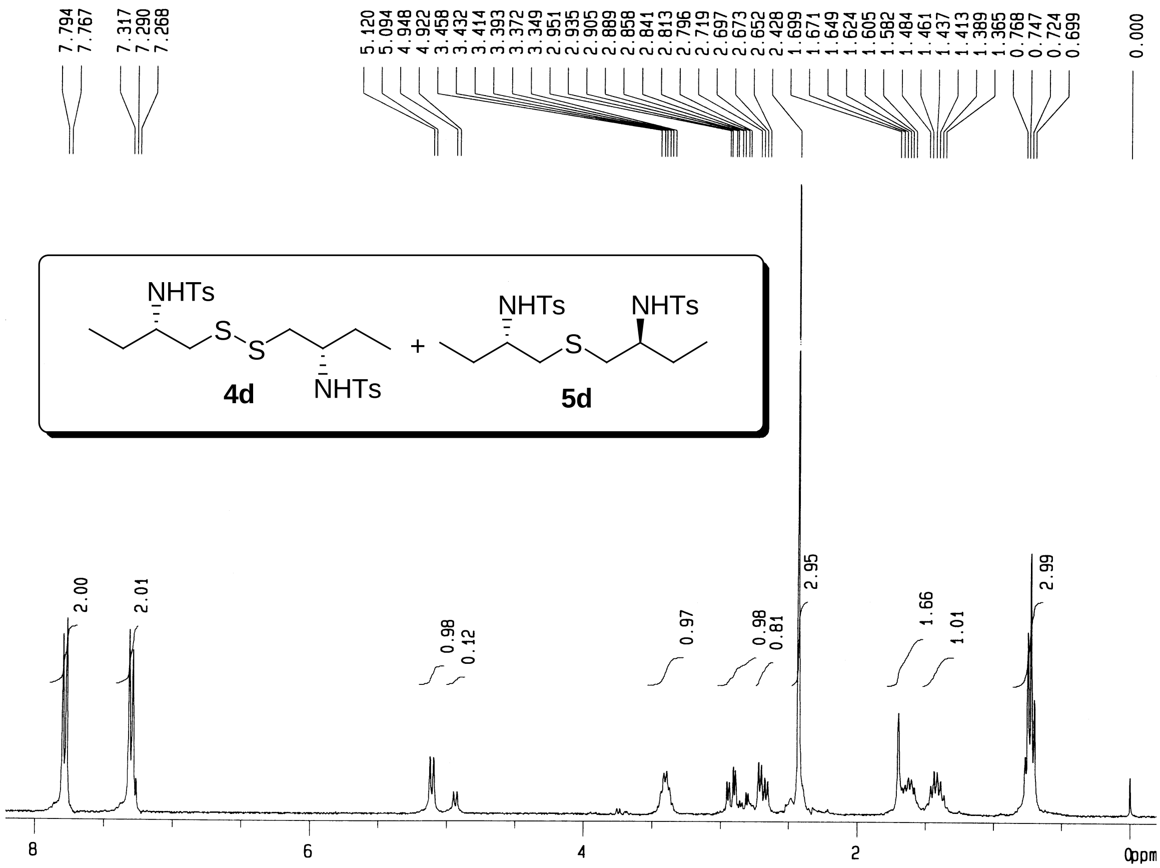

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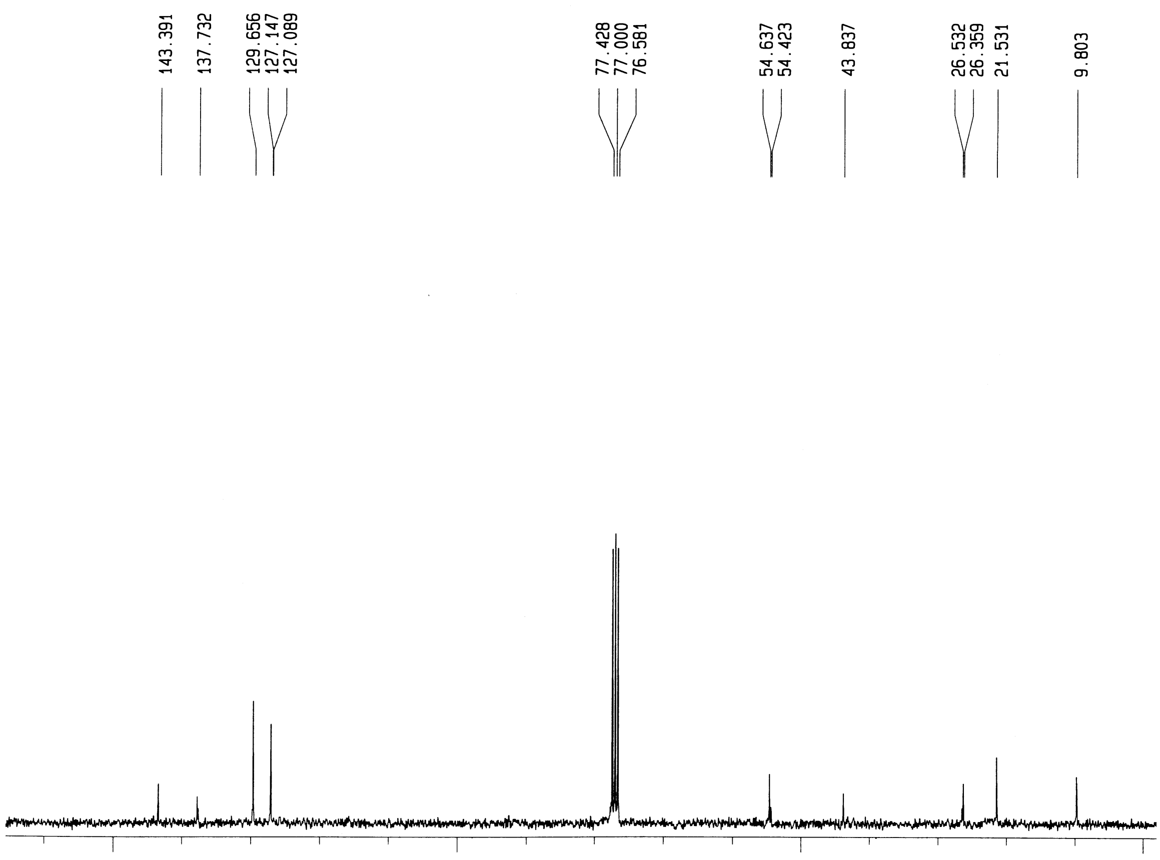
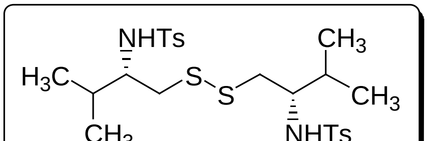
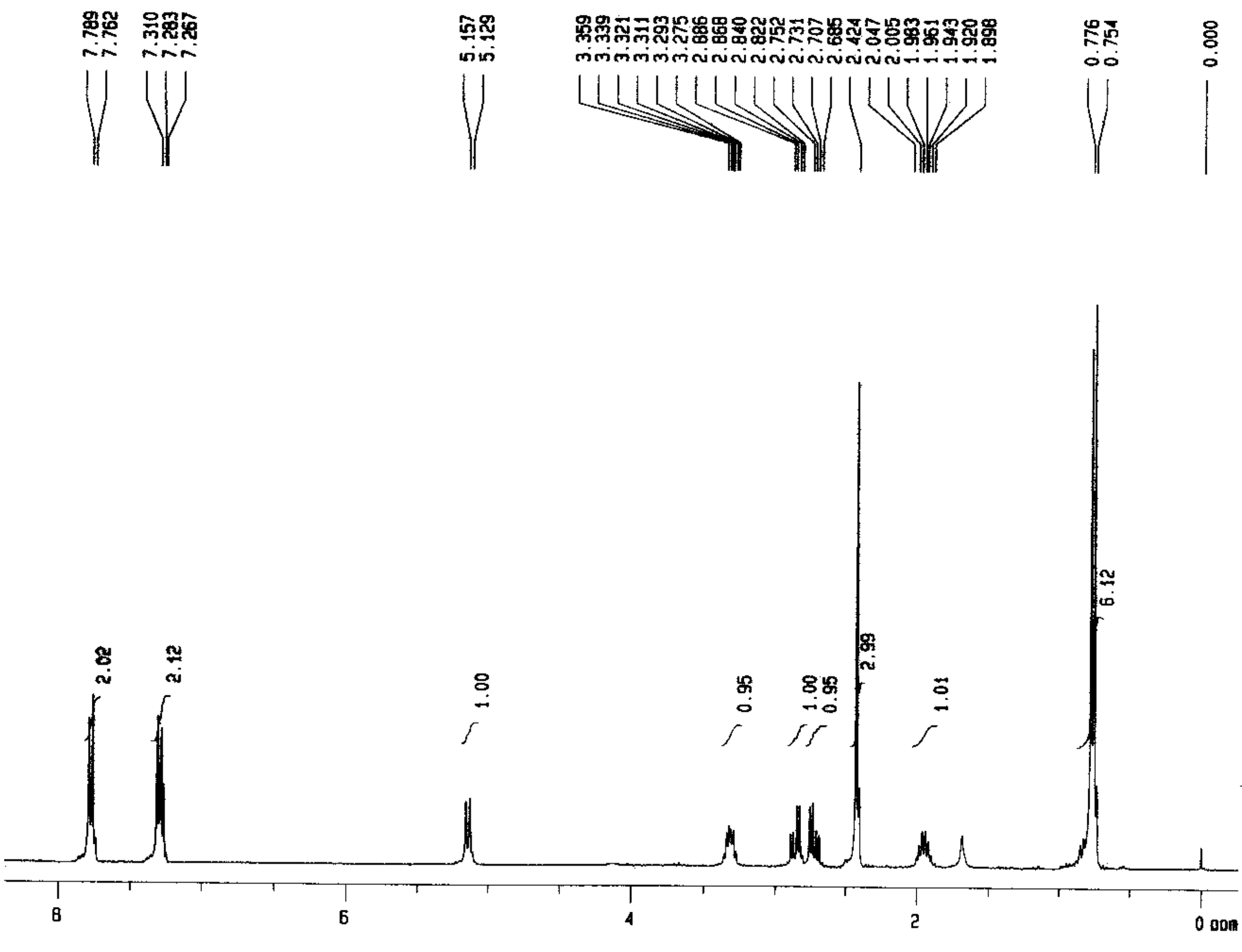


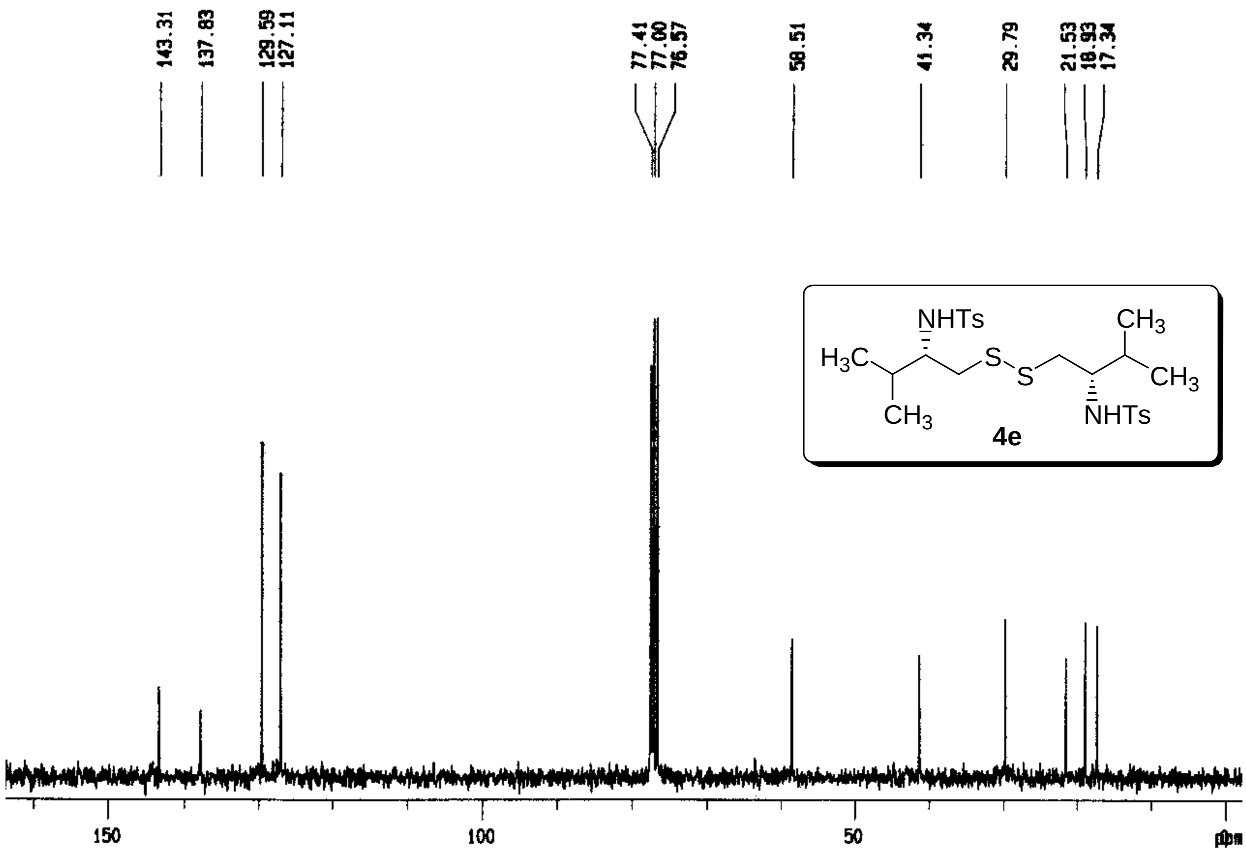


4e

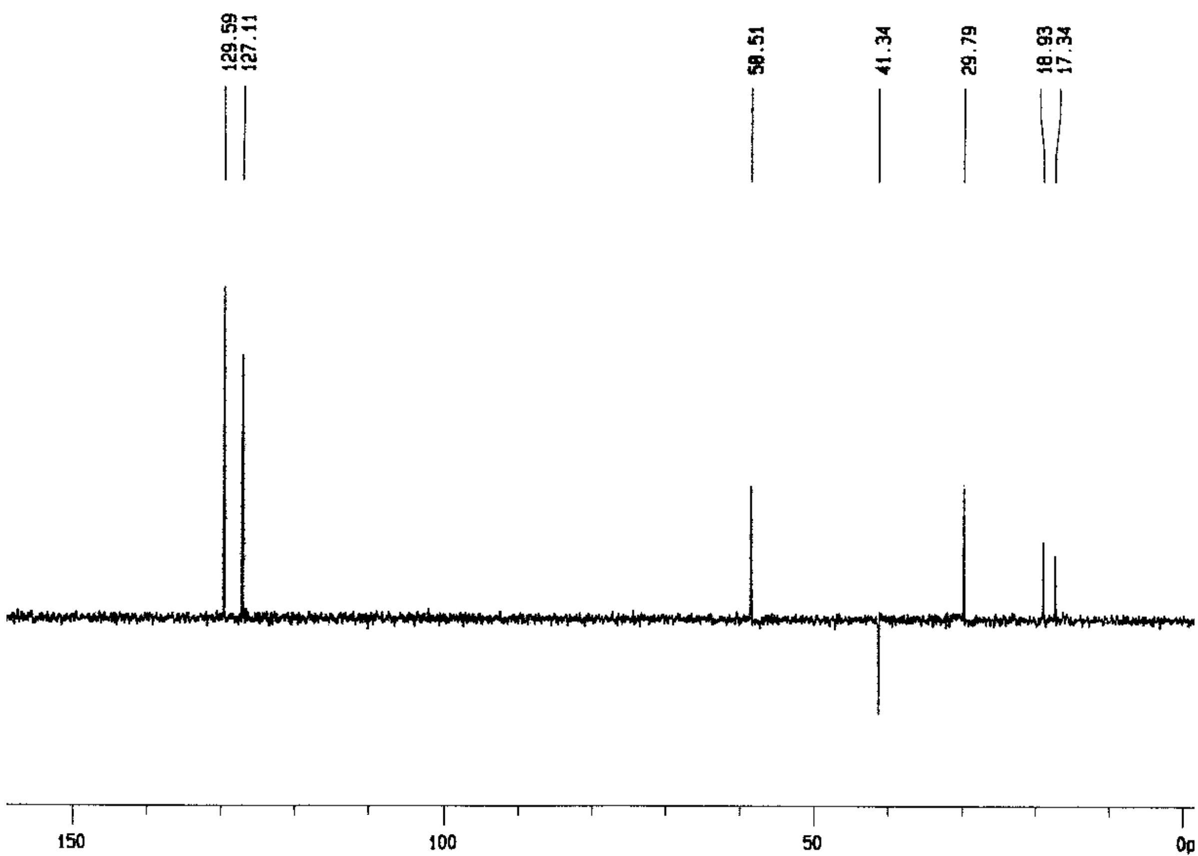
[1]H NMR – $CDCl_3$ (300 MHz)

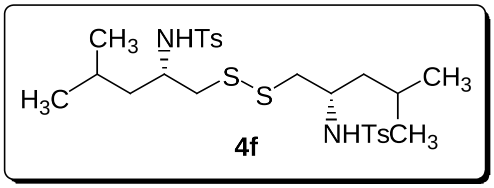


^{13}C NMR – $CDCl_3$ (75 MHz)

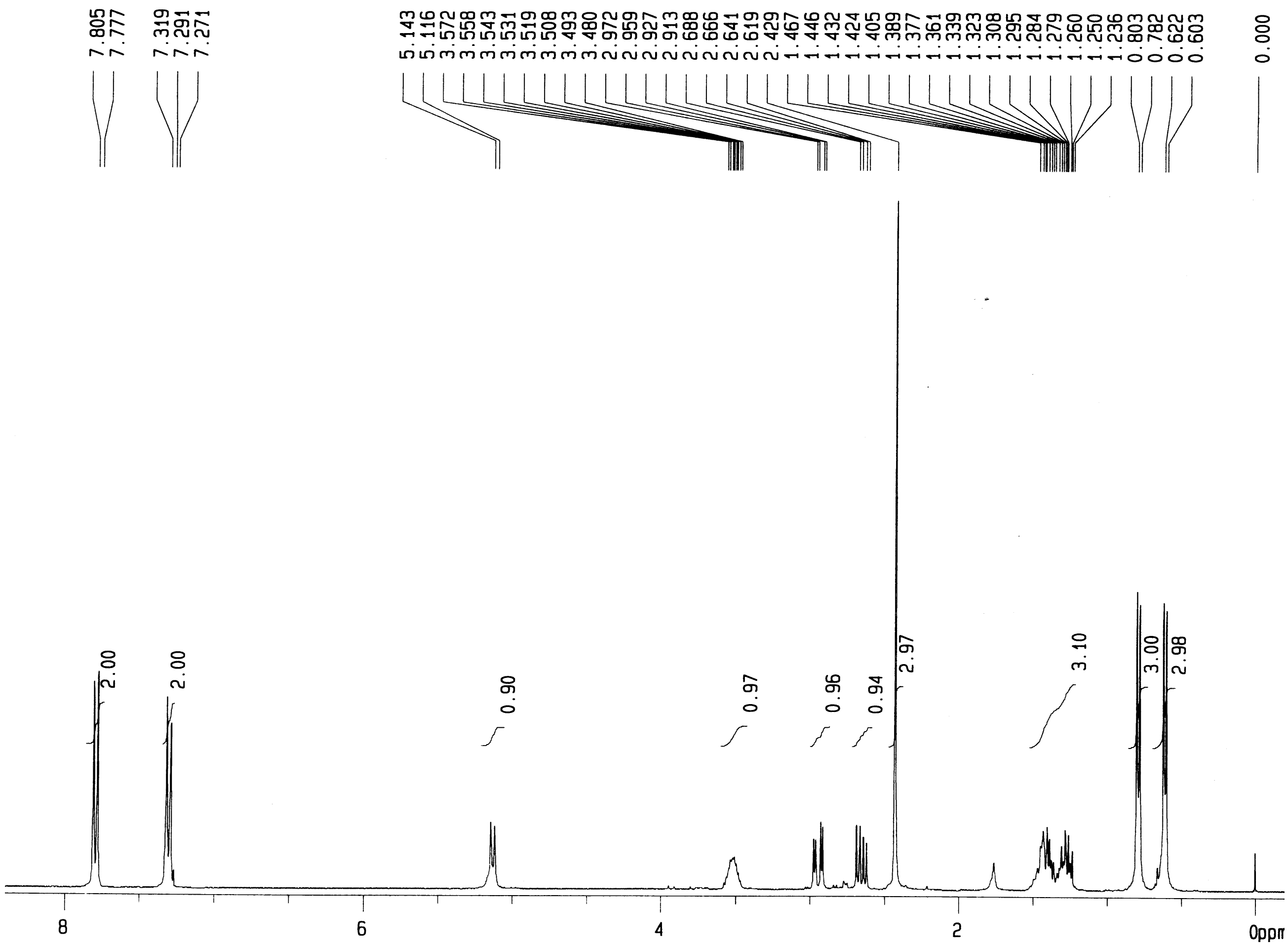


DEPT – $CDCl_3$ (75 MHz)





^{1}H NMR – $CDCl_3$ (300 MHz)



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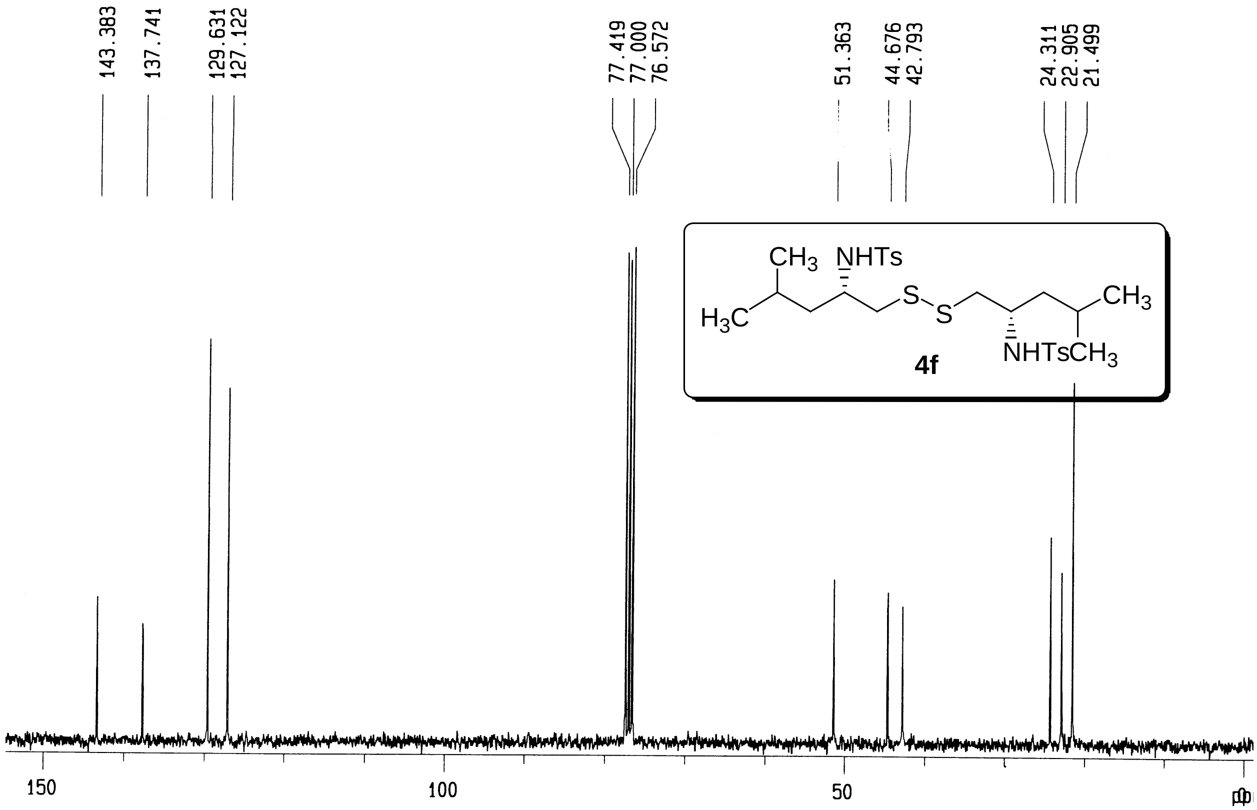

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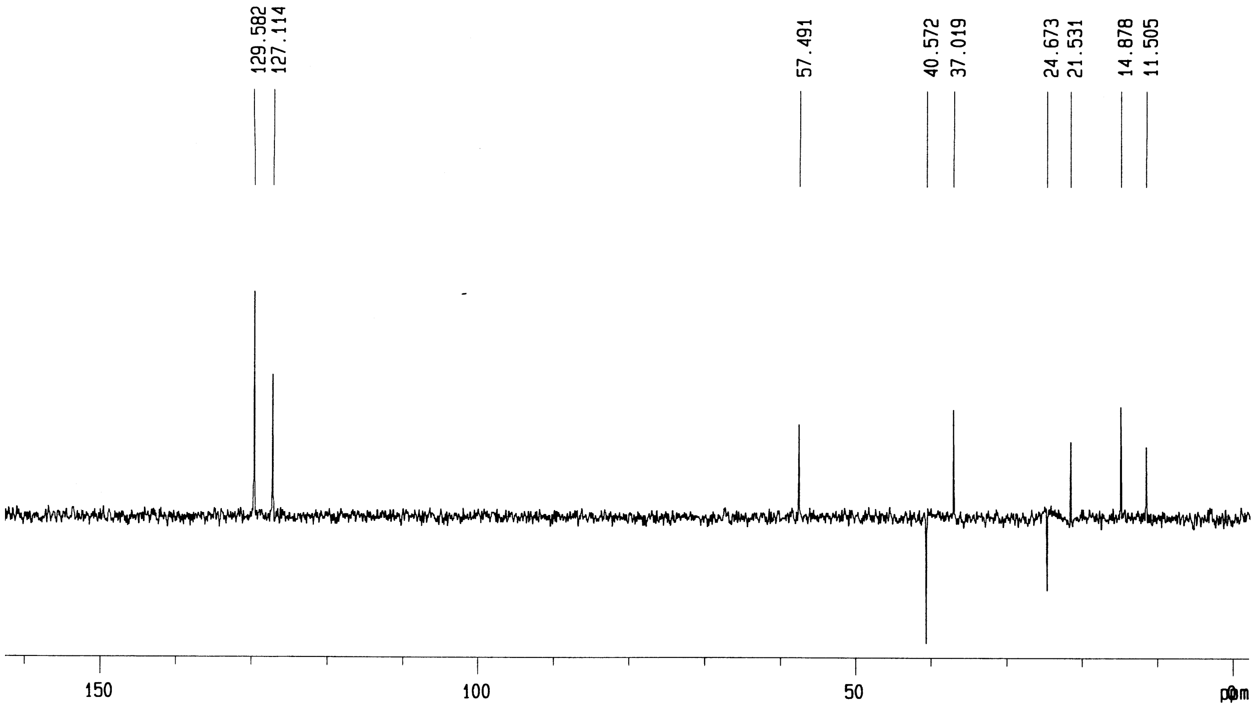

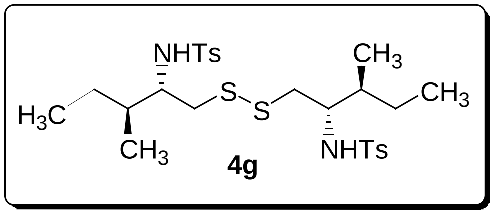

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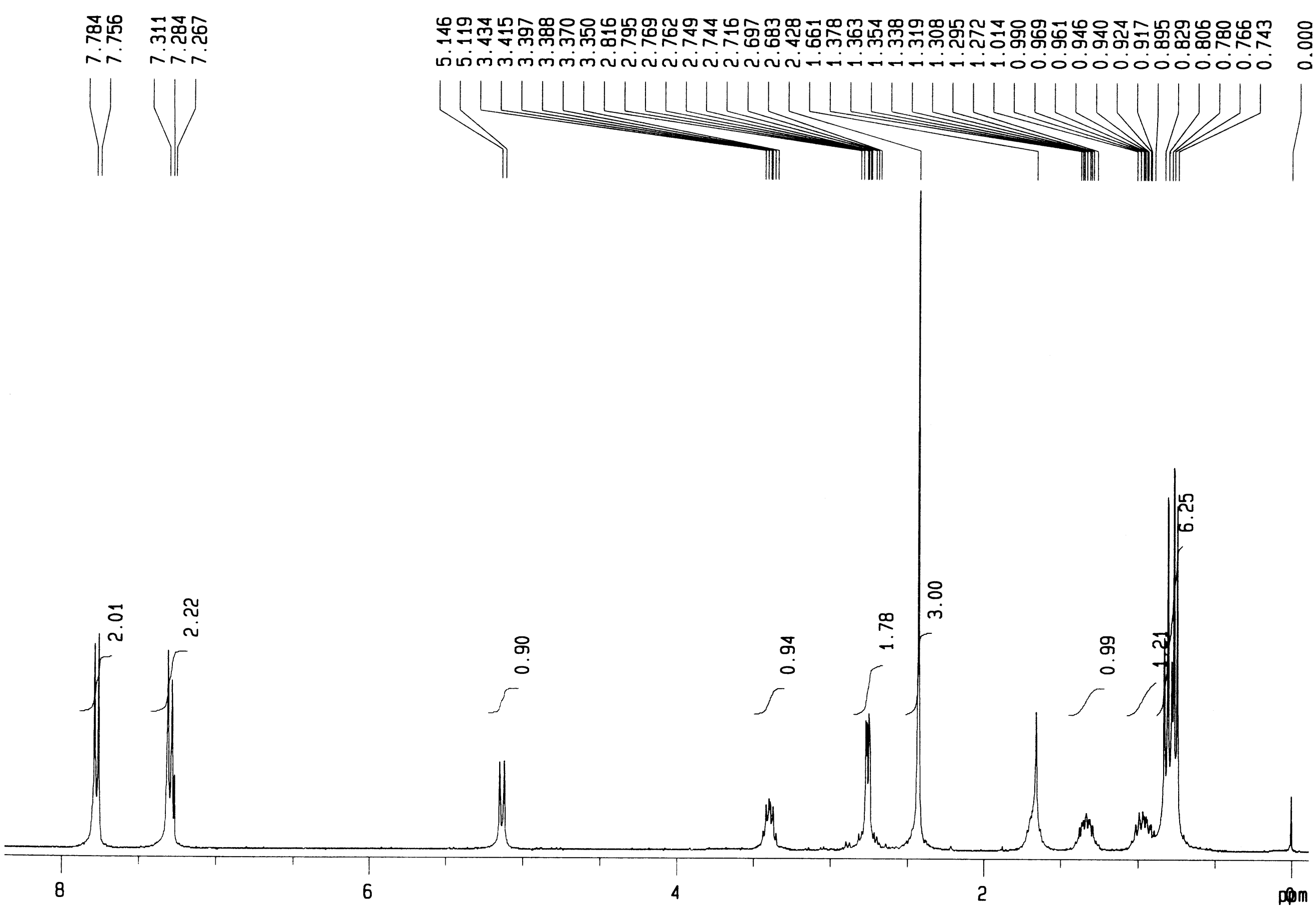

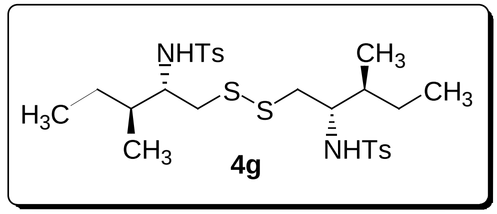

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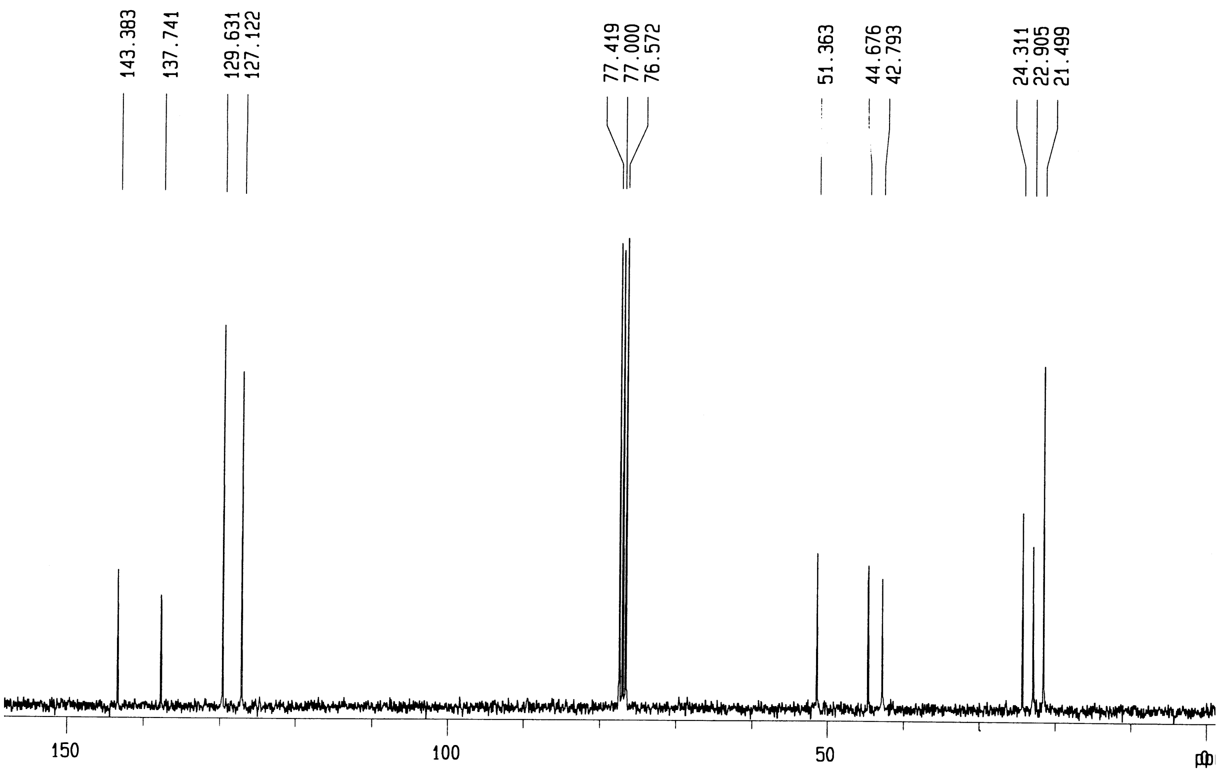
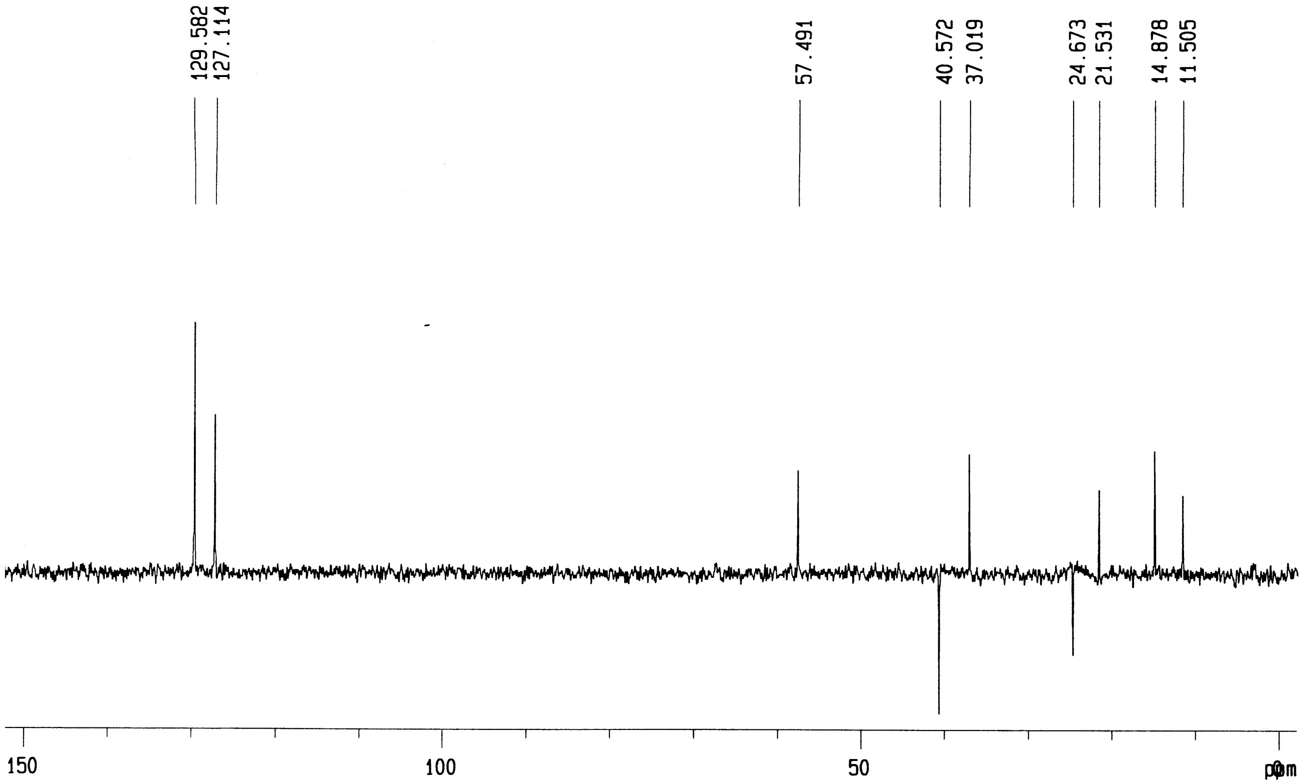
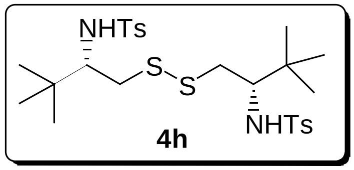
^{13}C NMR – $CDCl_3$ (75 MHz)



DEPT – $CDCl_3$ (75 MHz)





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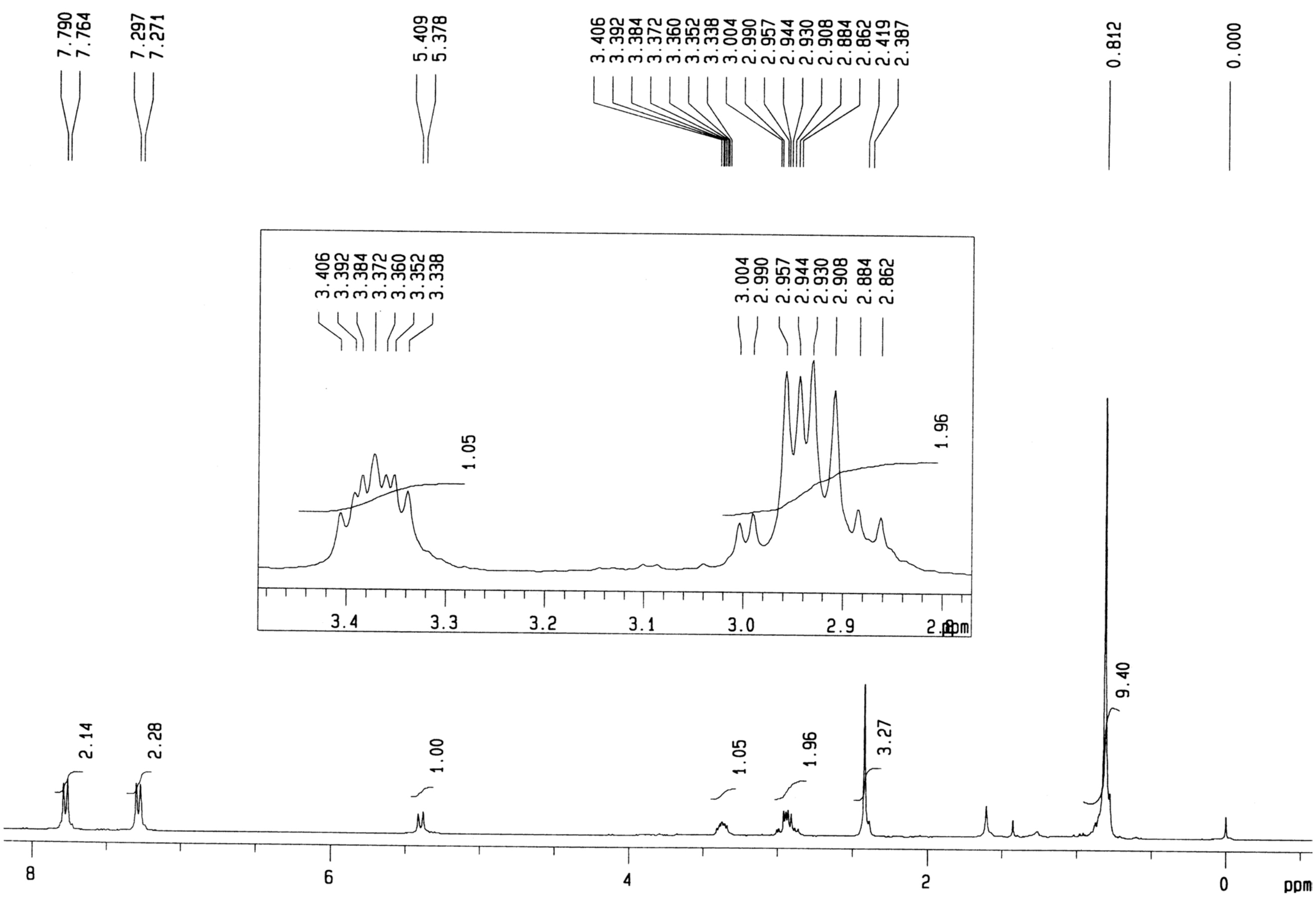
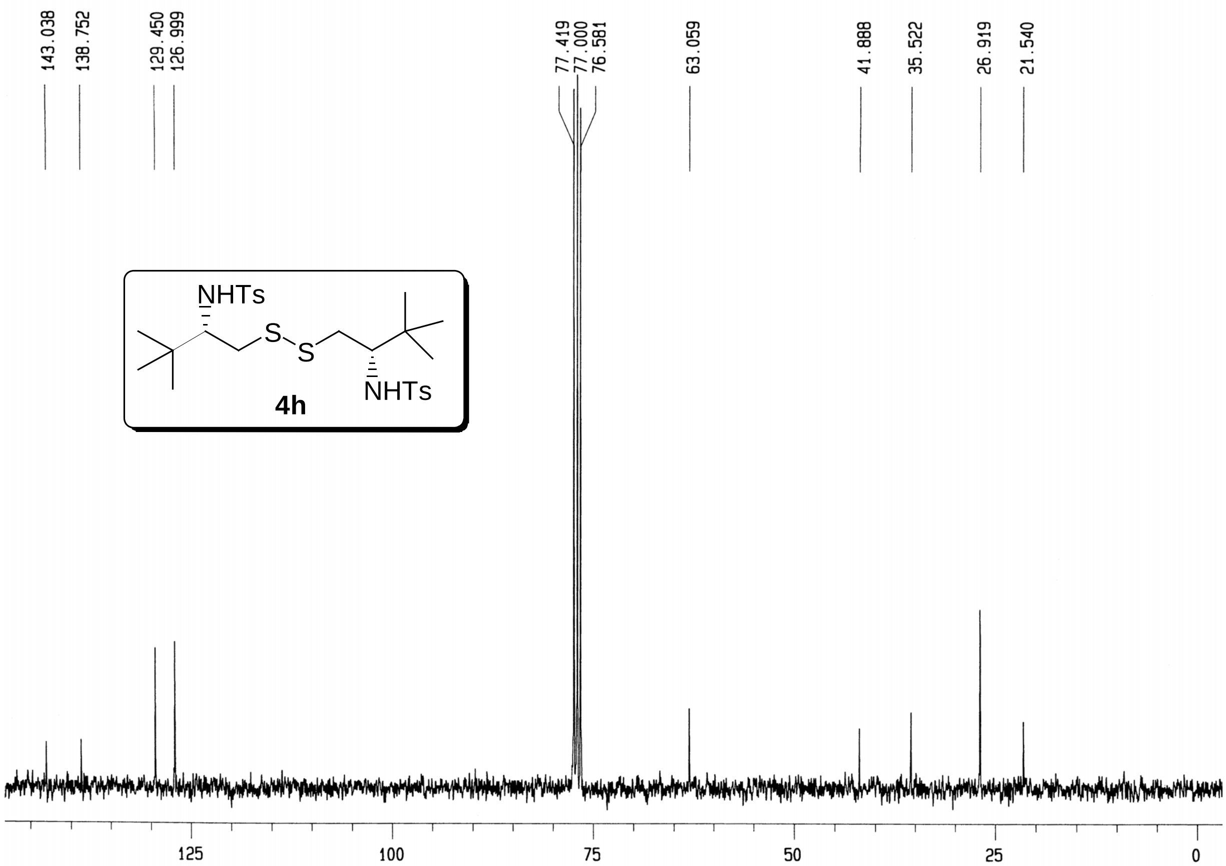
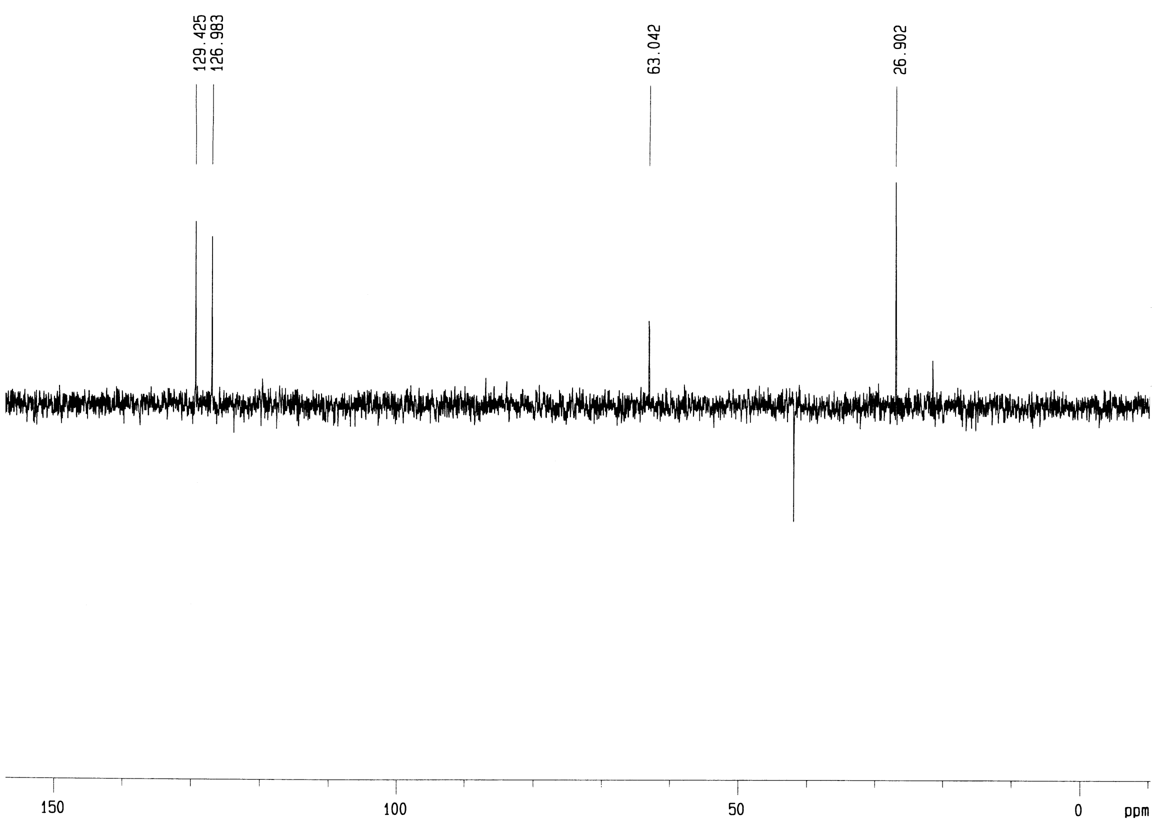
[1]H NMR – $CDCl_3$ (300 MHz)



^{13}C NMR – $CDCl_3$ (75 MHz)



DEPT – $CDCl_3$ (75 MHz)



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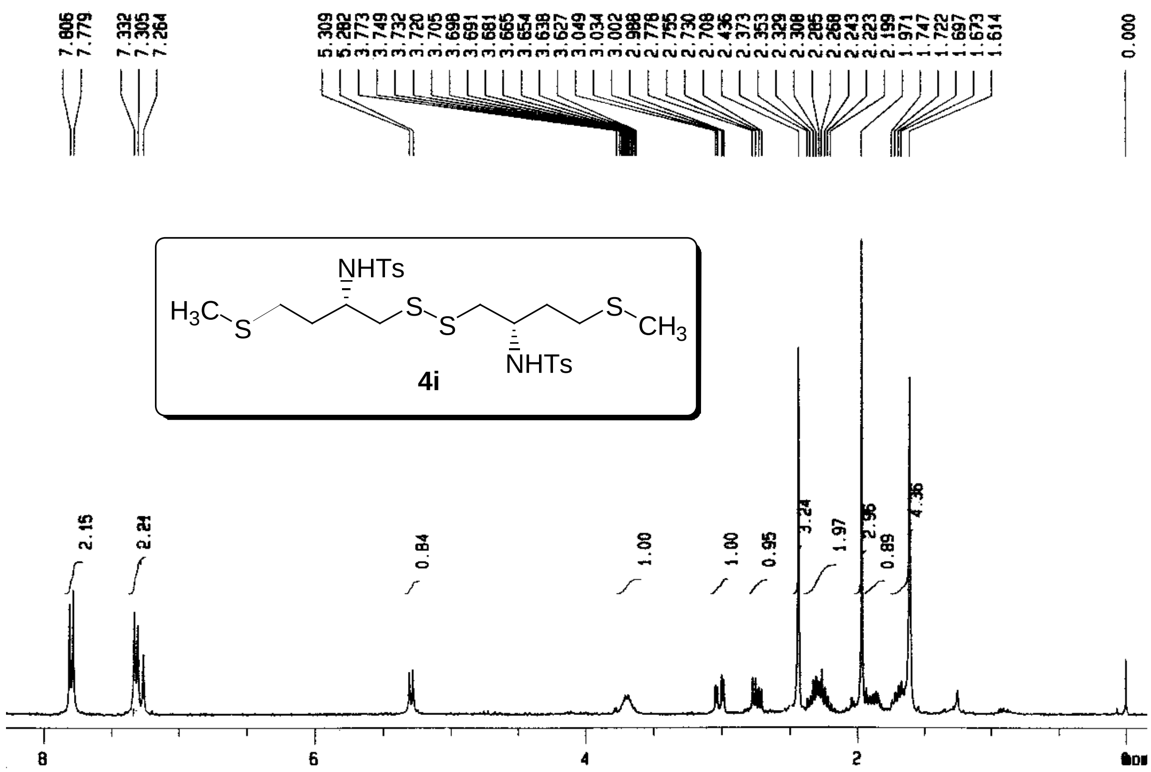

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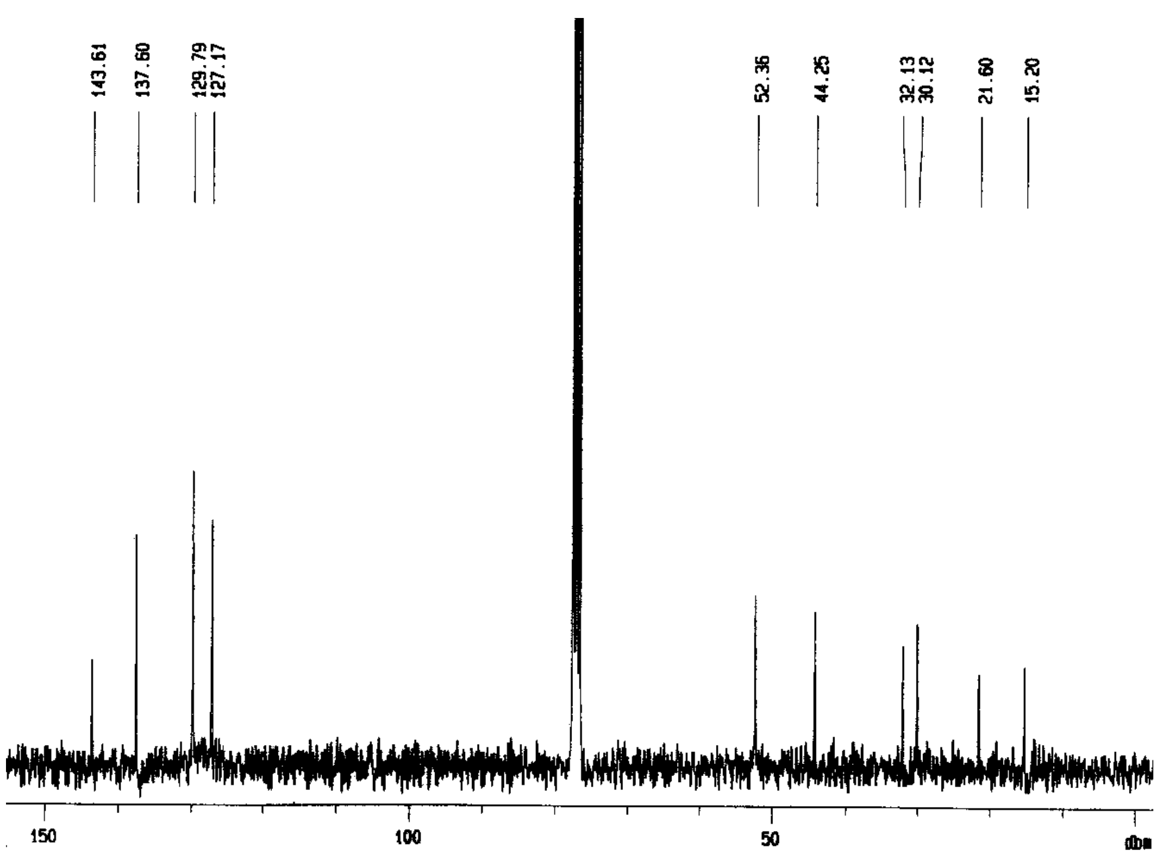

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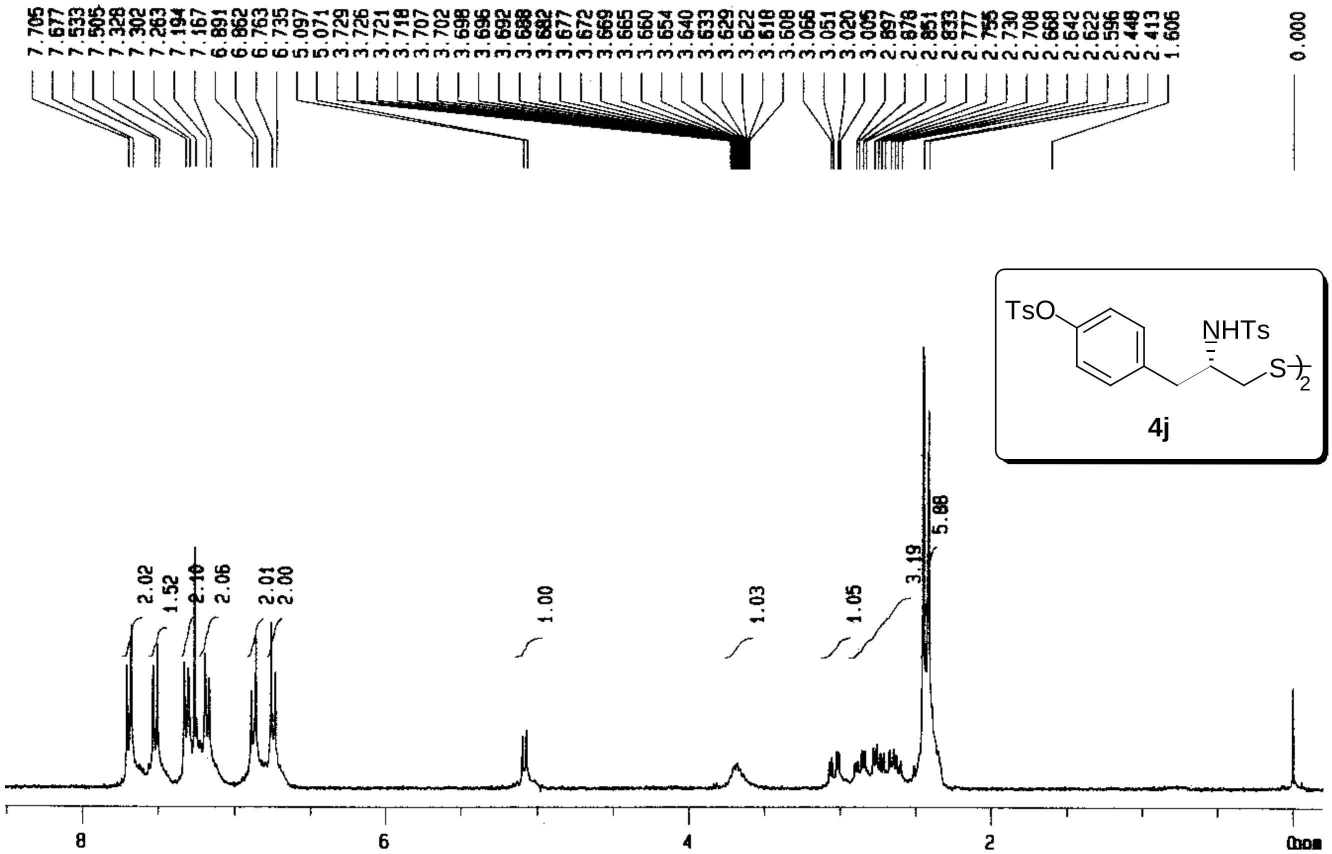
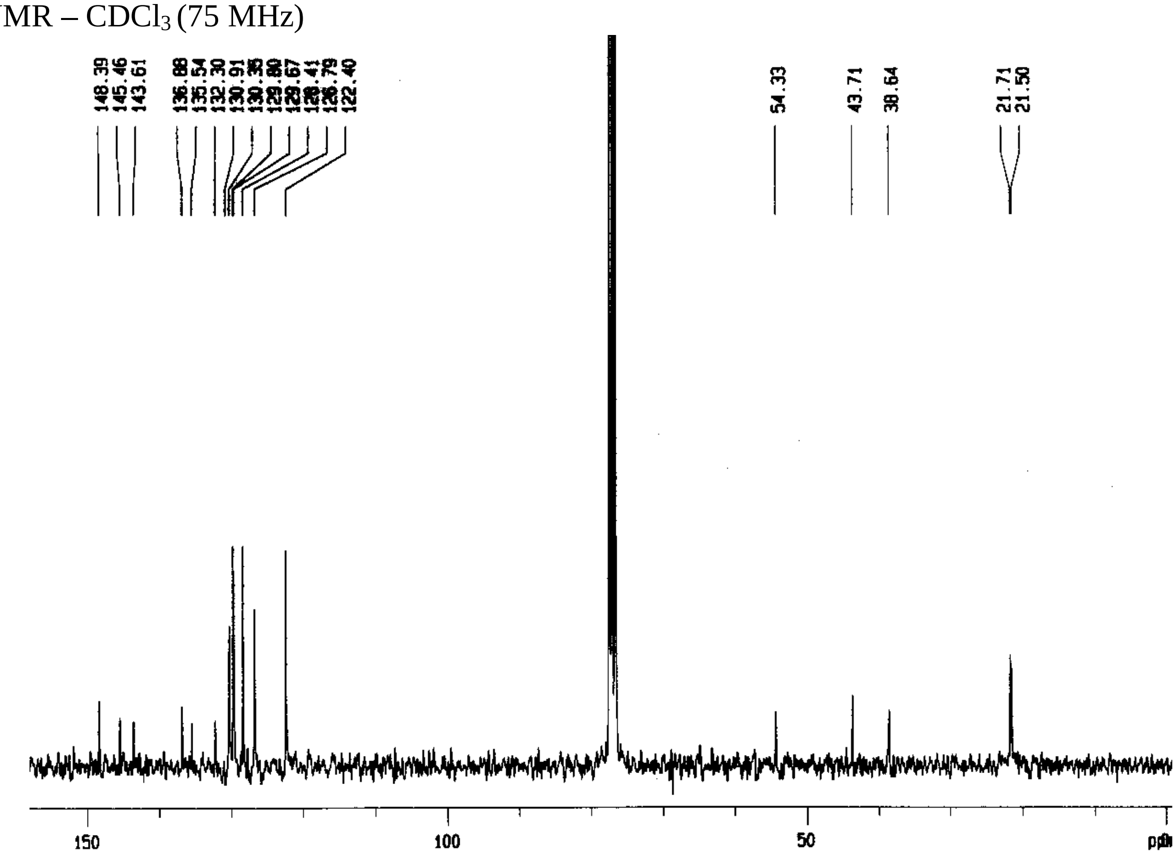


[13]C NMR – $CDCl_3$ (75 MHz)



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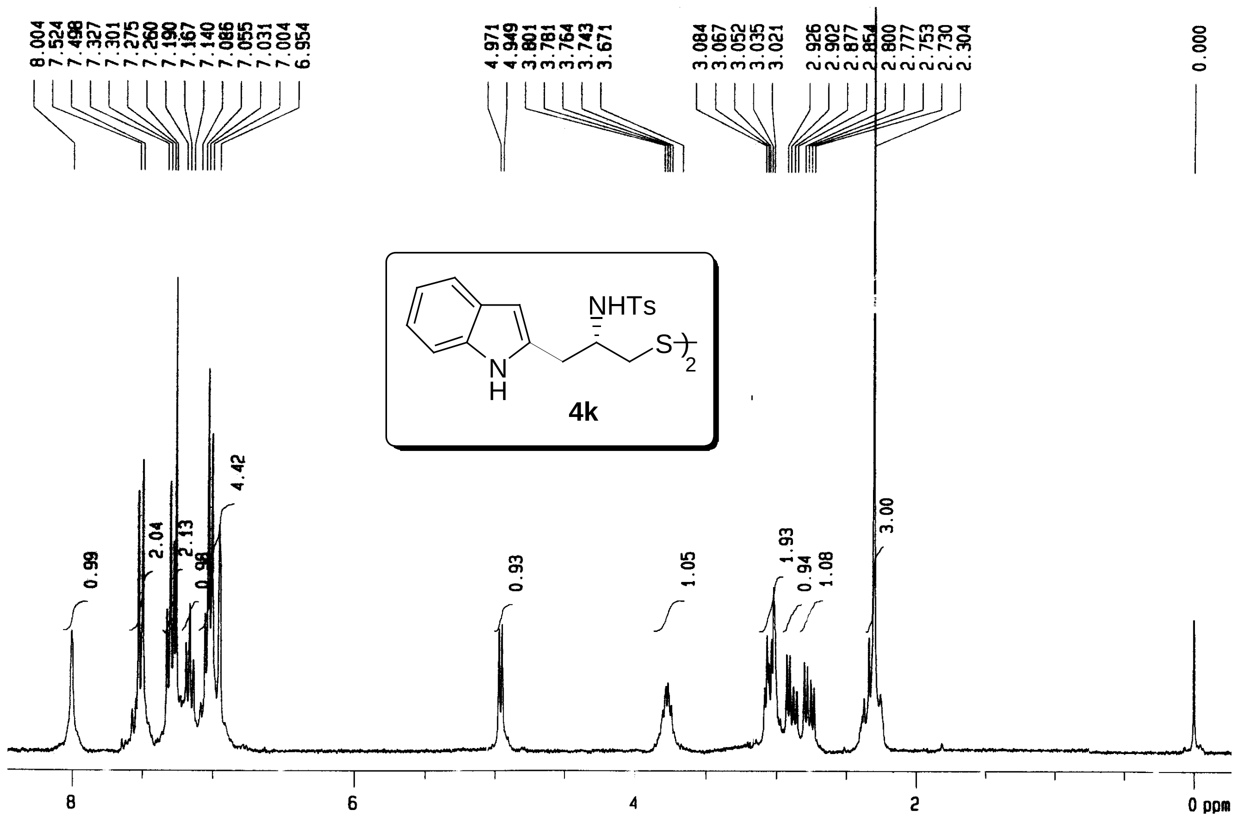
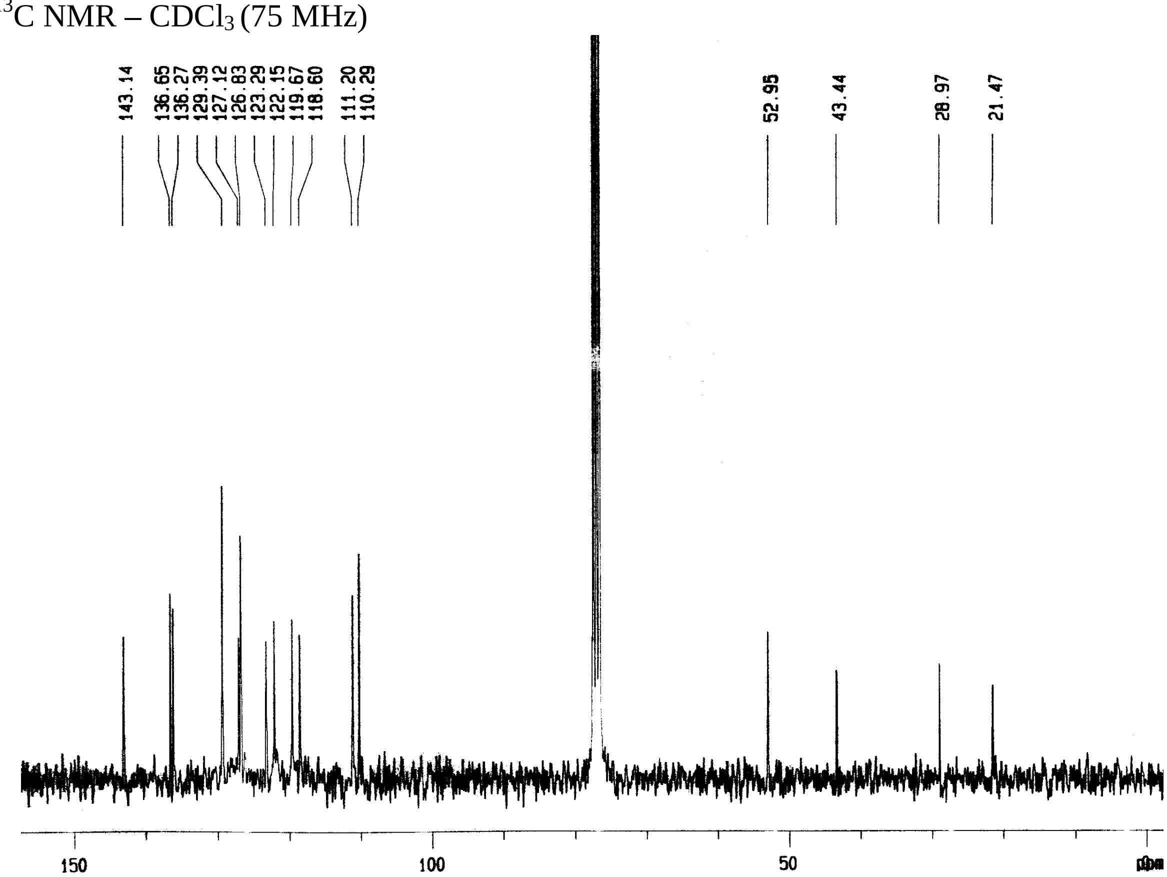
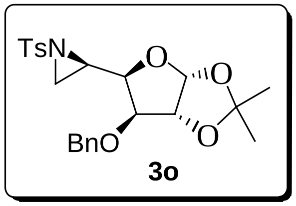


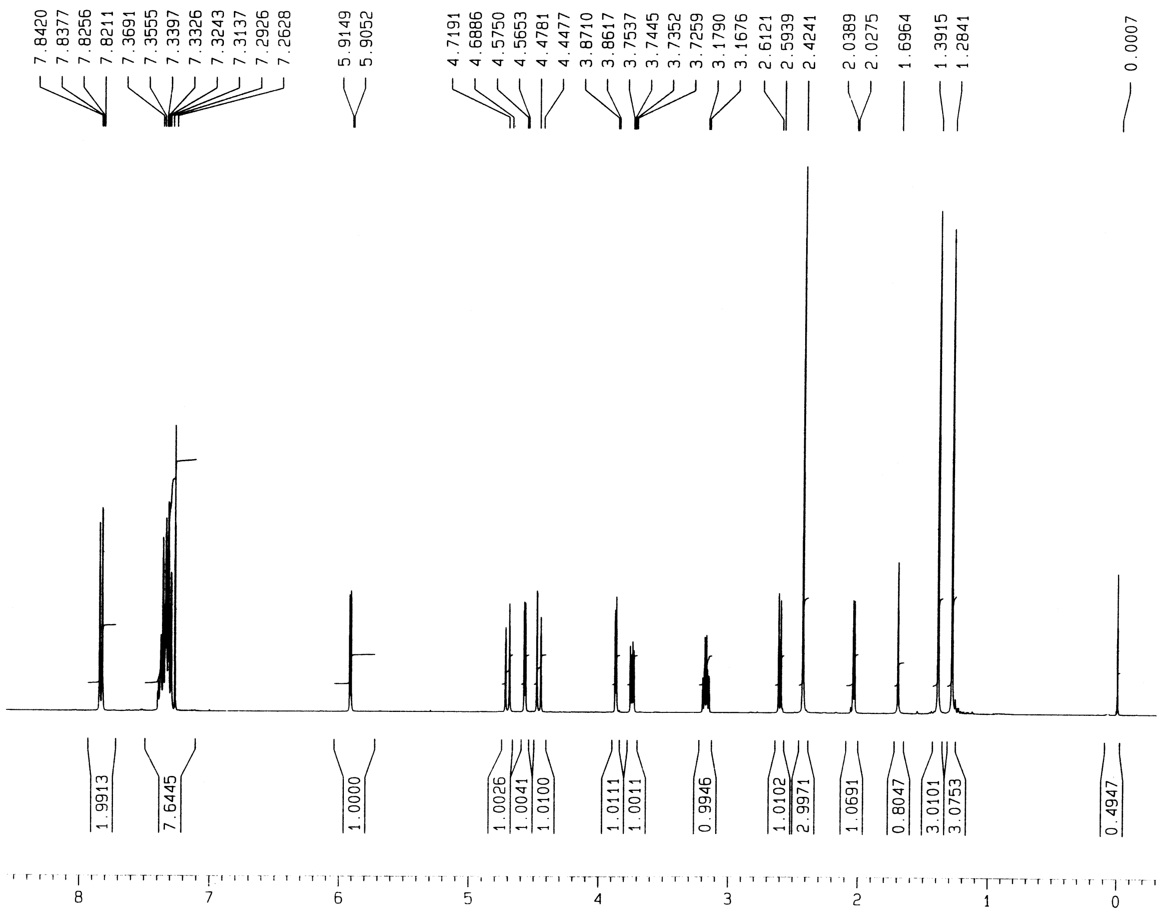
^{13}C NMR – $CDCl_3$ (75 MHz)

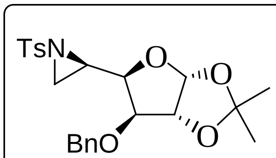




3o

[1]H NMR – $CDCl_3$ (400 MHz)





3o

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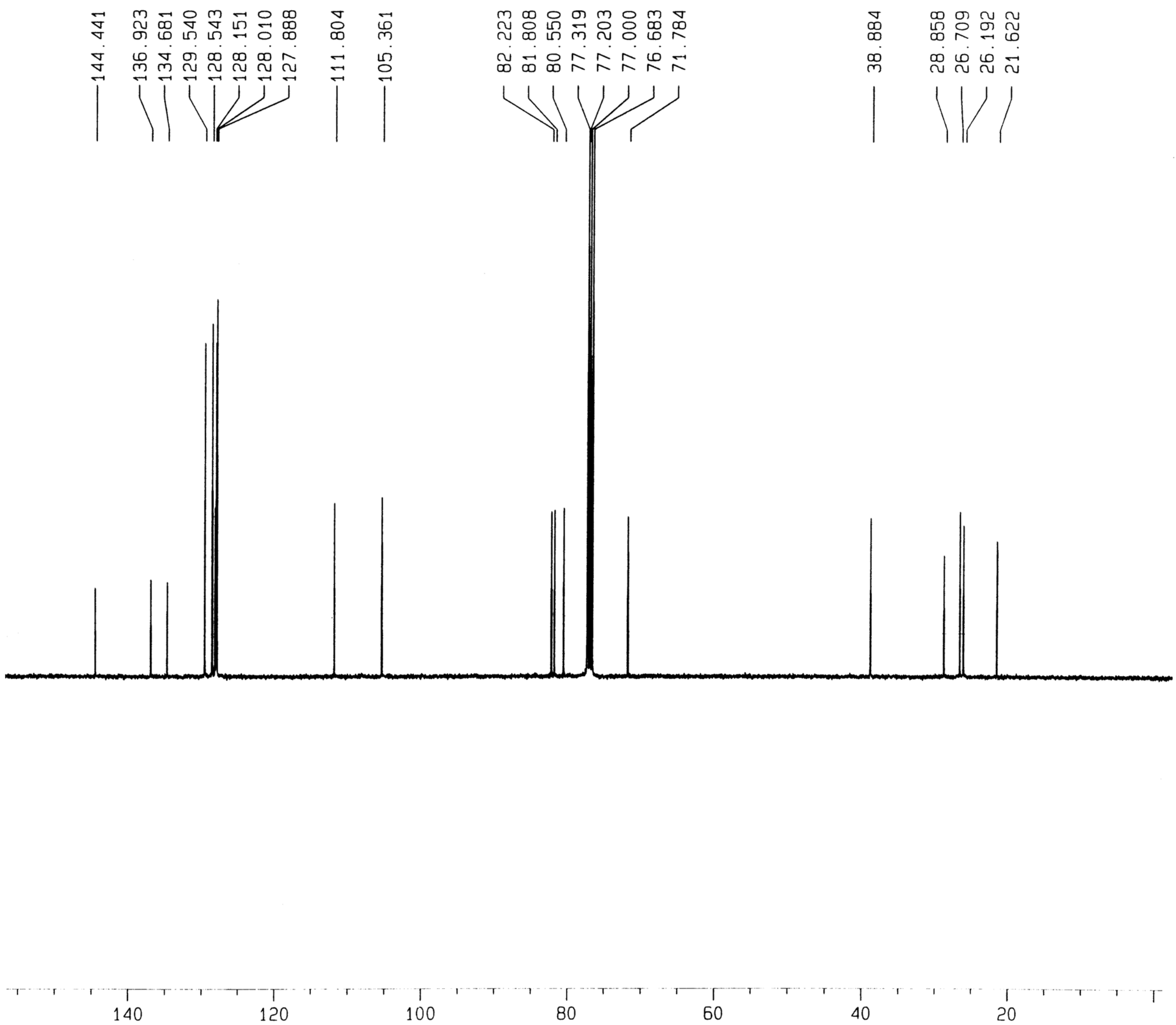

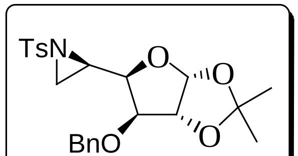

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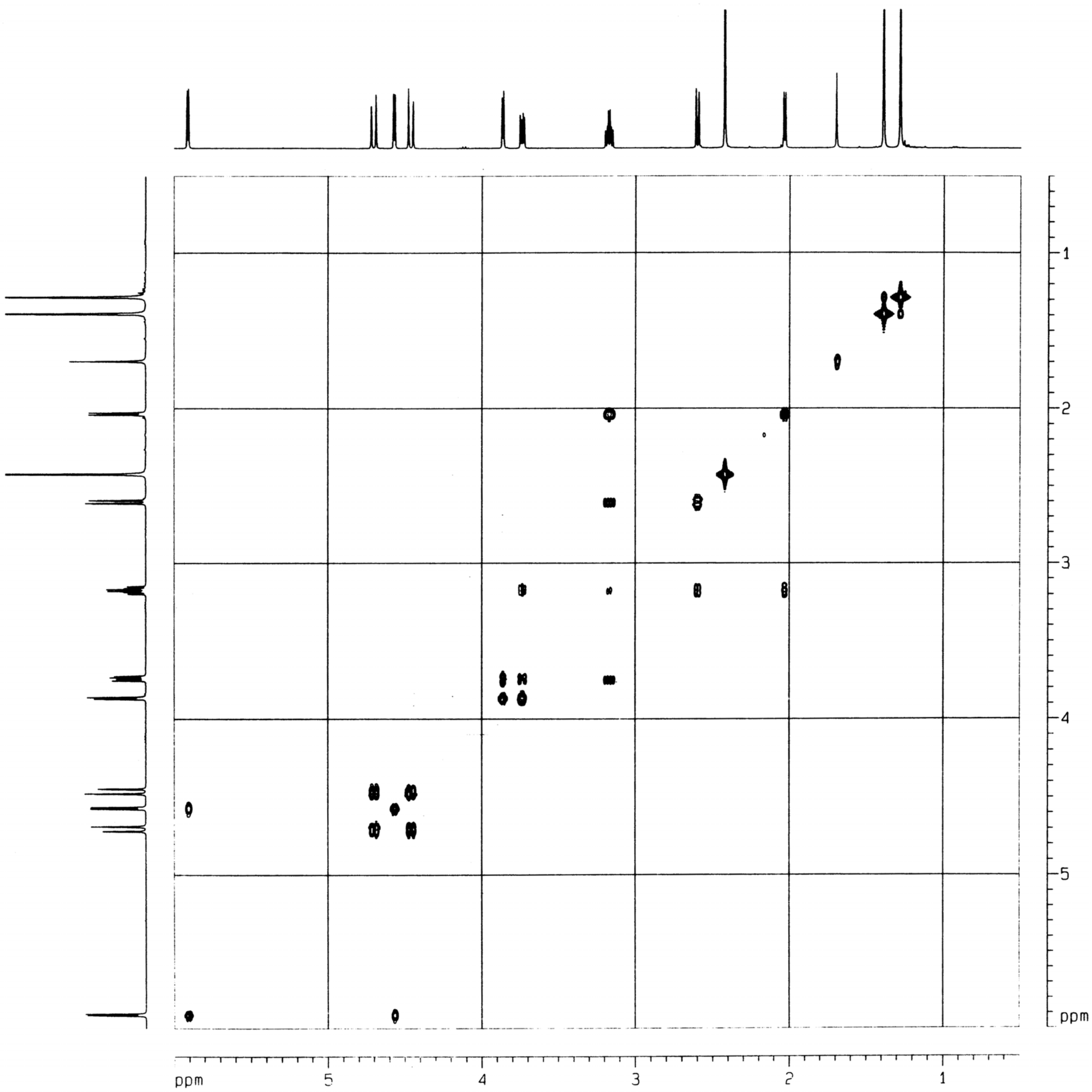

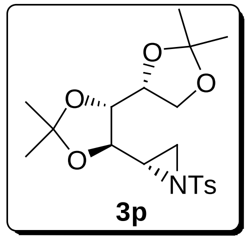

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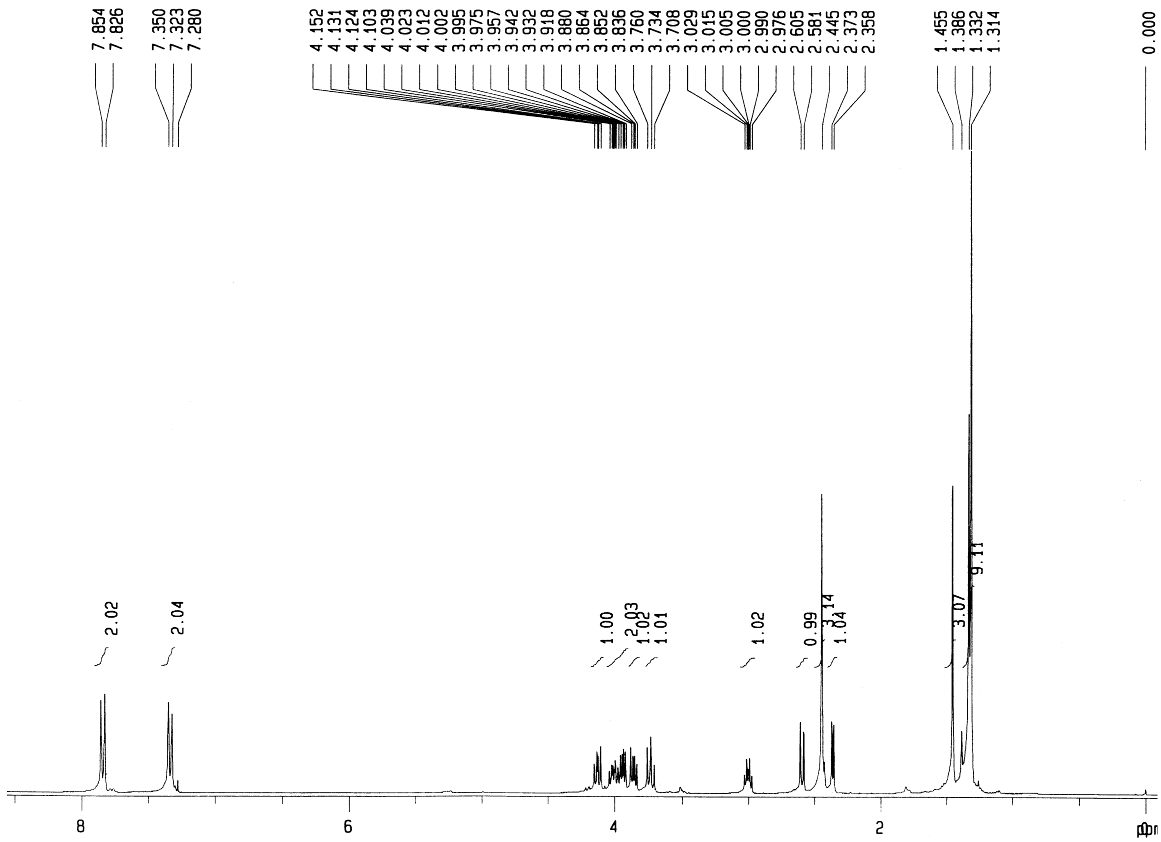

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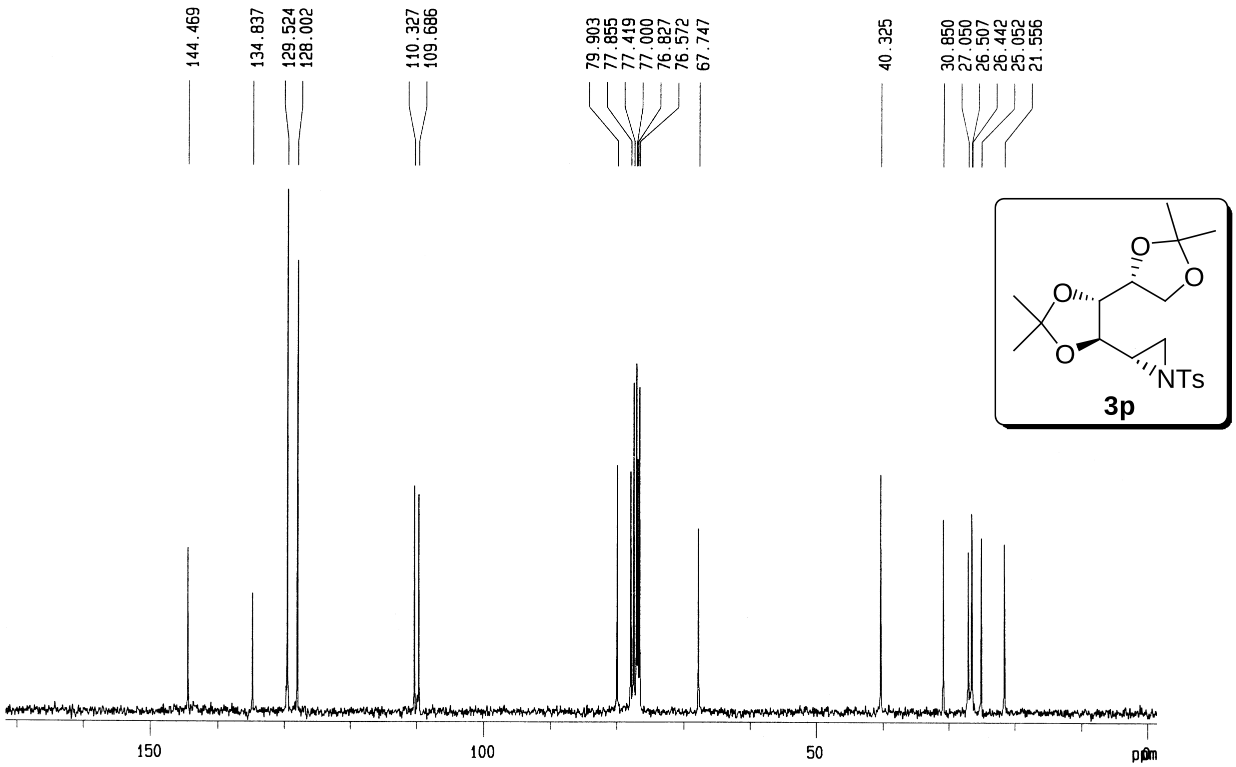
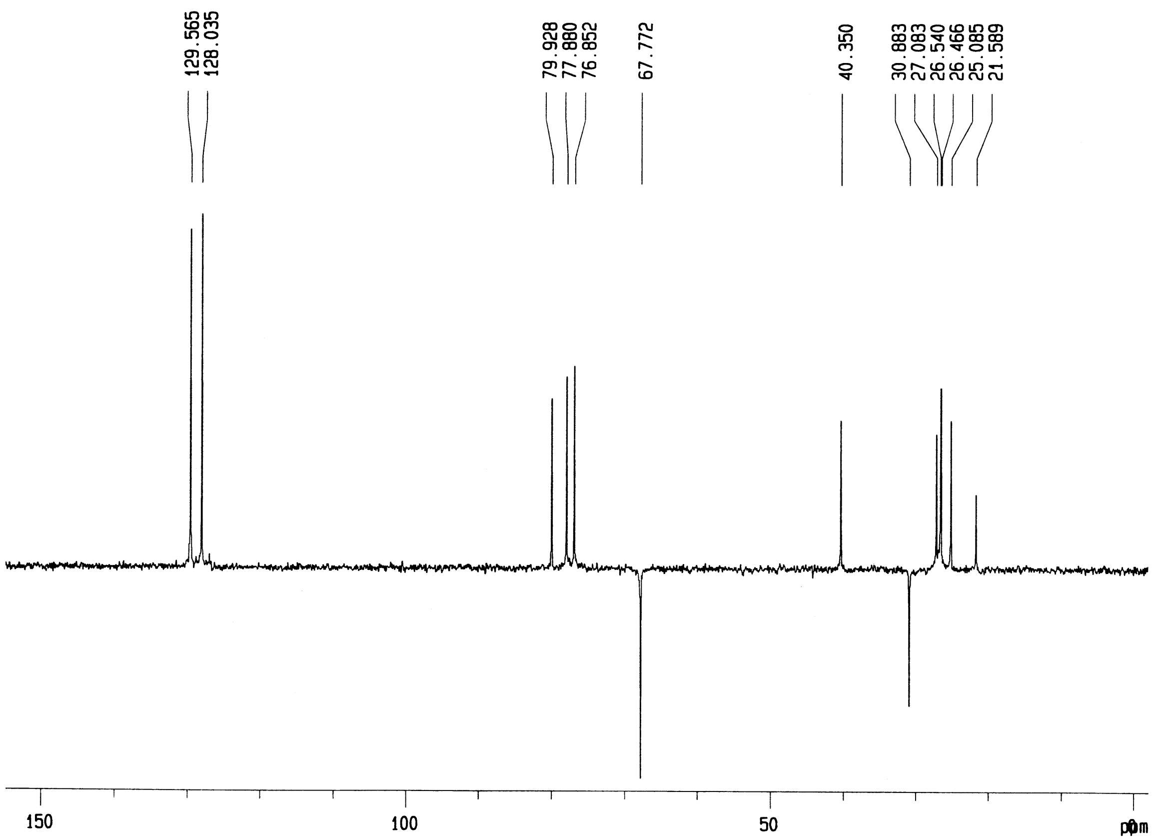
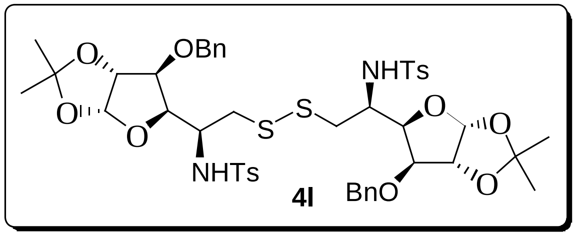
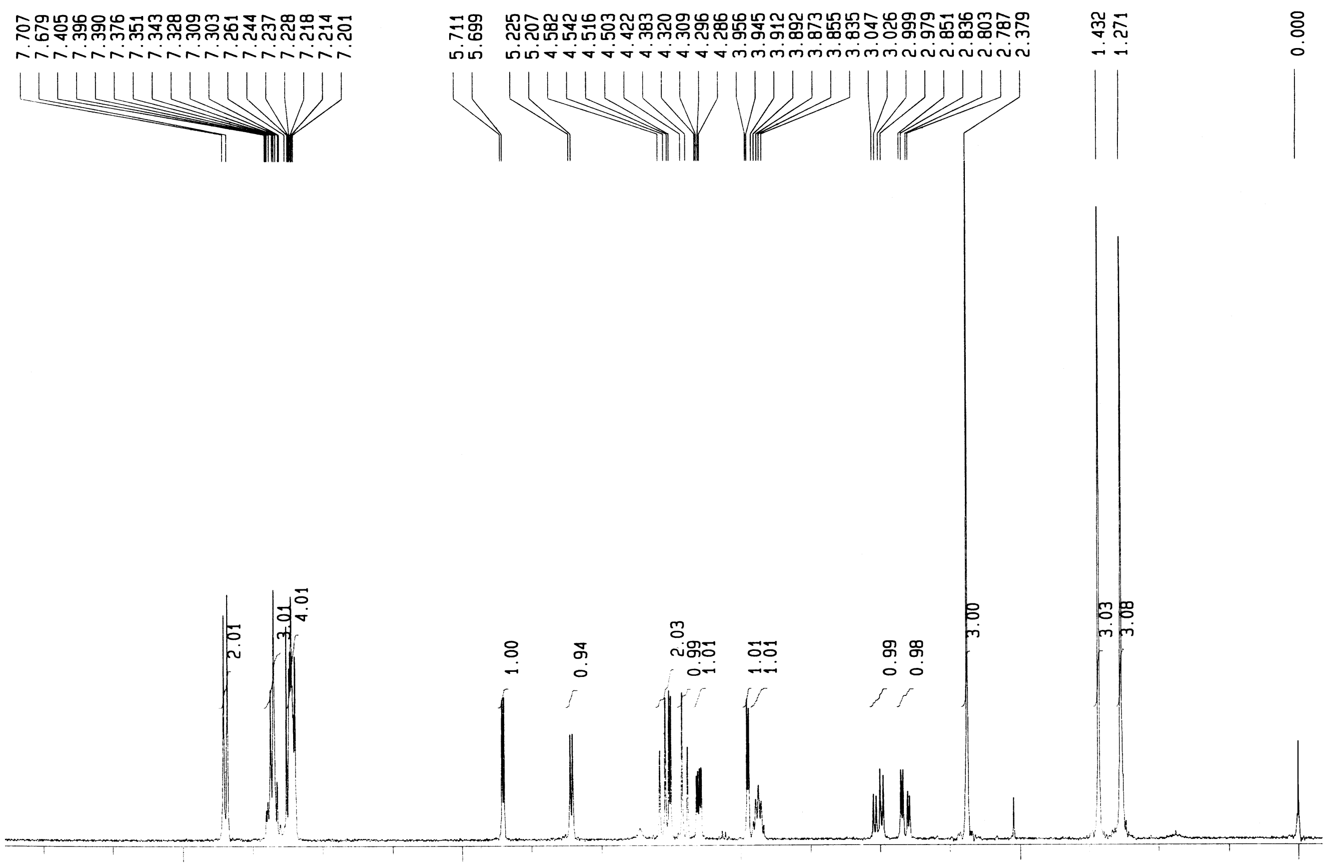


DEPT – $CDCl_3$ (75 MHz)

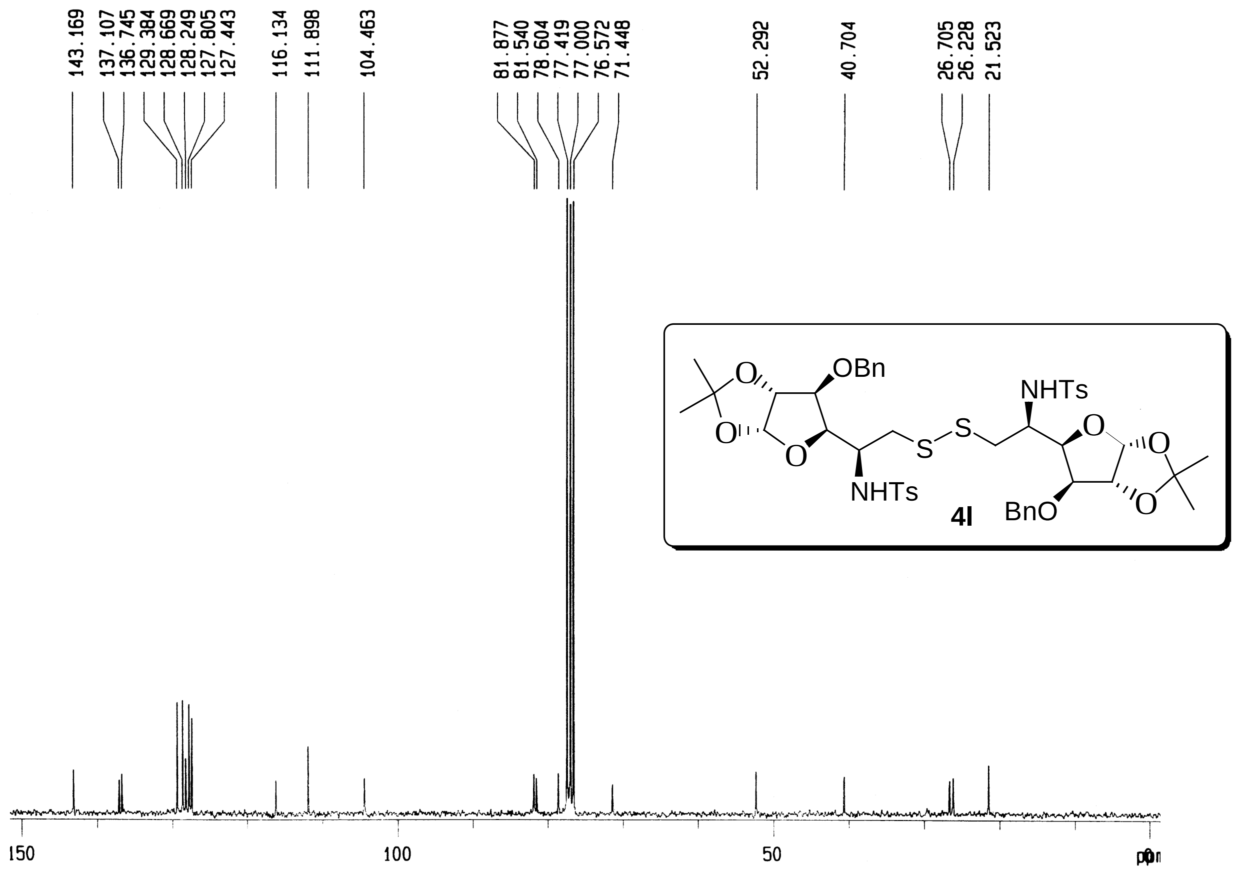




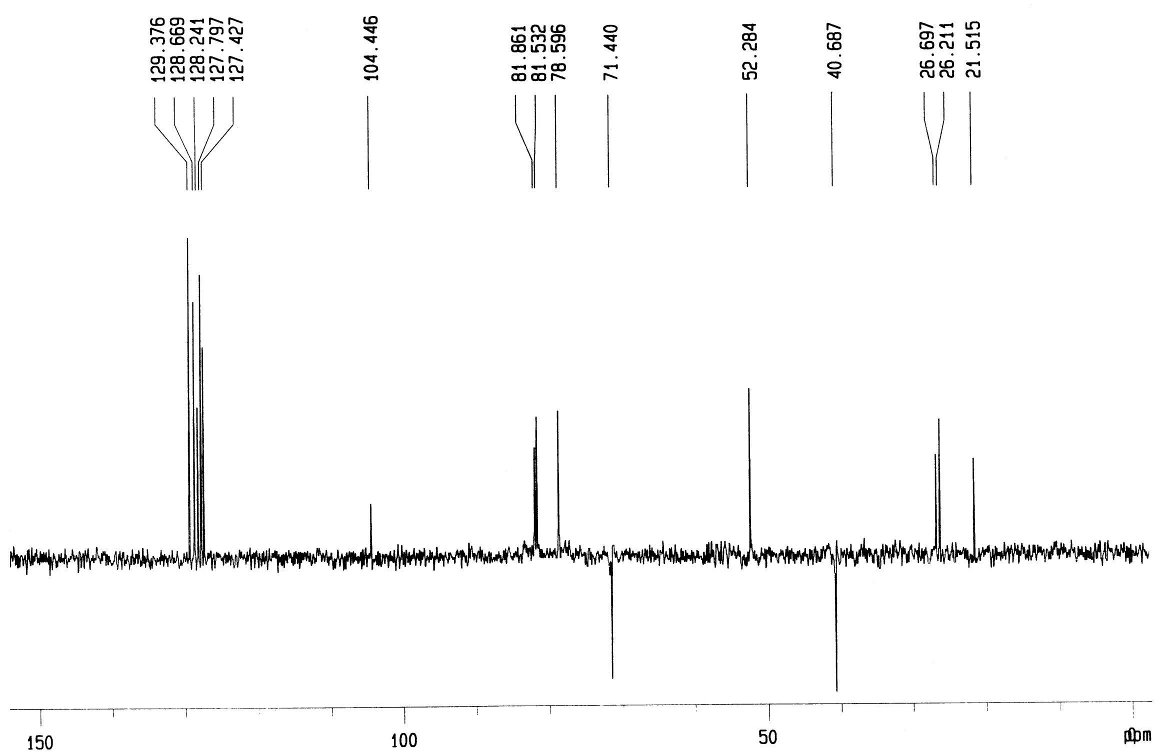
^1H NMR – $CDCl_3$ (300 MHz)

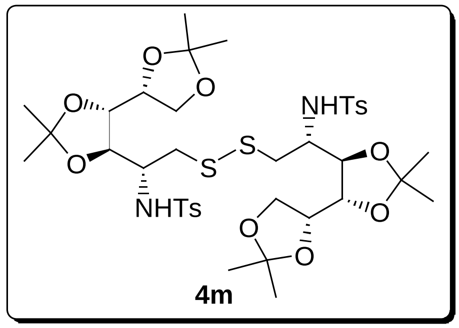


^{13}C NMR – $CDCl_3$ (75 MHz)



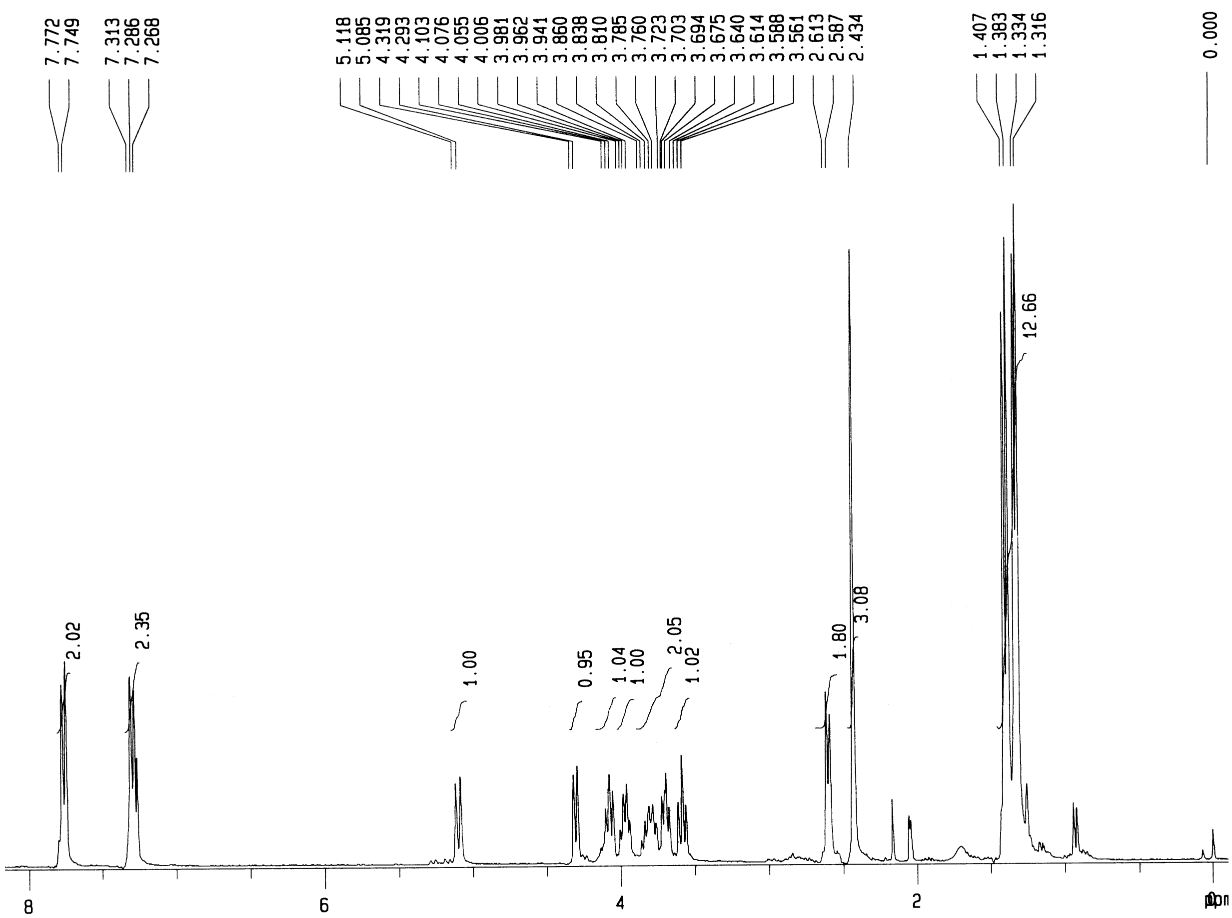
DEPT – $CDCl_3$ (75 MHz)



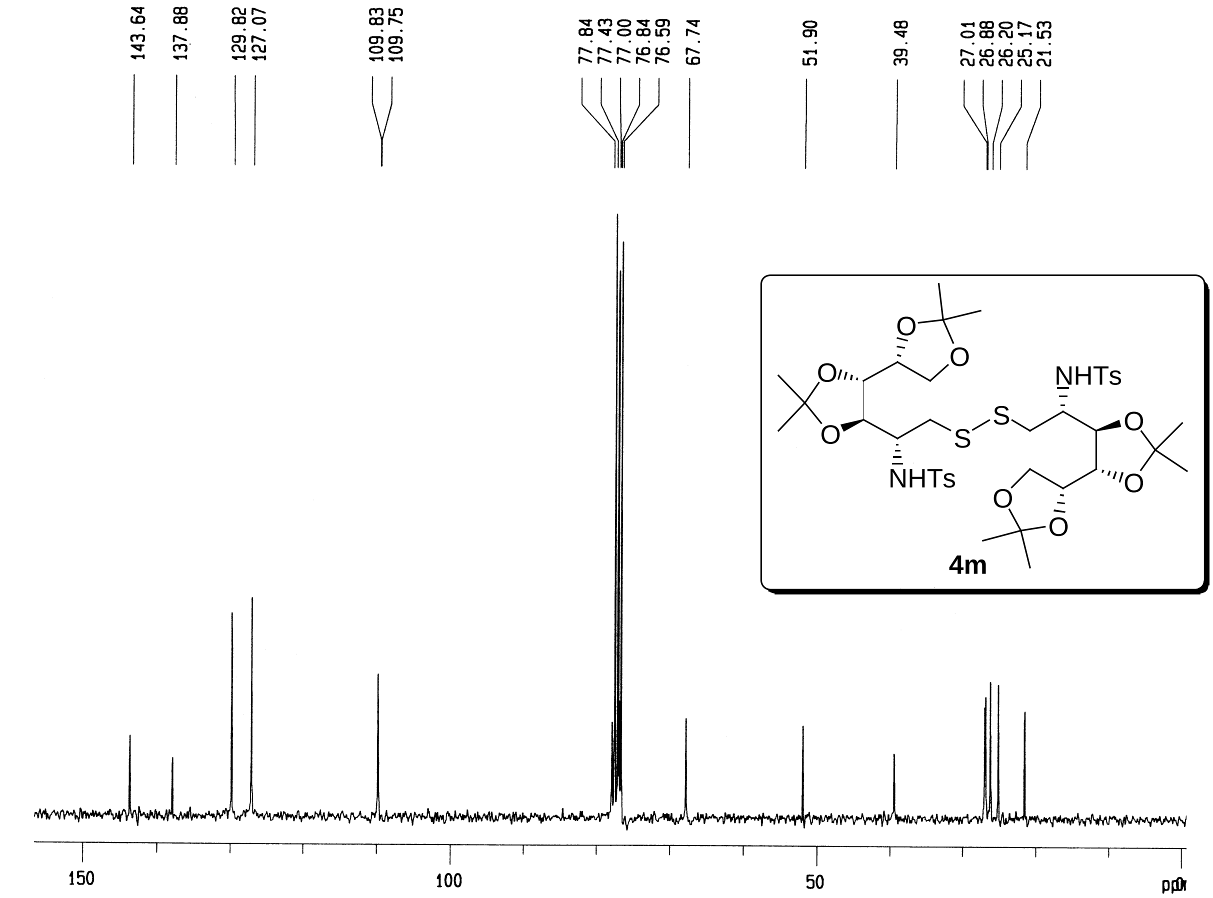


4m

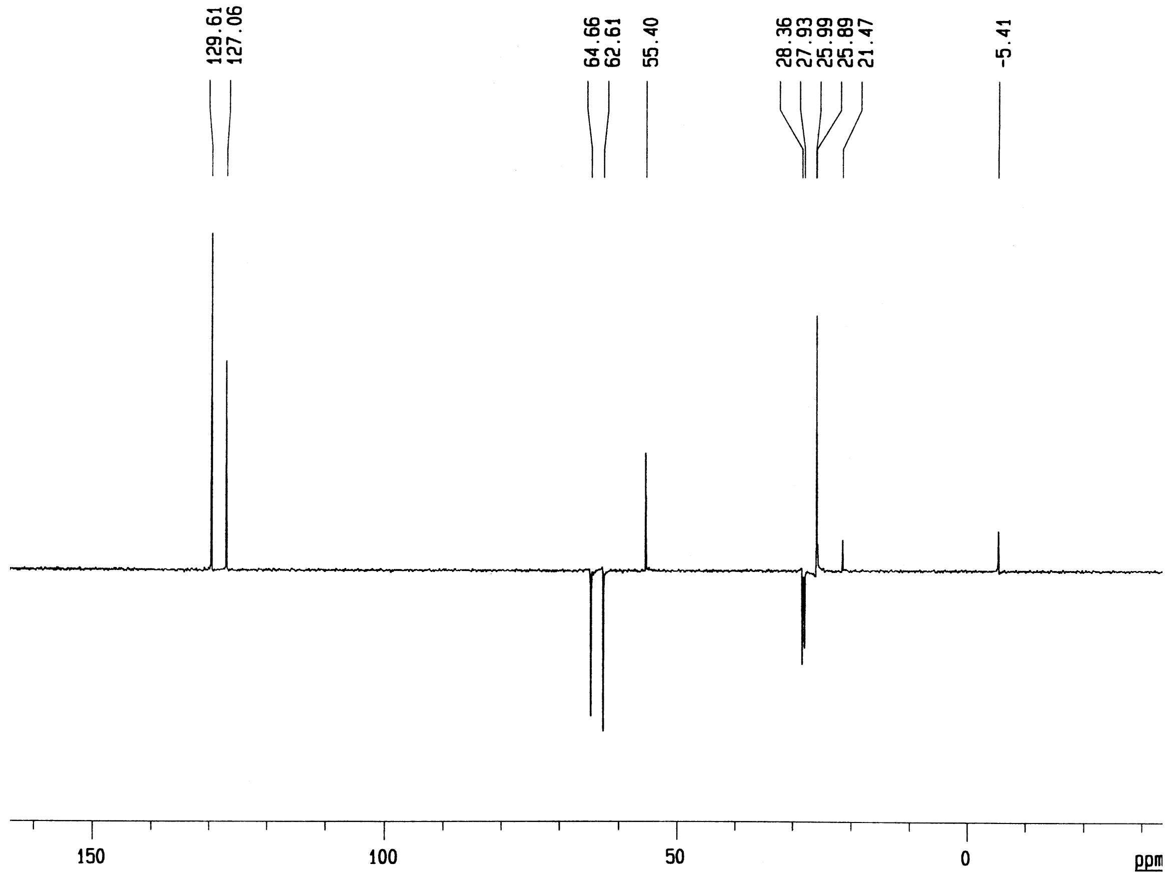
^{1}H NMR – $CDCl_3$ (300 MHz)

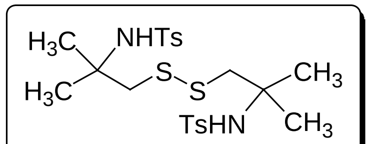


^{13}C NMR – $CDCl_3$ (75 MHz)



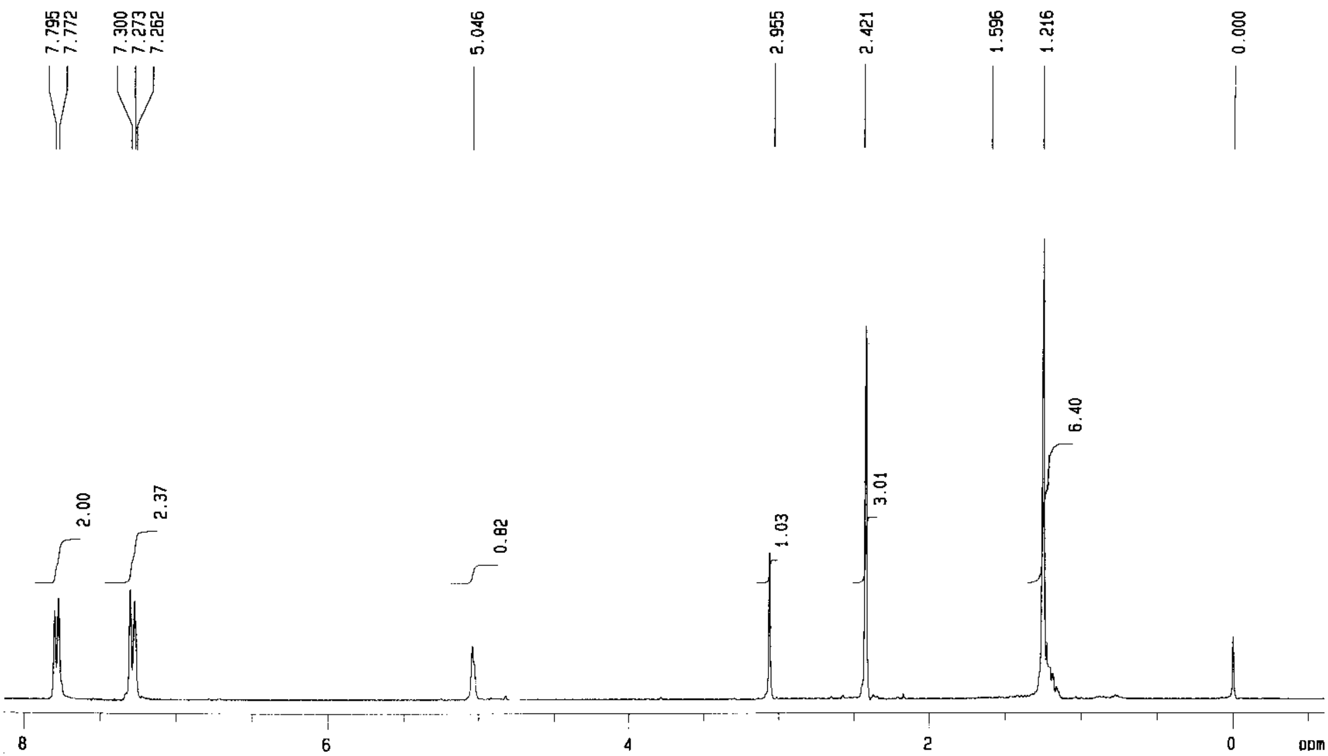
DEPT – $CDCl_3$ (75 MHz)



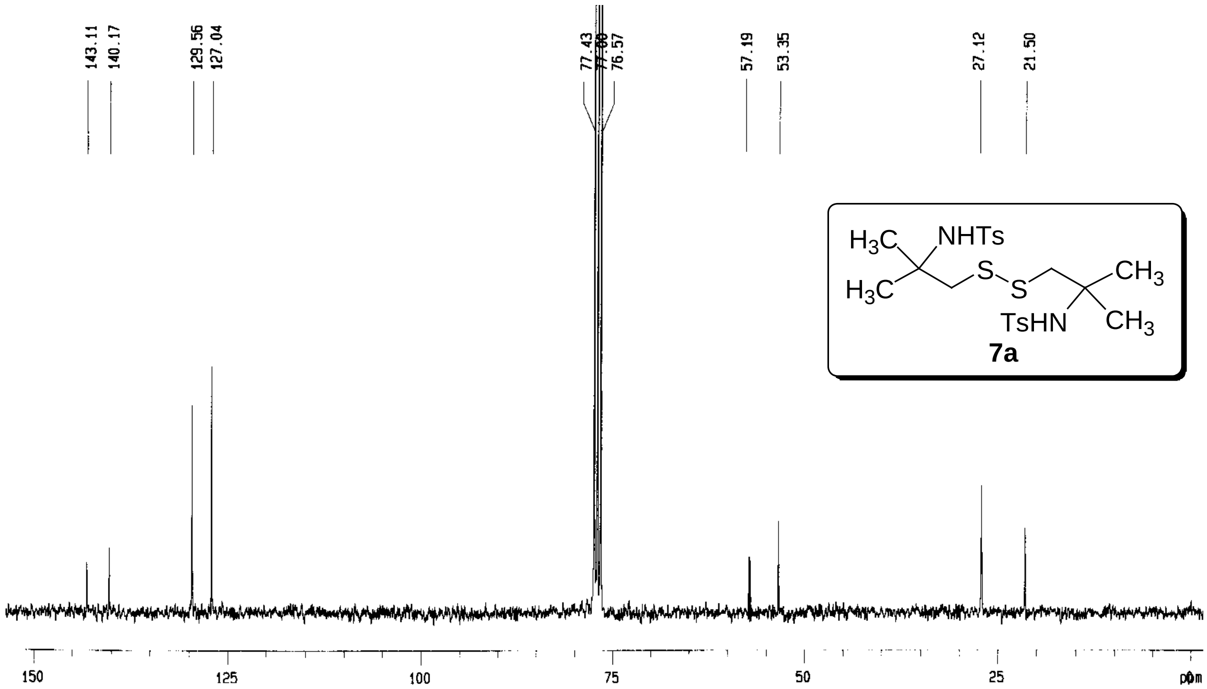


7a

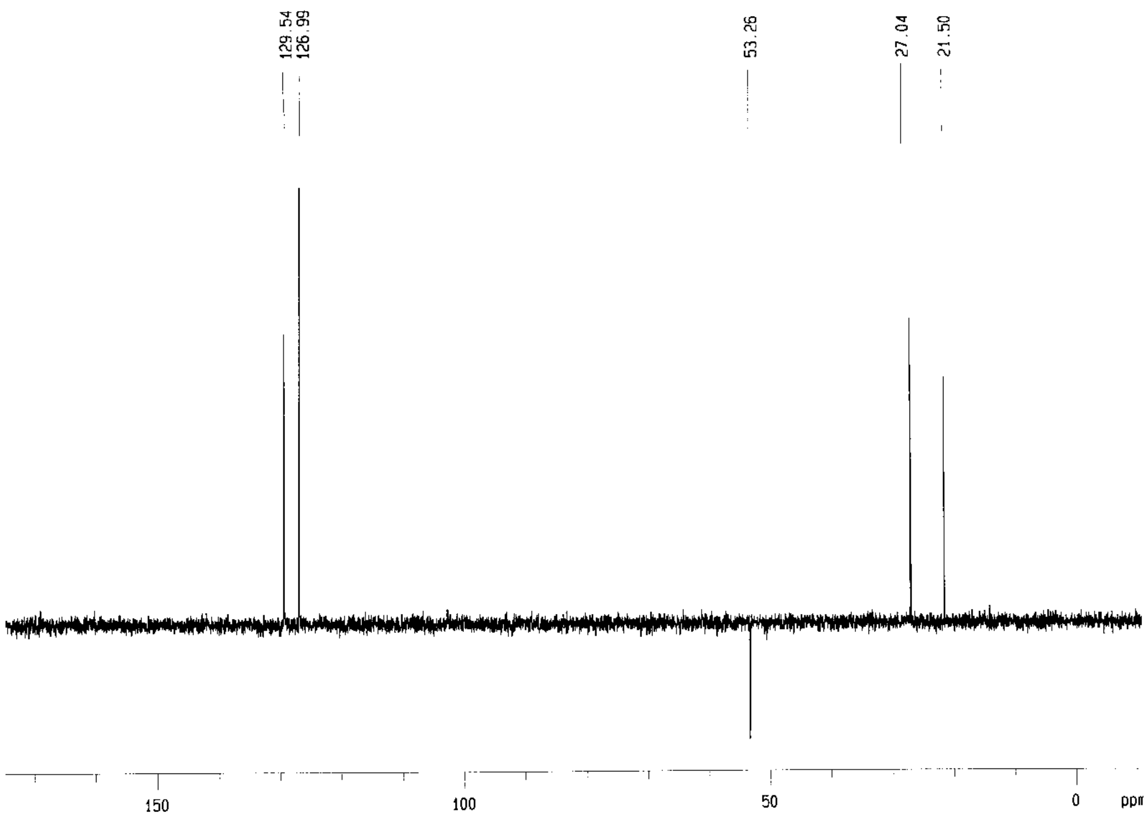
^{1}H NMR – $CDCl_3$ (300 MHz)



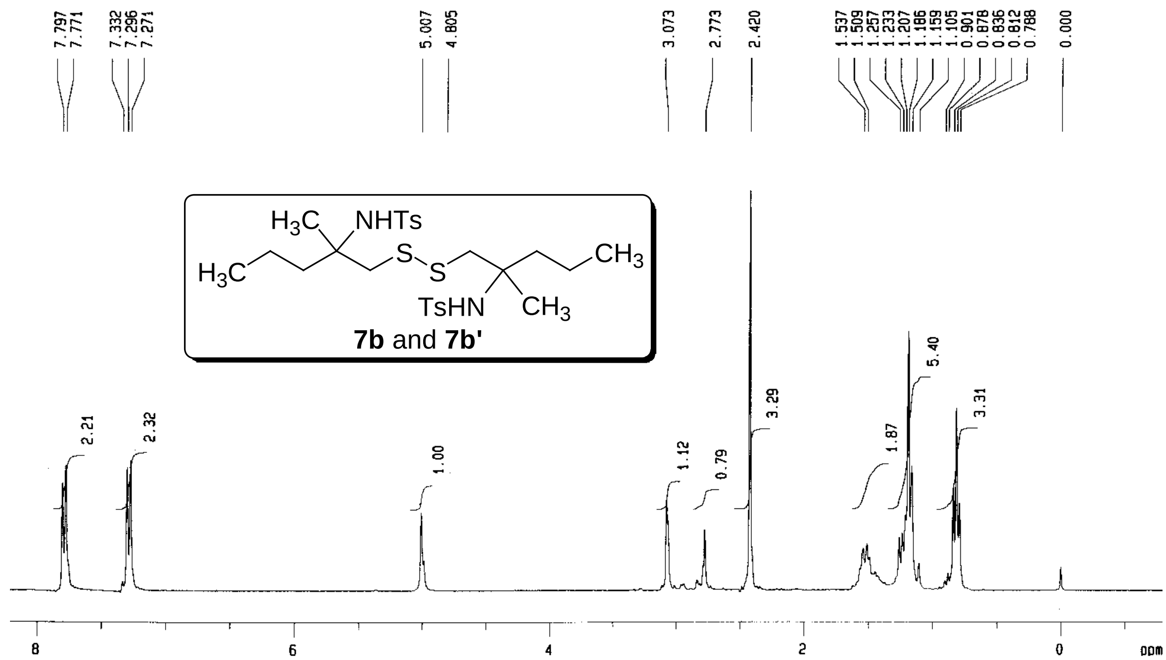
^{13}C NMR – $CDCl_3$ (75 MHz)



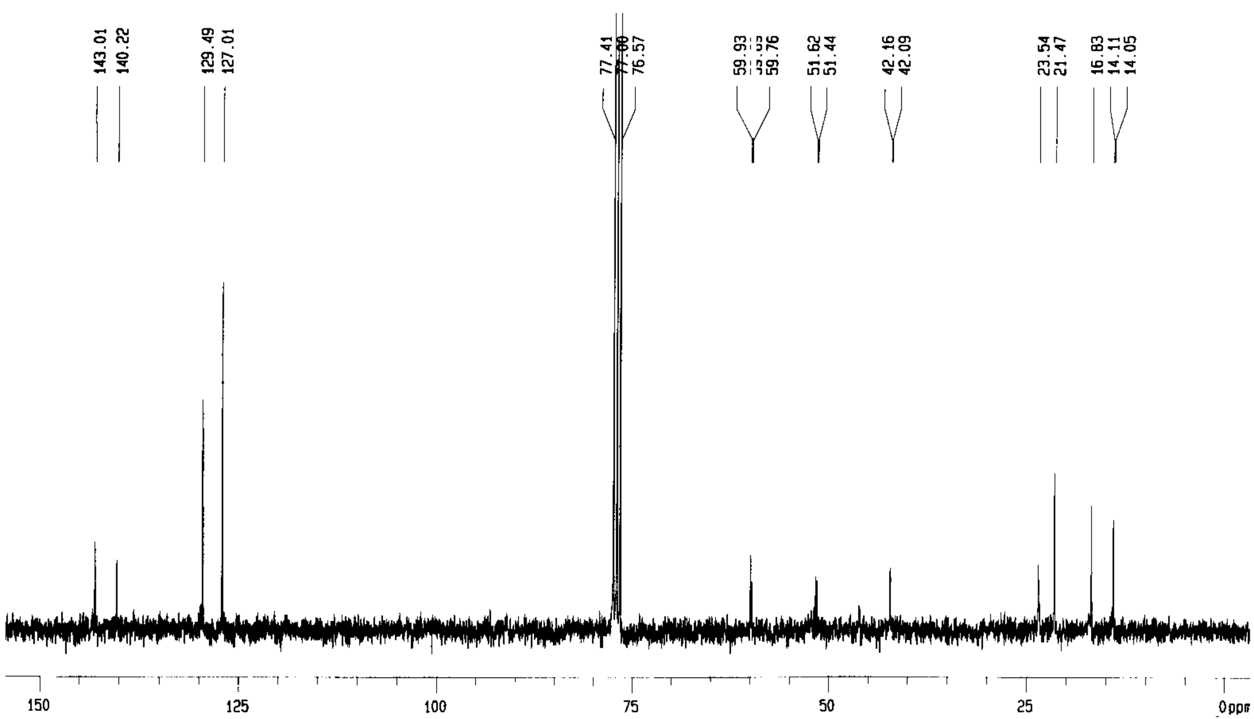
DEPT – $CDCl_3$ (75 MHz)



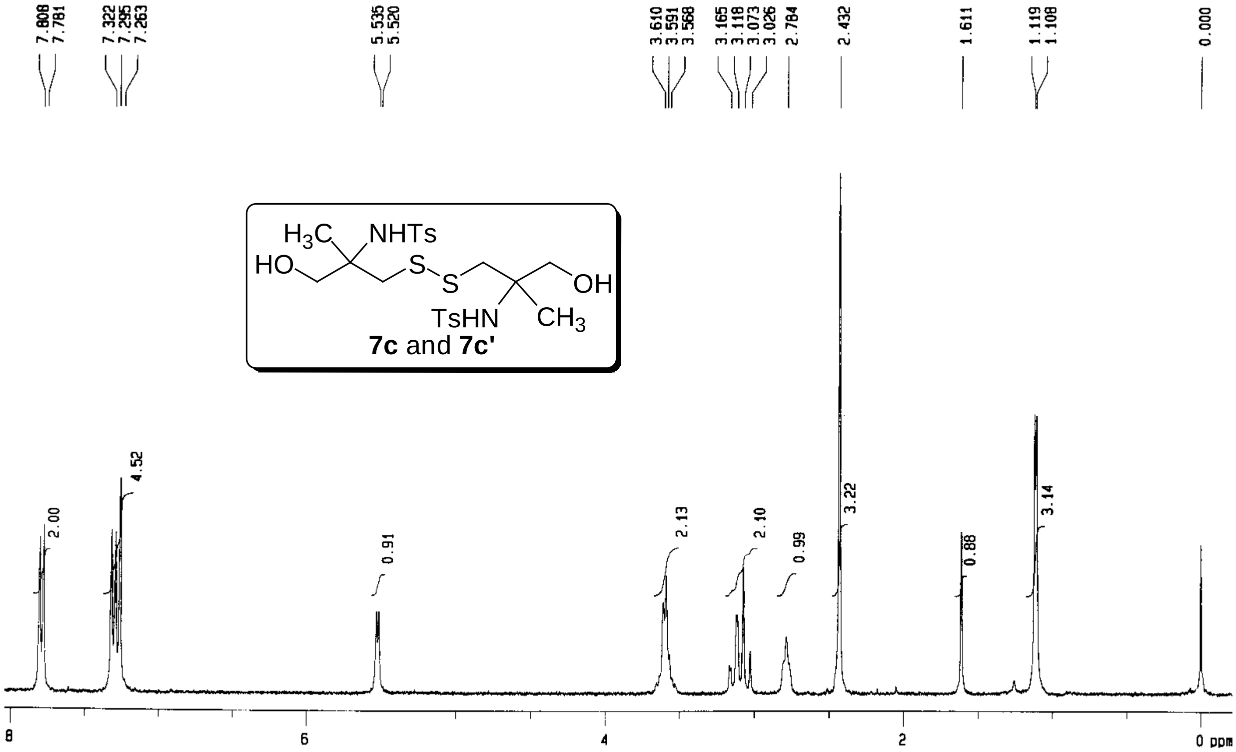
^{1}H NMR – $CDCl_3$ (300 MHz)



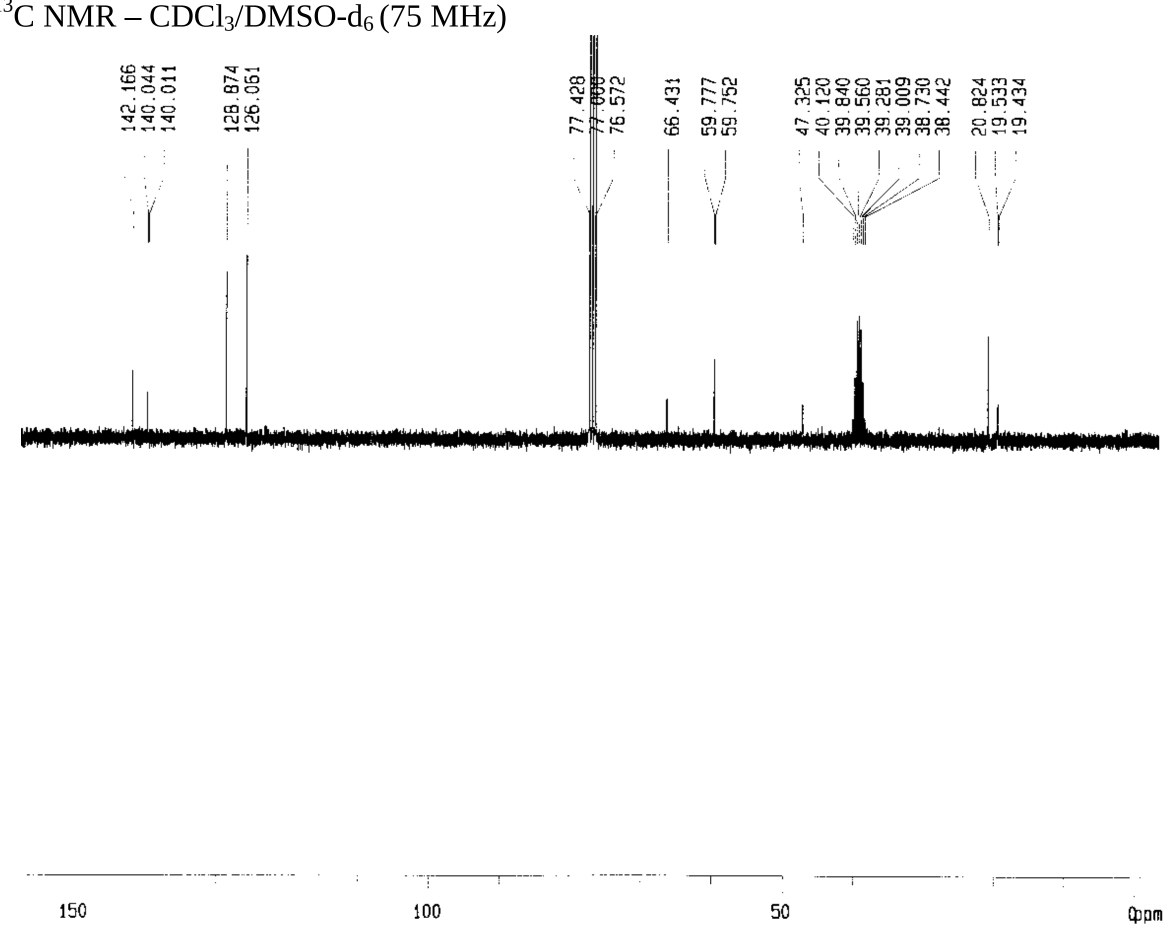
^{13}C NMR – $CDCl_3$ (75 MHz)

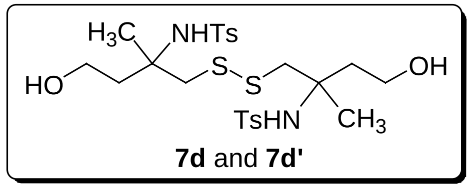


^{1}H NMR – $CDCl_3$/DMSO-d_6 (300 MHz)

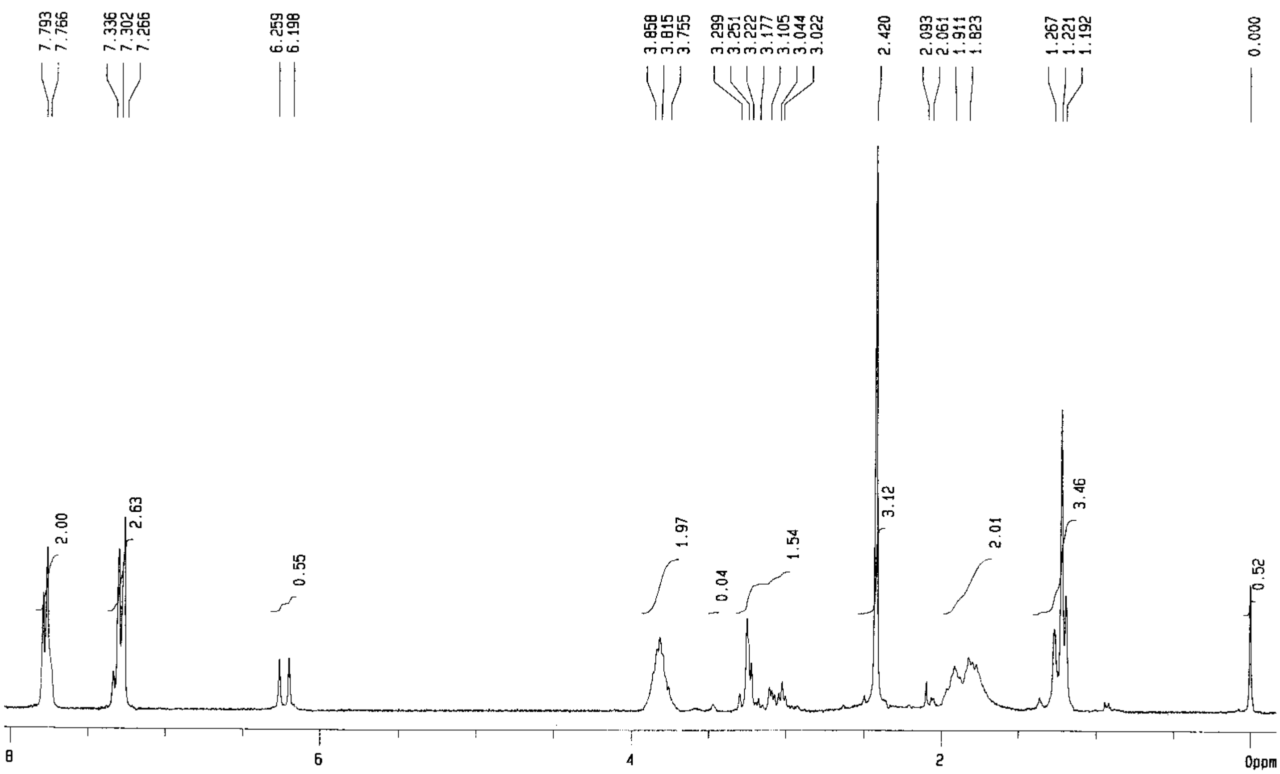


^{13}C NMR – $CDCl_3$/DMSO-d_6 (75 MHz)

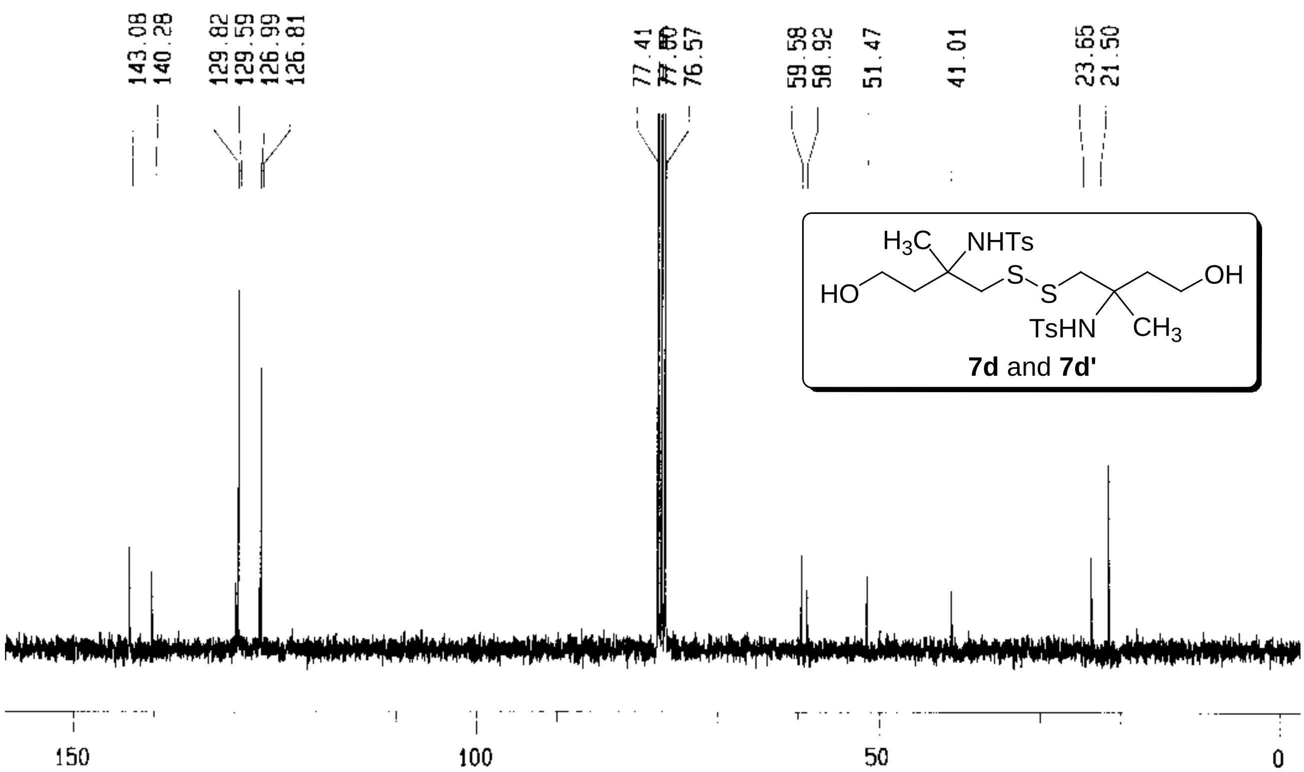




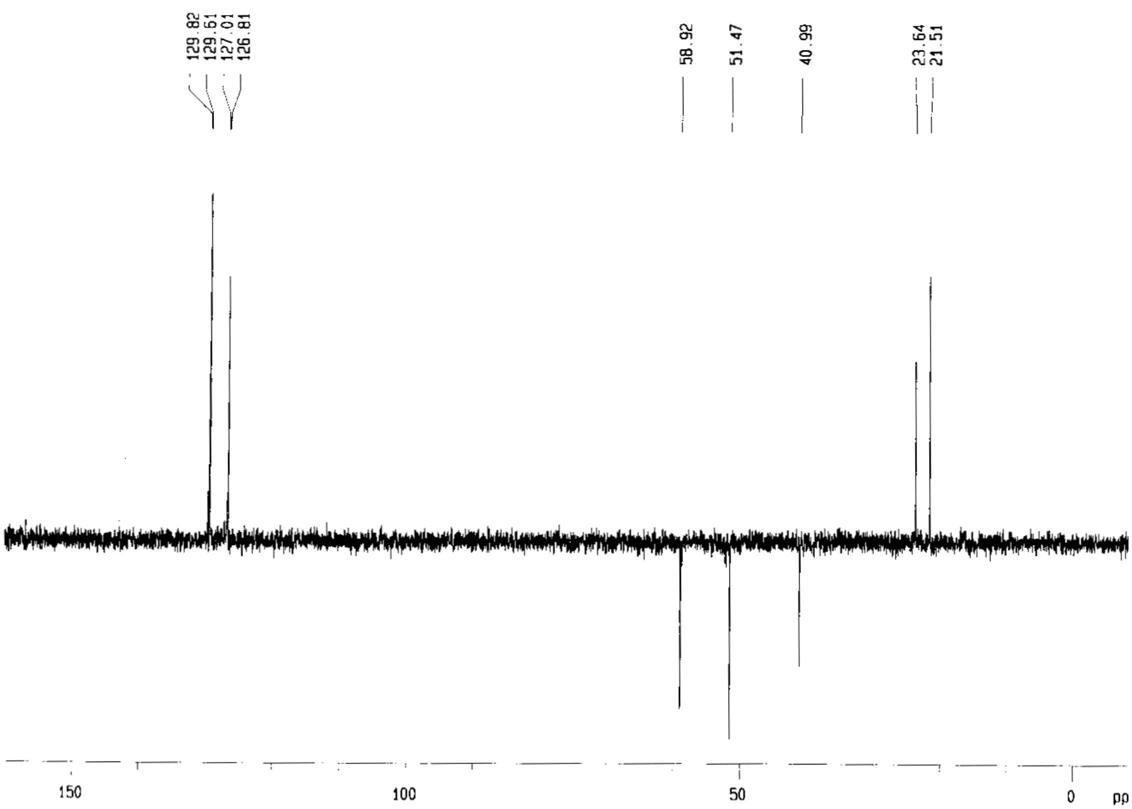
^{1}H NMR – $CDCl_3$ (300 MHz)



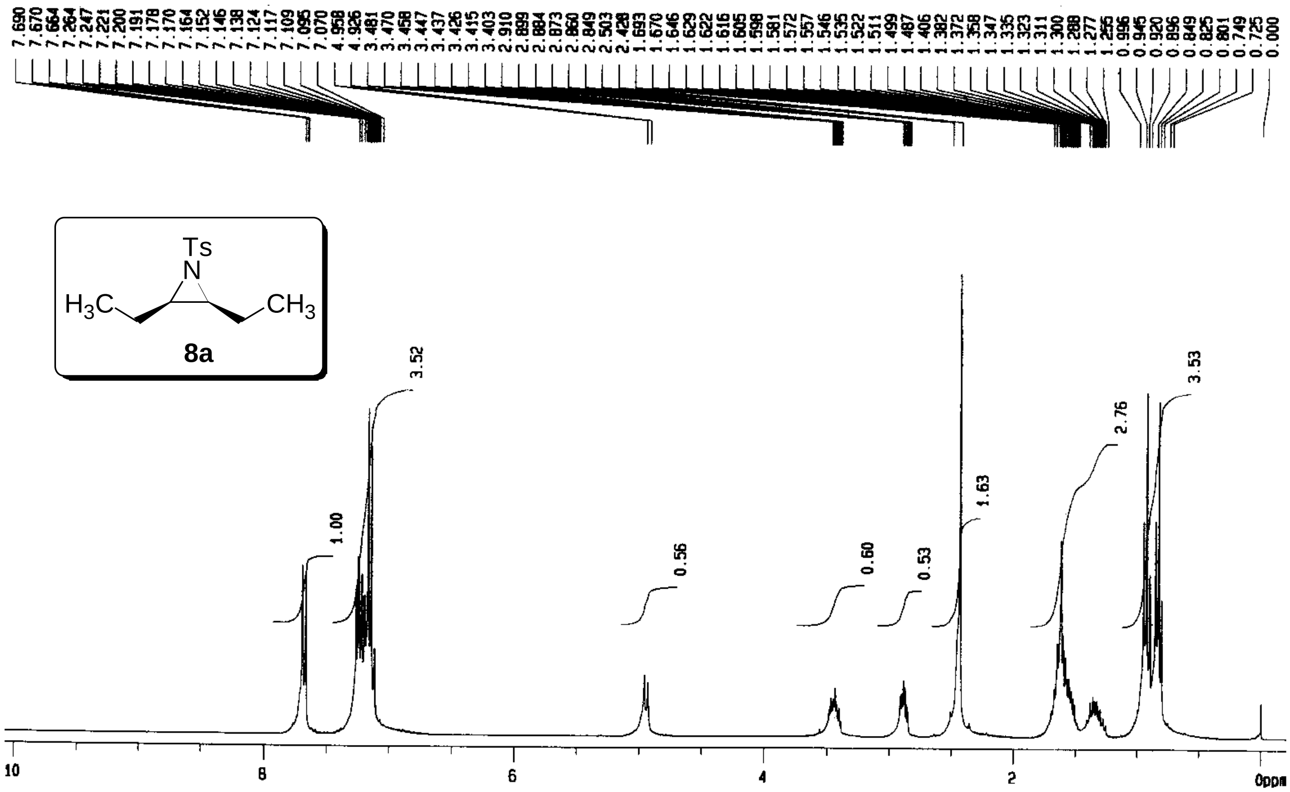
^{13}C NMR – $CDCl_3$ (75 MHz)



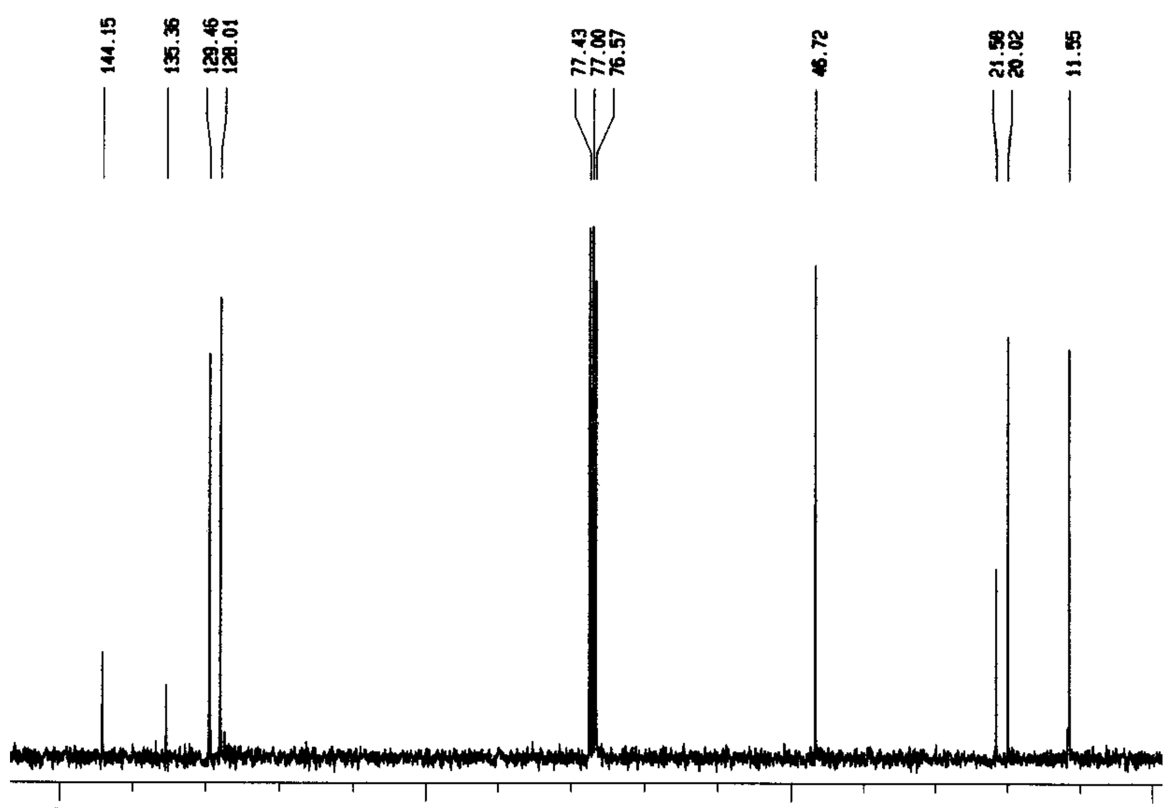
DEPT – $CDCl_3$ (75 MHz)



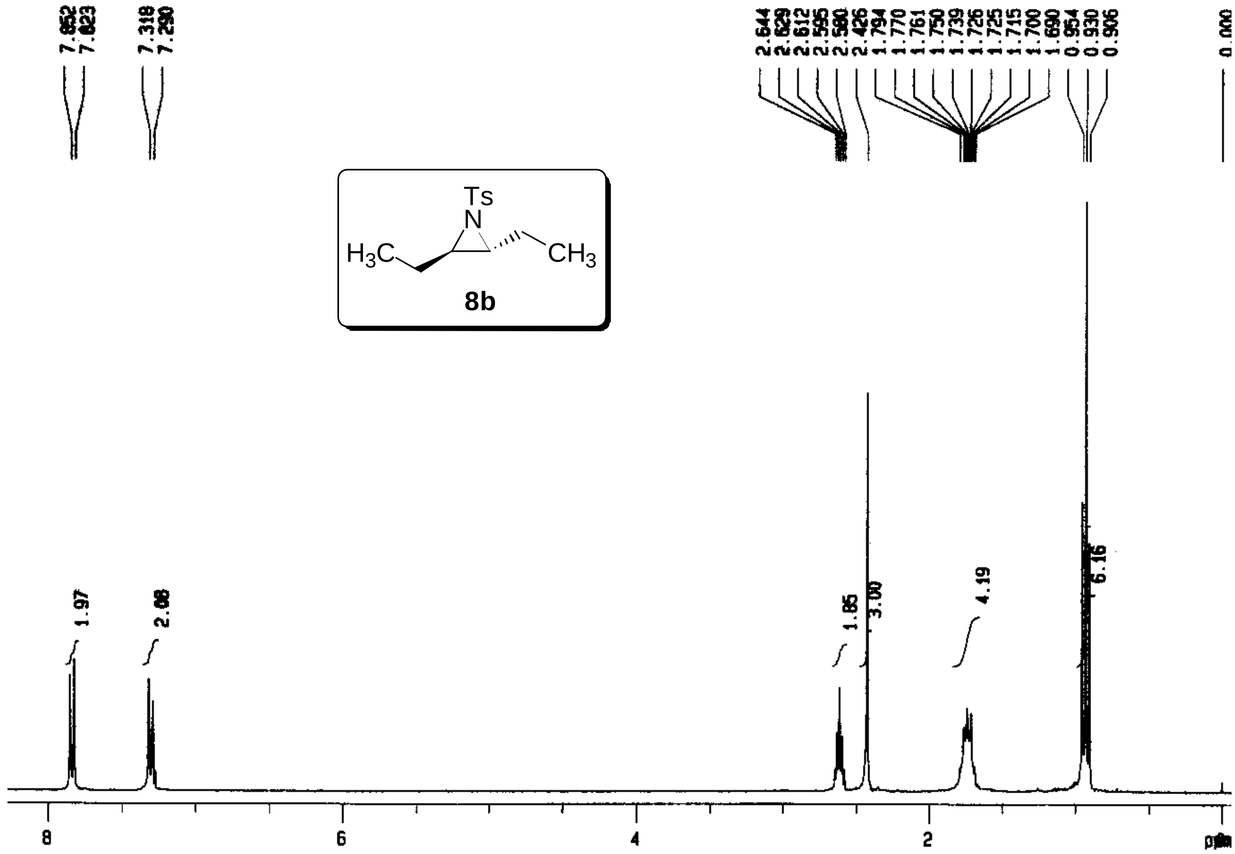
^{1}H NMR – $CDCl_3$ (300 MHz)



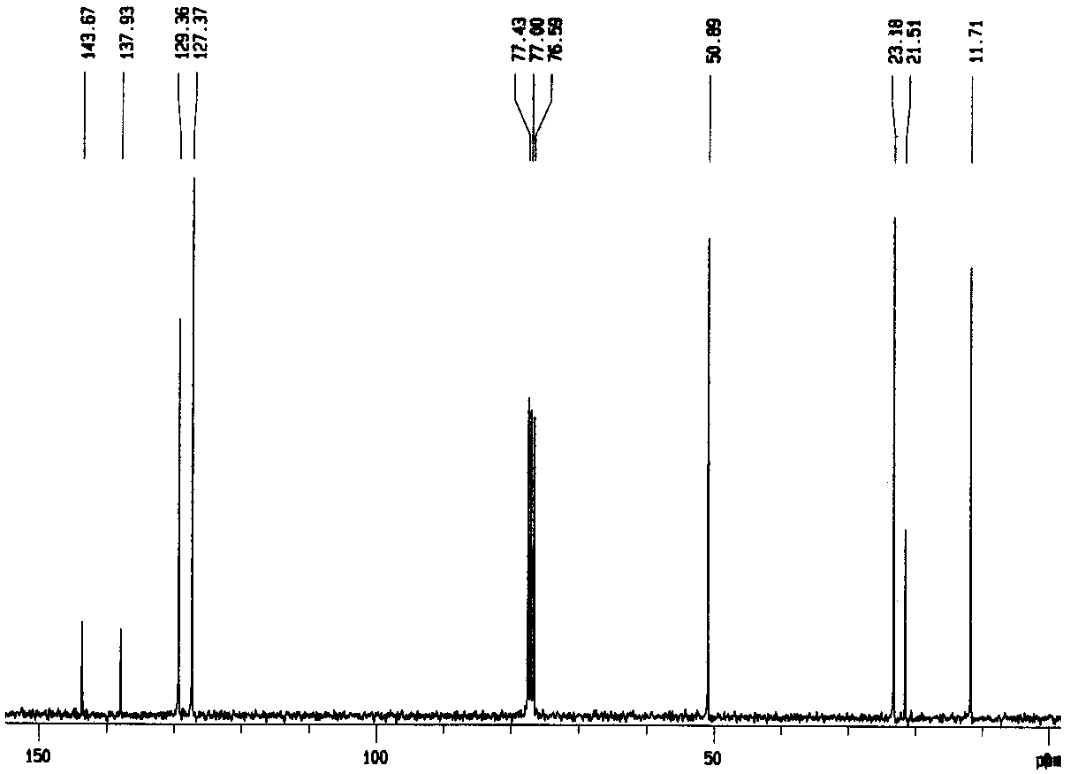
^{13}C NMR – $CDCl_3$ (75 MHz)



[1]H NMR – $CDCl_3$ (300 MHz)

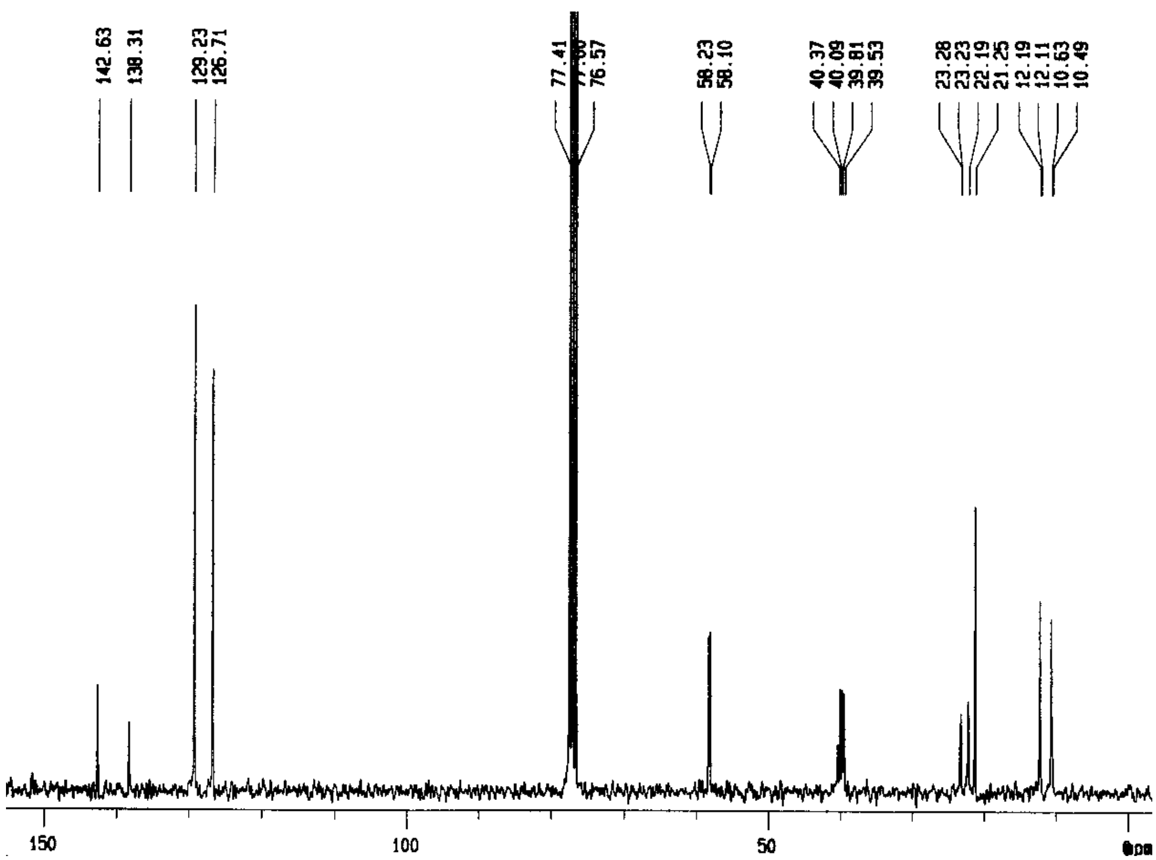


[13]C NMR – $CDCl_3$ (75 MHz)

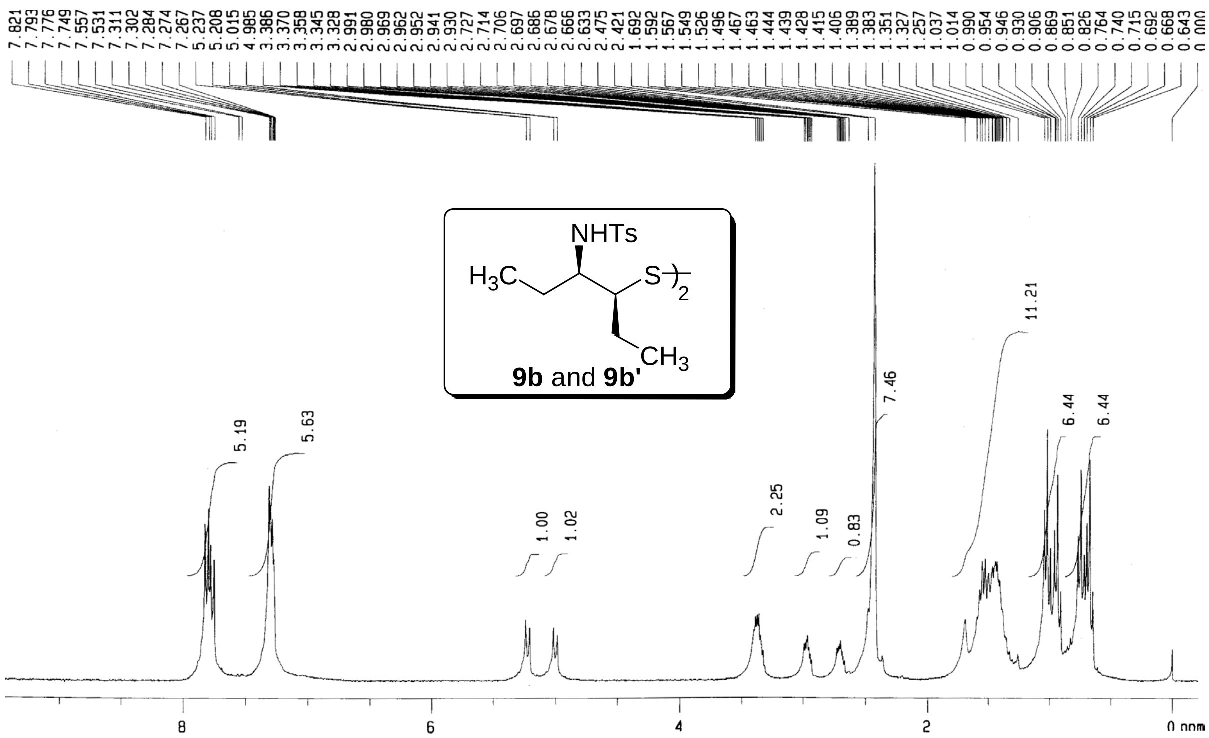


^{1}H NMR – $CDCl_3$ (300 MHz)

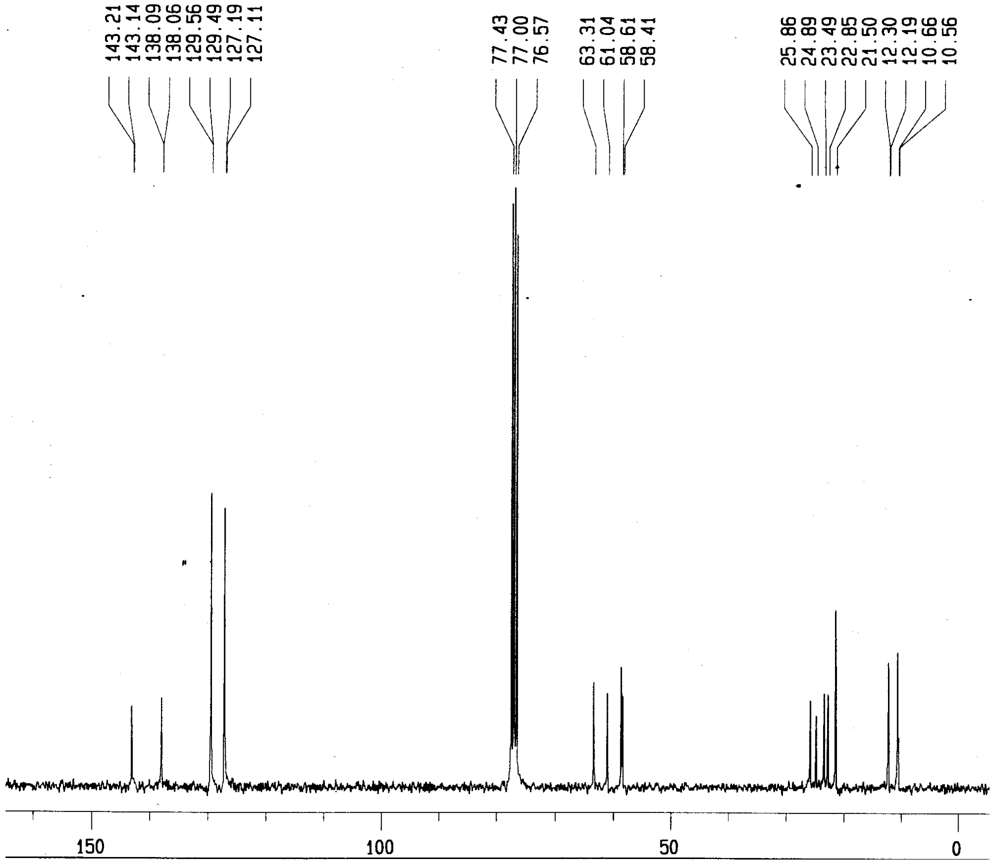
^{13}C NMR – $CDCl_3$ (75 MHz)



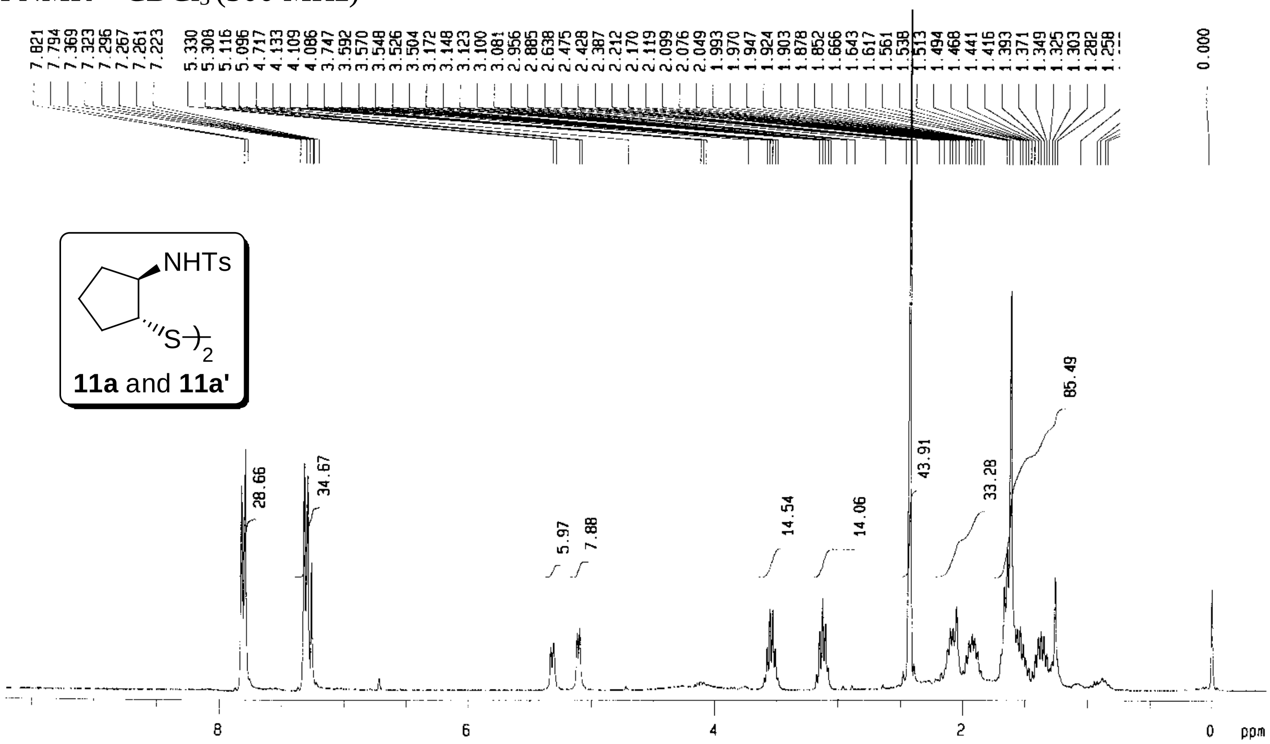
^1H NMR – $CDCl_3$ (300 MHz)



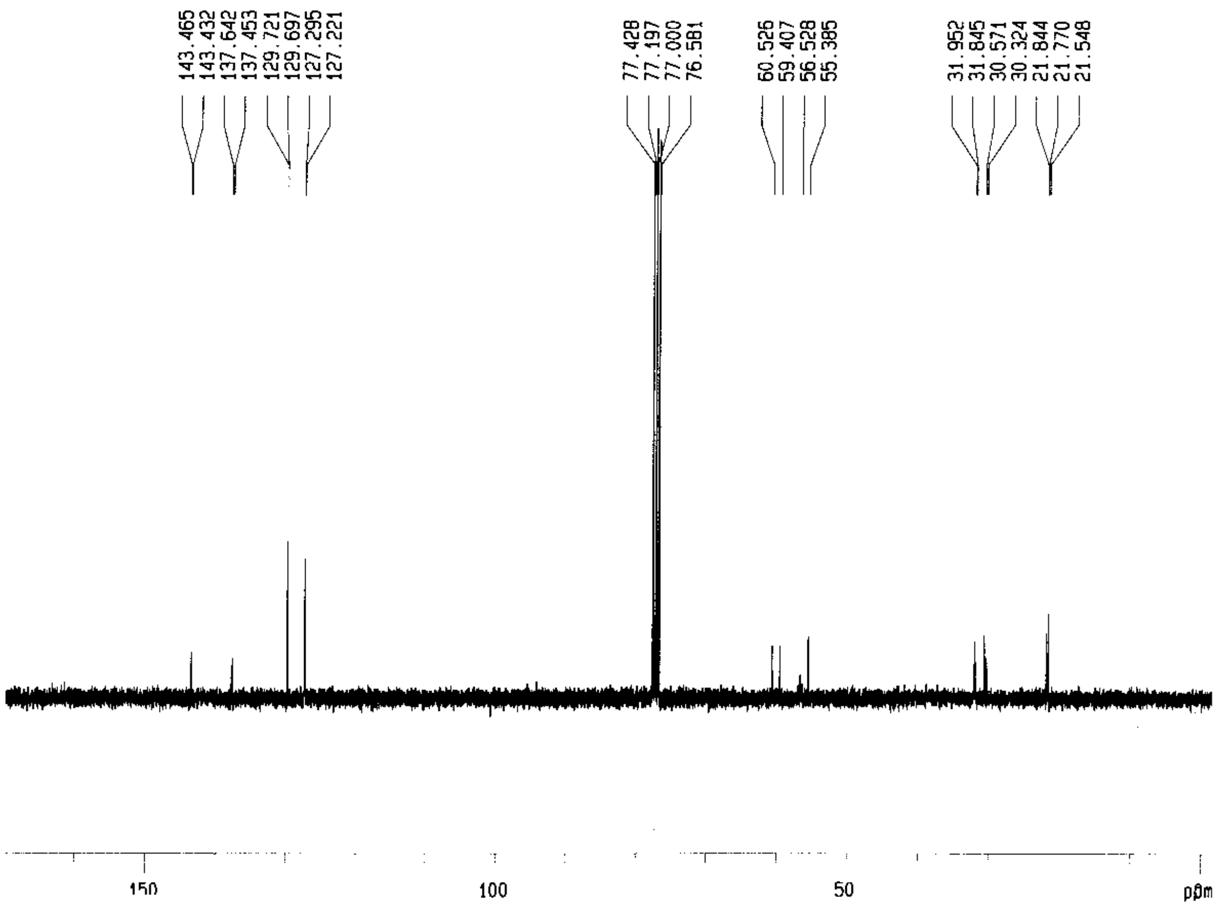
^{13}C NMR – $CDCl_3$ (75 MHz)



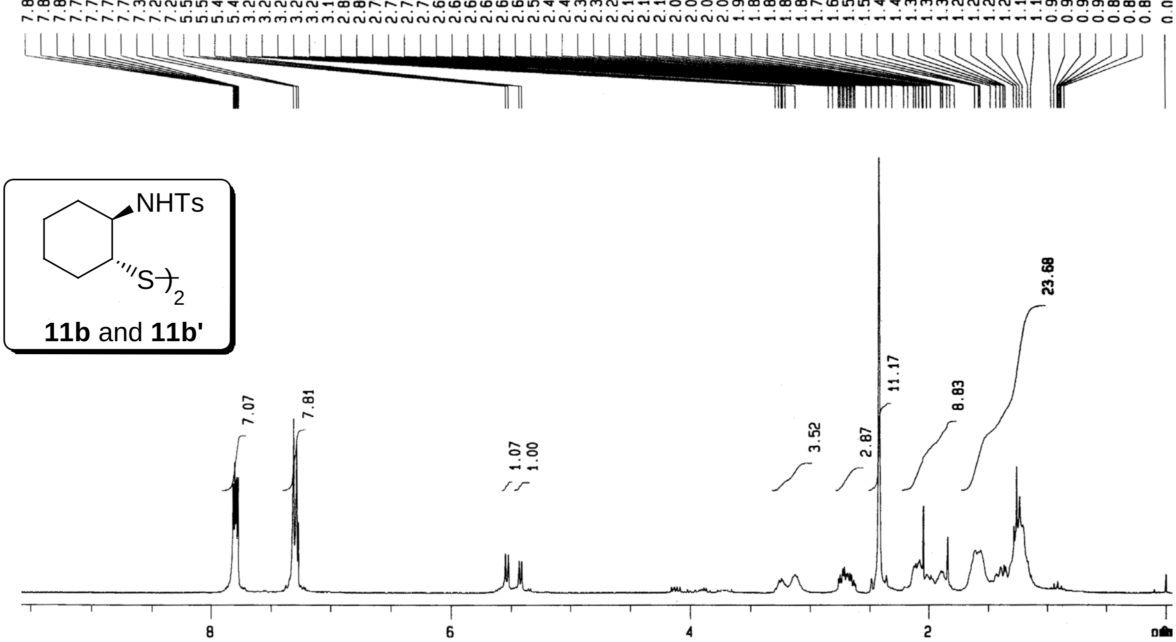
^{1}H NMR – $CDCl_3$ (300 MHz)



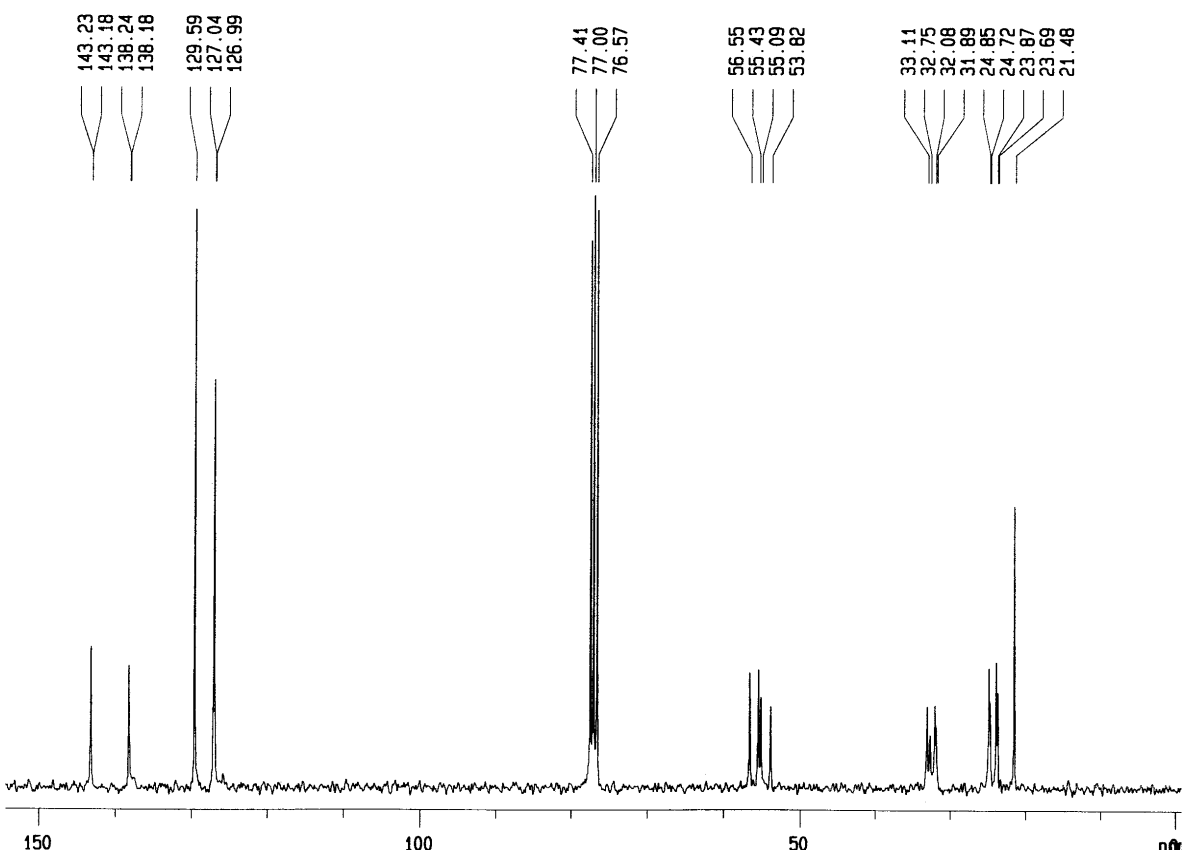
^{13}C NMR – $CDCl_3$ (75 MHz)



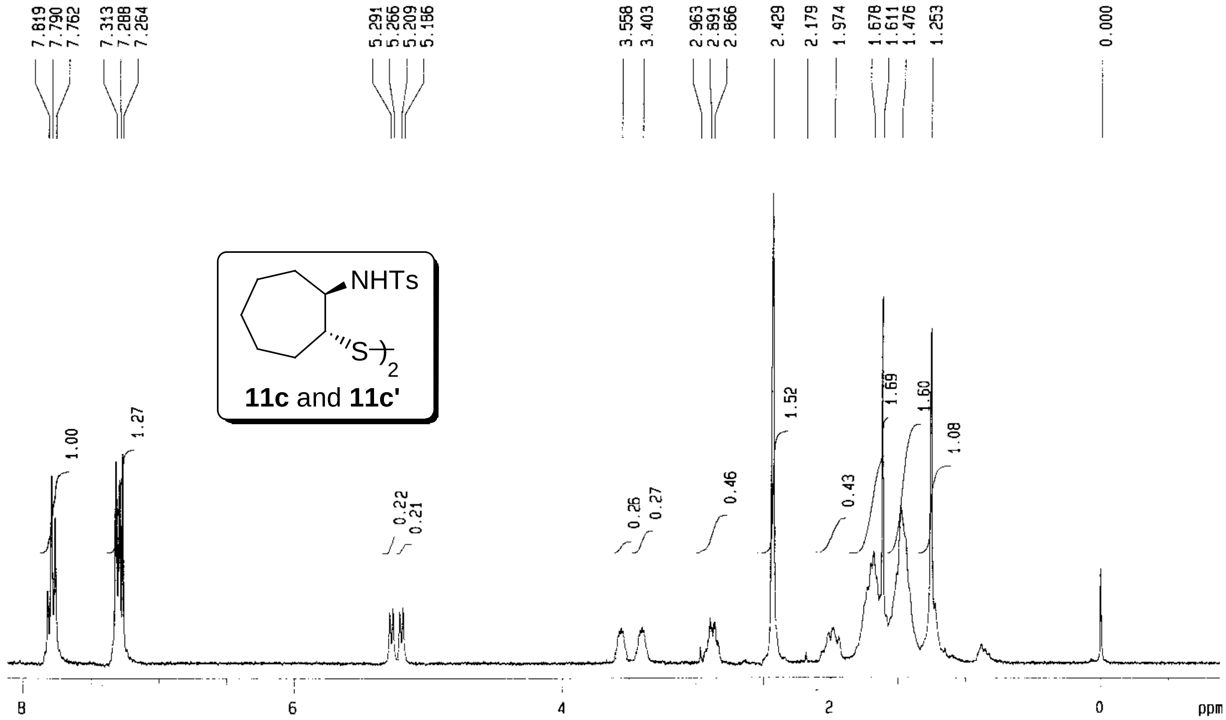
^{1}H NMR – $CDCl_3$ (300 MHz)



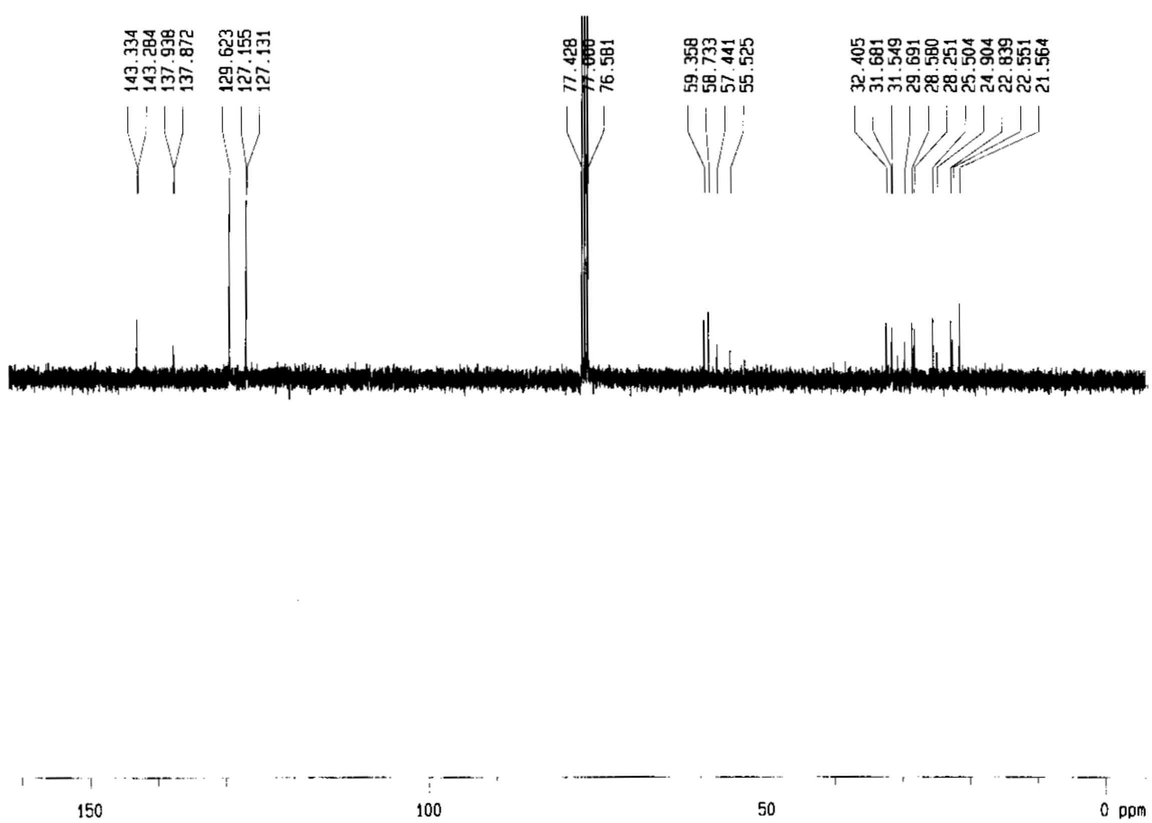
^{13}C NMR – $CDCl_3$ (75 MHz)



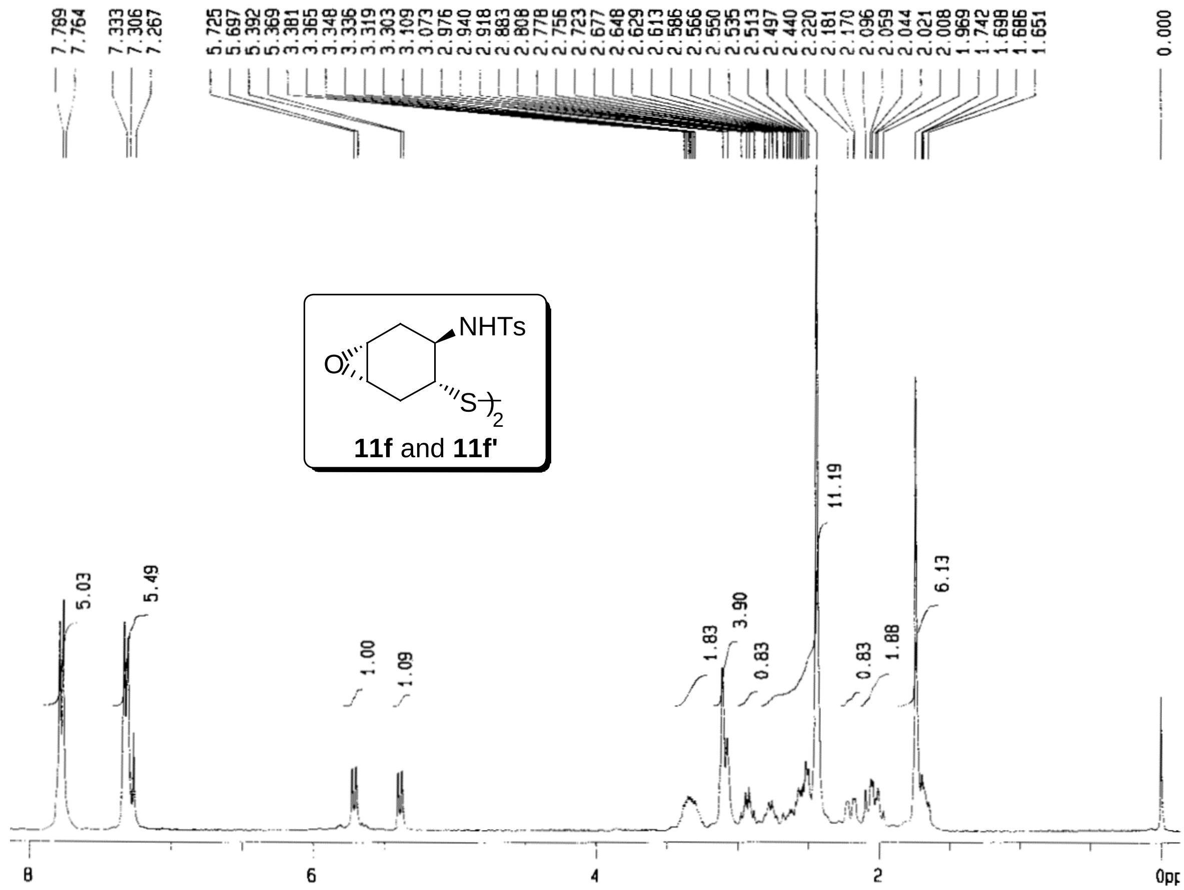
^{1}H NMR – $CDCl_3$ (300 MHz)



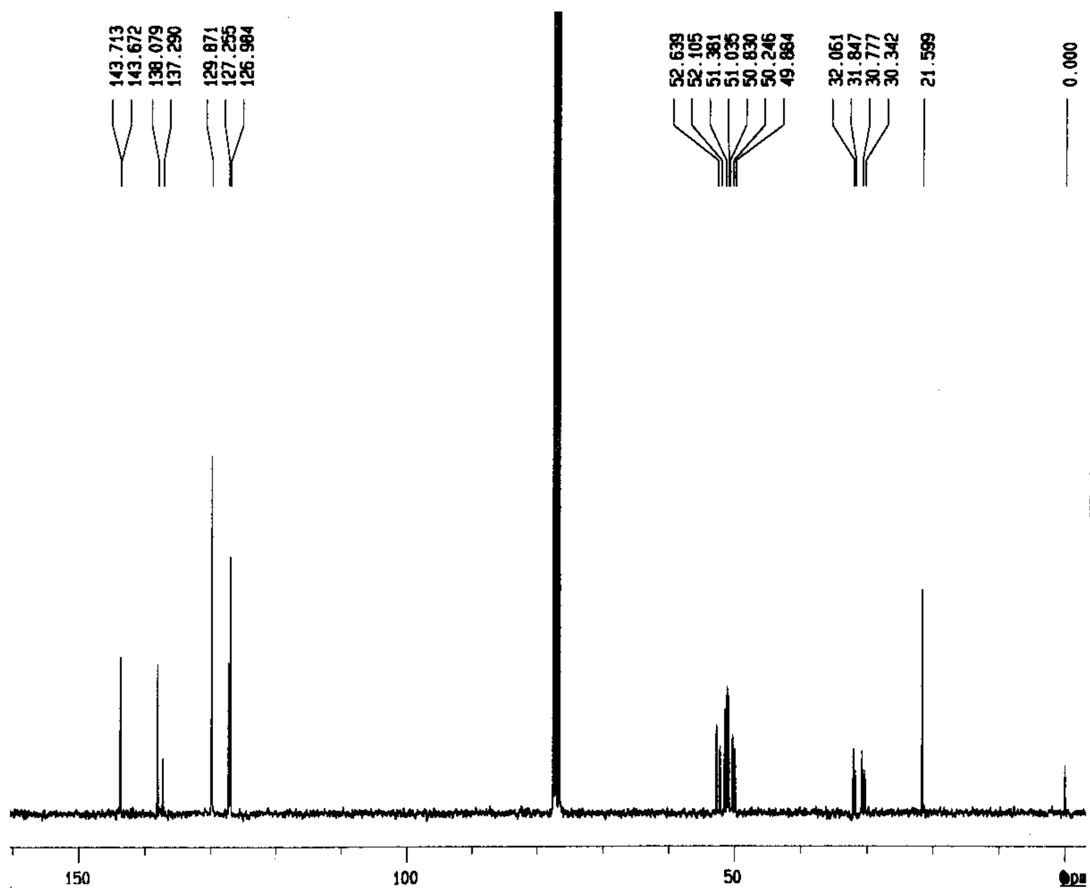
^{13}C NMR – $CDCl_3$ (75 MHz)



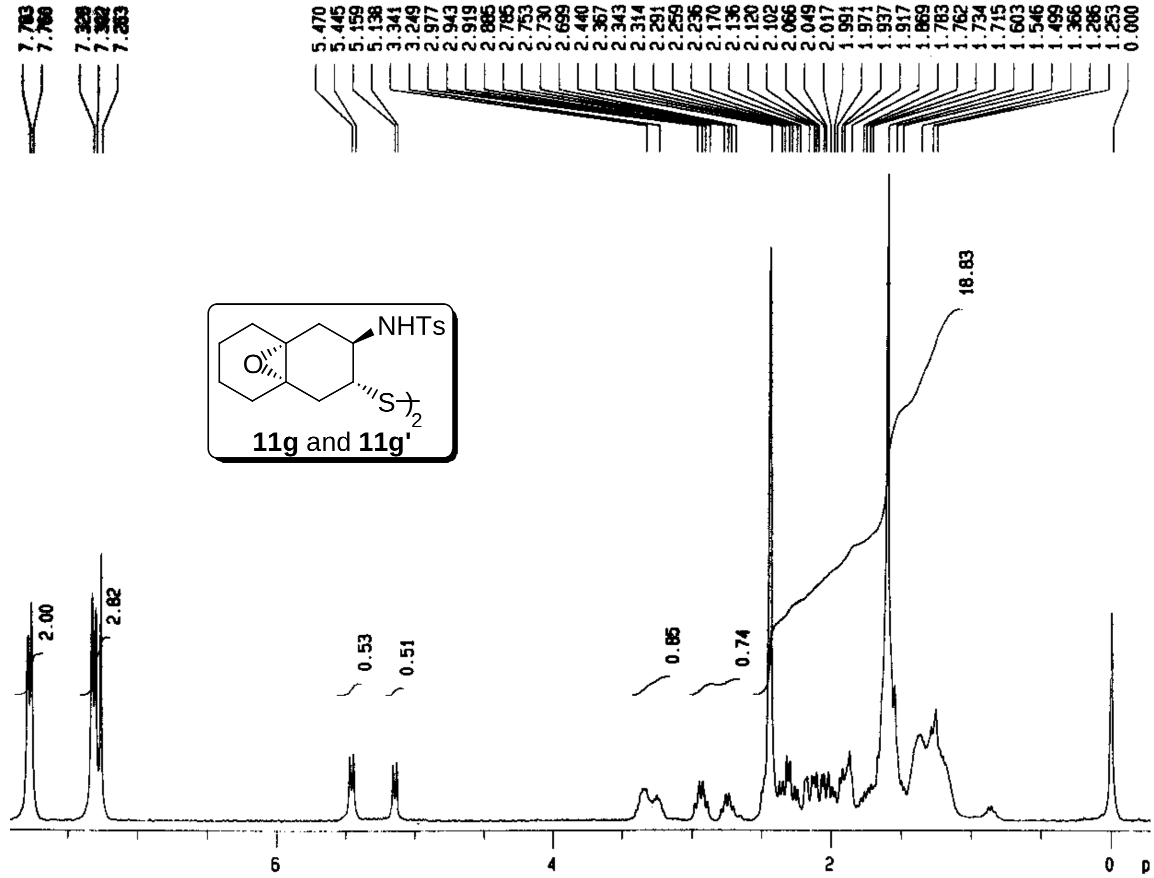
[1]H NMR – $CDCl_3$ (300 MHz)



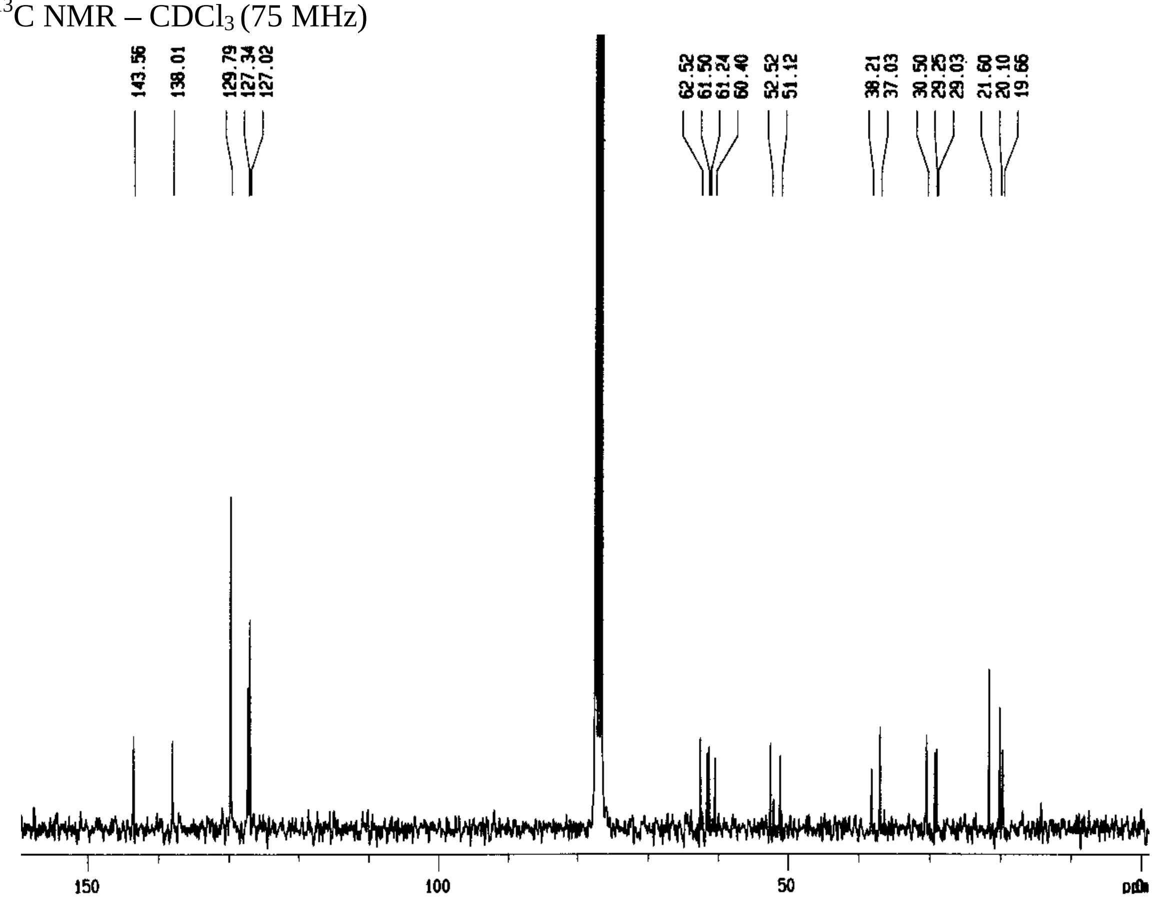
[13]C NMR – $CDCl_3$ (75 MHz)



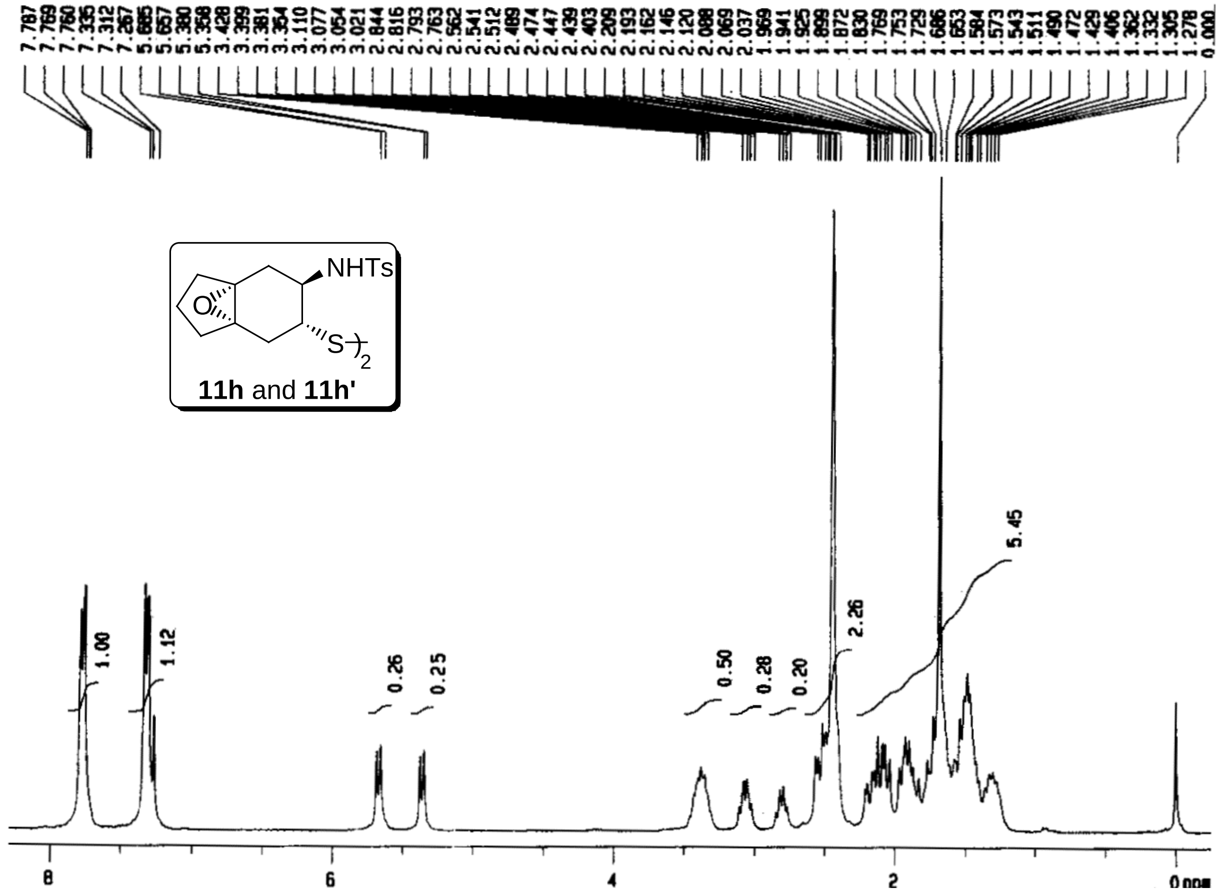
[1]H NMR – $CDCl_3$ (300 MHz)



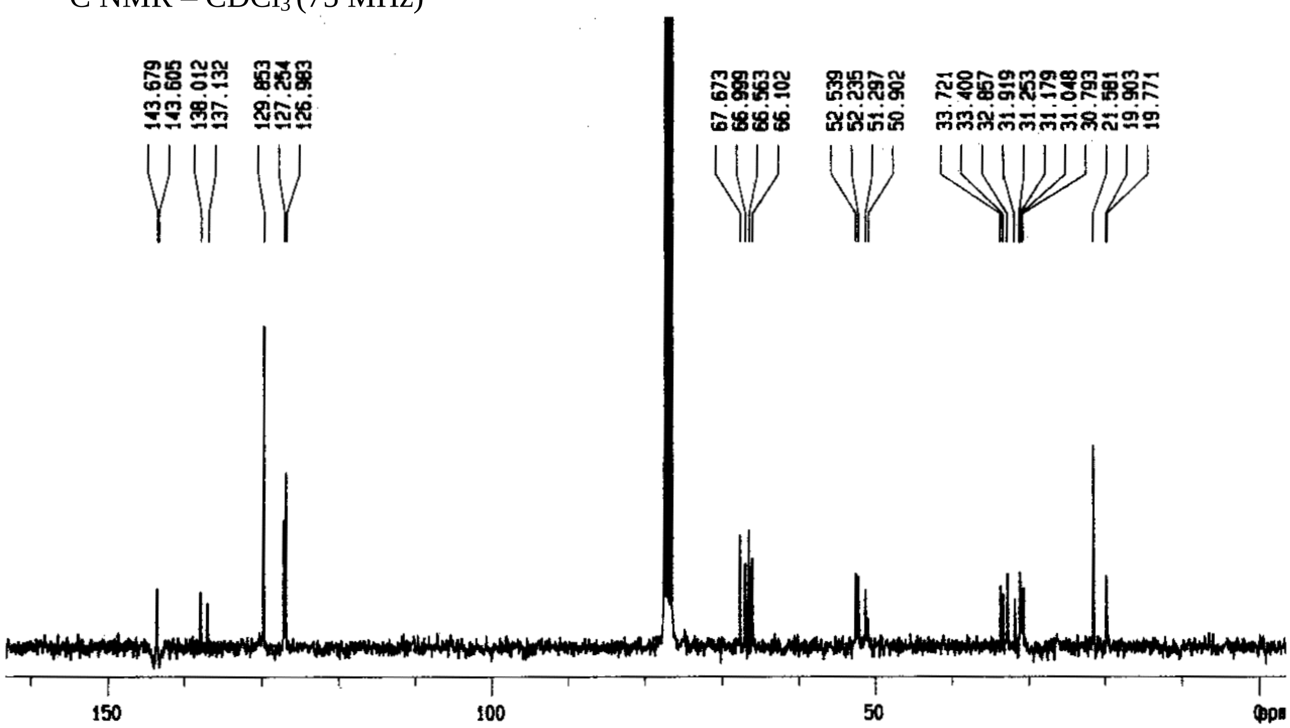
[13]C NMR – $CDCl_3$ (75 MHz)

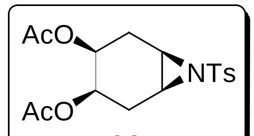


^{1}H NMR – $CDCl_3$ (300 MHz)



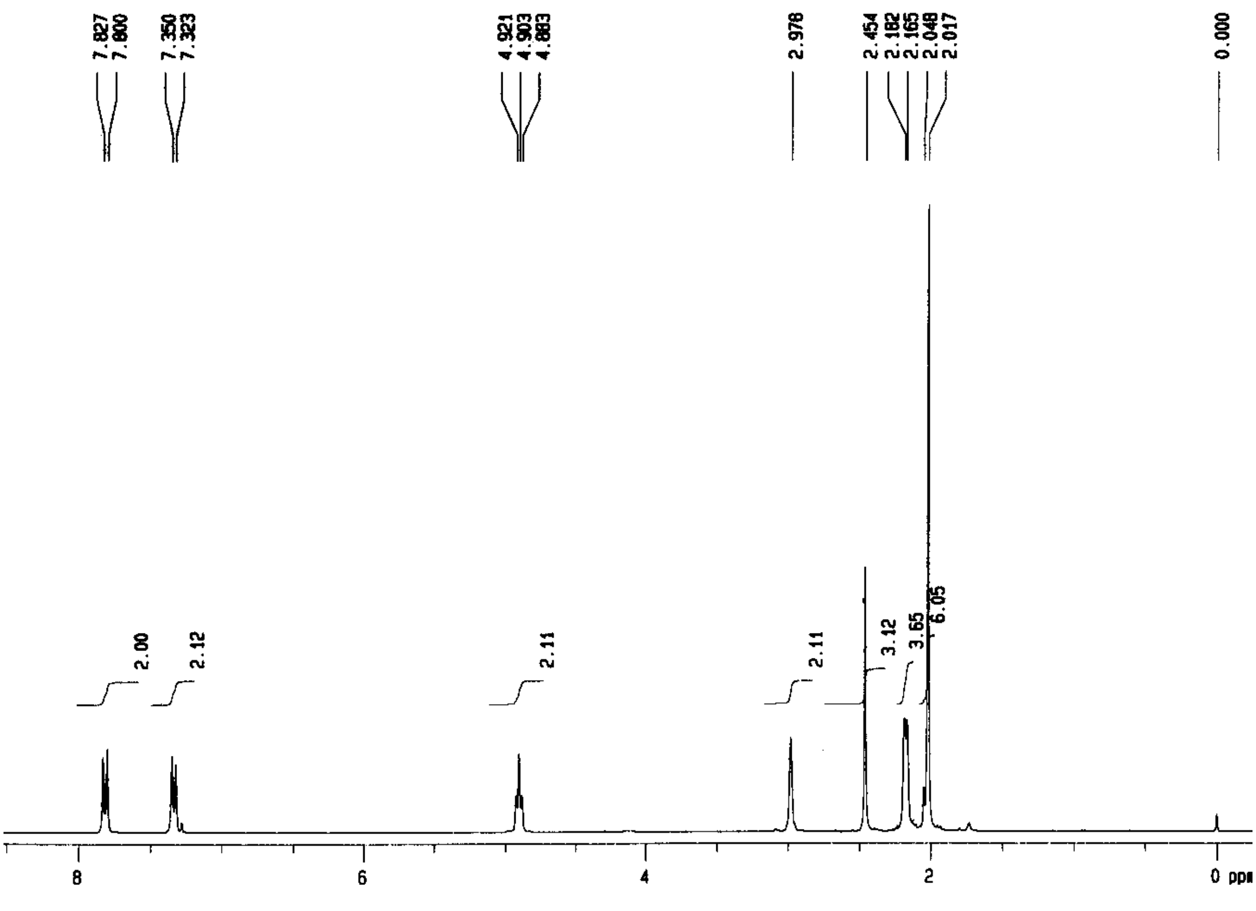
^{13}C NMR – $CDCl_3$ (75 MHz)



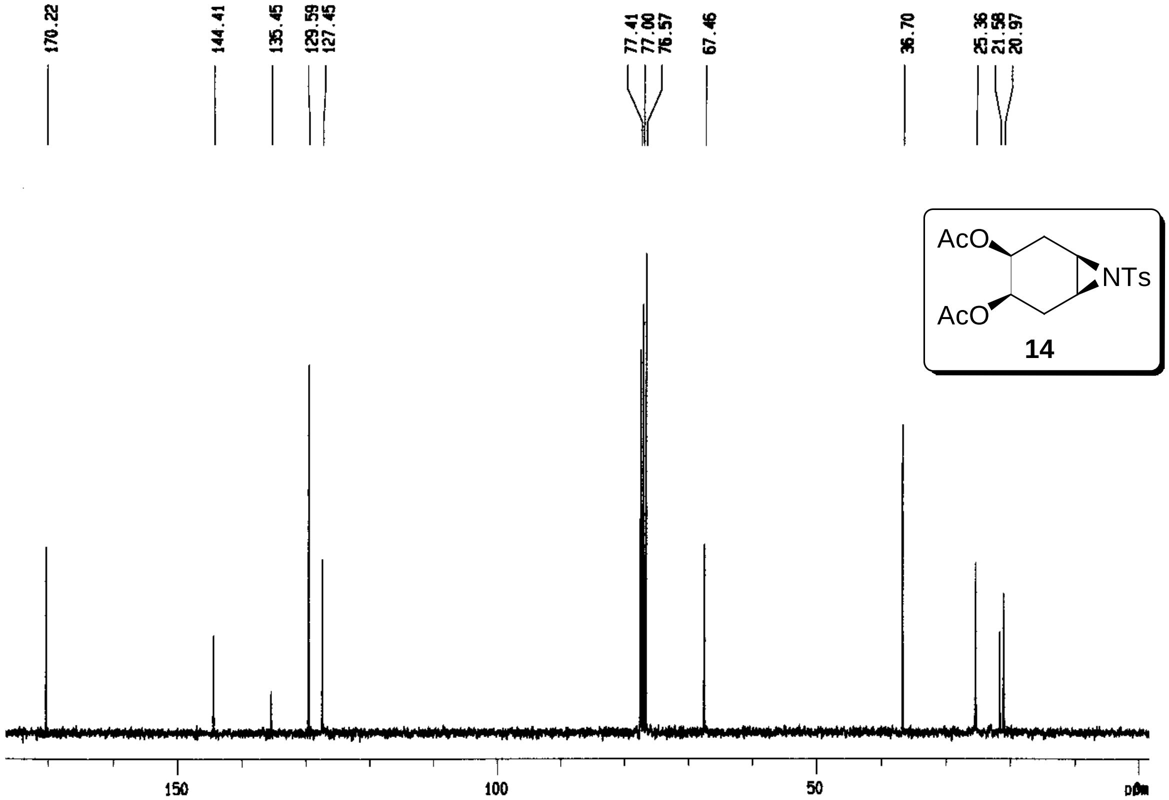


14

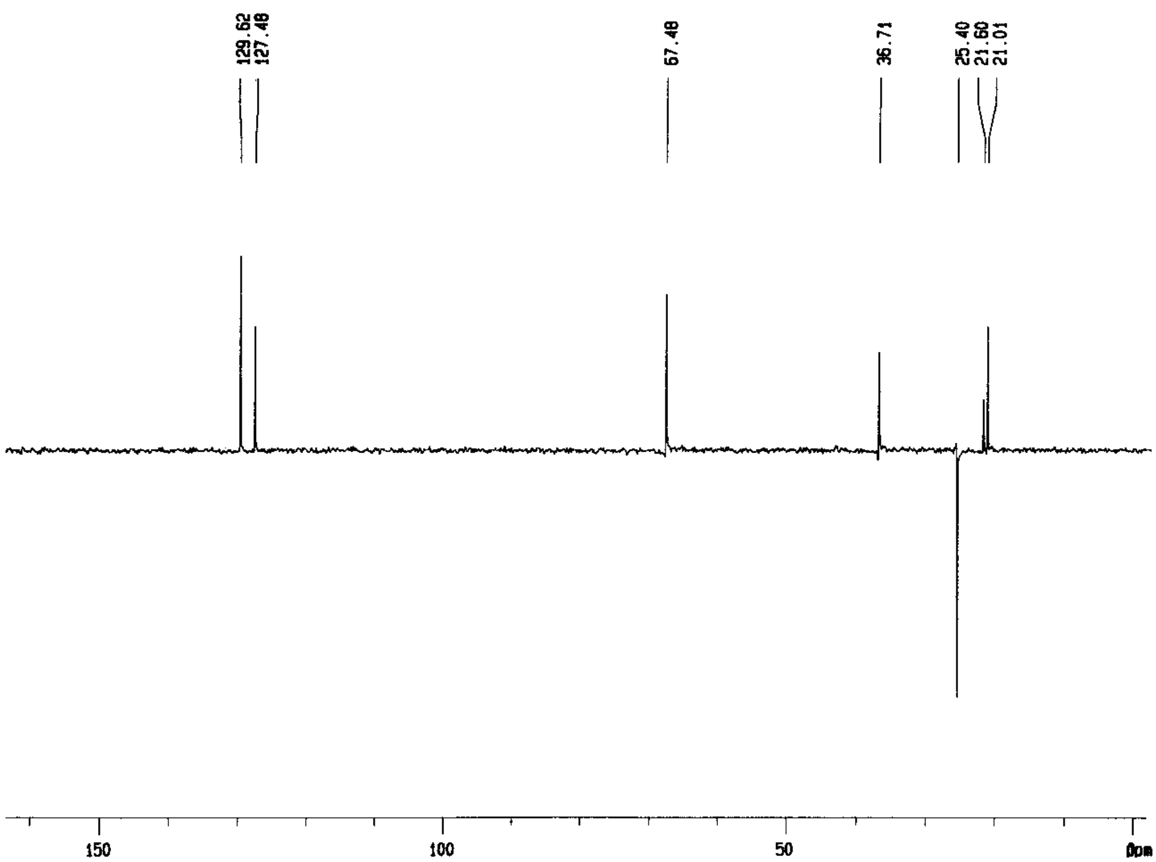
^1H NMR – $CDCl_3$ (300 MHz)



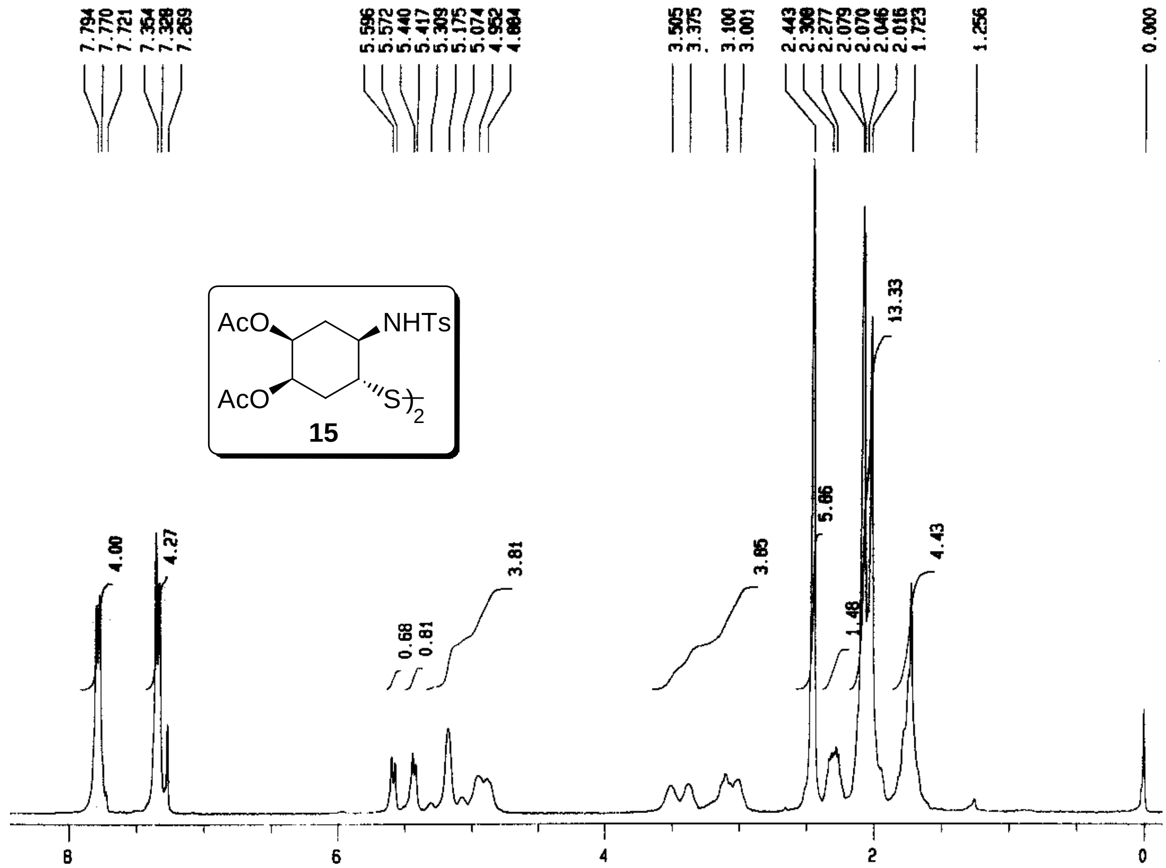
^{13}C NMR – $CDCl_3$ (75 MHz)



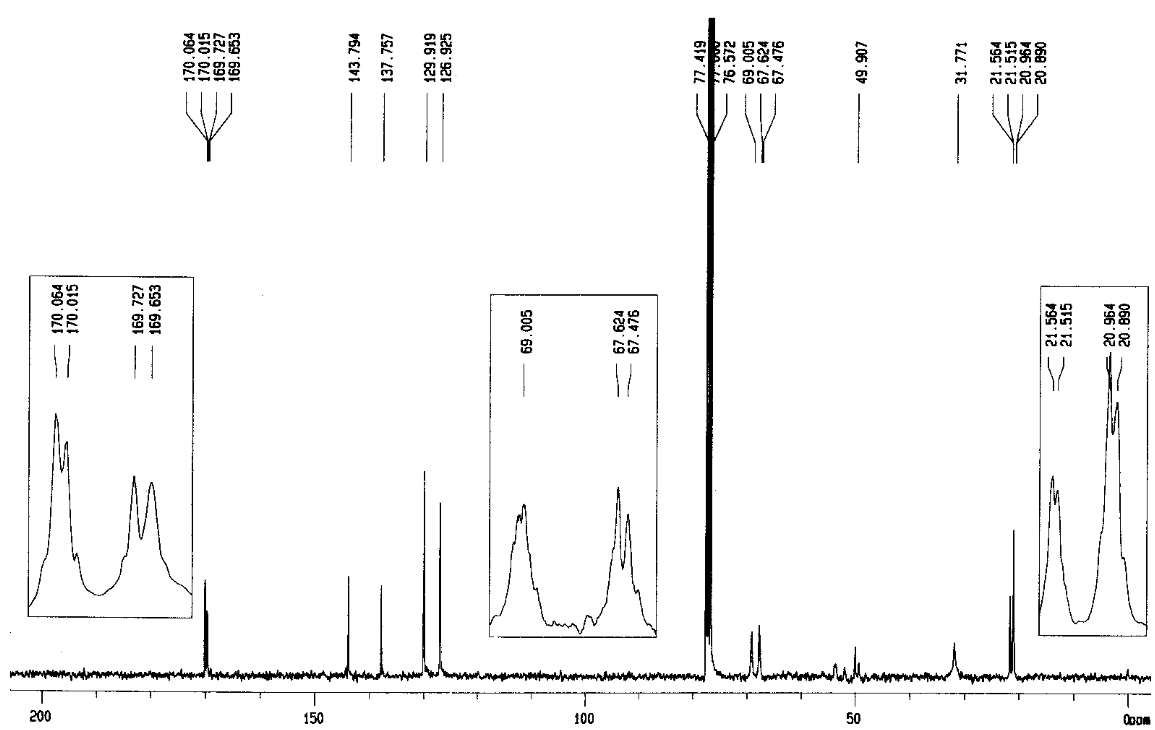
DEPT – $CDCl_3$ (75 MHz)

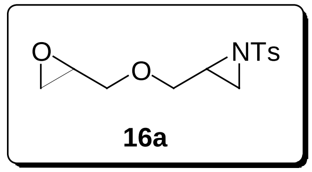


^{1}H NMR – $CDCl_3$ (300 MHz)

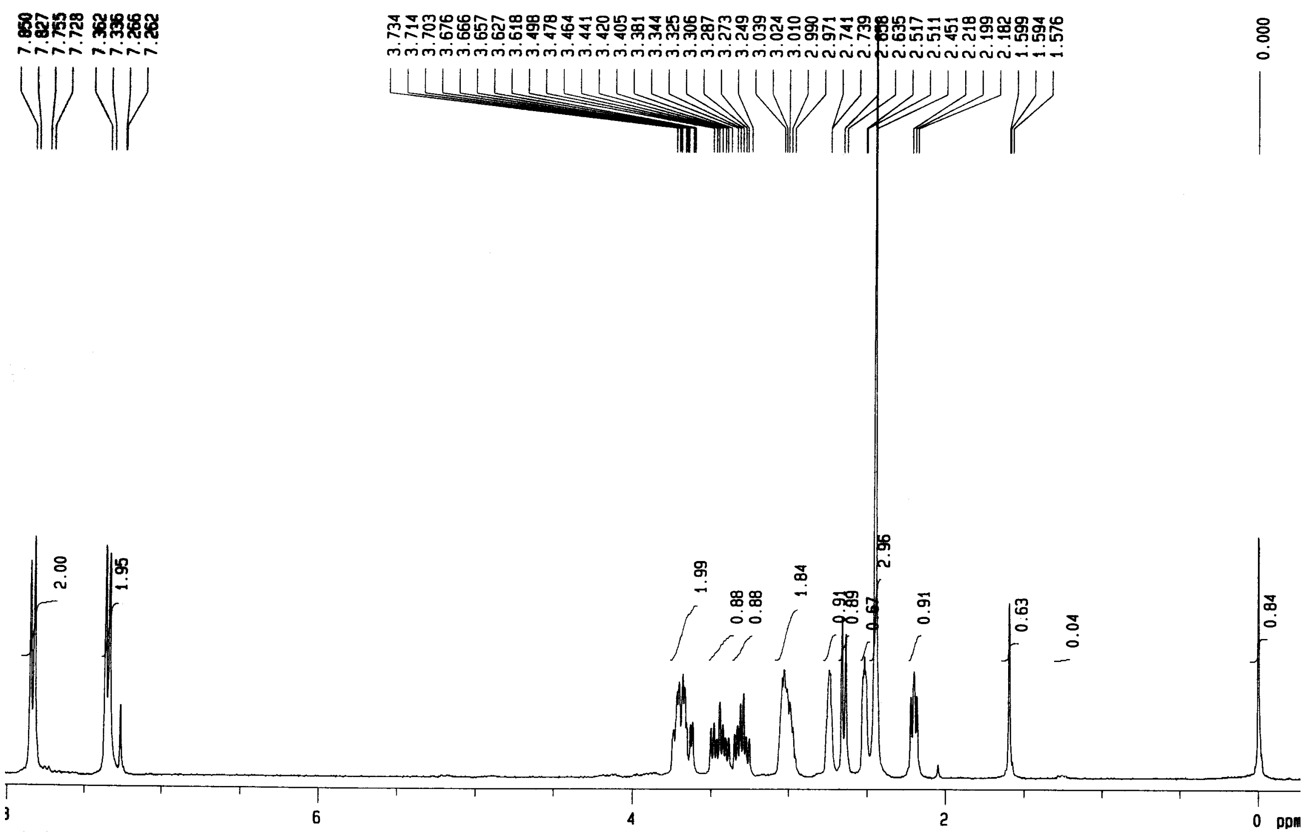


^{13}C NMR – $CDCl_3$ (75 MHz)

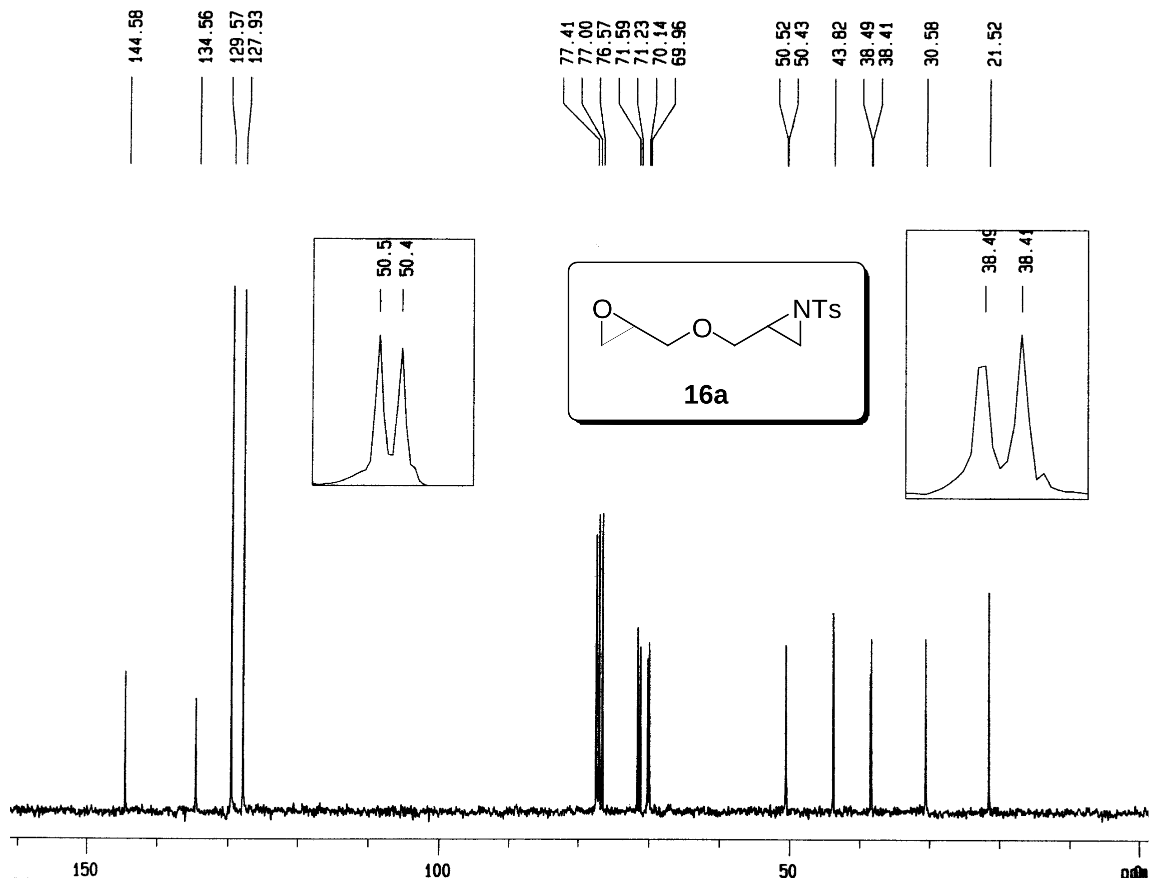




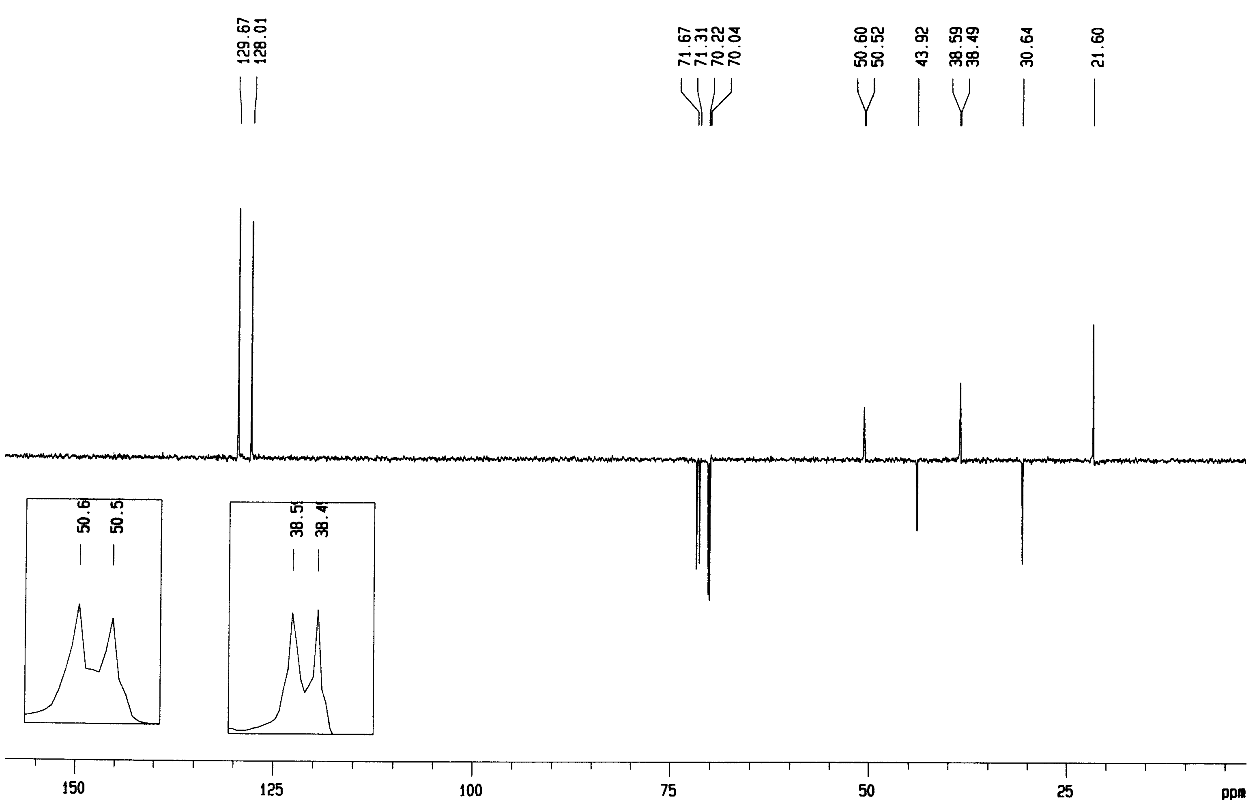
^1H NMR – $CDCl_3$ (300 MHz)



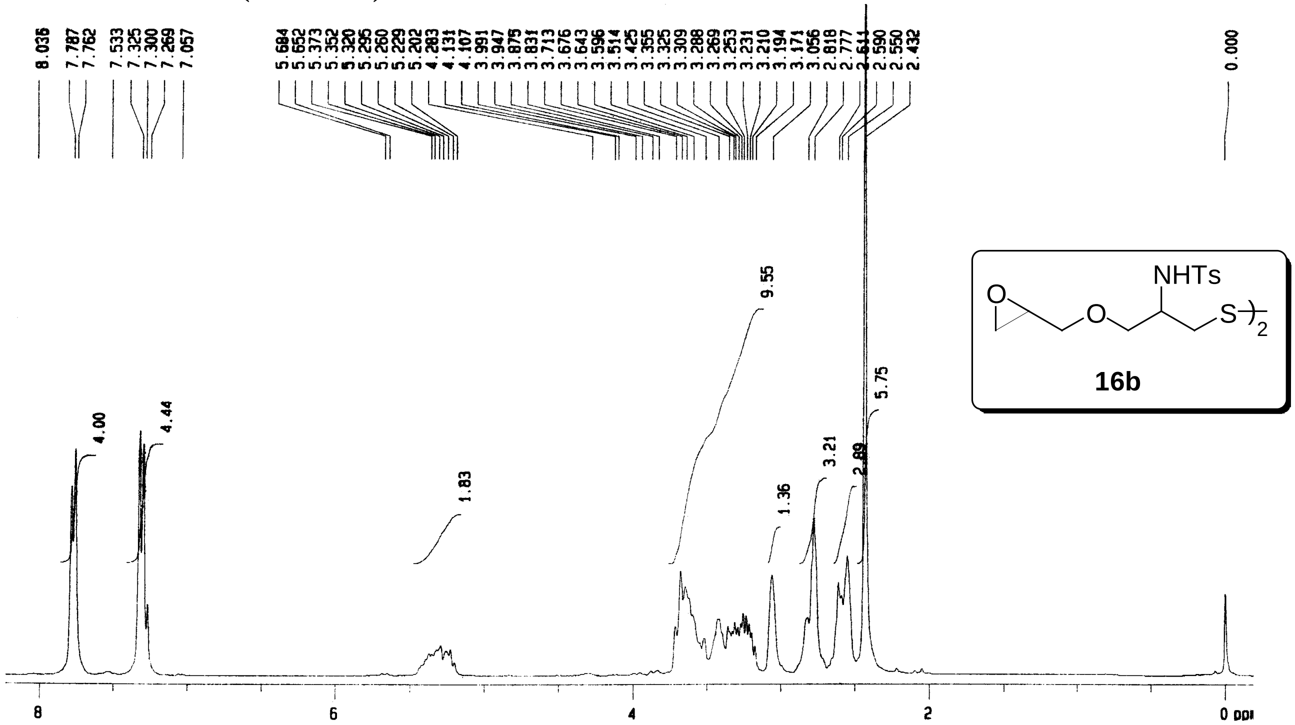
^{13}C NMR – $CDCl_3$ (75 MHz)



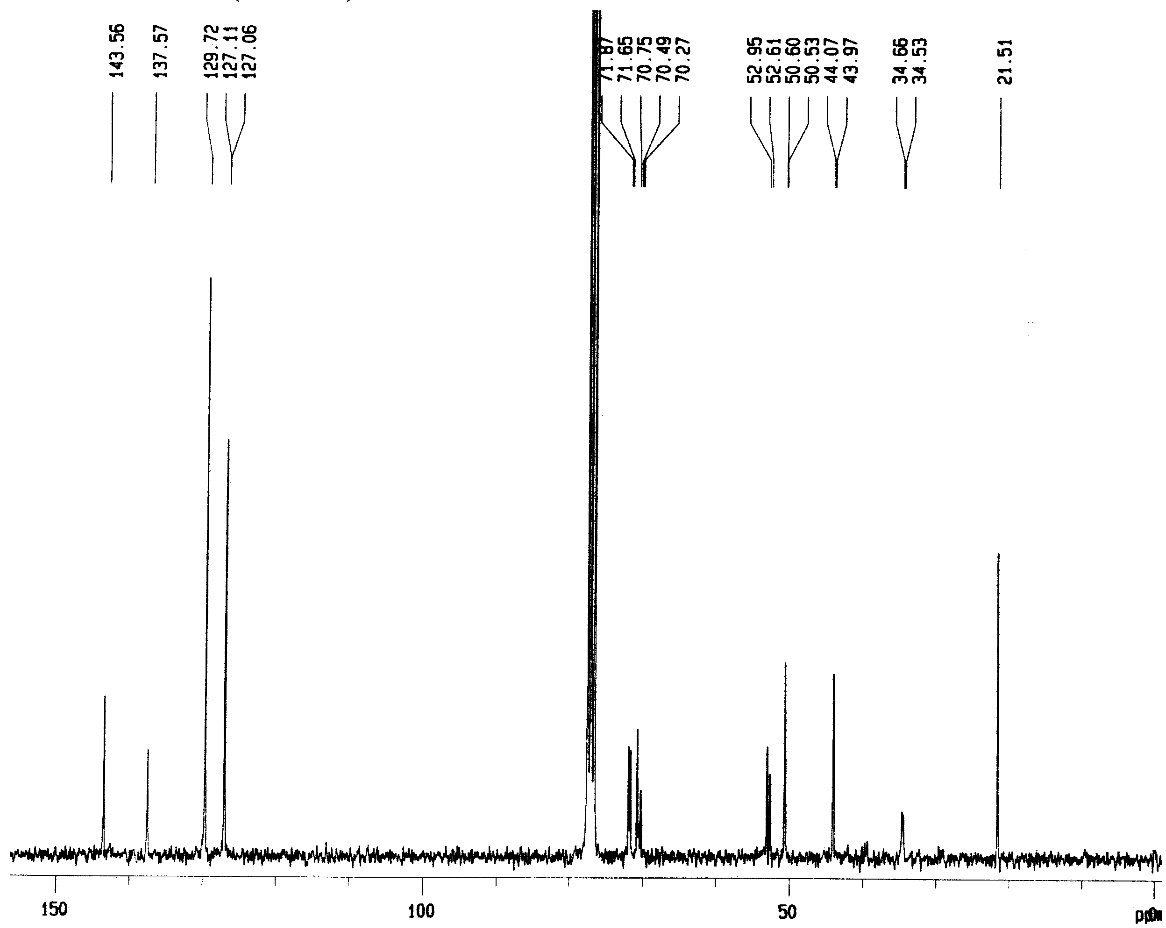
DEPT – $CDCl_3$ (75 MHz)



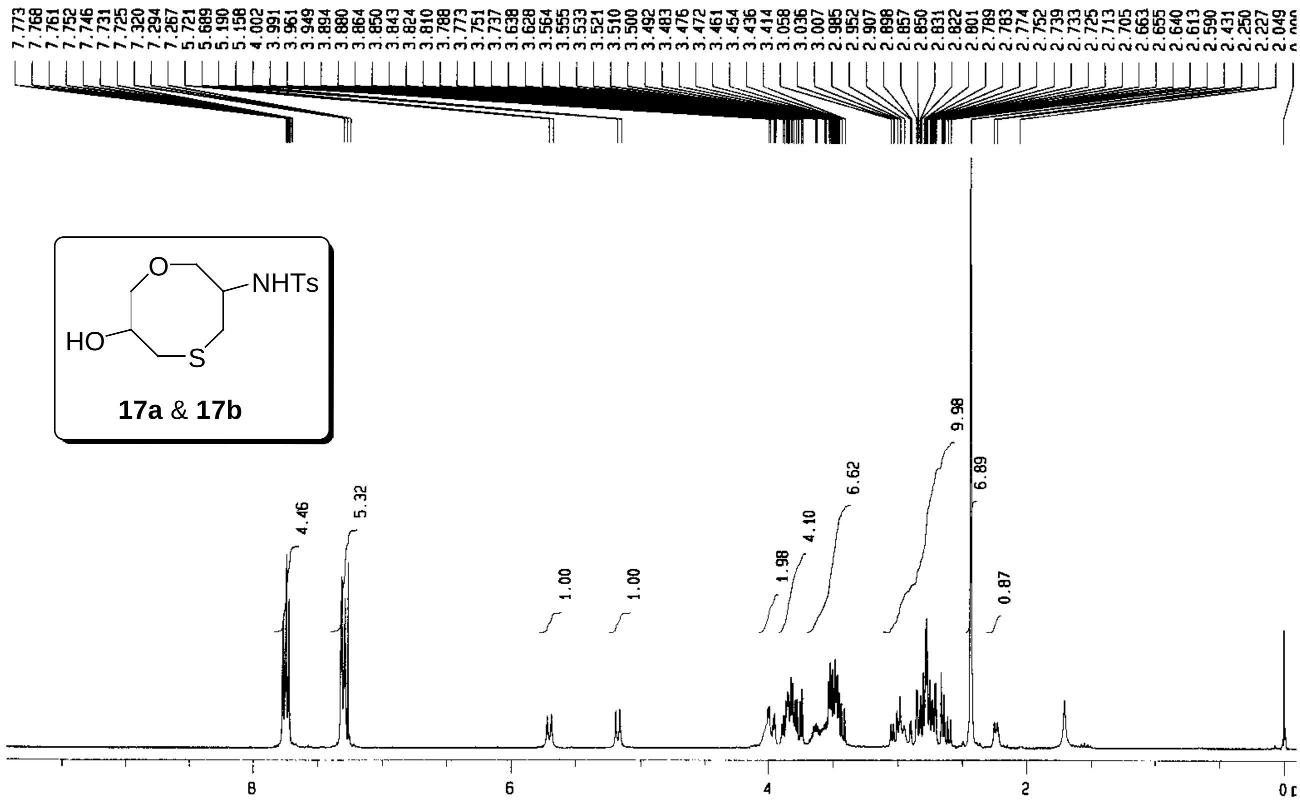
[1]H NMR – $CDCl_3$ (300 MHz)



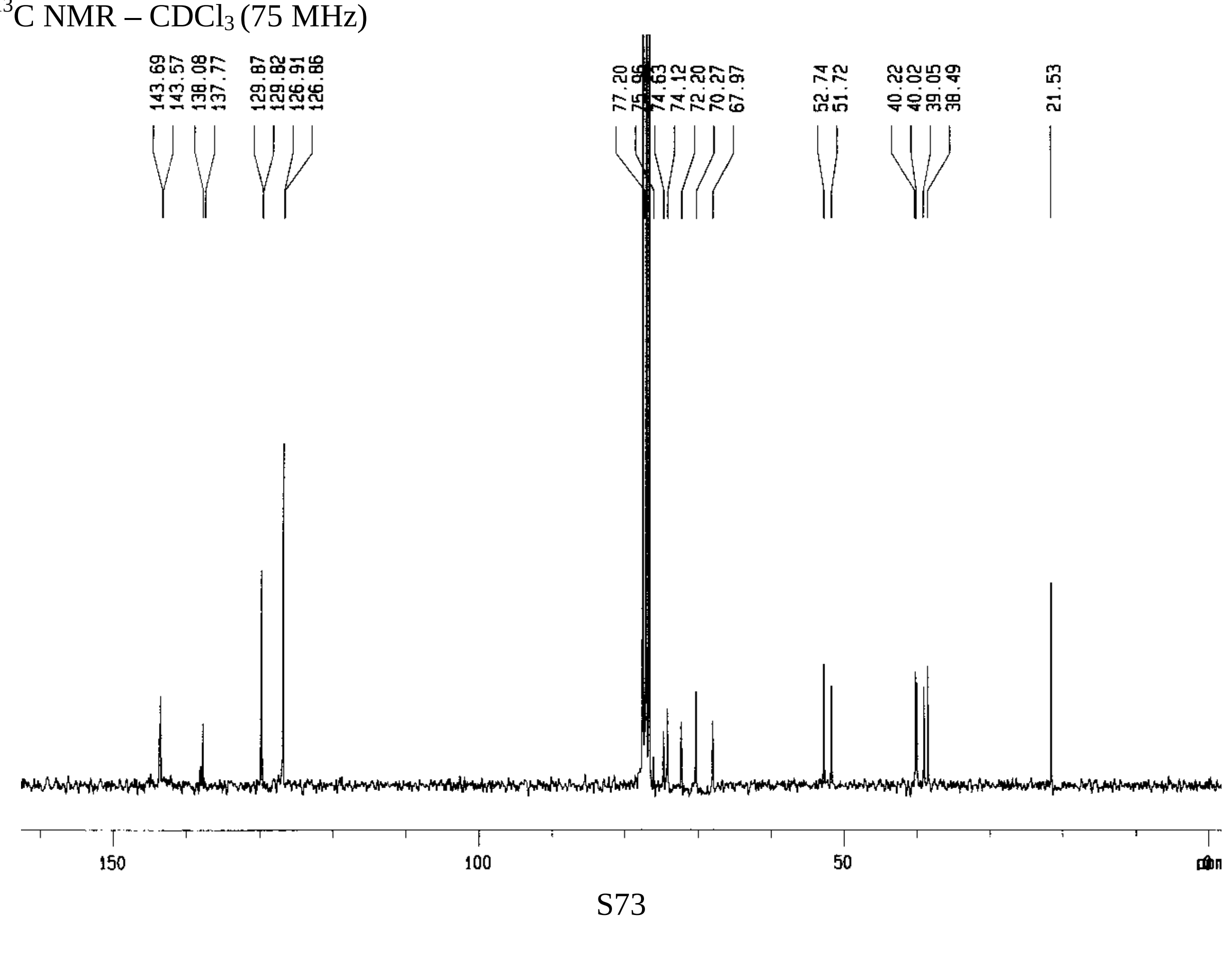
[13]C NMR – $CDCl_3$ (75 MHz)



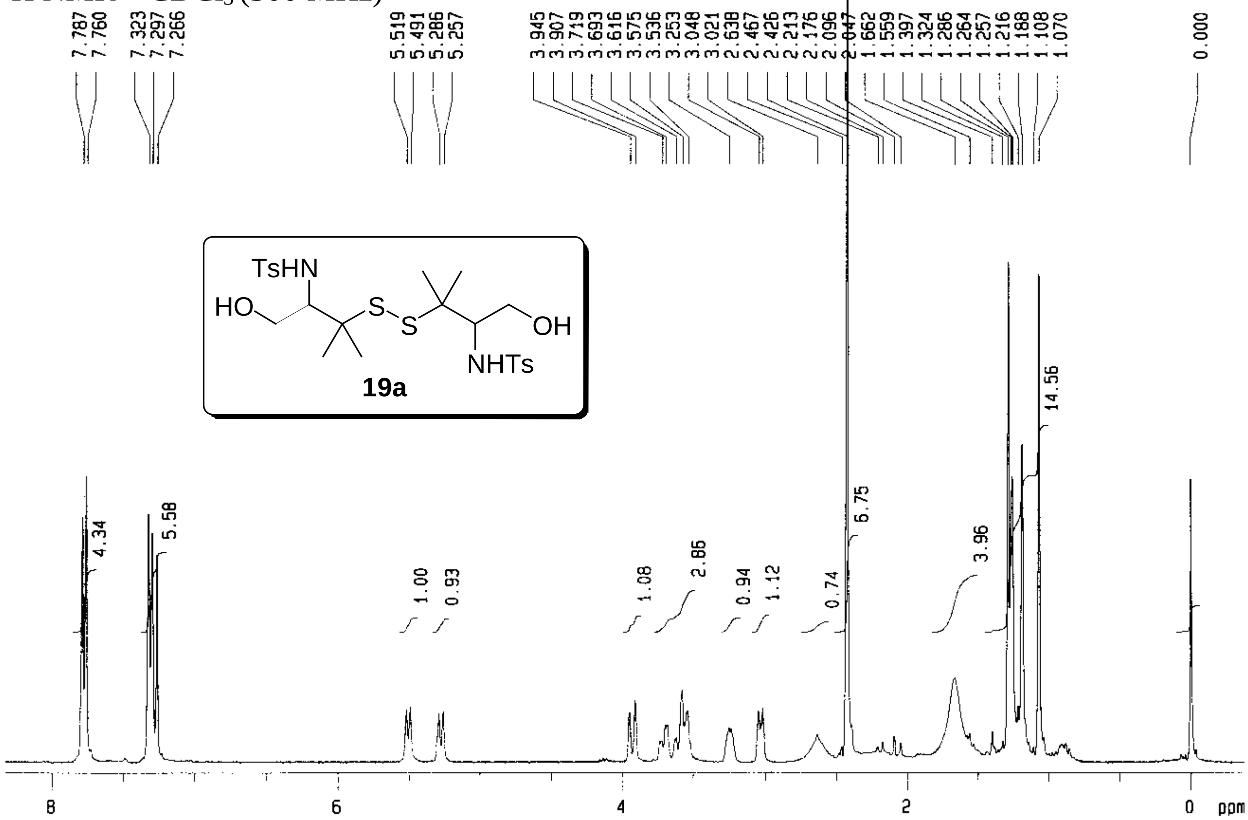
[1]H NMR – $CDCl_3$ (300 MHz)



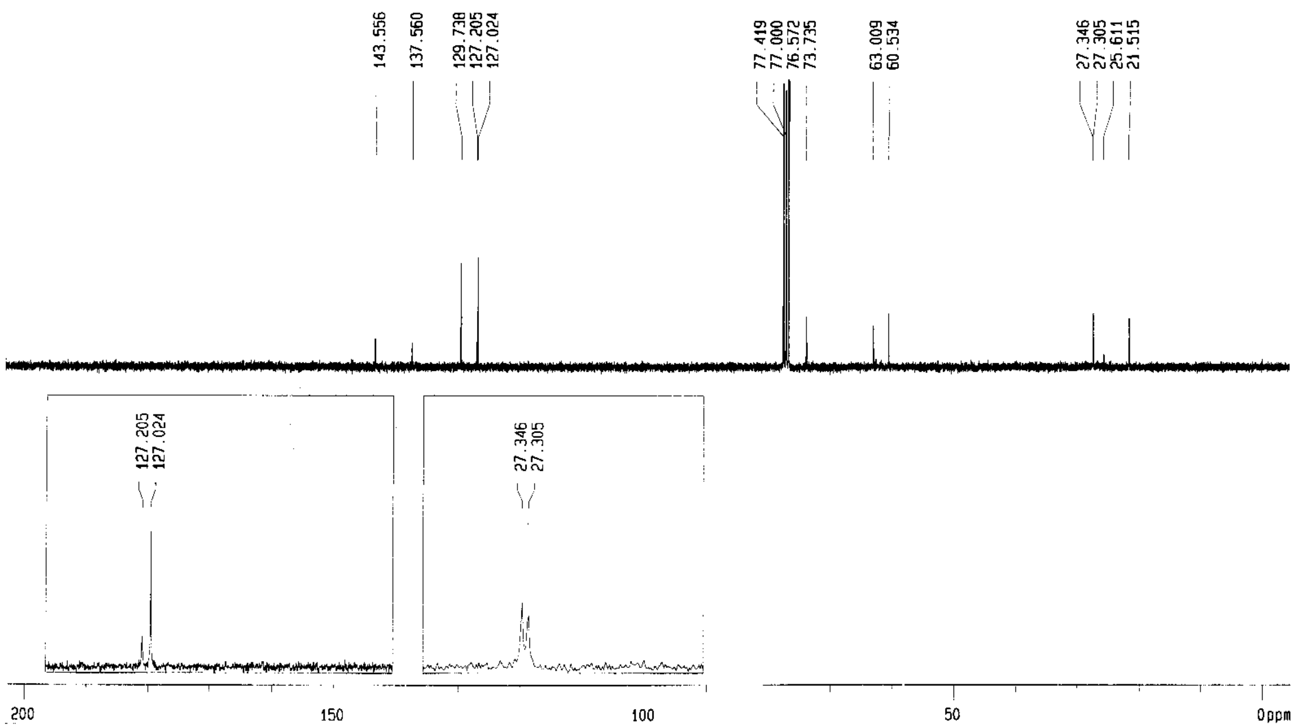
[13]C NMR – $CDCl_3$ (75 MHz)

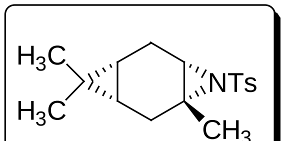


^{1}H NMR – $CDCl_3$ (300 MHz)



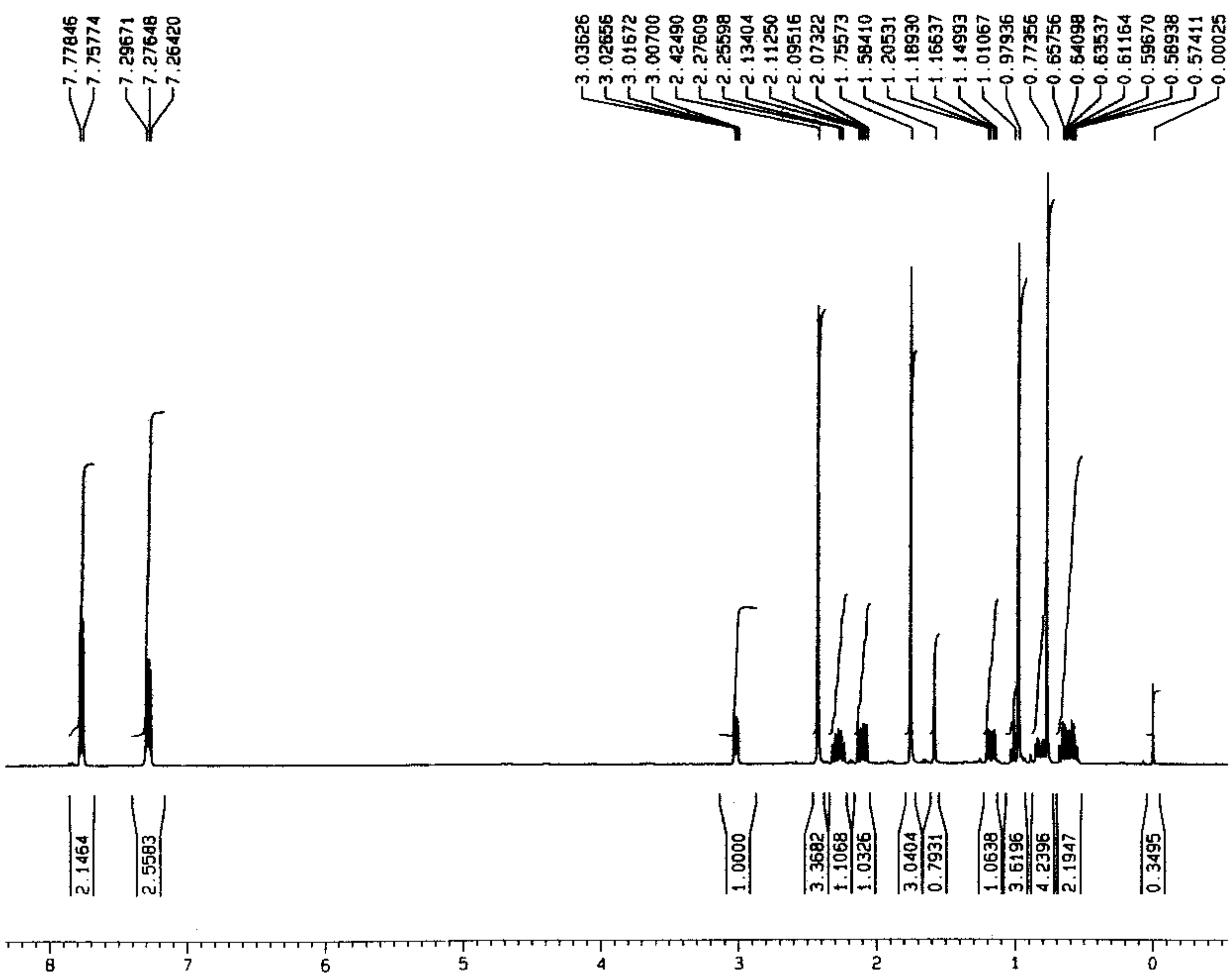
^{13}C NMR – $CDCl_3$ (75 MHz)



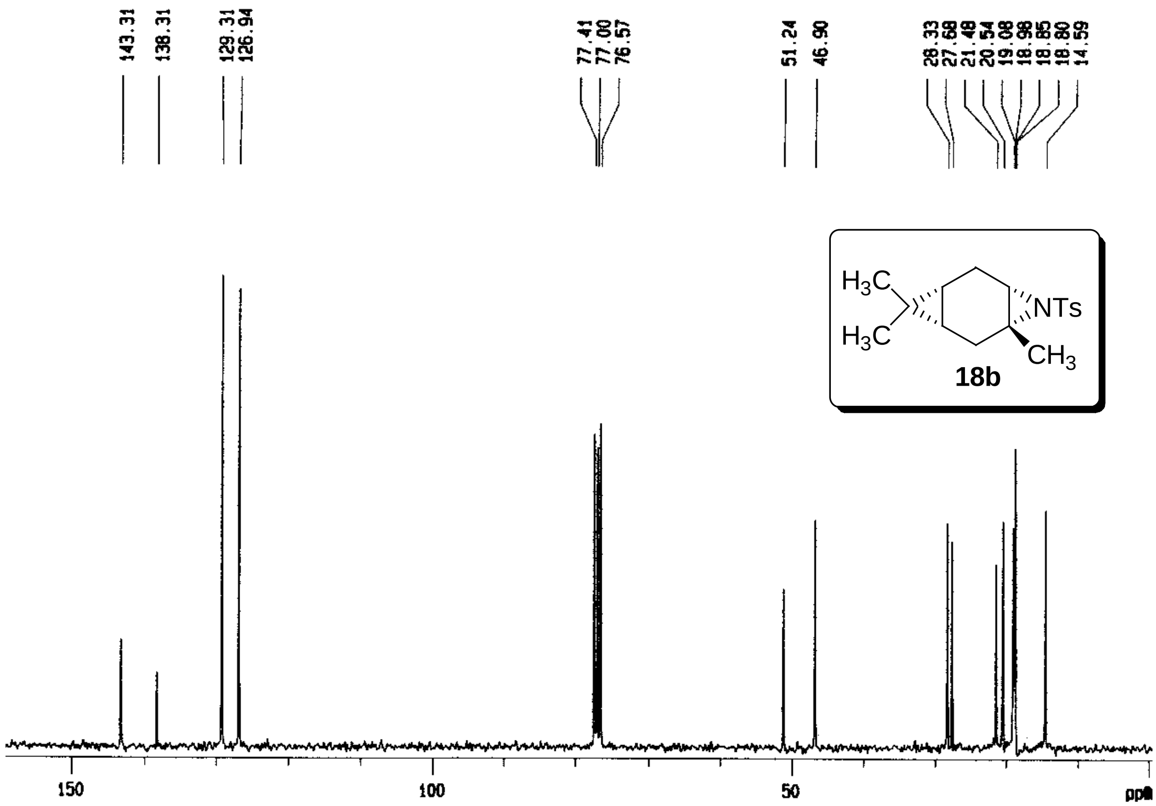


18b

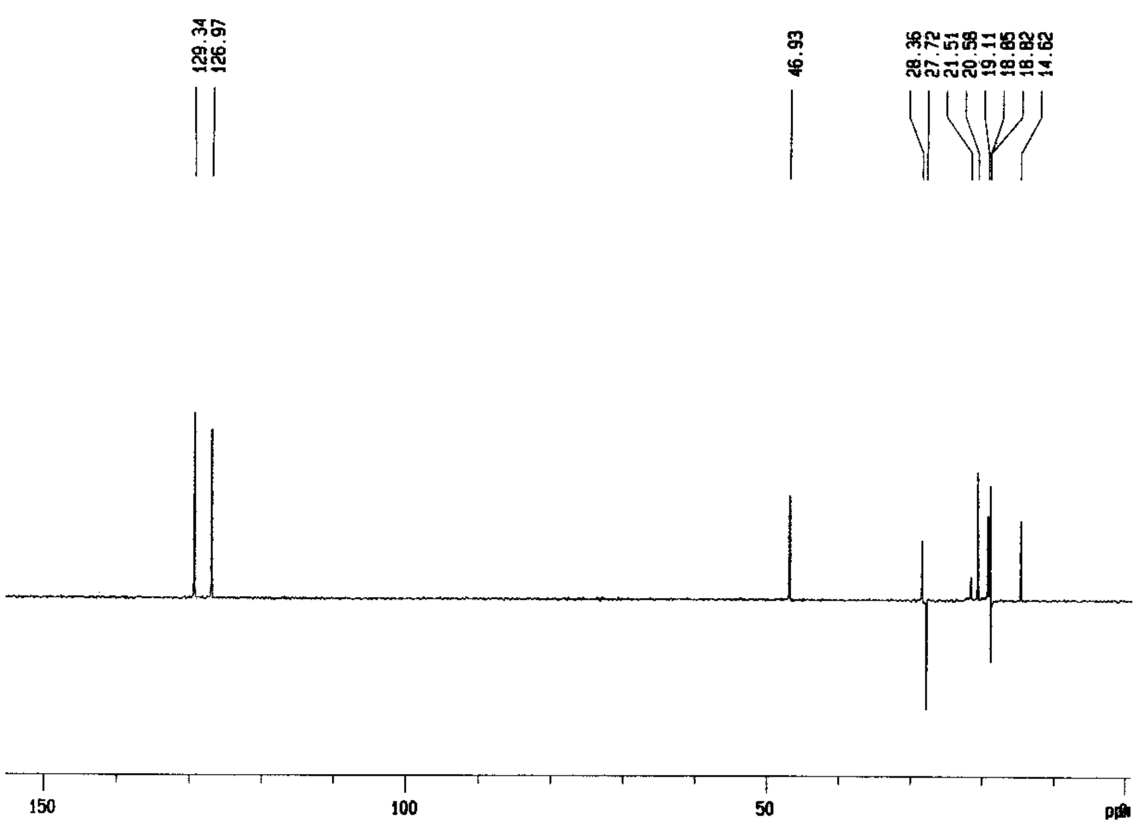
^{1}H NMR – $CDCl_3$ (400 MHz)



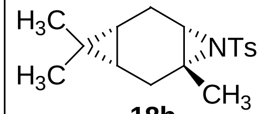
^{13}C NMR – $CDCl_3$ (75 MHz)



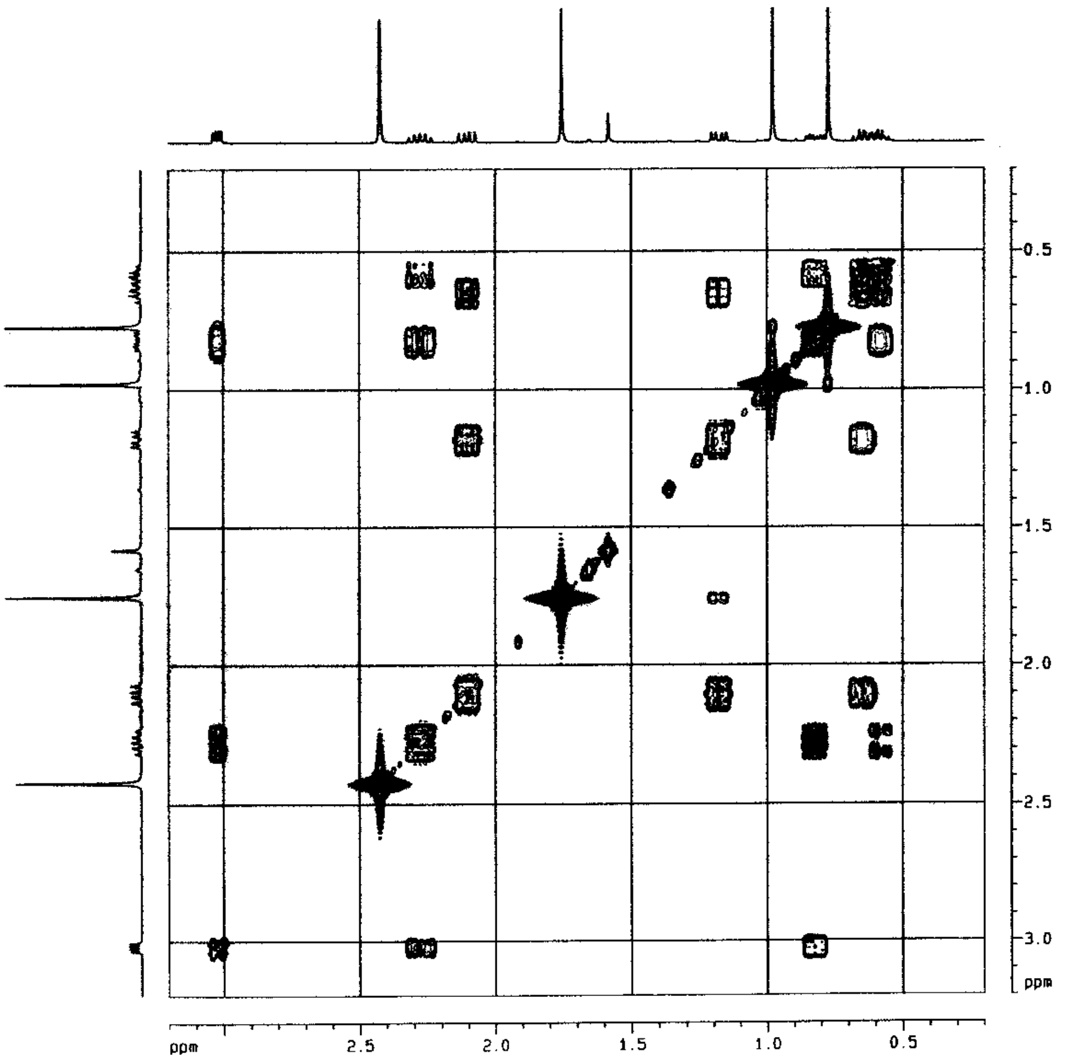
DEPT – $CDCl_3$ (75 MHz)



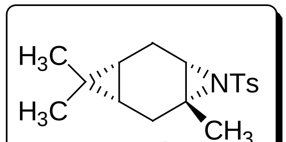
[1]H-[1]H COSY NMR – $CDCl_3$



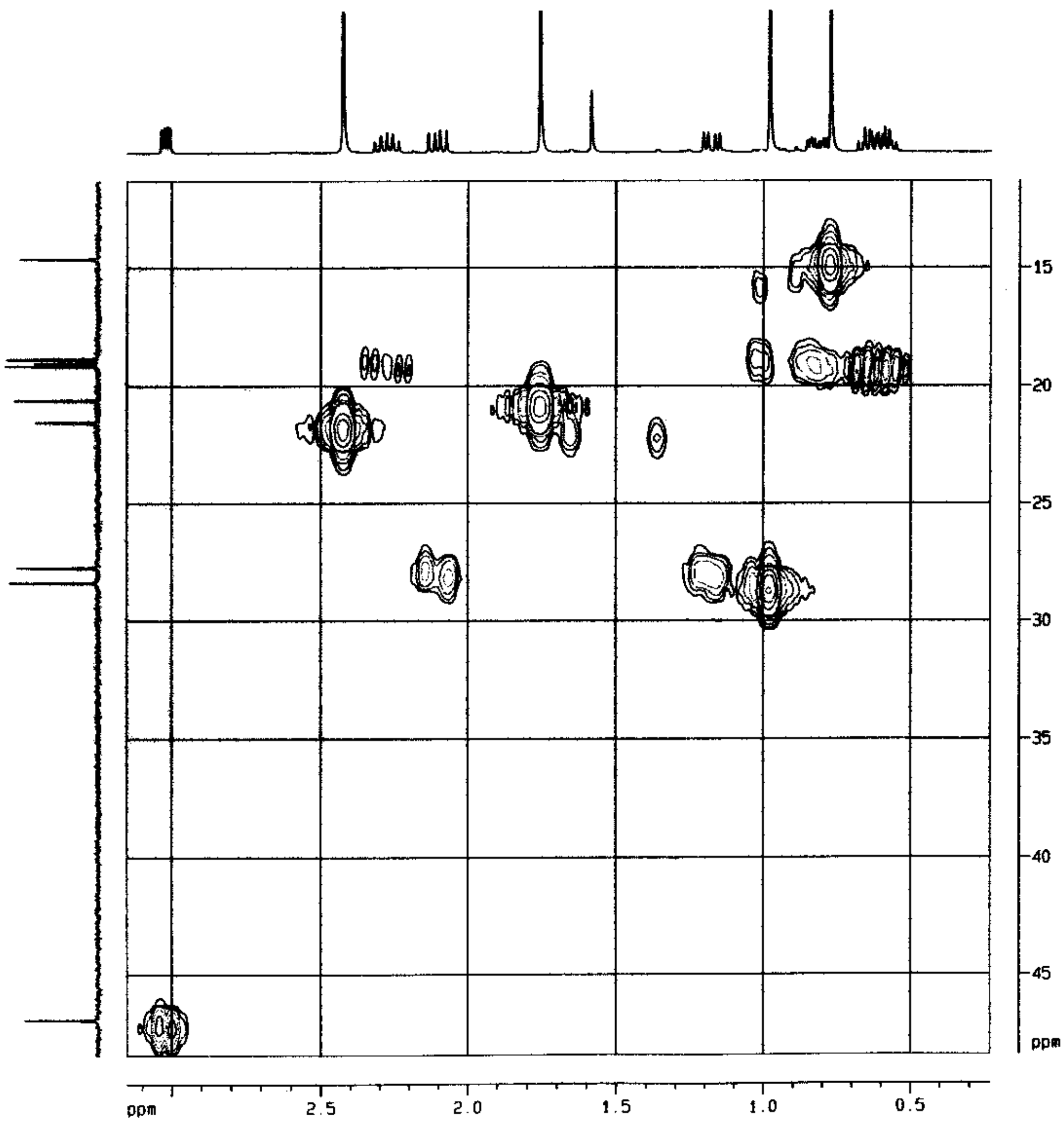
18b

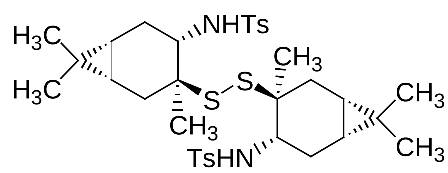


^{1}H-^{13}C COSY NMR – $CDCl_3$



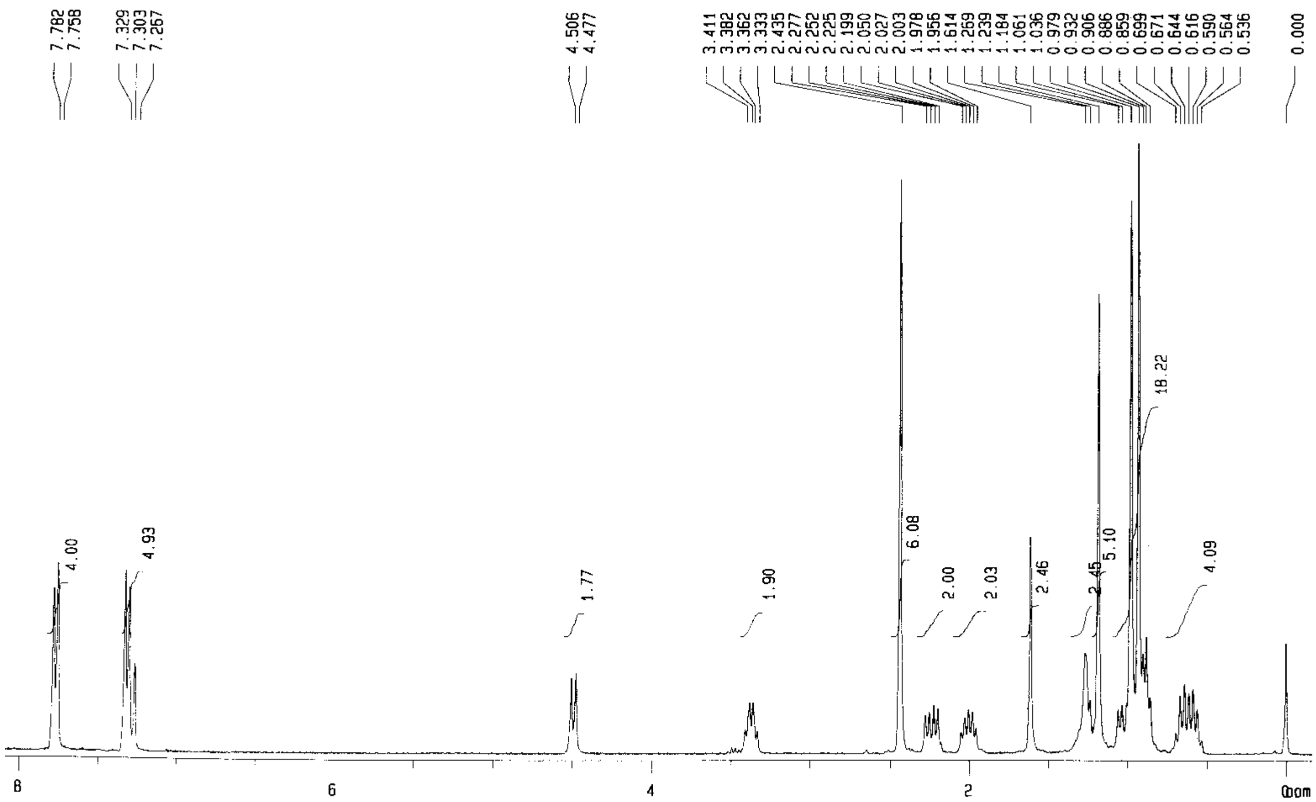
18b



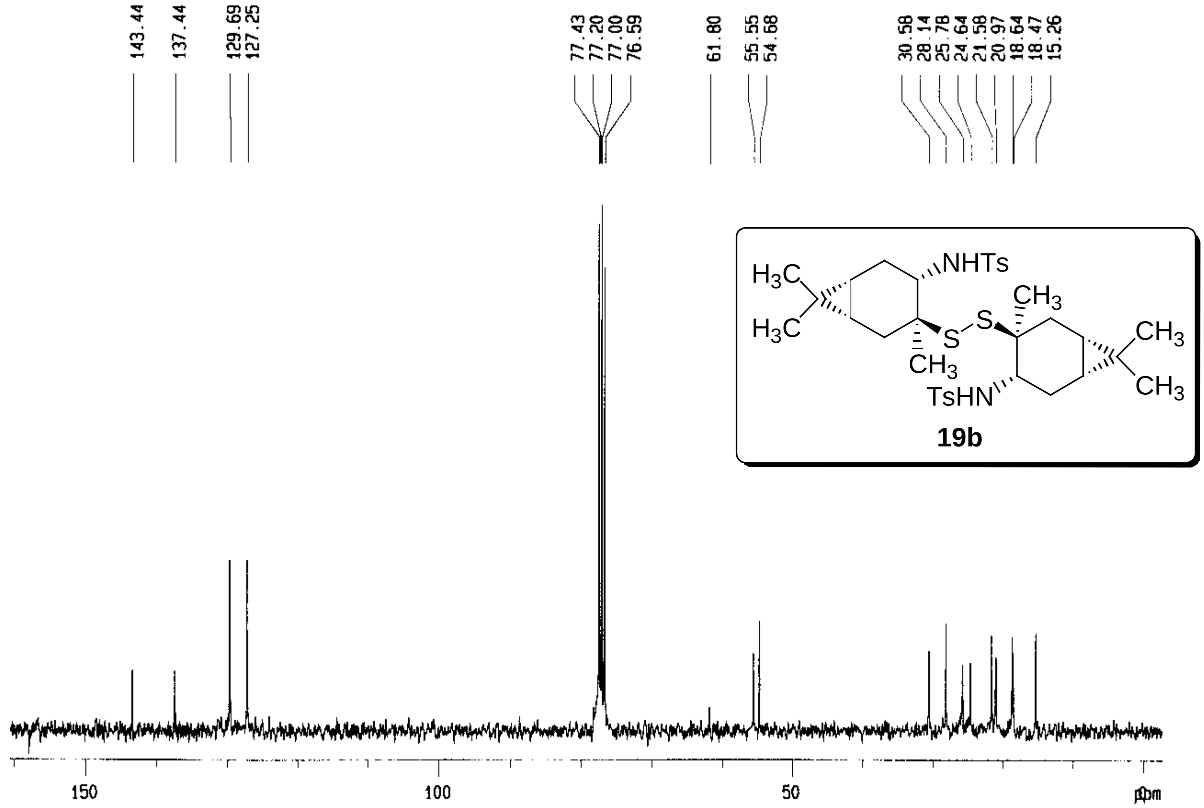


19b

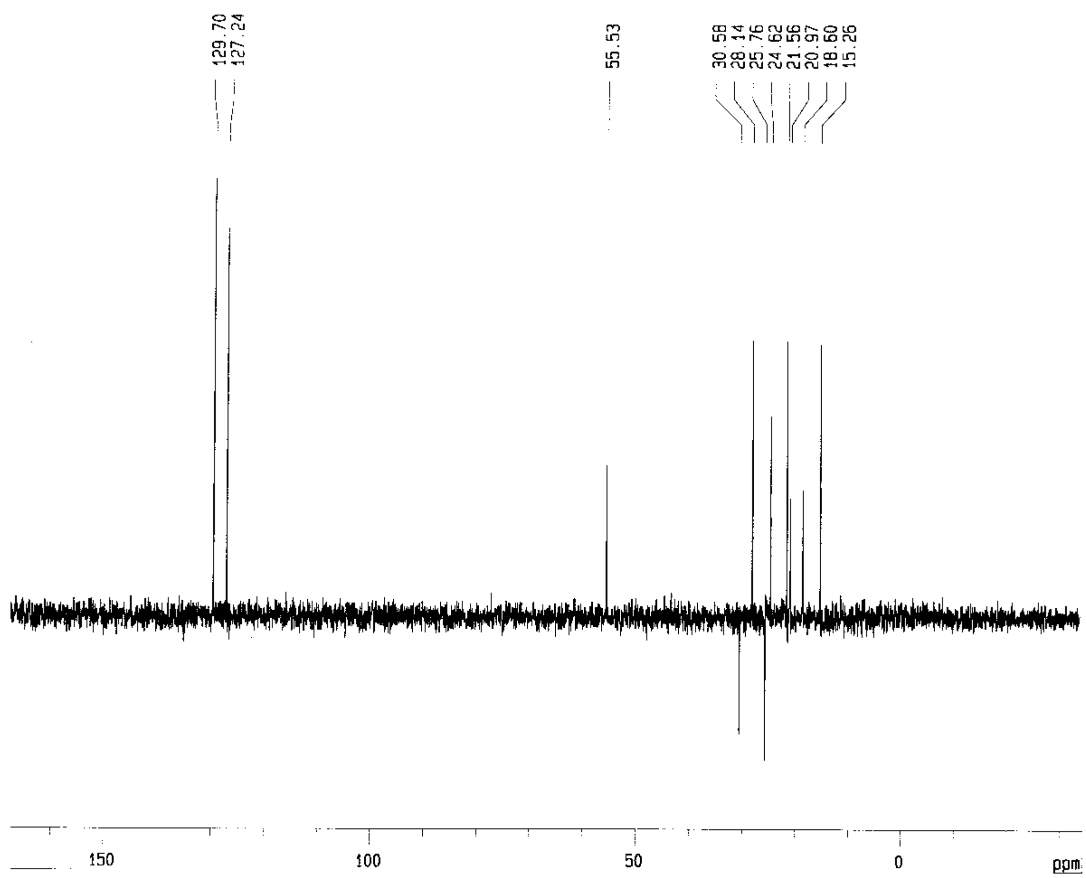
^{1}H NMR – $CDCl_3$ (300 MHz)

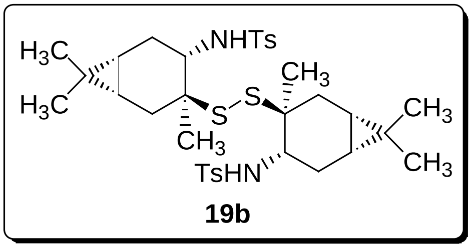


^{13}C NMR – $CDCl_3$ (75 MHz)

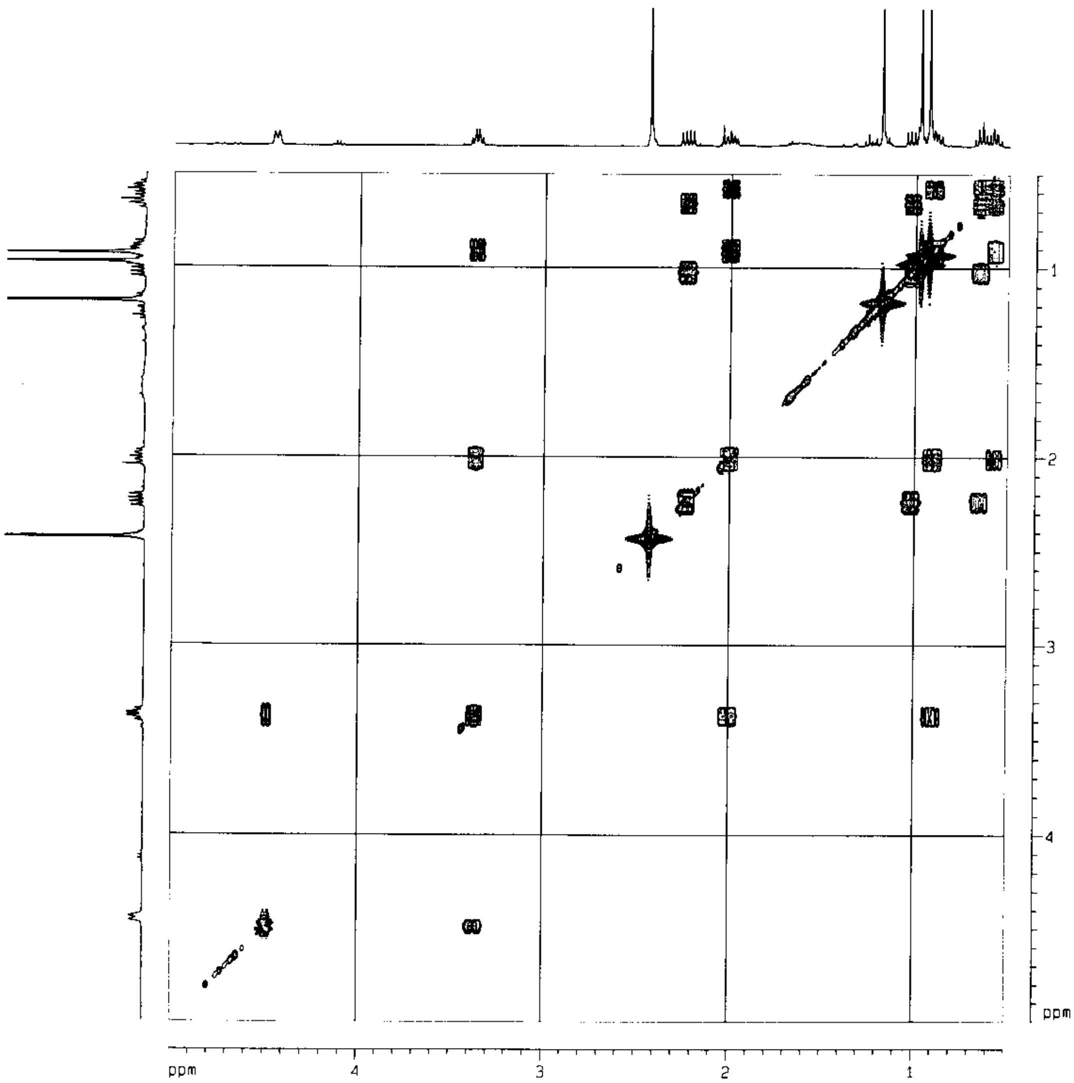


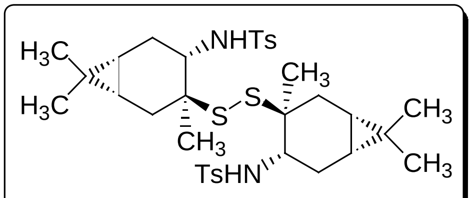
DEPT – $CDCl_3$ (75 MHz)





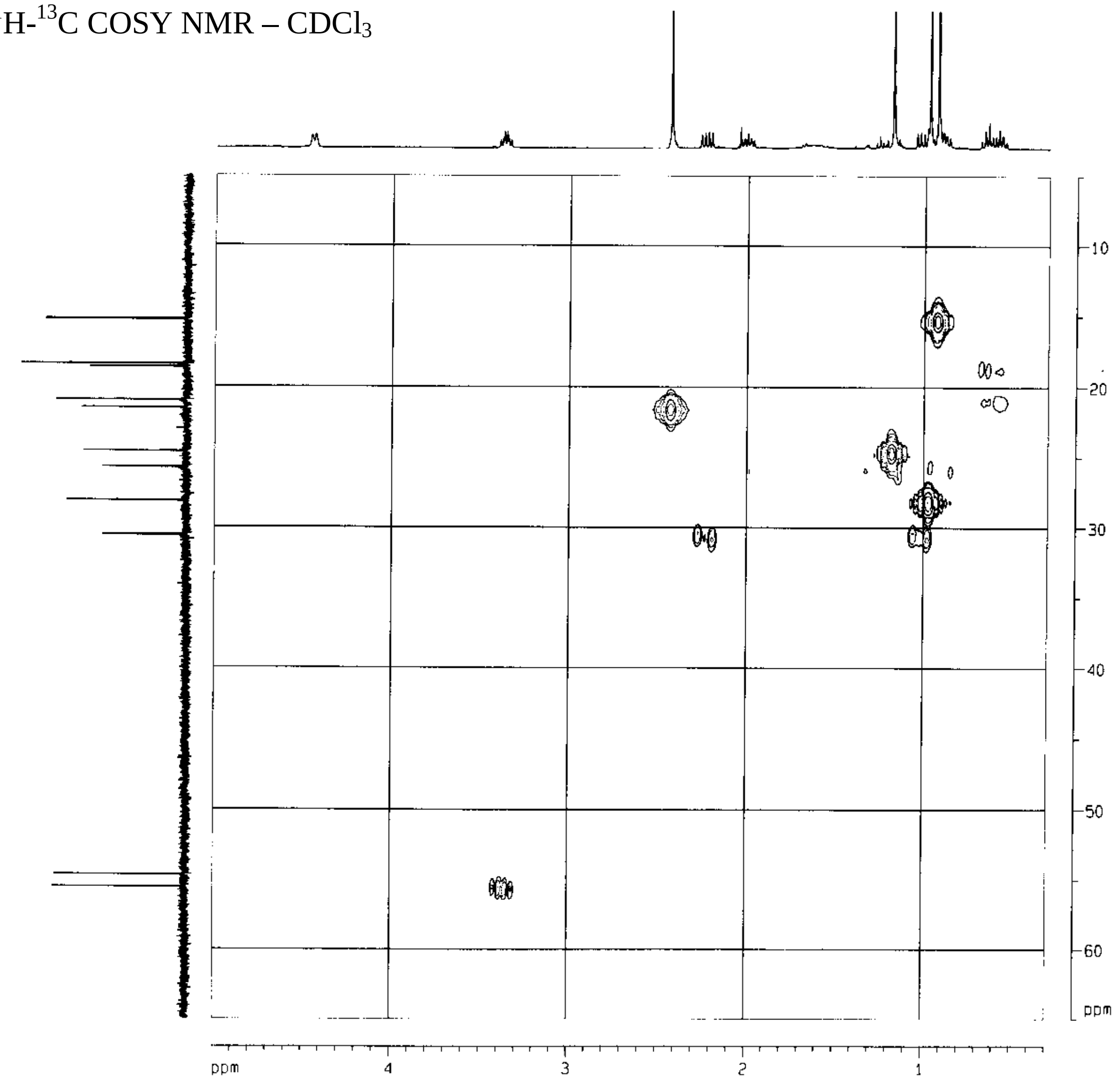
^1H-^1H COSY NMR – $CDCl_3$

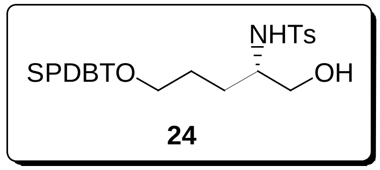




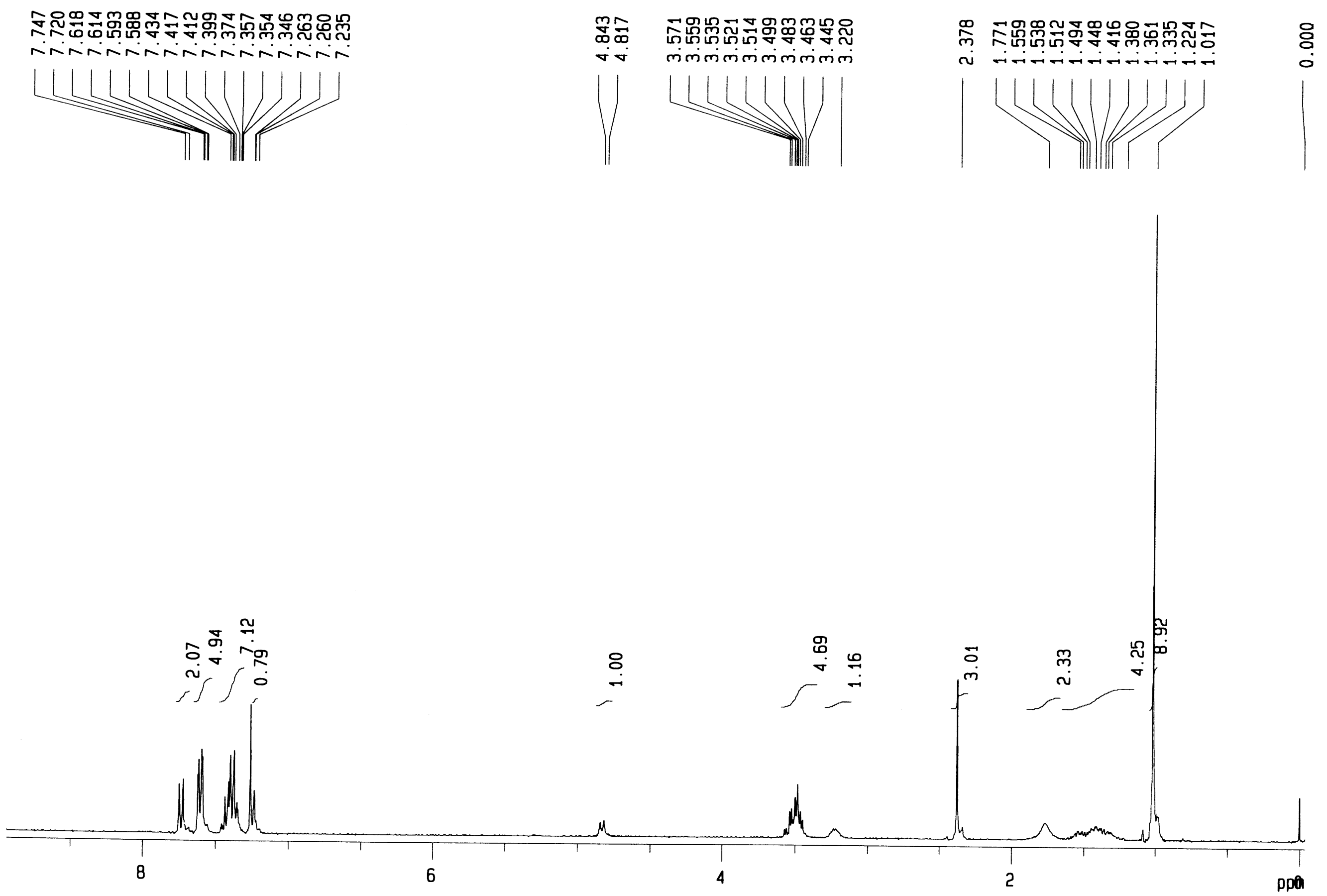
19b

^{1}H-^{13}C COSY NMR – $CDCl_3$

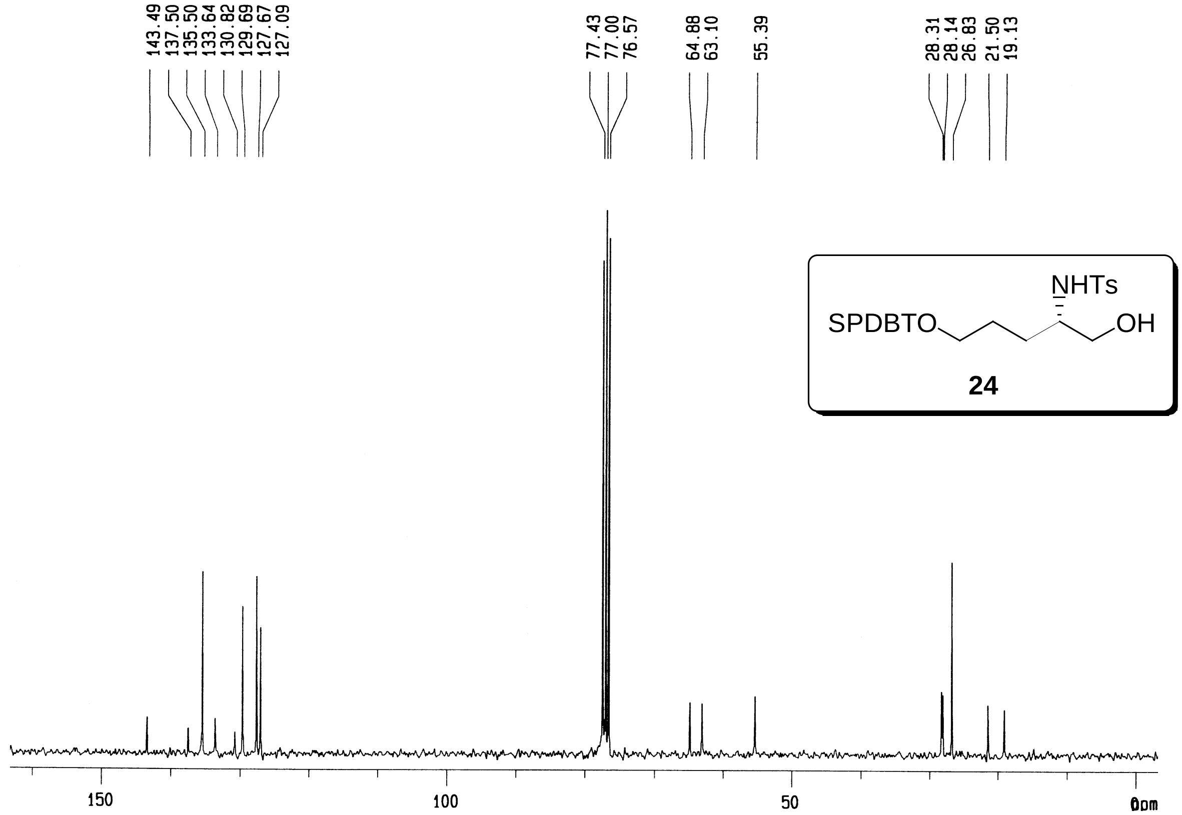




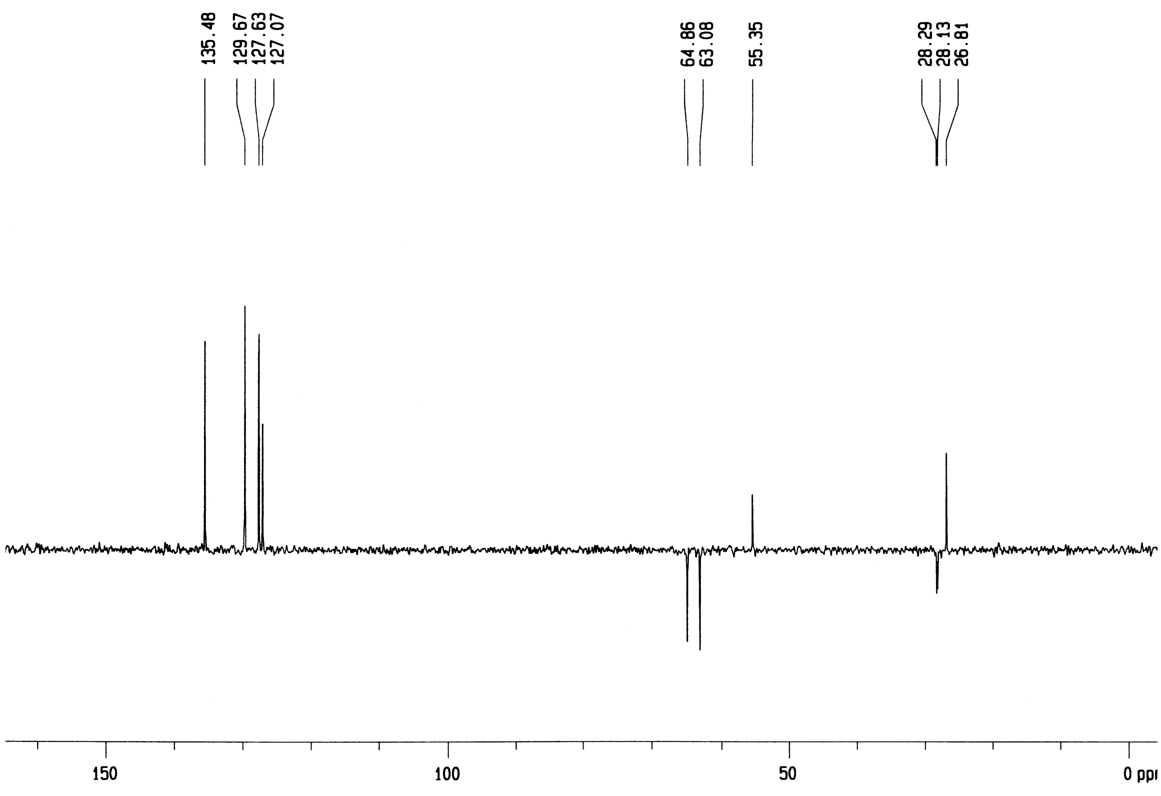
^{1}H NMR – $CDCl_3$ (300 MHz)

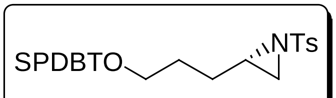


^{13}C NMR – $CDCl_3$ (75 MHz)



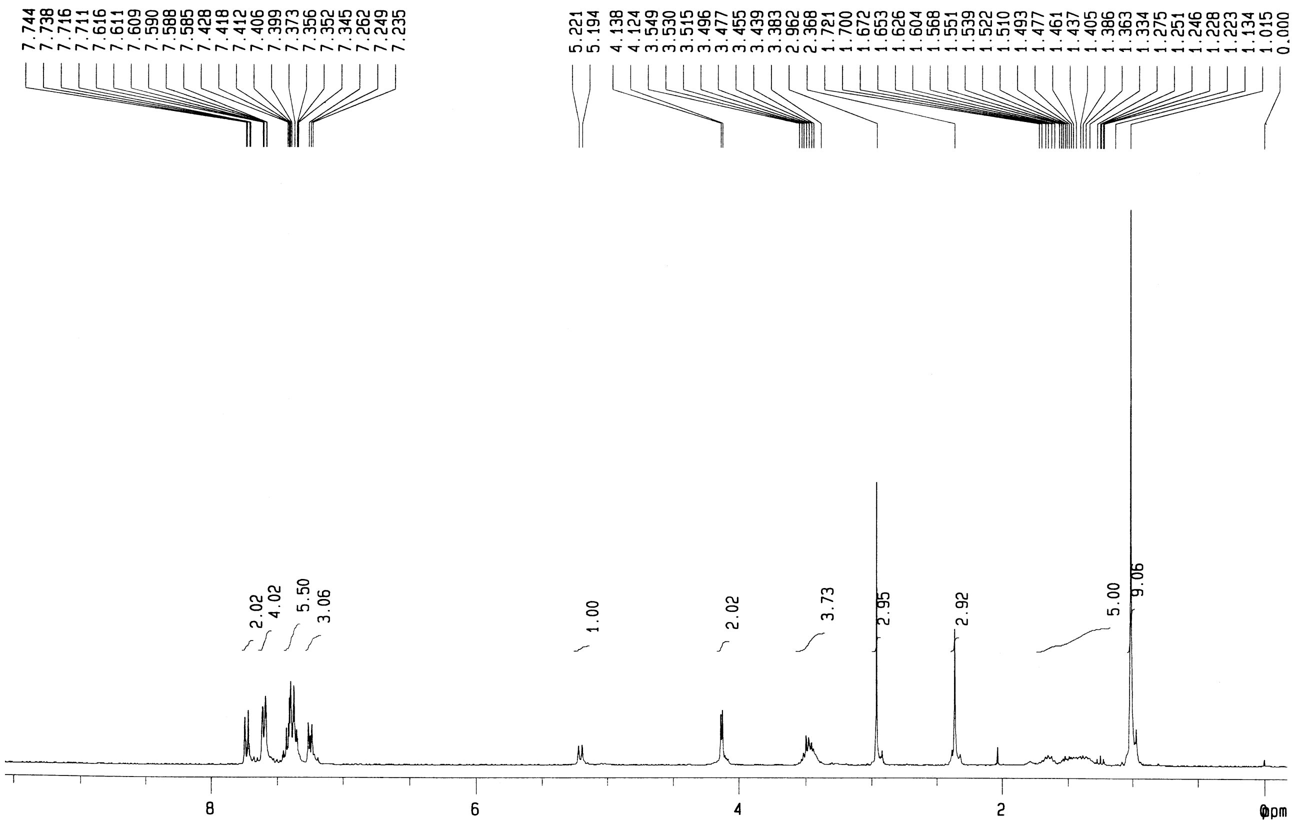
DEPT – $CDCl_3$ (75 MHz)



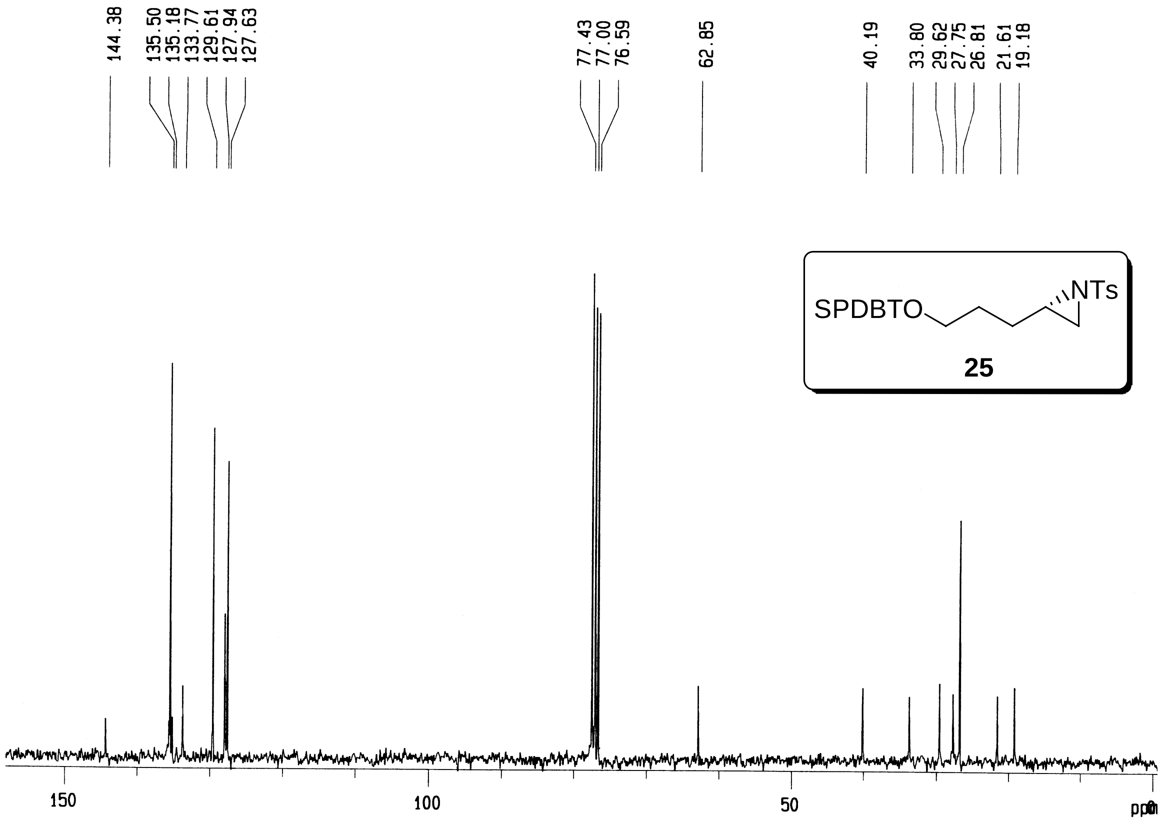


25

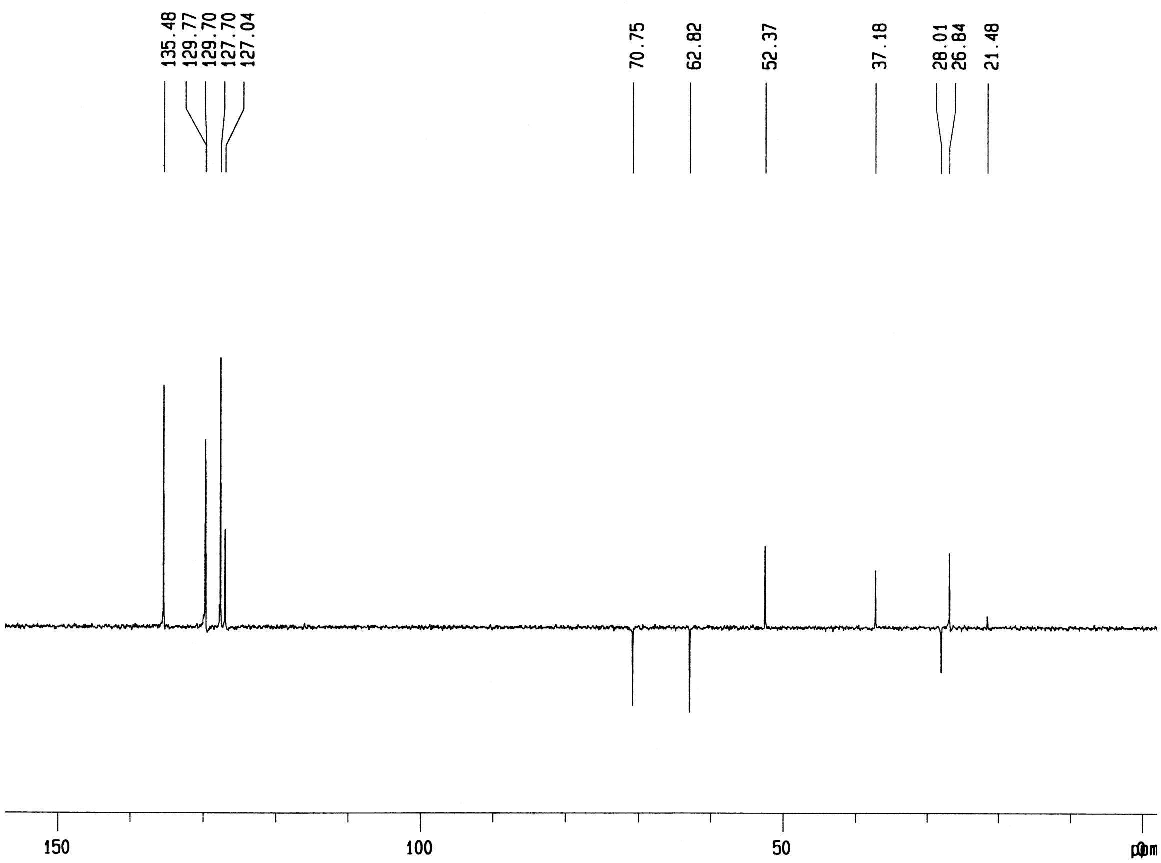
^{1}H NMR – $CDCl_3$ (300 MHz)

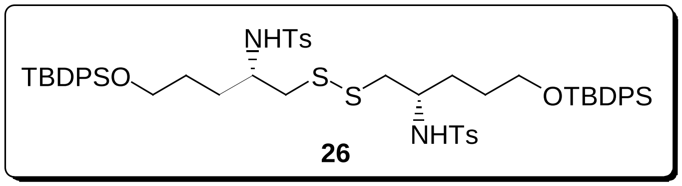


^{13}C NMR – $CDCl_3$ (75 MHz)



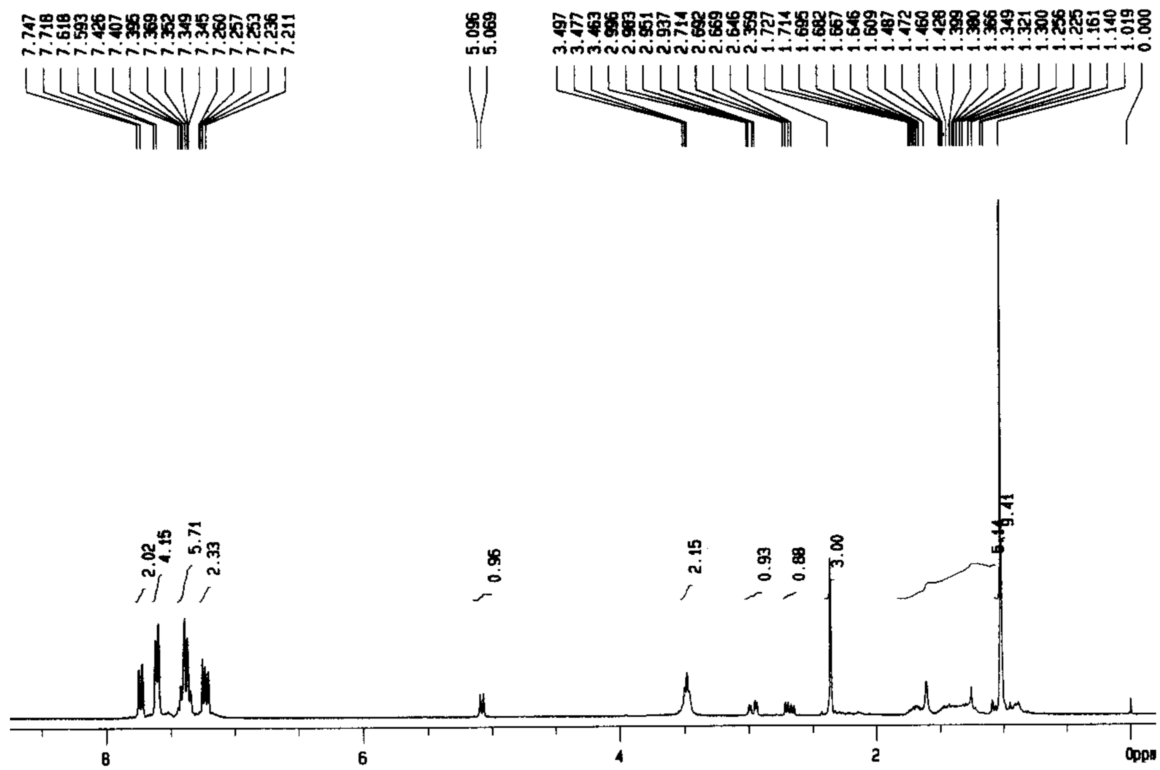
DEPT – $CDCl_3$ (75 MHz)



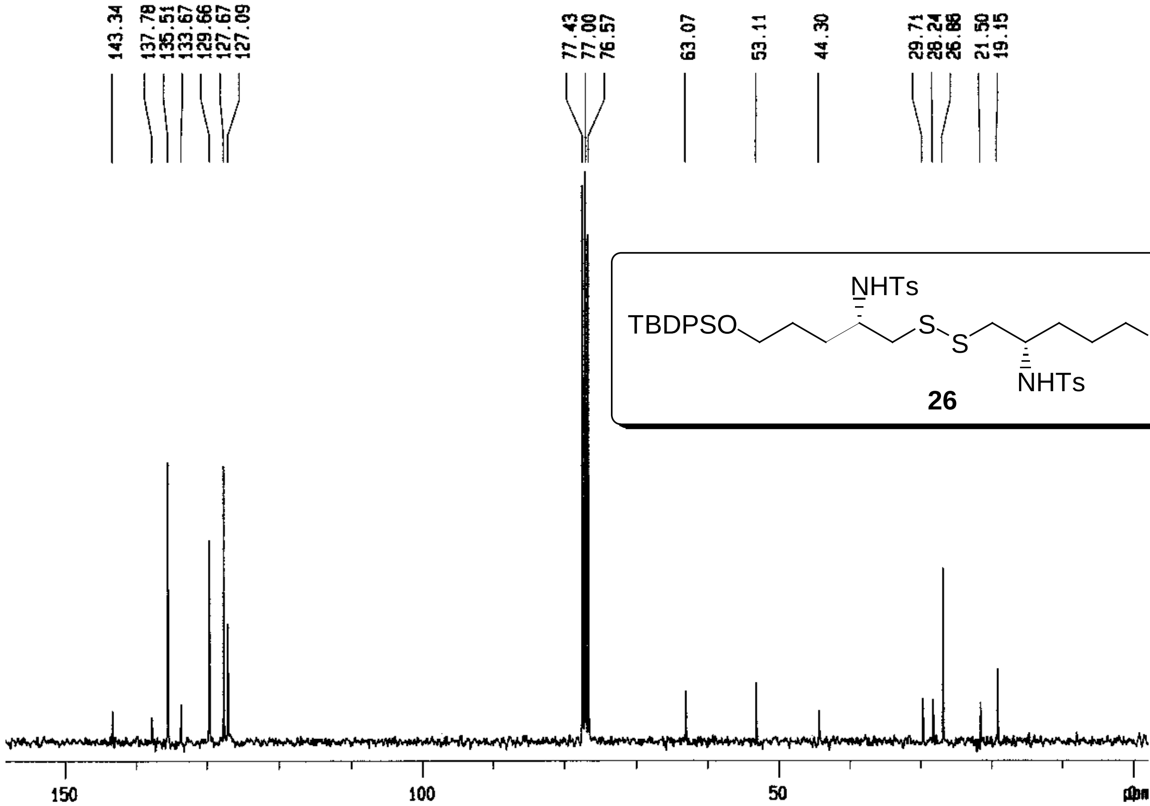


26

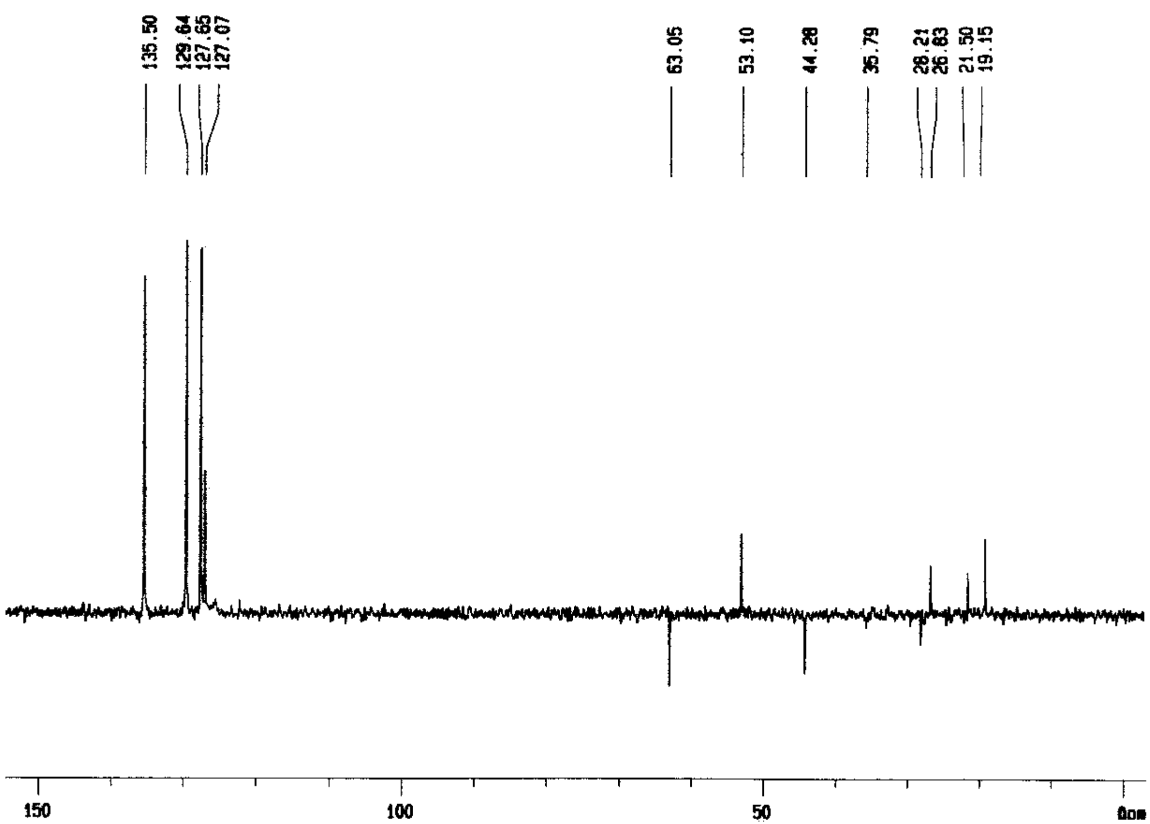
^{1}H NMR – $CDCl_3$ (300 MHz)

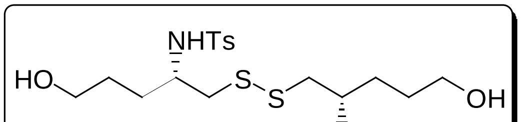


^{13}C NMR – $CDCl_3$ (75 MHz)



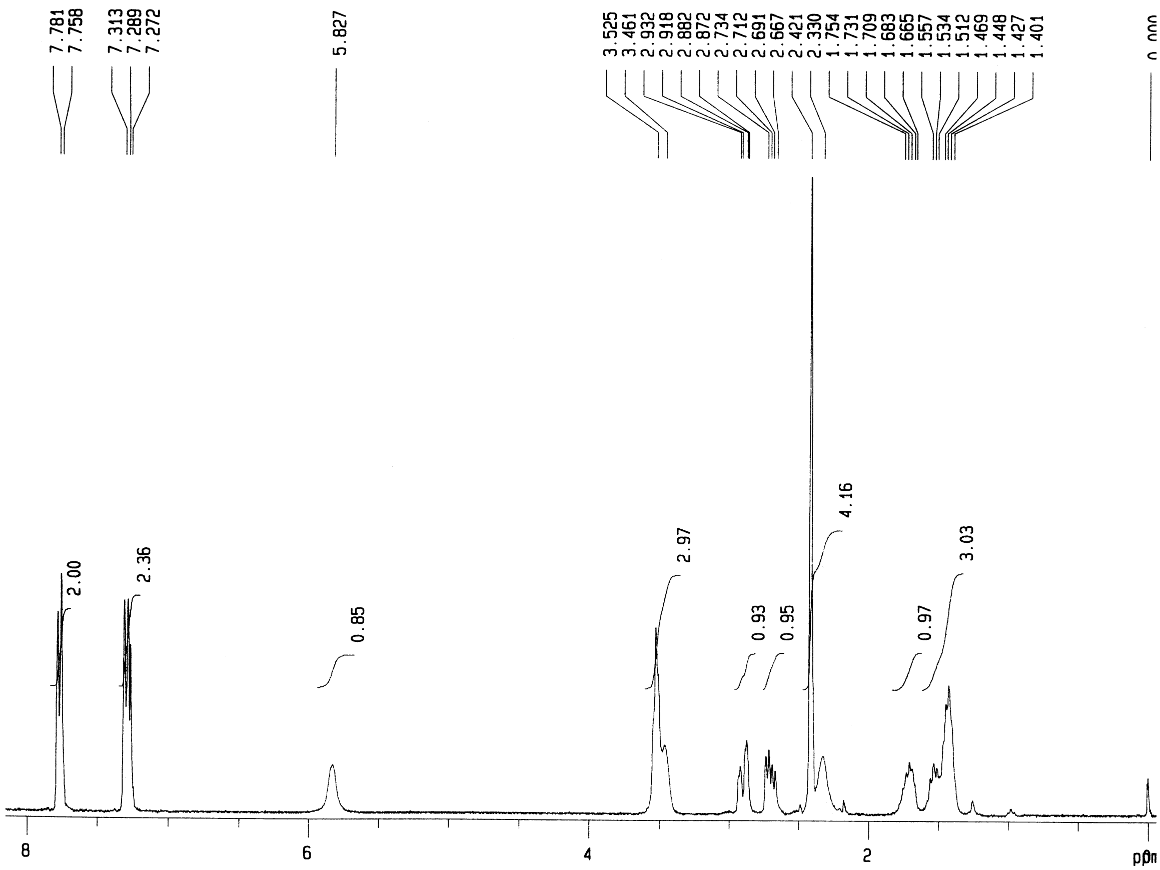
DEPT – $CDCl_3$ (75 MHz)



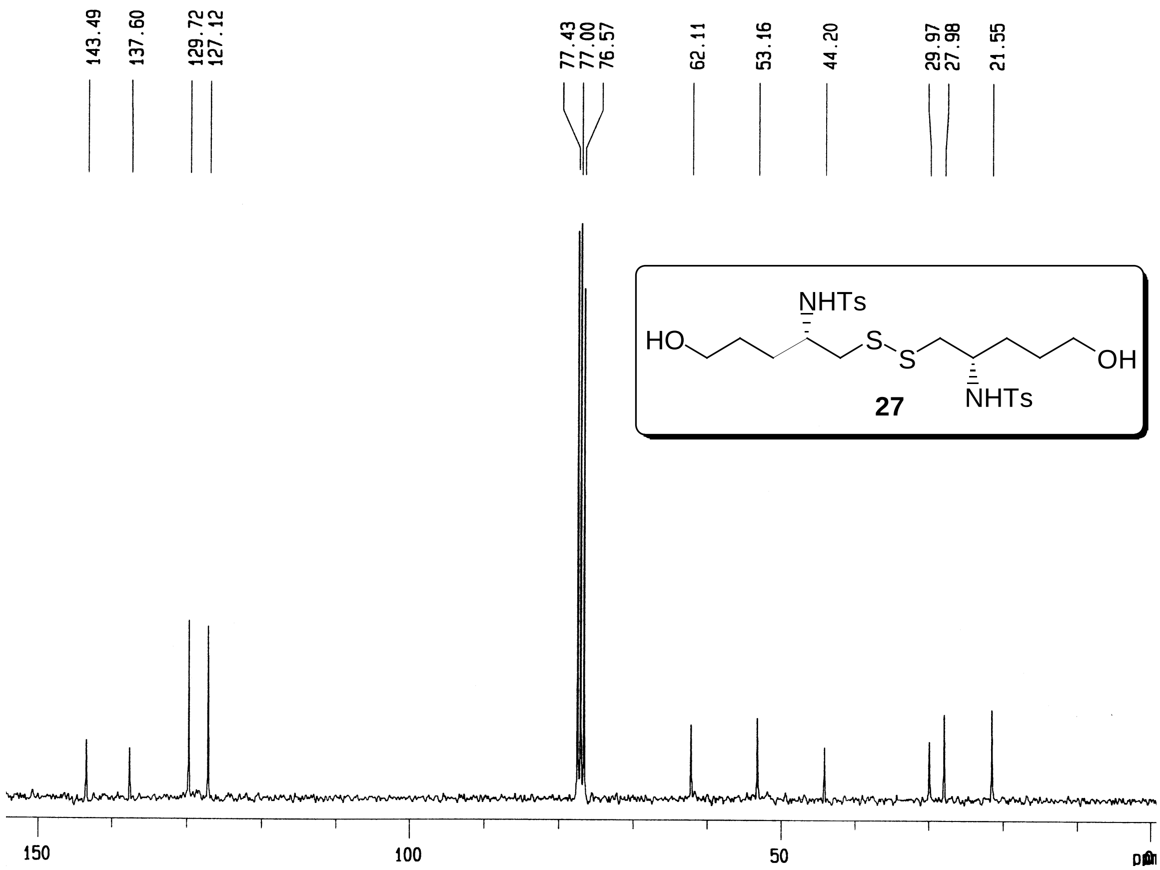


27

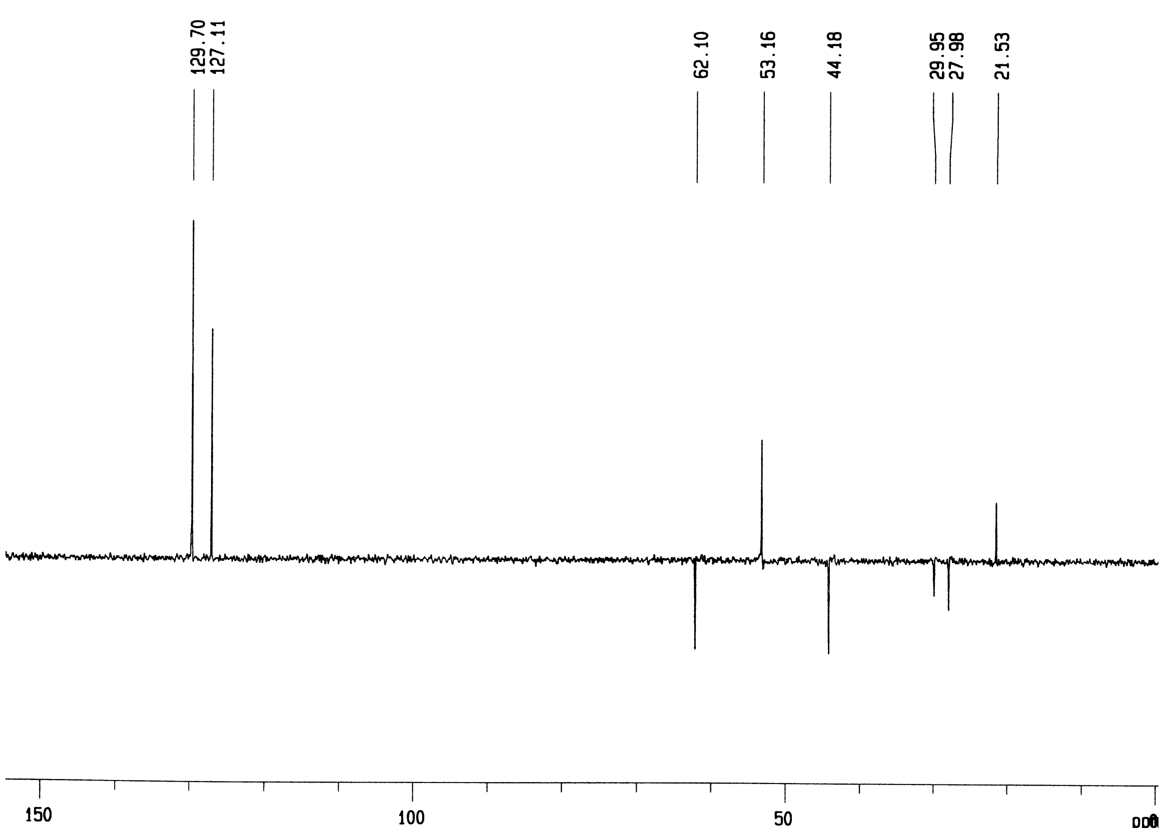
[1]H NMR – $CDCl_3$ (300 MHz)

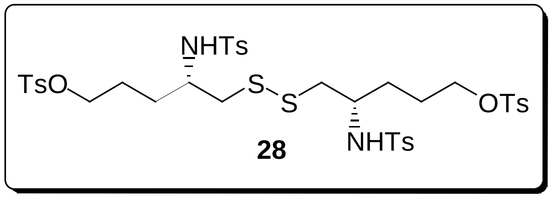


^{13}C NMR – $CDCl_3$ (75 MHz)

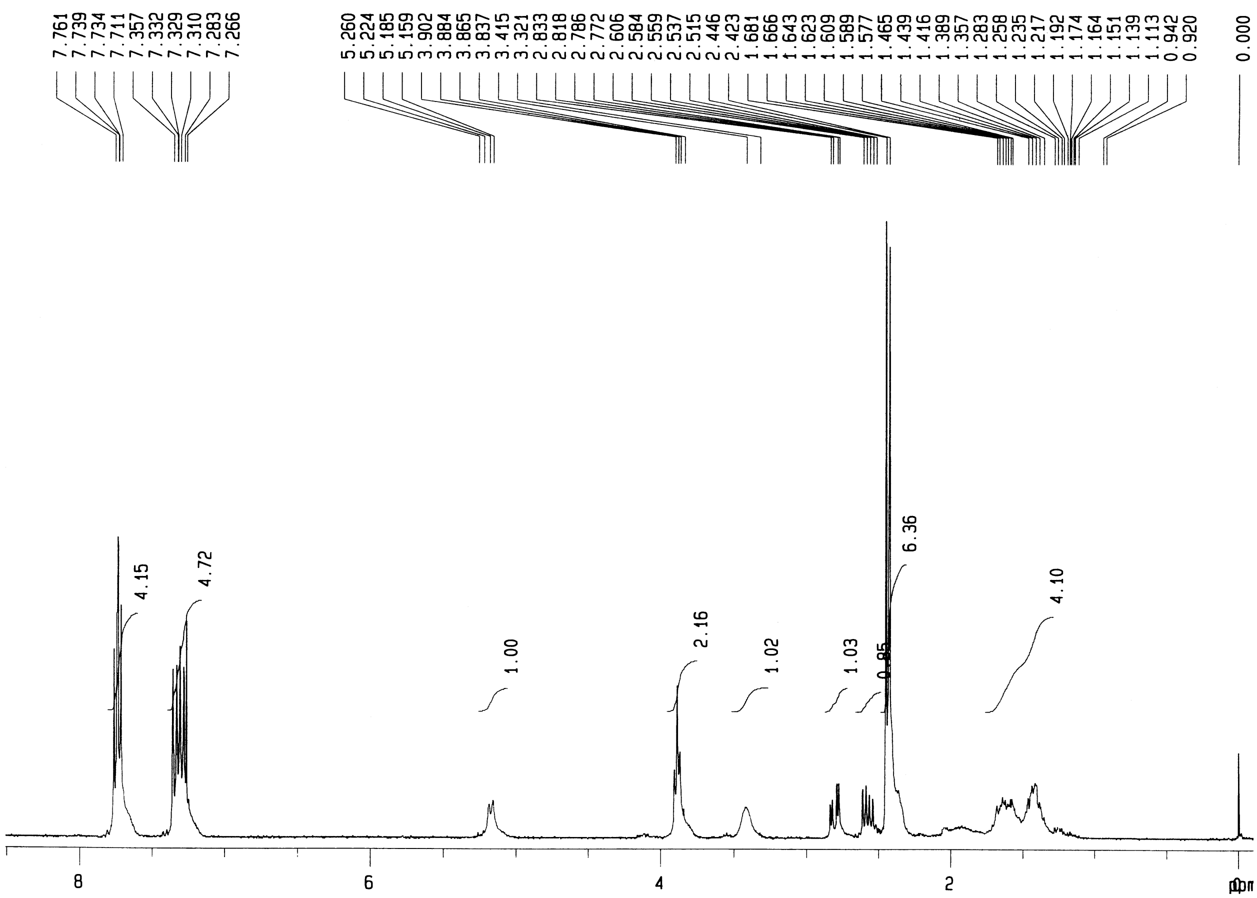


DEPT – $CDCl_3$ (75 MHz)

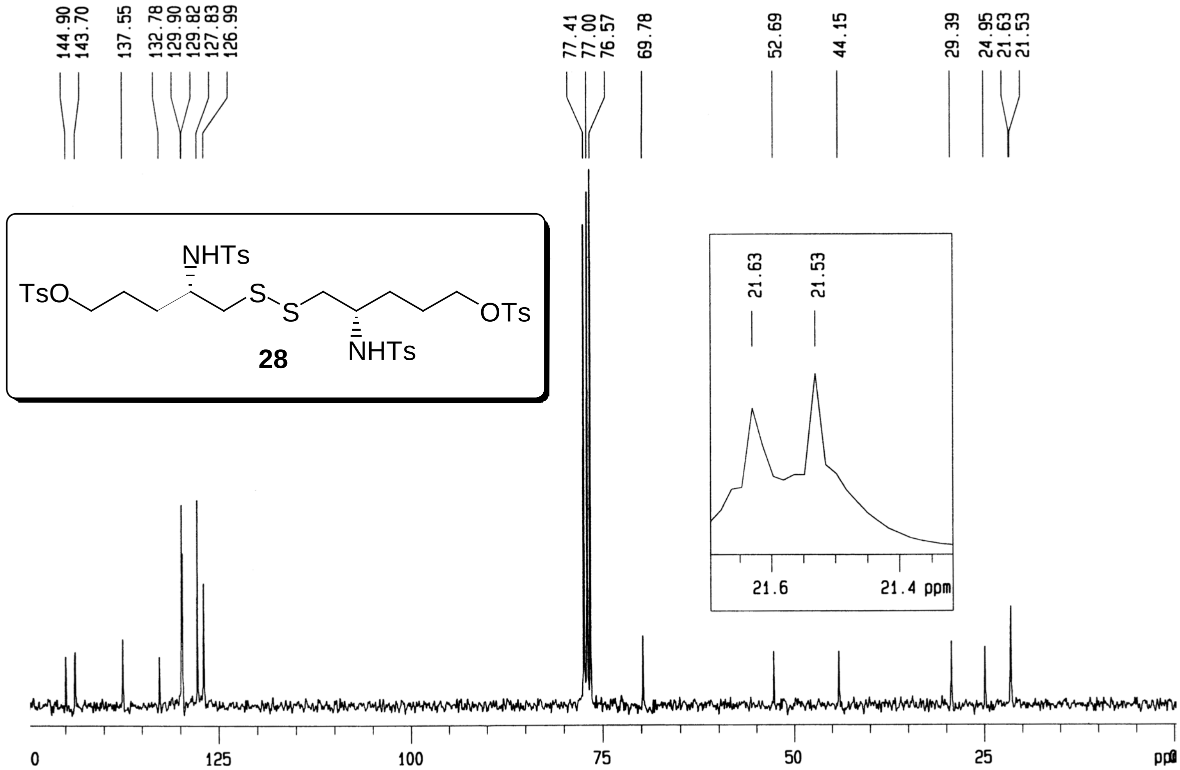




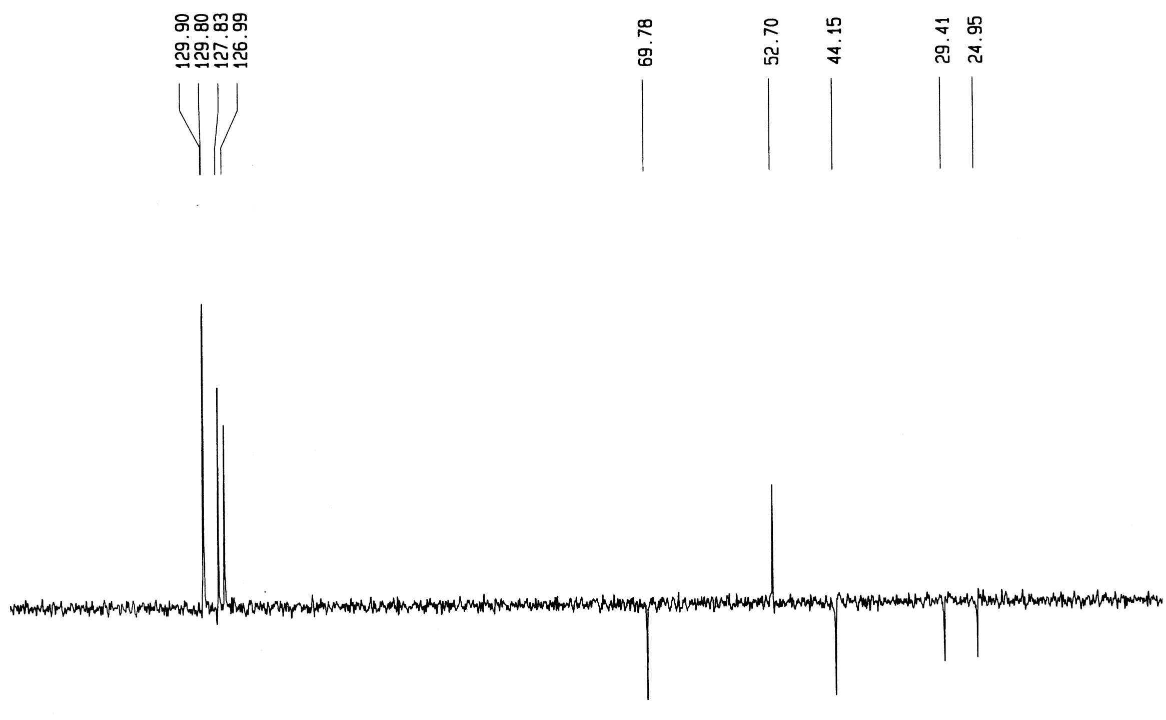
^{1}H NMR – $CDCl_3$ (300 MHz)

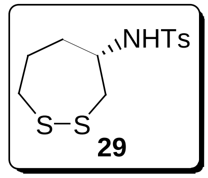


^{13}C NMR – $CDCl_3$ (75 MHz)

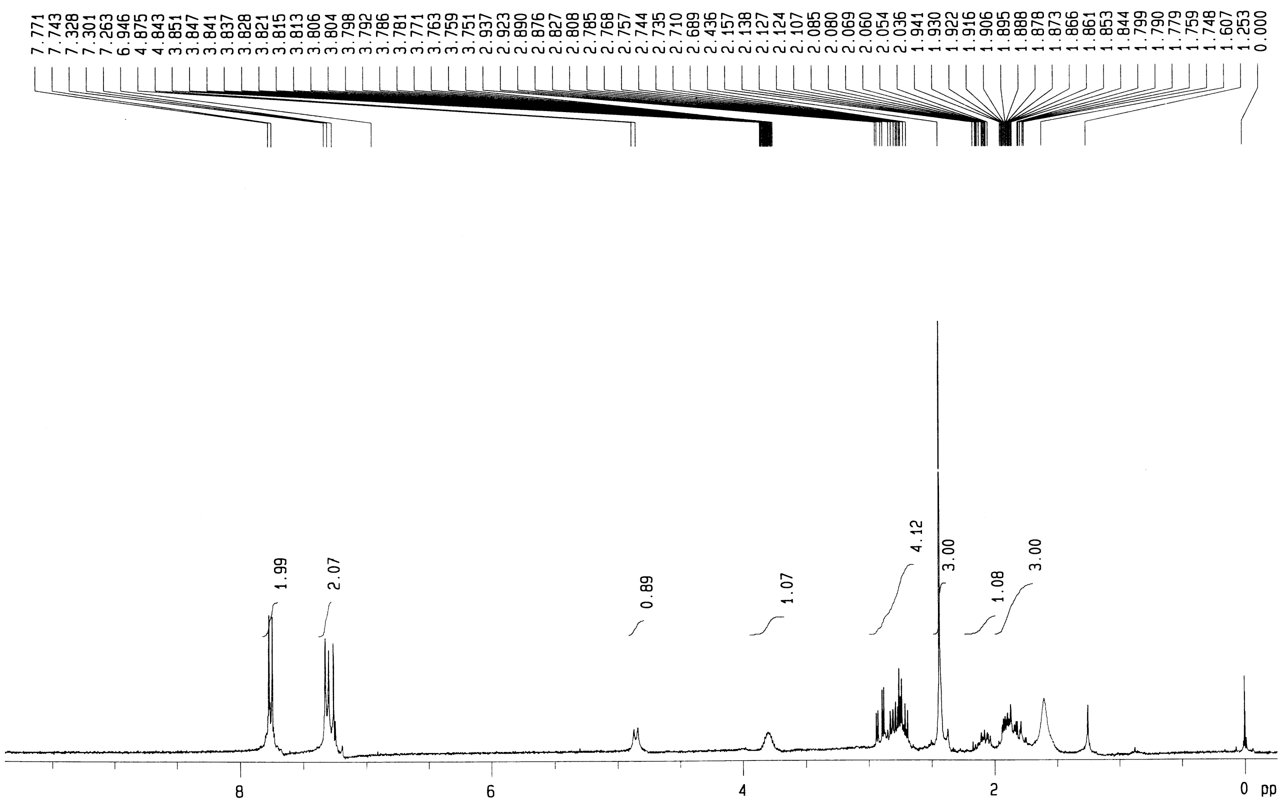


DEPT – $CDCl_3$ (75 MHz)

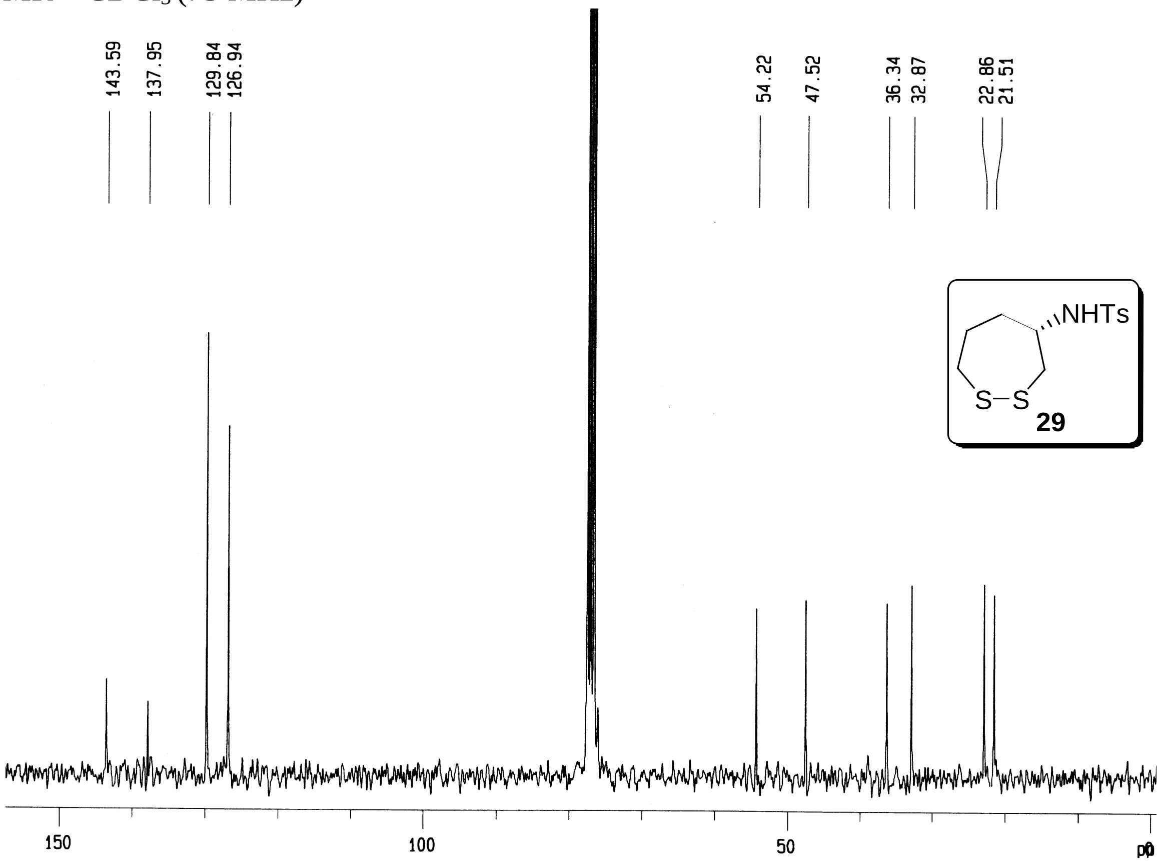




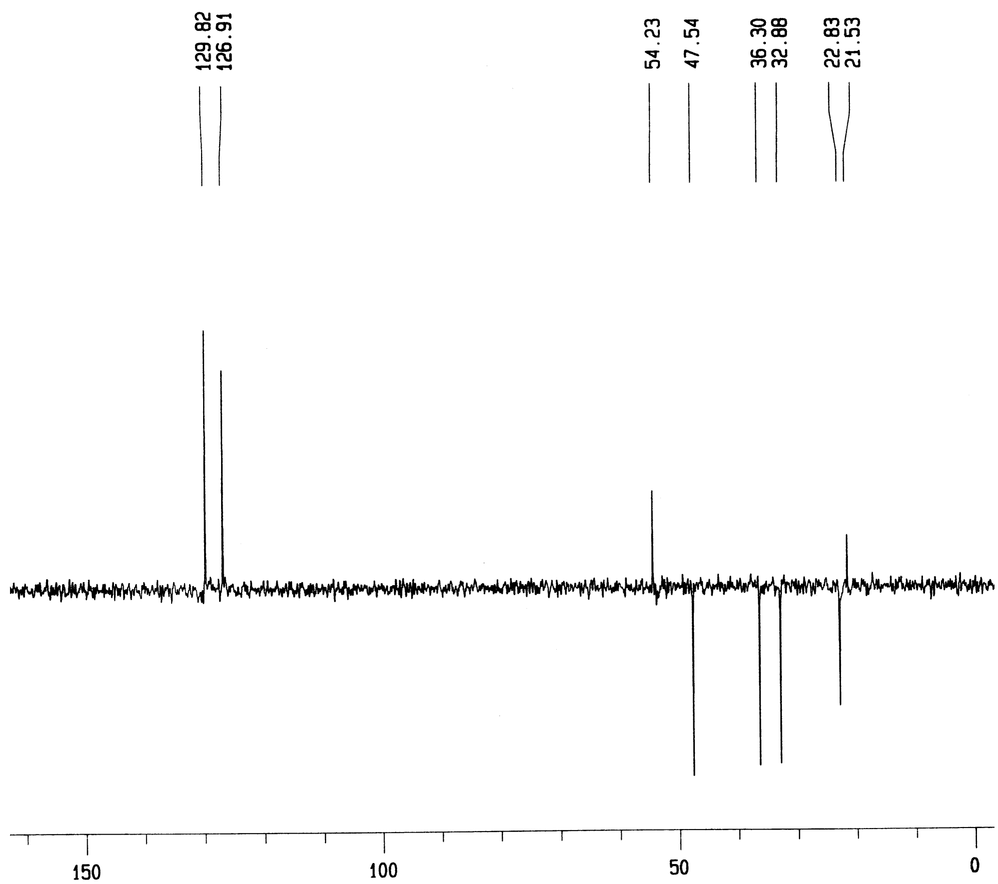
^{1}H NMR – $CDCl_3$ (300 MHz)

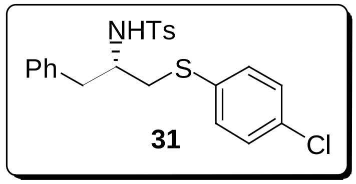


^{13}C NMR – $CDCl_3$ (75 MHz)

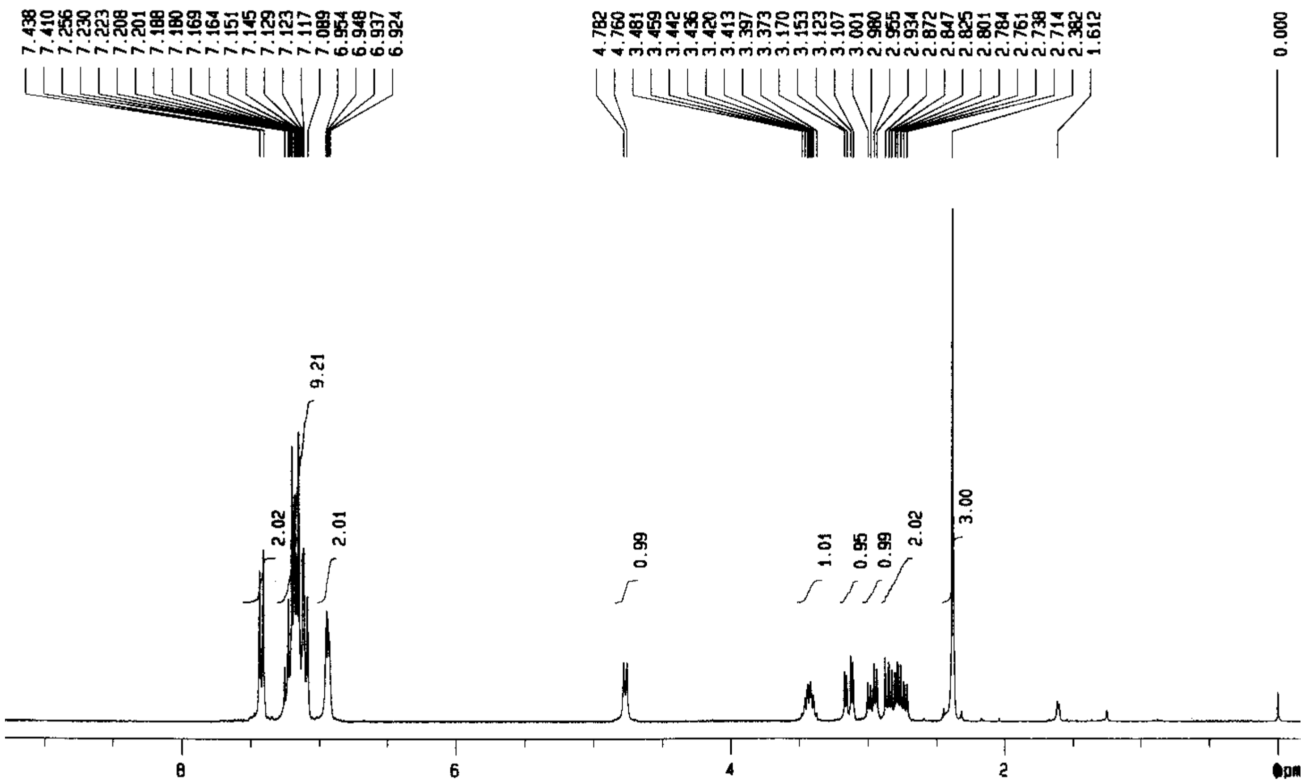


DEPT – $CDCl_3$ (75 MHz)

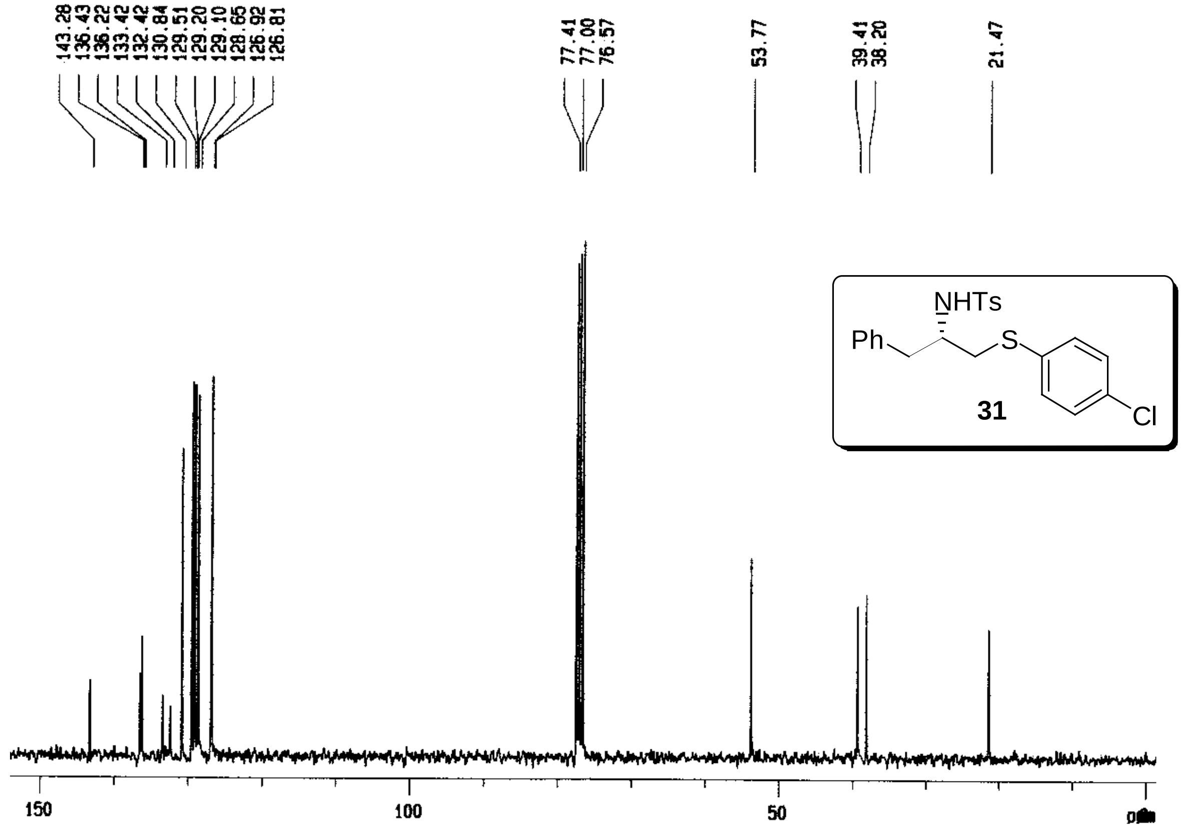




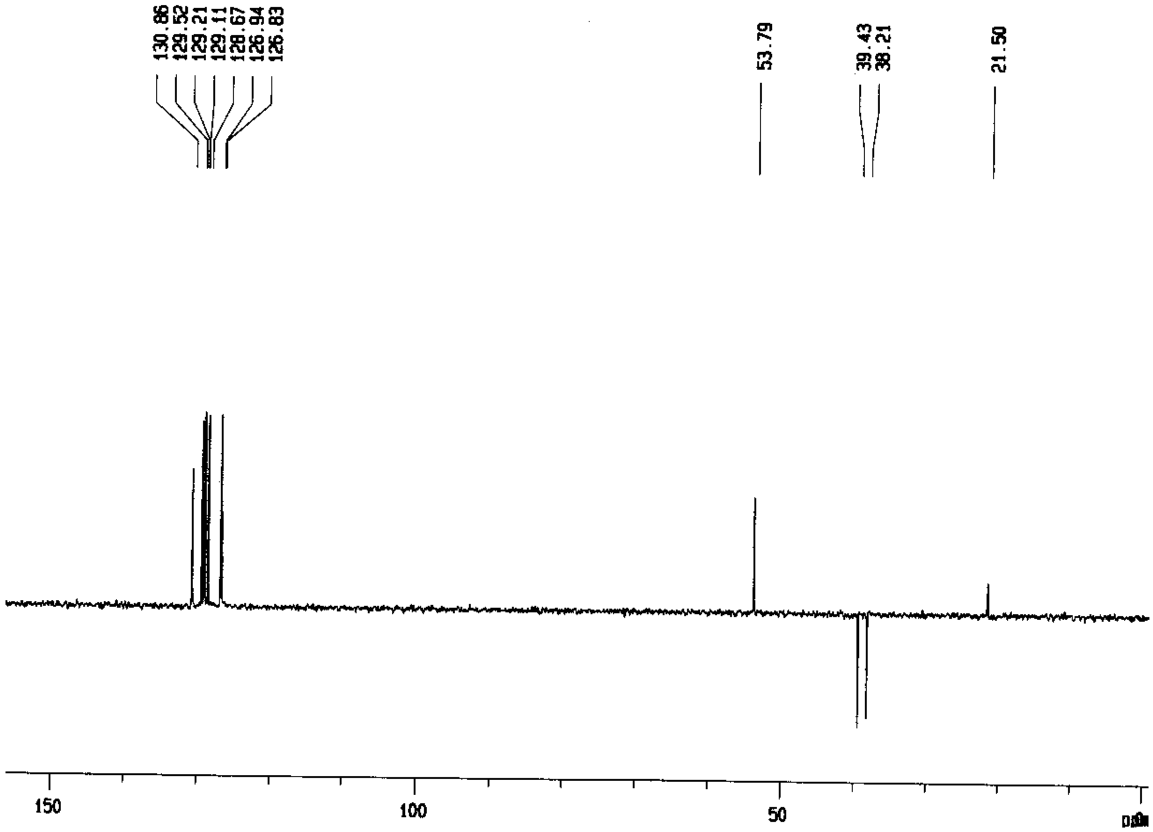
^{1}H NMR – $CDCl_3$ (300 MHz)

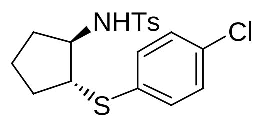


^{13}C NMR – $CDCl_3$ (75 MHz)



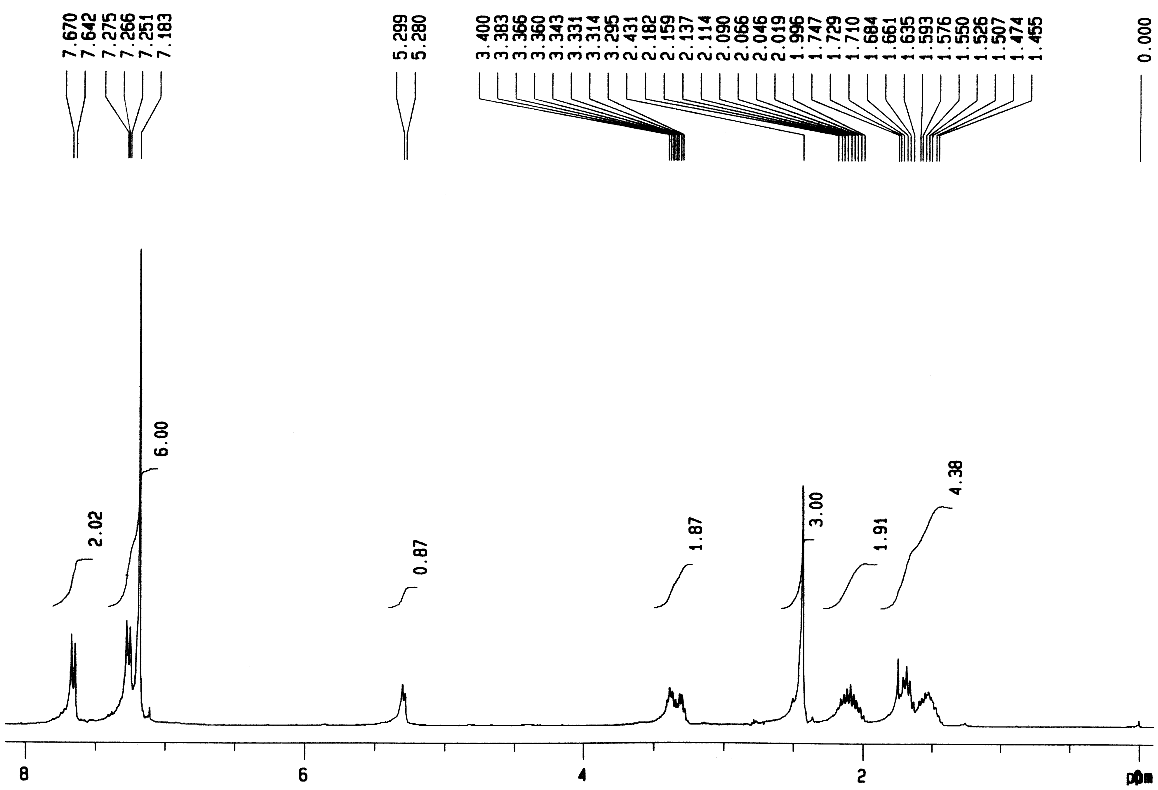
DEPT – $CDCl_3$ (75 MHz)



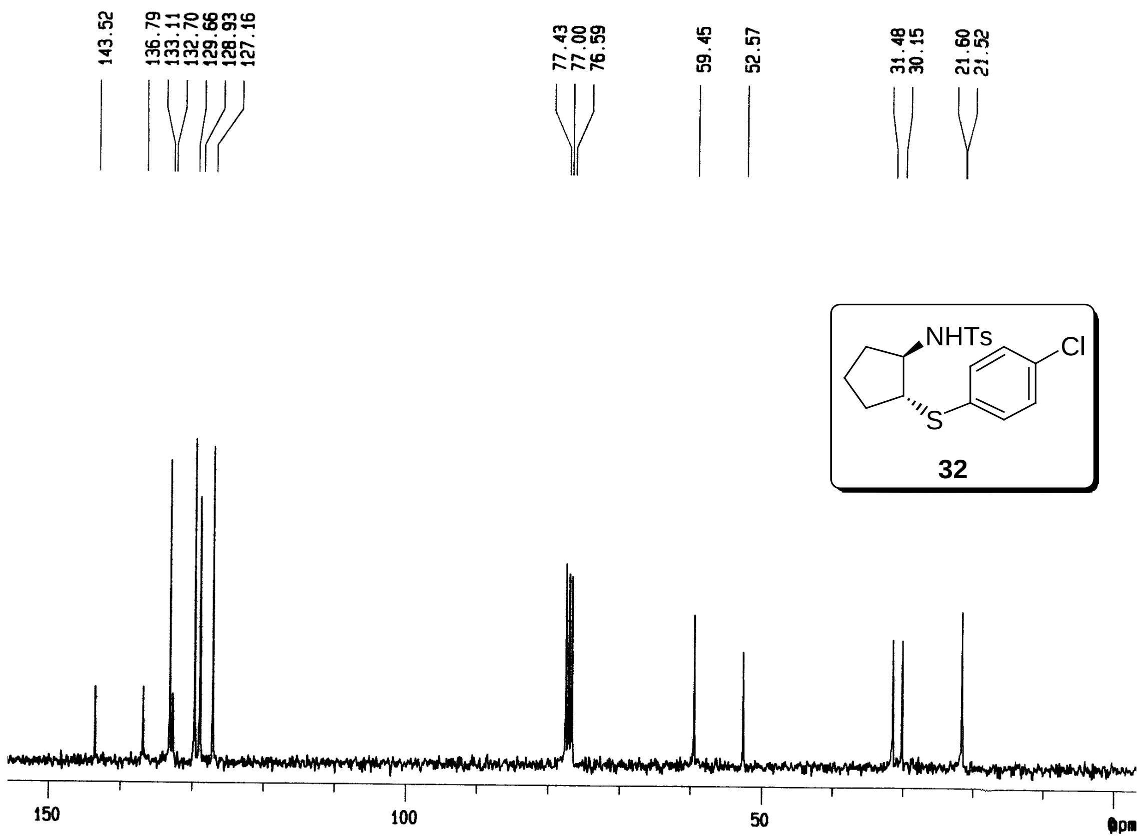


32

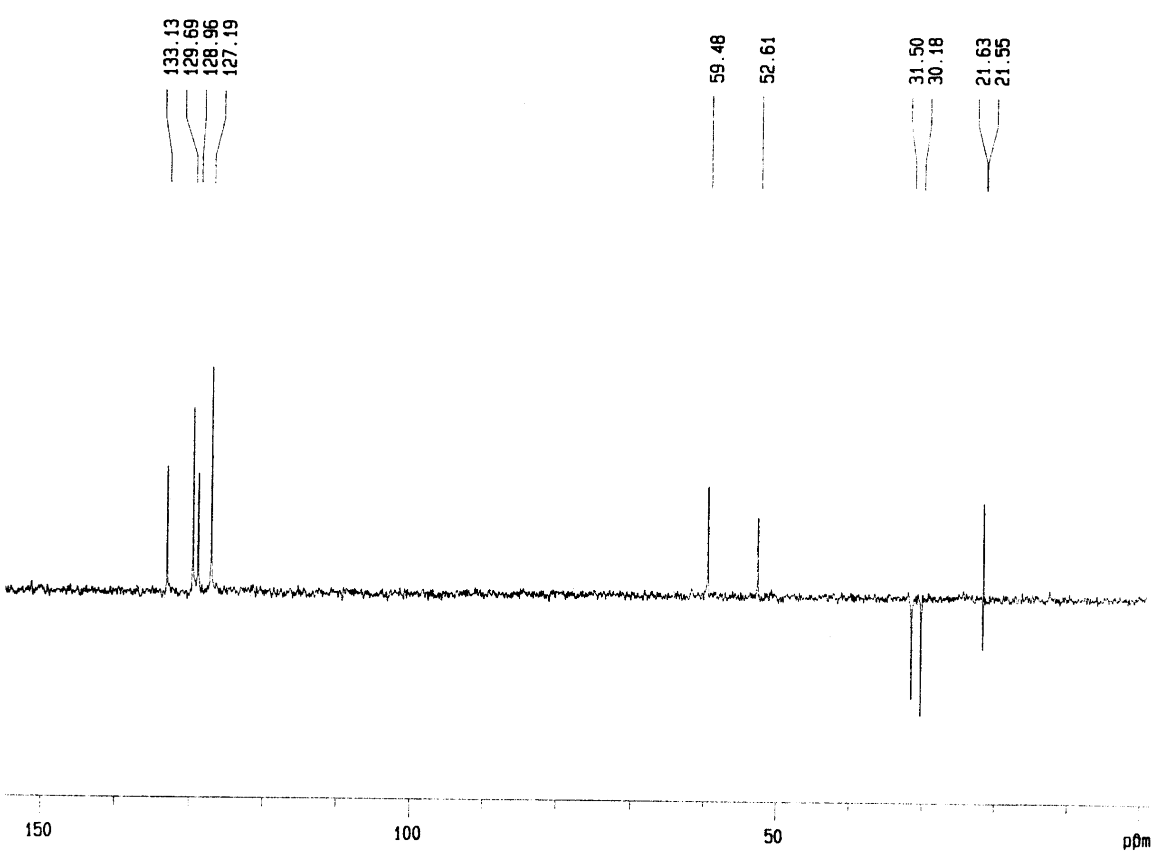
^{1}H NMR – $CDCl_3$ (300 MHz)



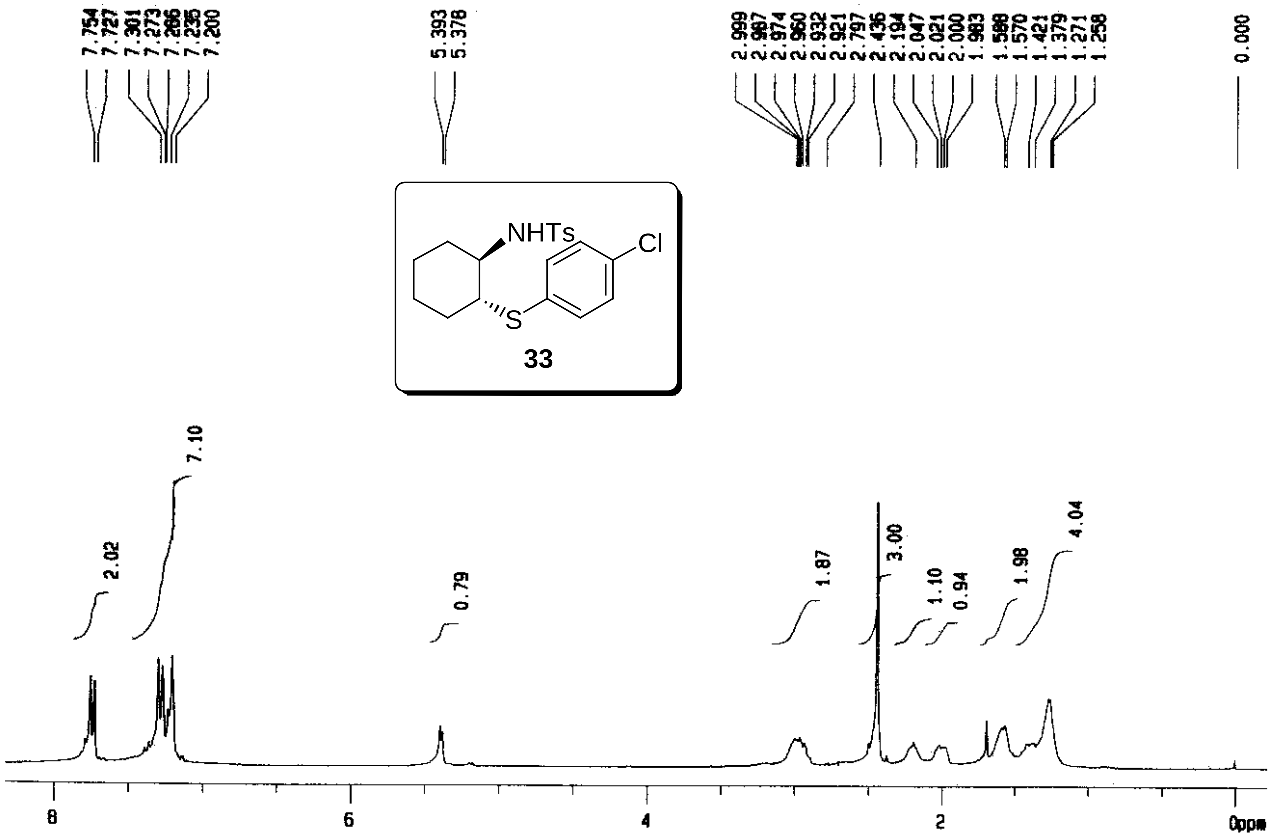
^{13}C NMR – $CDCl_3$ (75 MHz)



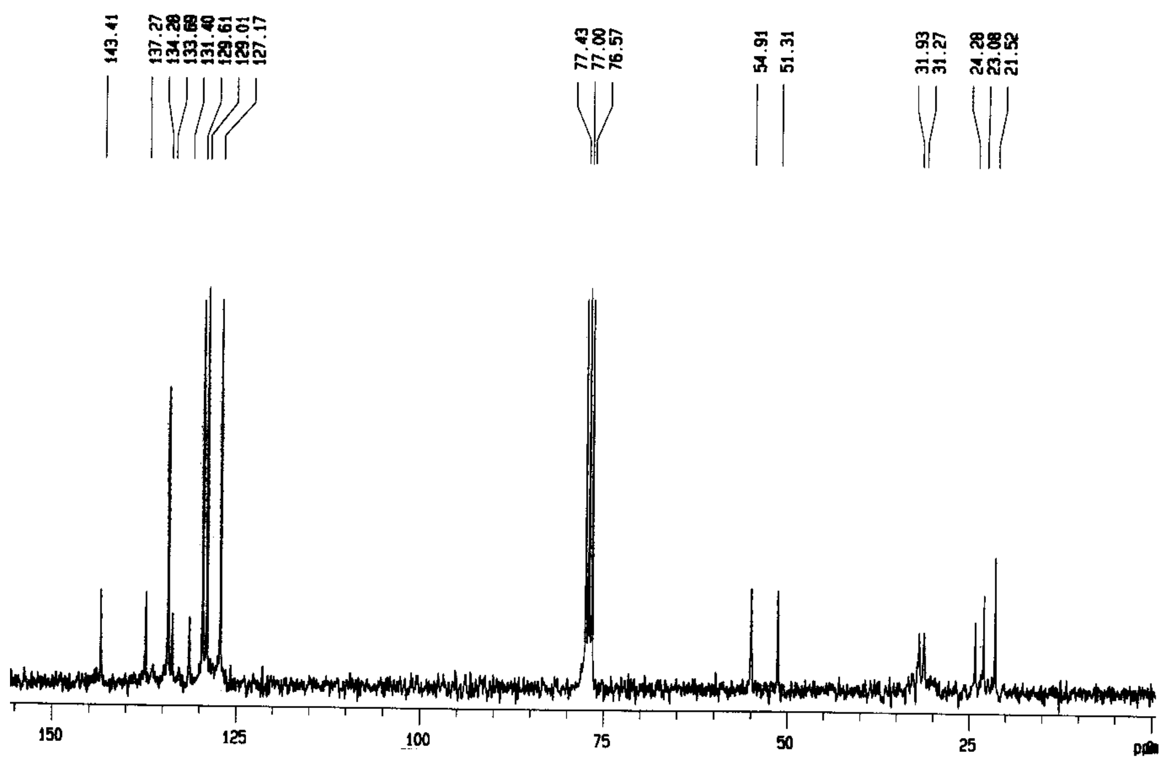
DEPT – $CDCl_3$ (75 MHz)

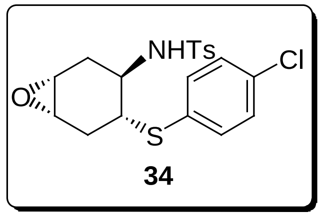


^{1}H NMR – $CDCl_3$ (300 MHz)

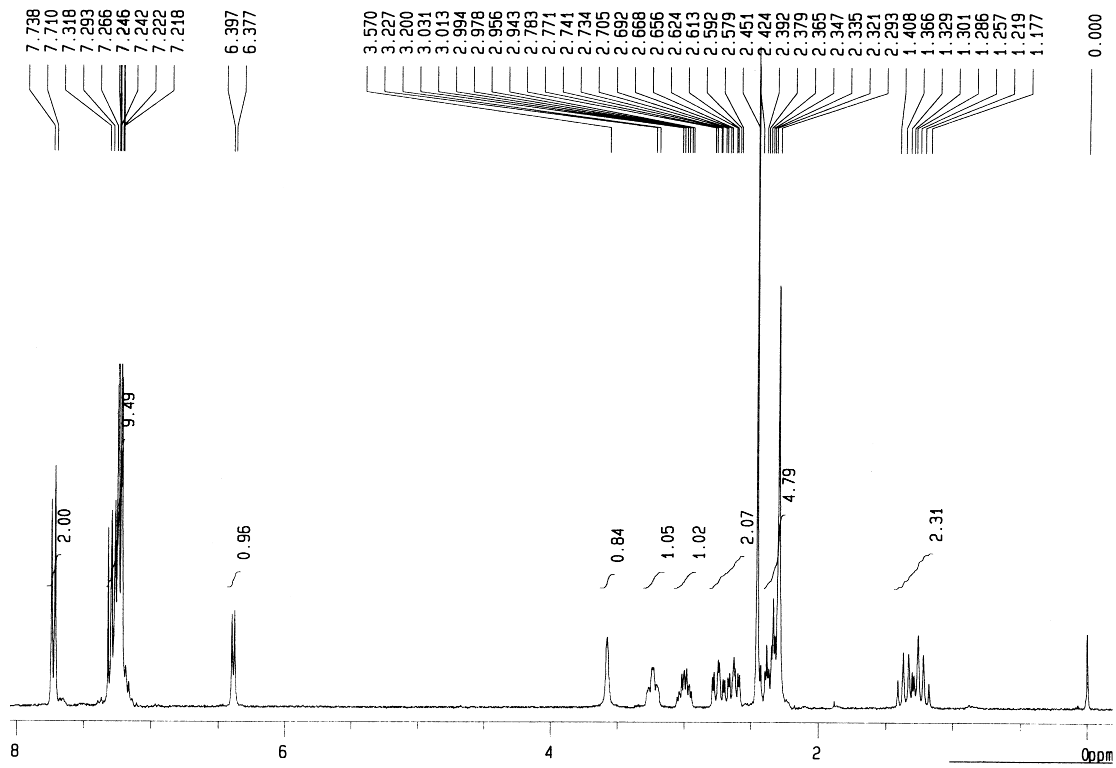


^{13}C NMR – $CDCl_3$ (75 MHz)

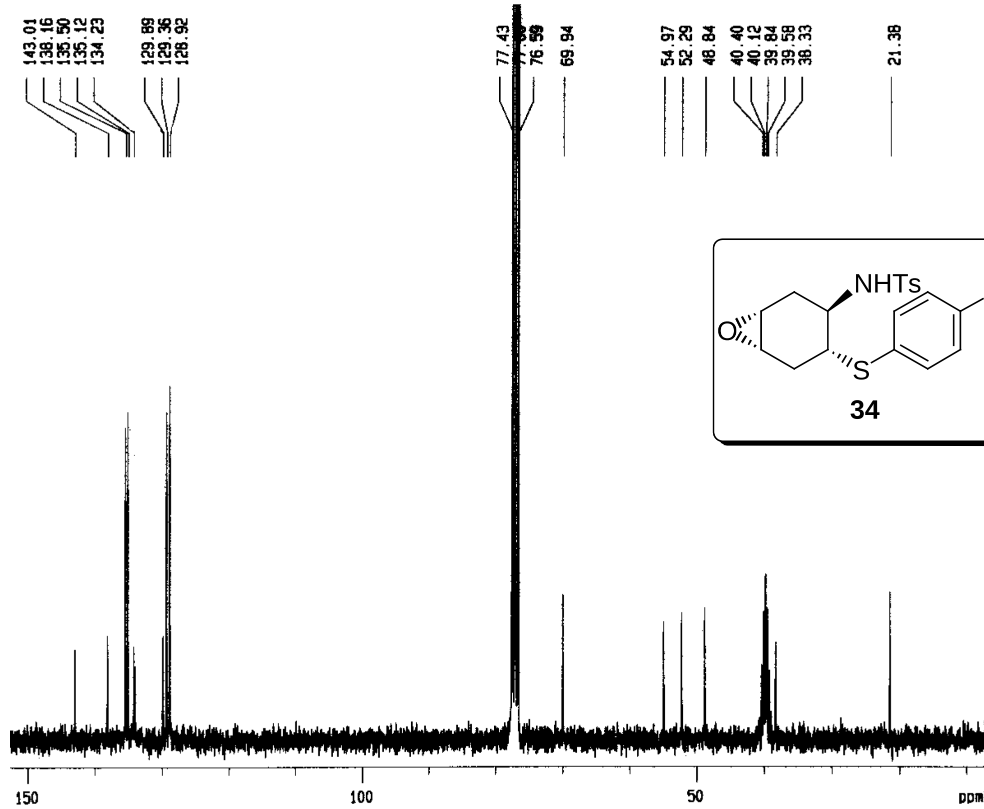




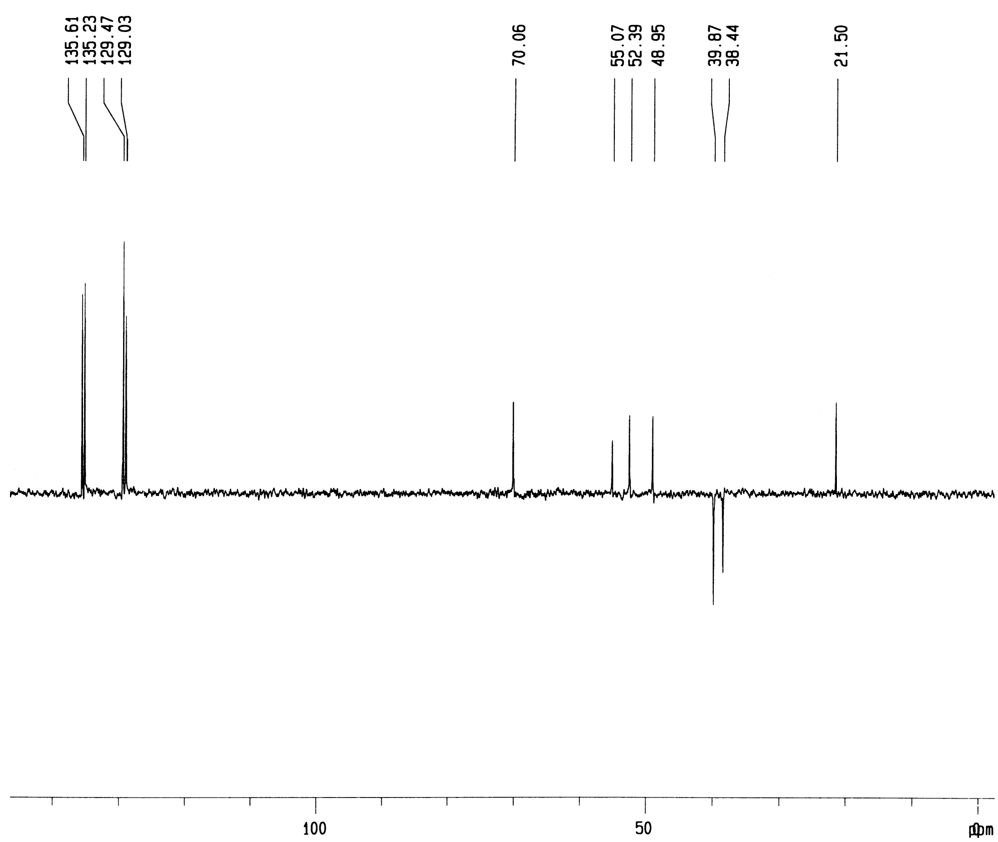
^{1}H NMR – $CDCl_3$/DMSO-d_6 (300 MHz)

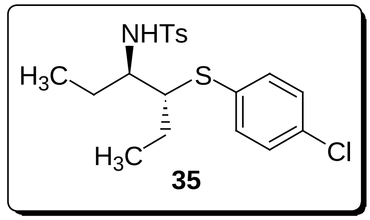


^{13}C NMR – $CDCl_3$/DMSO-d_6 (75 MHz)

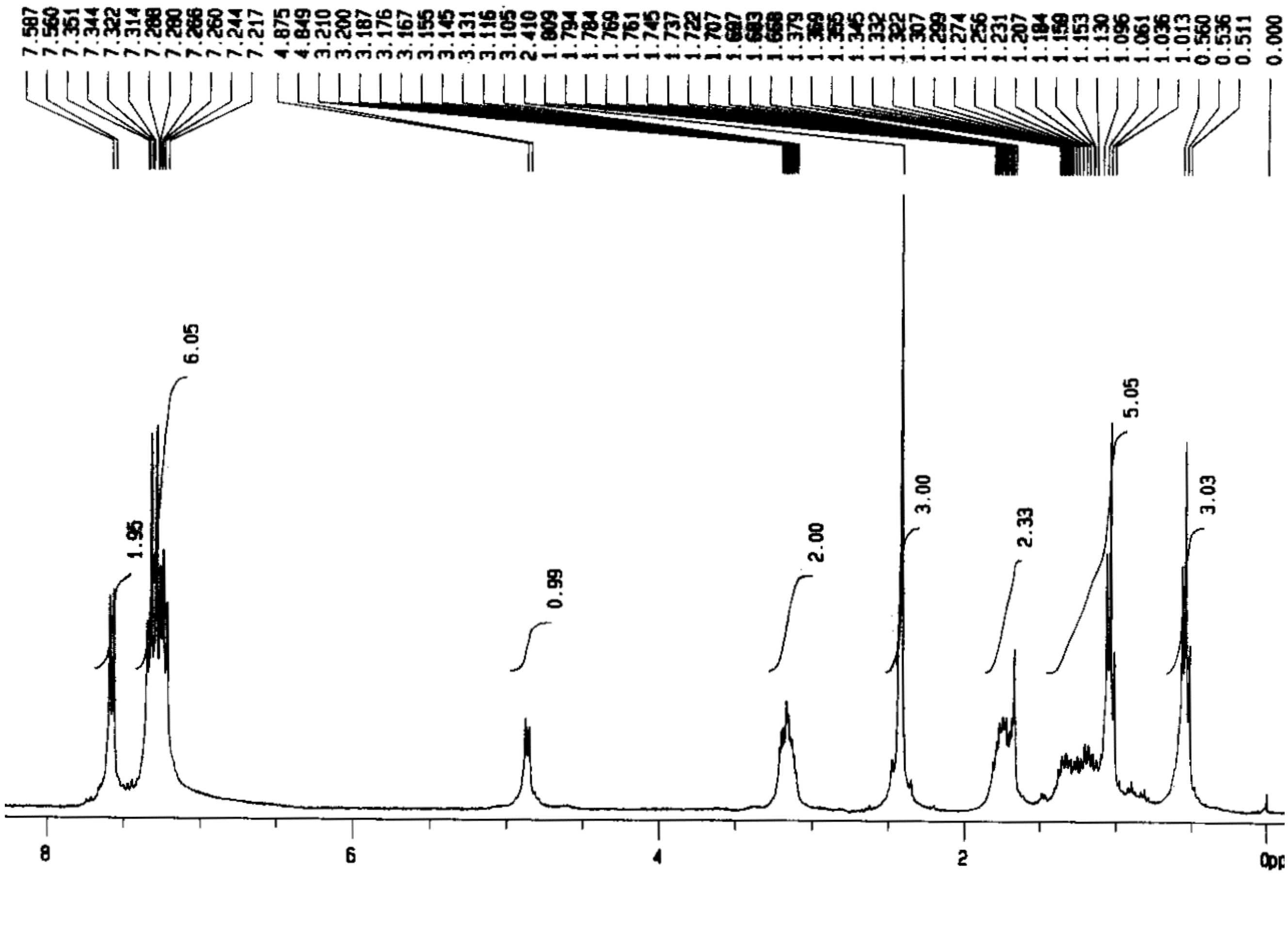


DEPT – $CDCl_3$/DMSO-d_6 (75 MHz)

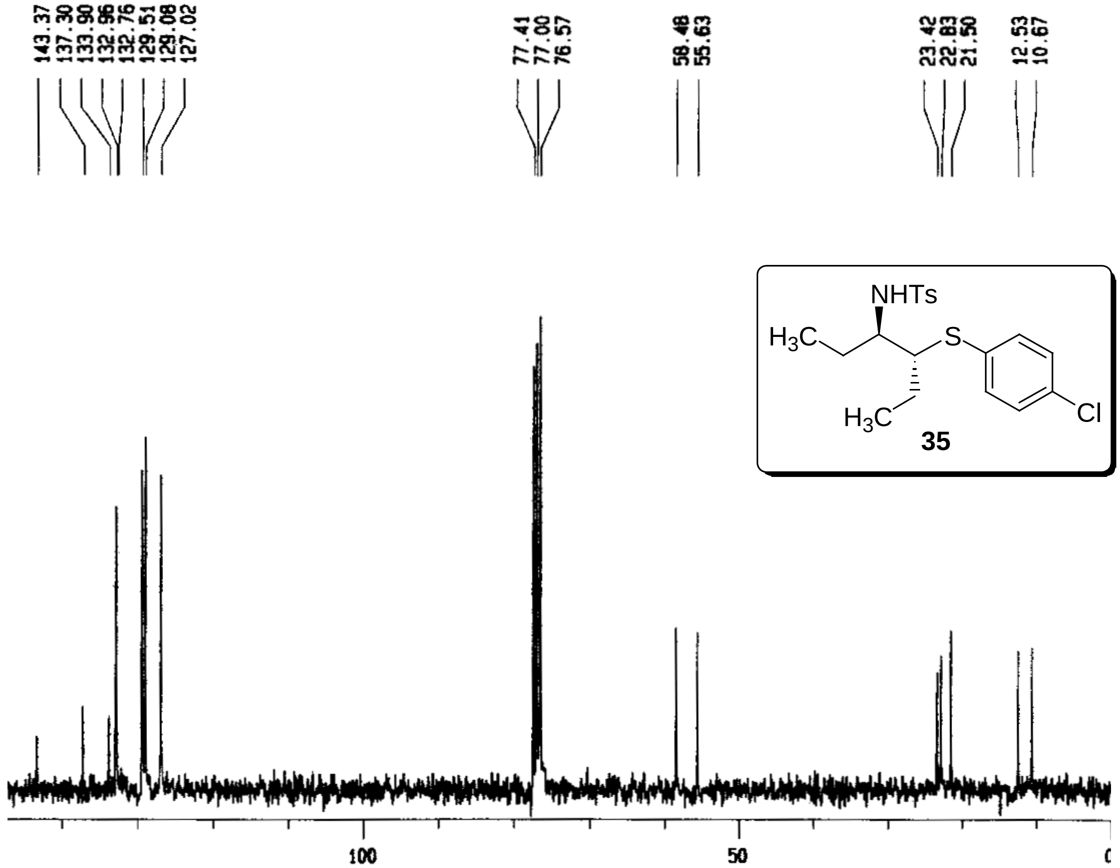




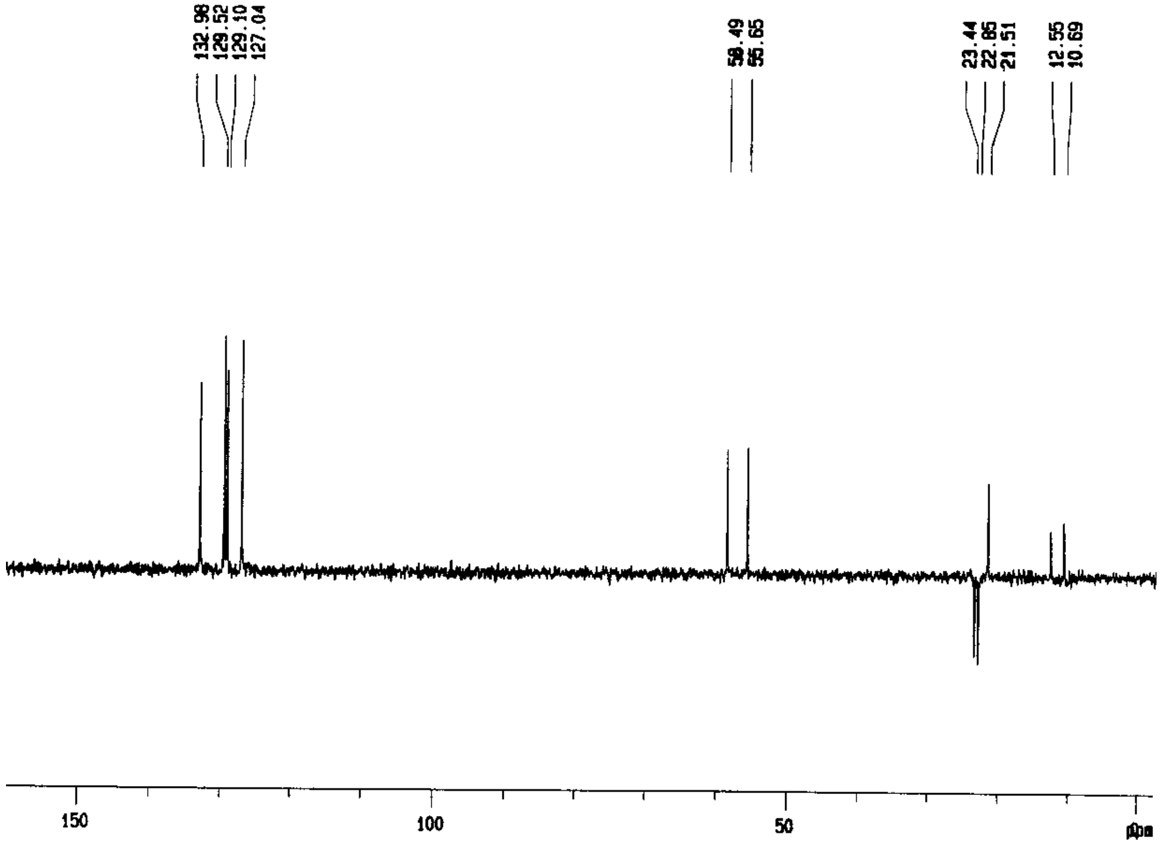
^{1}H NMR – $CDCl_3$ (300 MHz)

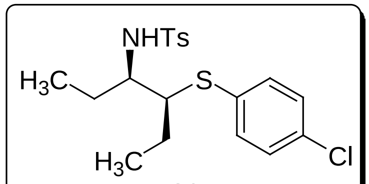


^{13}C NMR – $CDCl_3$ (75 MHz)



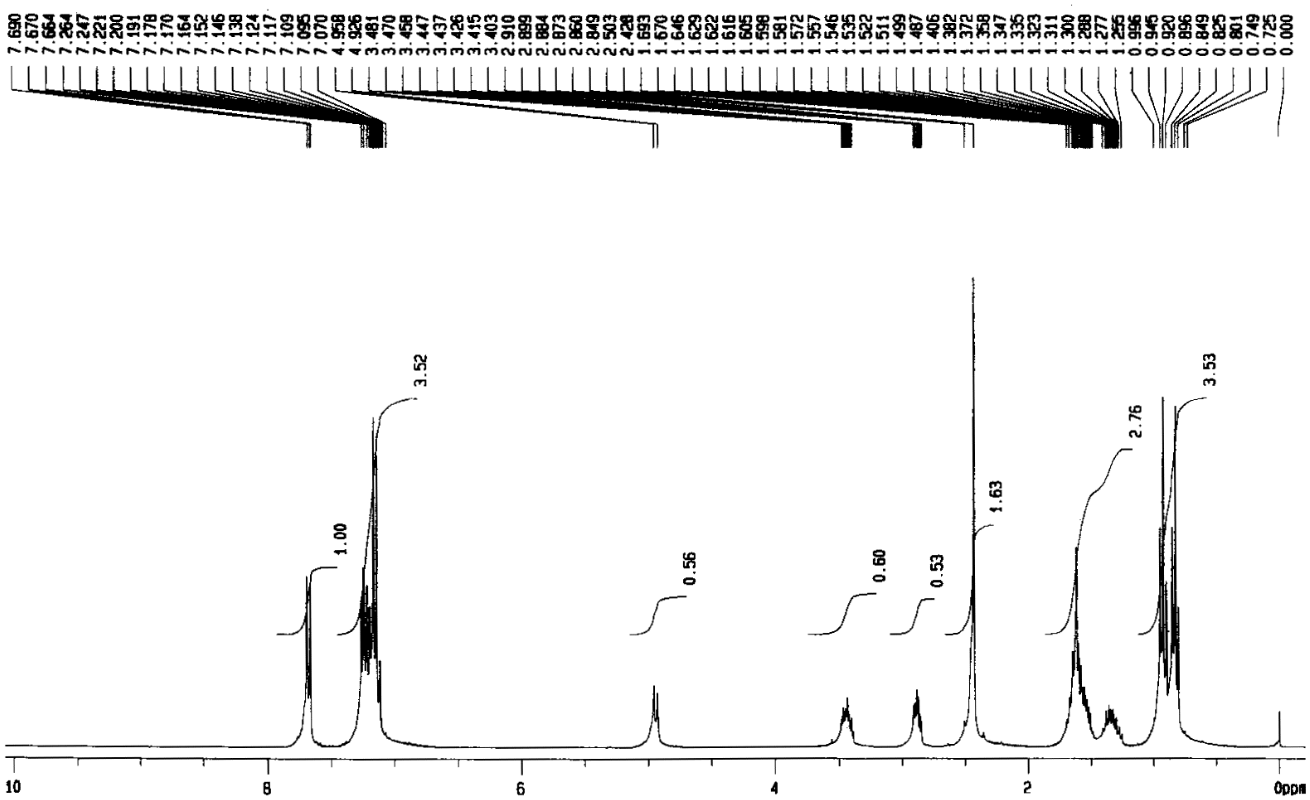
DEPT – $CDCl_3$ (75 MHz)



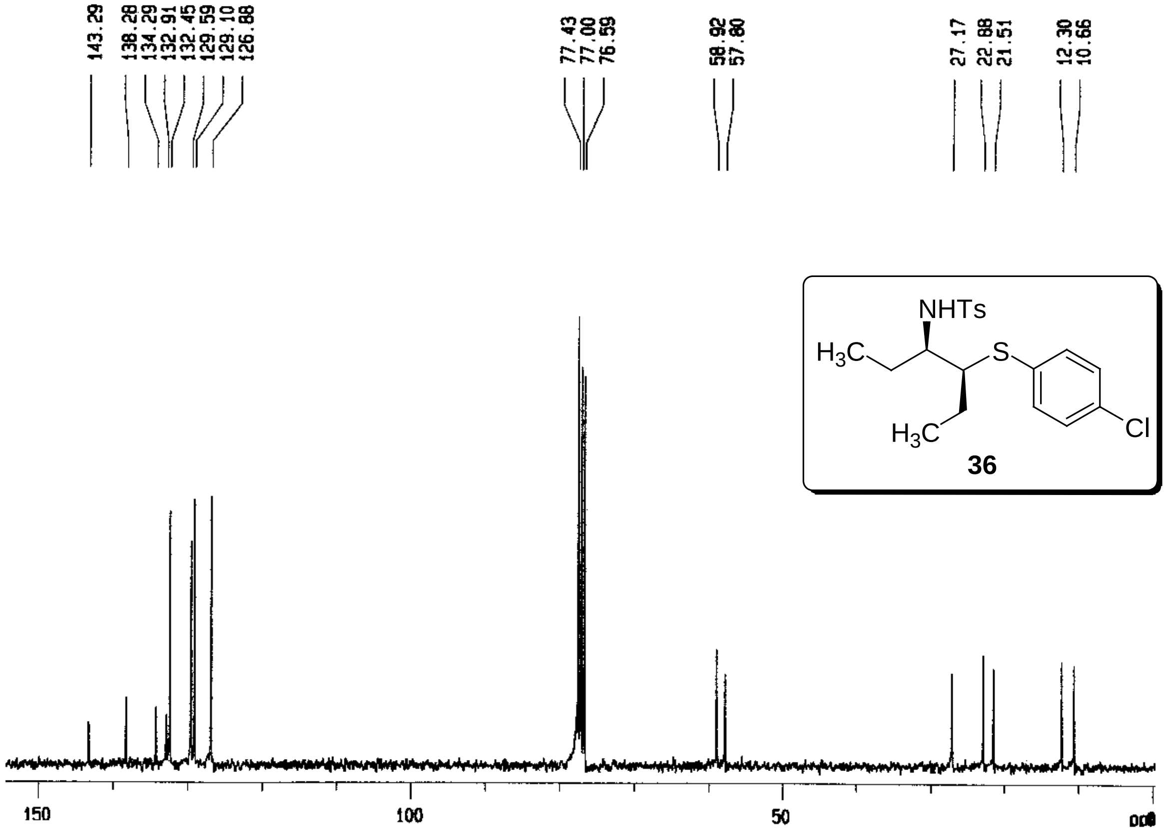


36

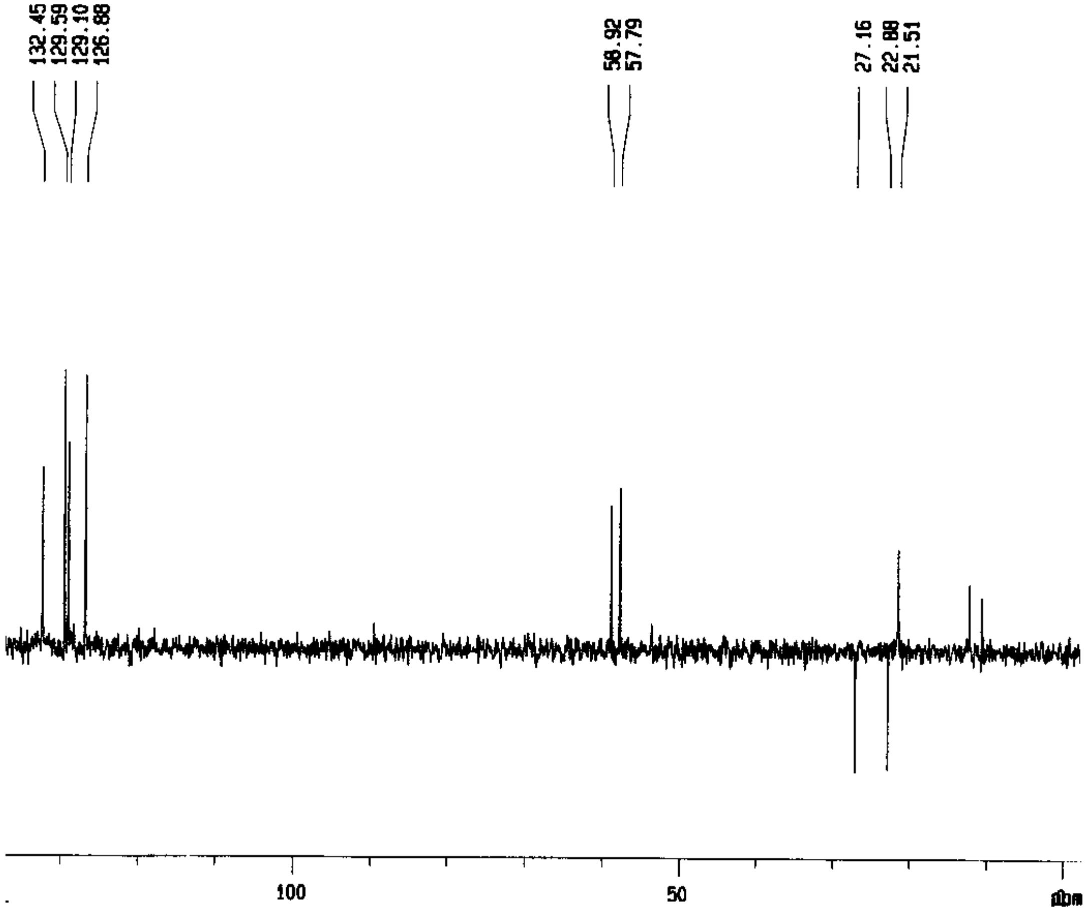
^{1}H NMR – $CDCl_3$ (300 MHz)

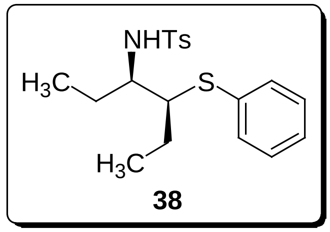


^{13}C NMR – $CDCl_3$ (75 MHz)

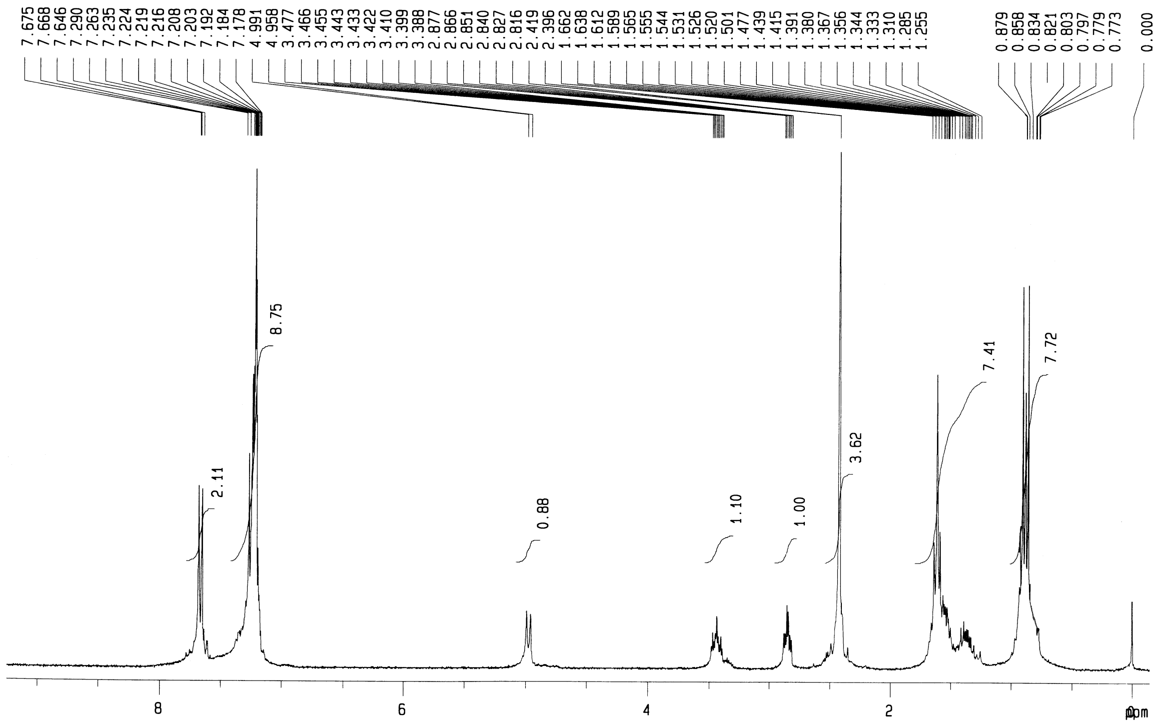


DEPT – $CDCl_3$ (75 MHz)

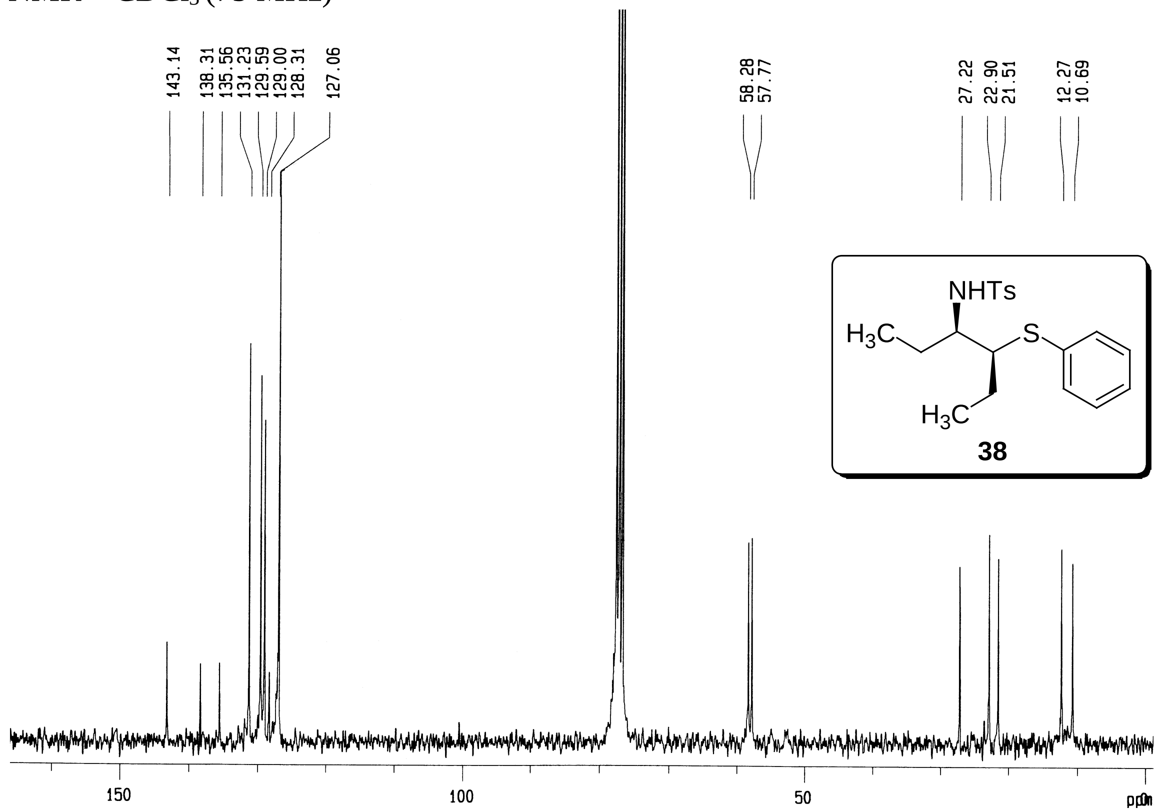




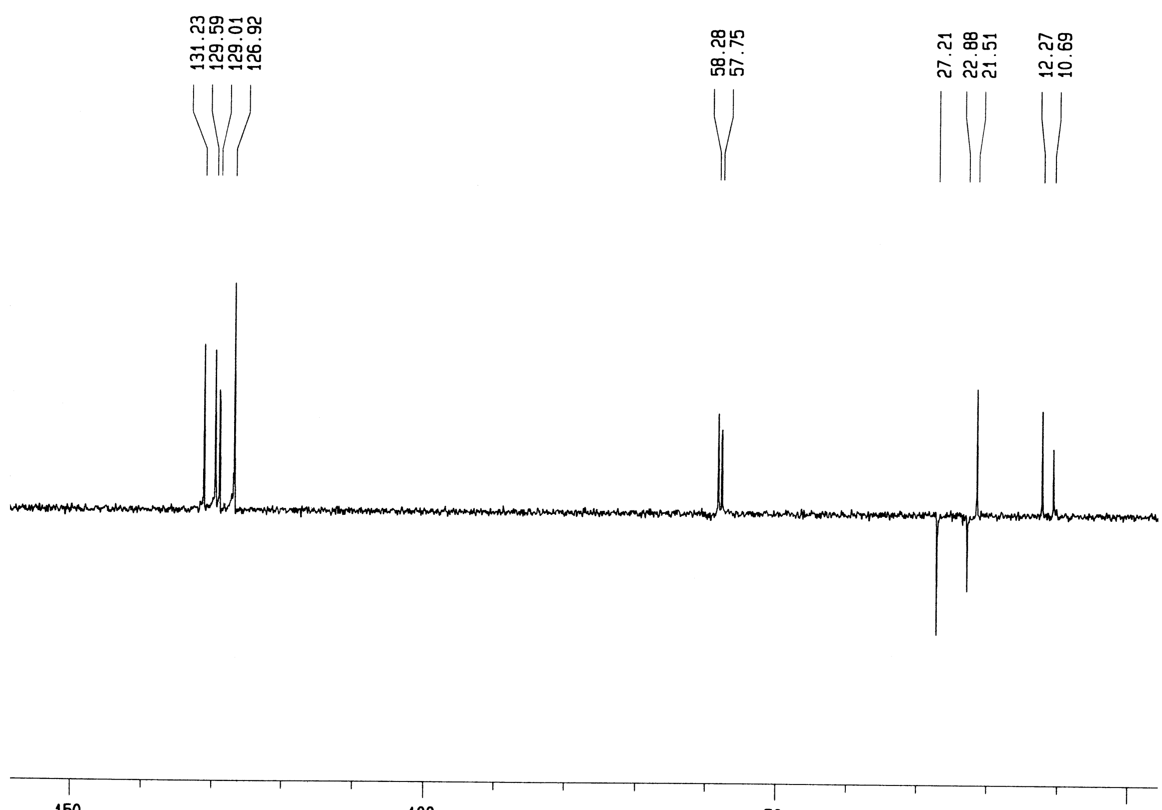
^{1}H NMR – $CDCl_3$ (300 MHz)



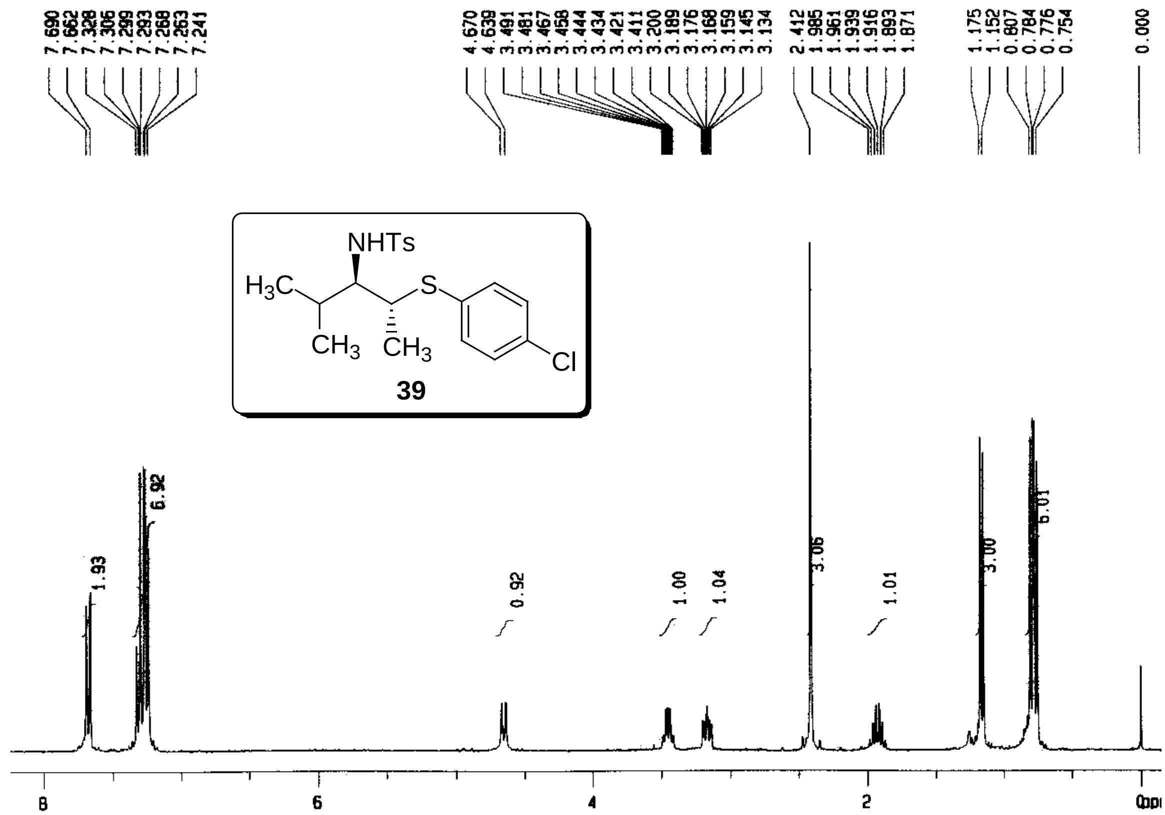
^{13}C NMR – $CDCl_3$ (75 MHz)



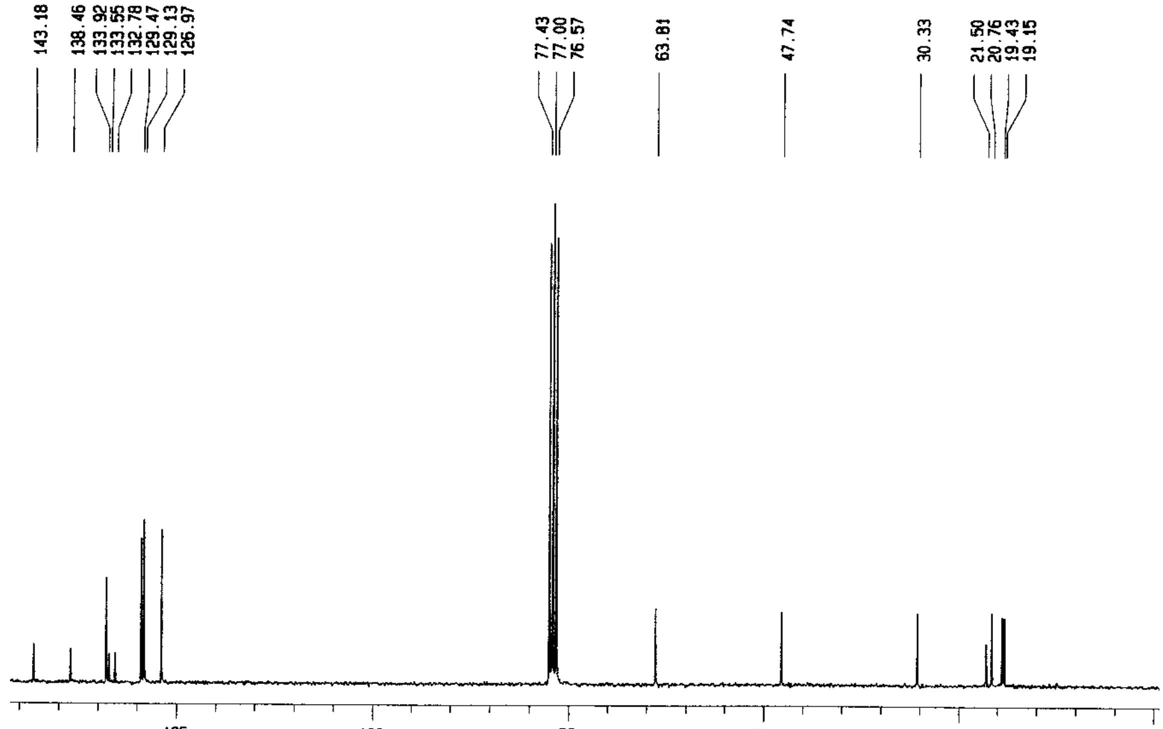
DEPT – $CDCl_3$ (75 MHz)



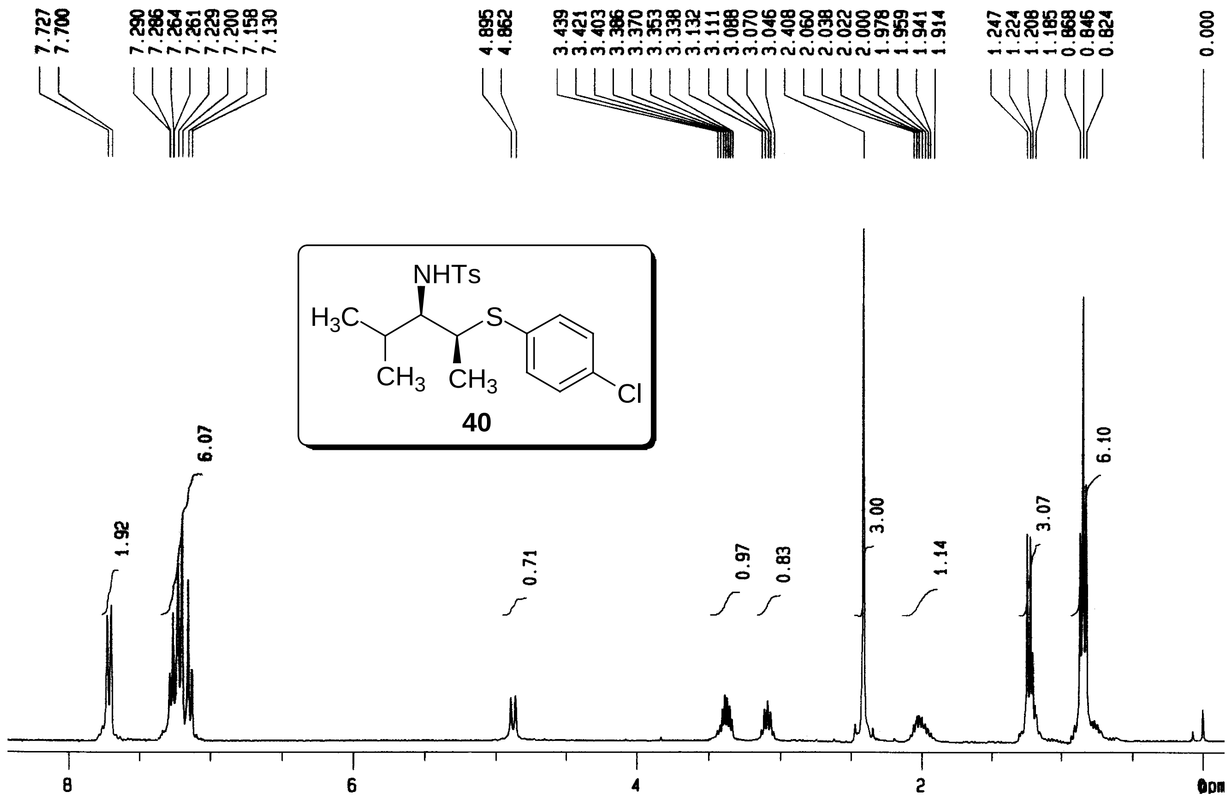
^{1}H NMR – $CDCl_3$ (300 MHz)



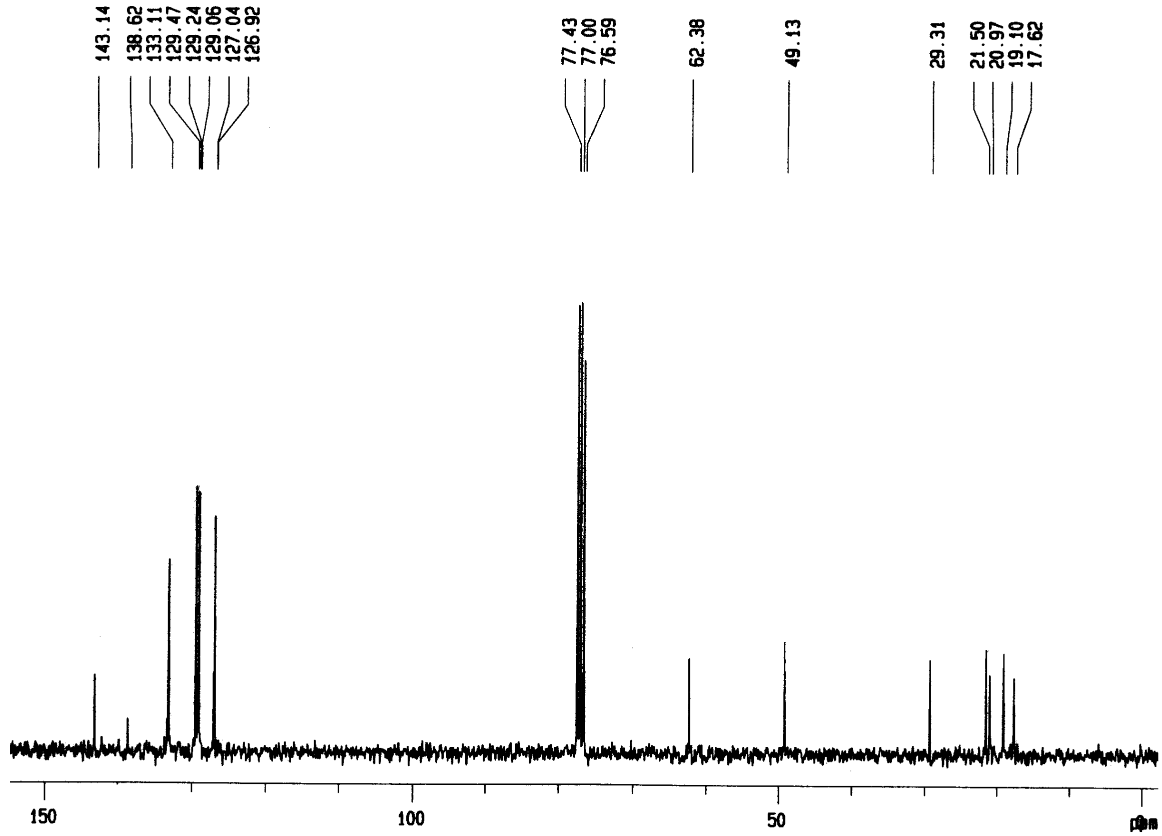
^{13}C NMR – $CDCl_3$ (75 MHz)

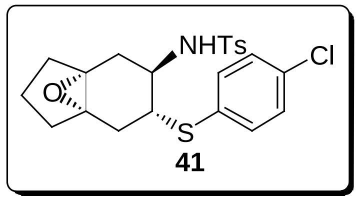


^{1}H NMR – $CDCl_3$ (300MHz)

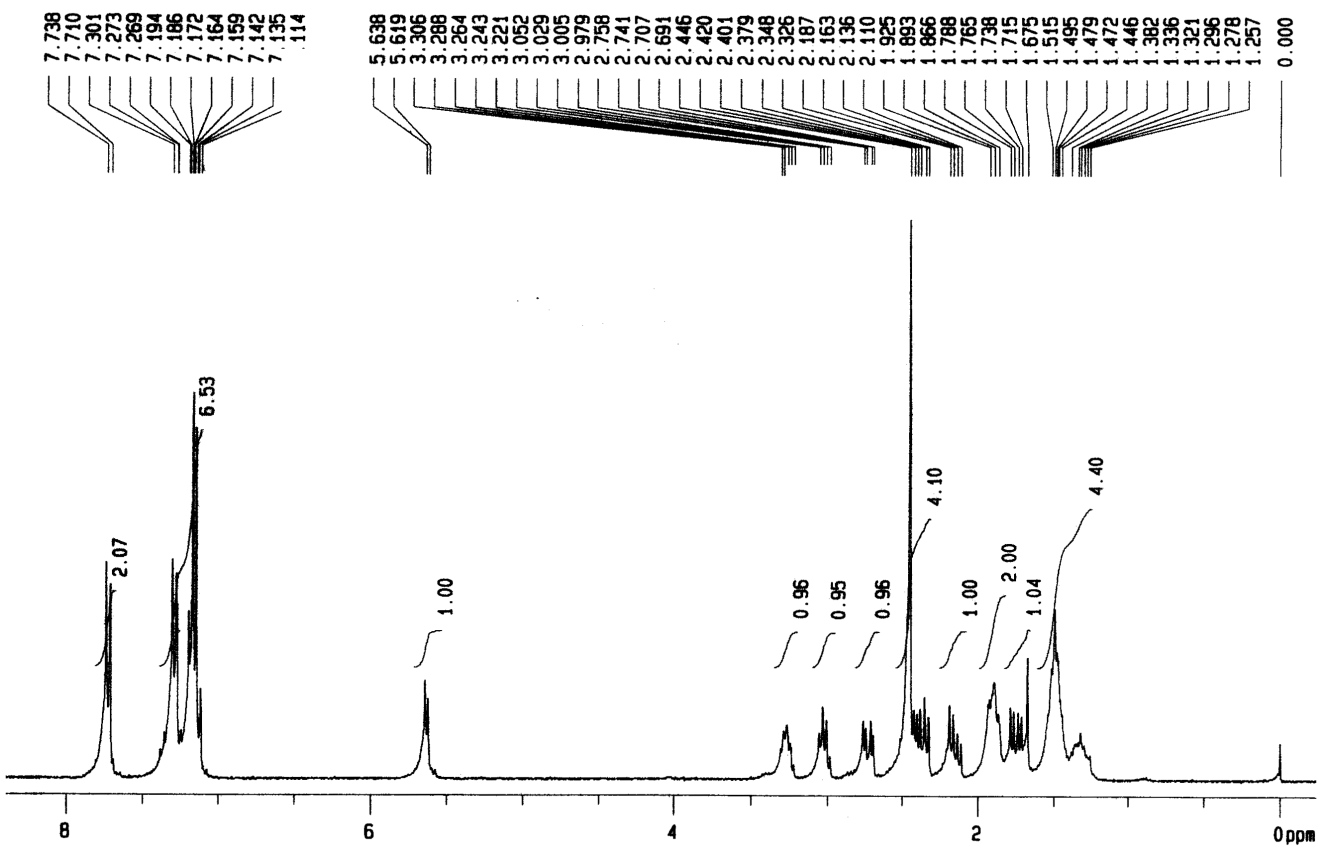


^{13}C NMR – $CDCl_3$ (75 MHz)

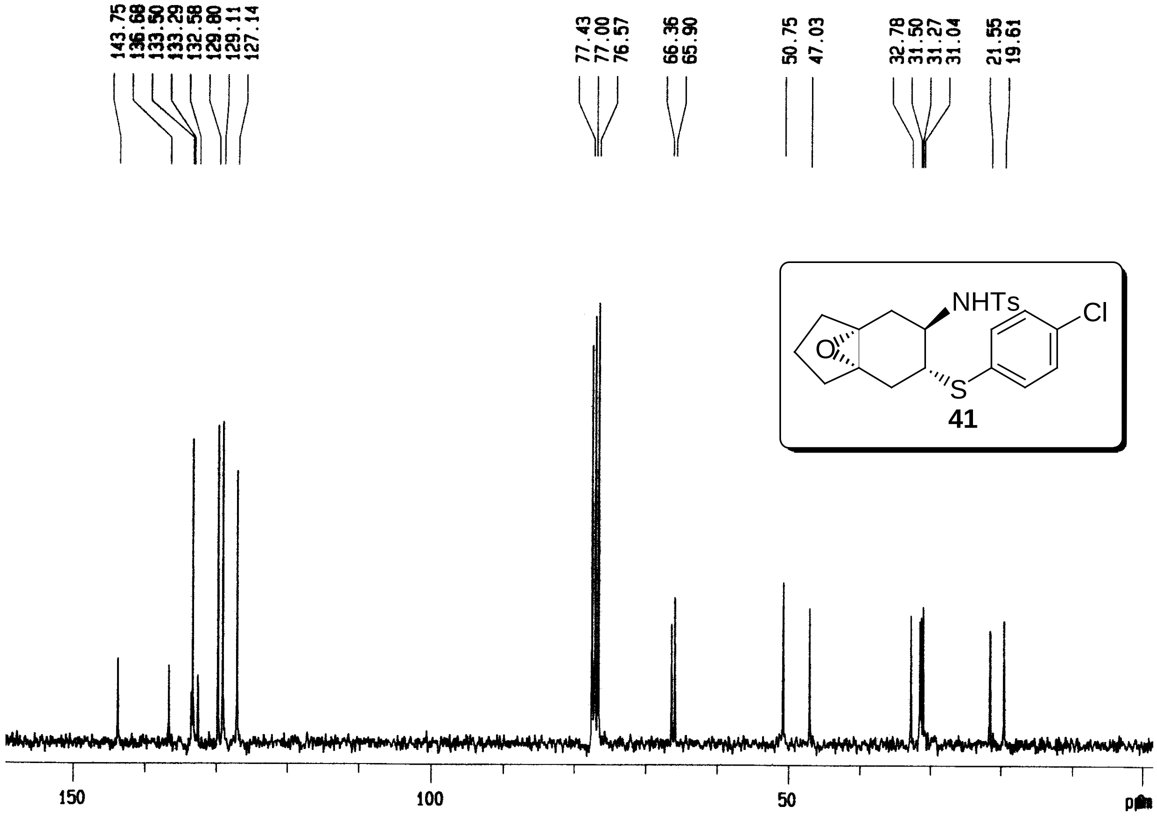




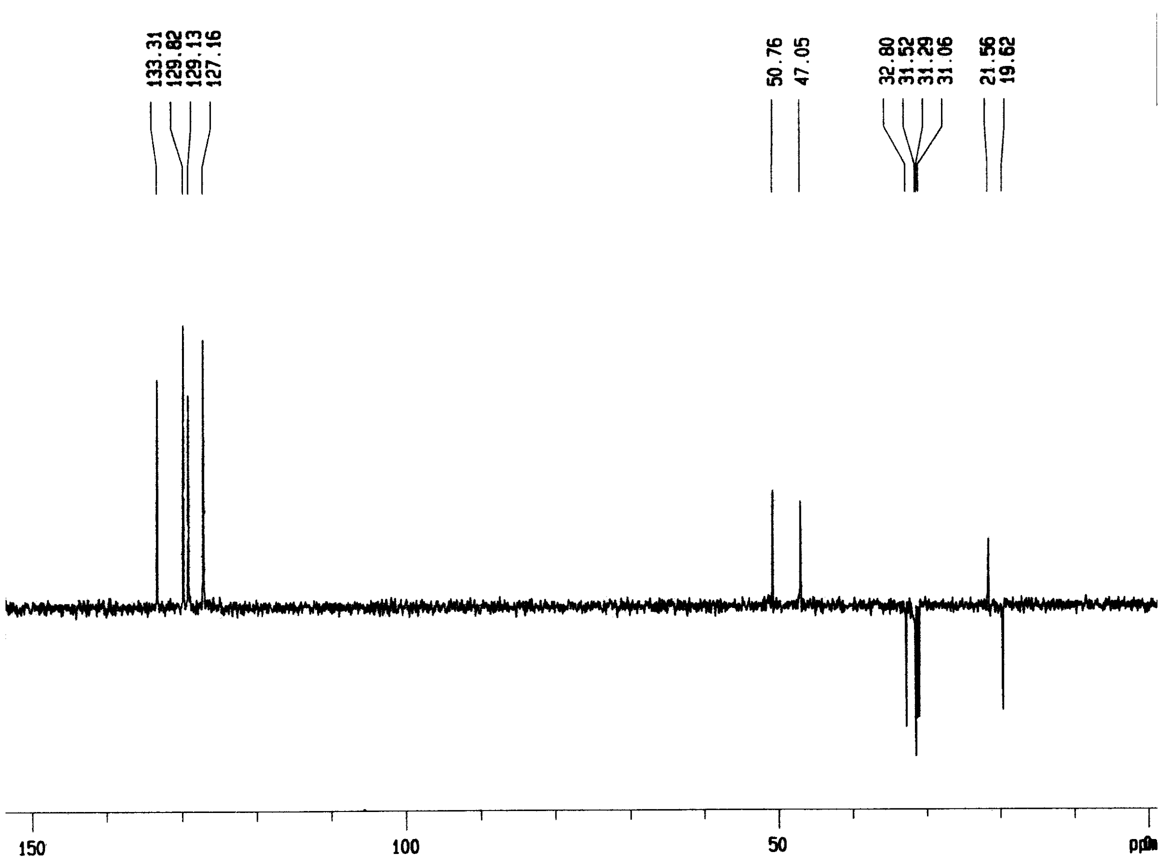
^{1}H NMR – $CDCl_3$ (300 MHz)

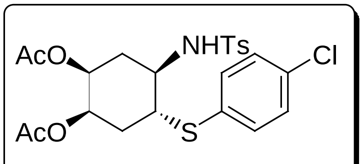


^{13}C NMR – $CDCl_3$ (75 MHz)



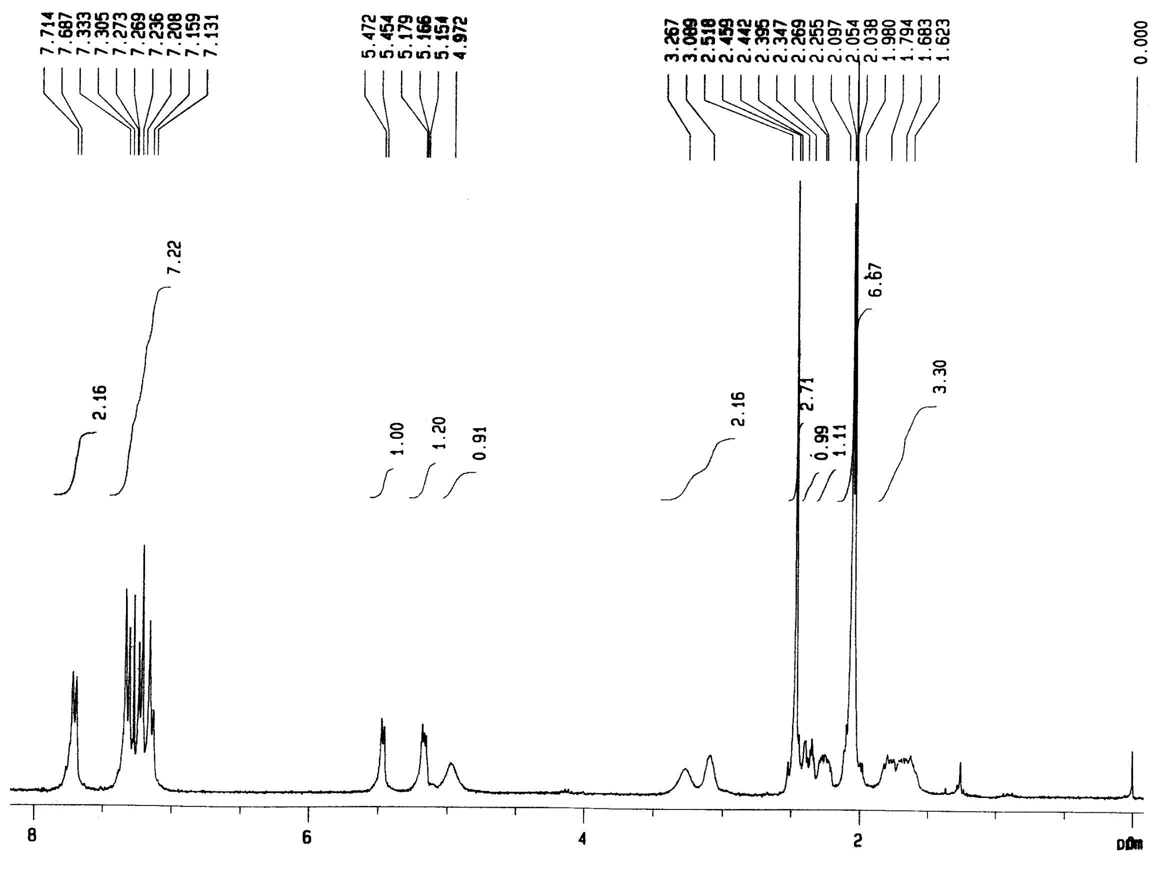
DEPT – $CDCl_3$ (75 MHz)



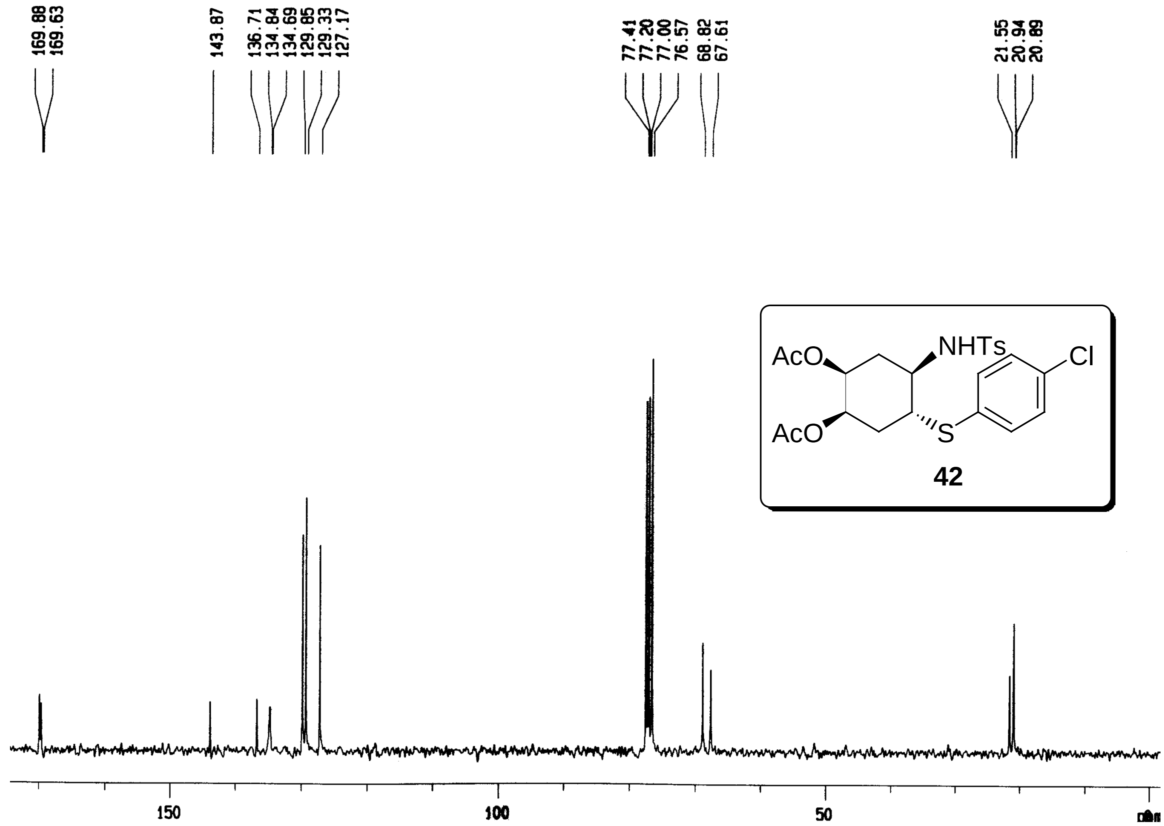


42

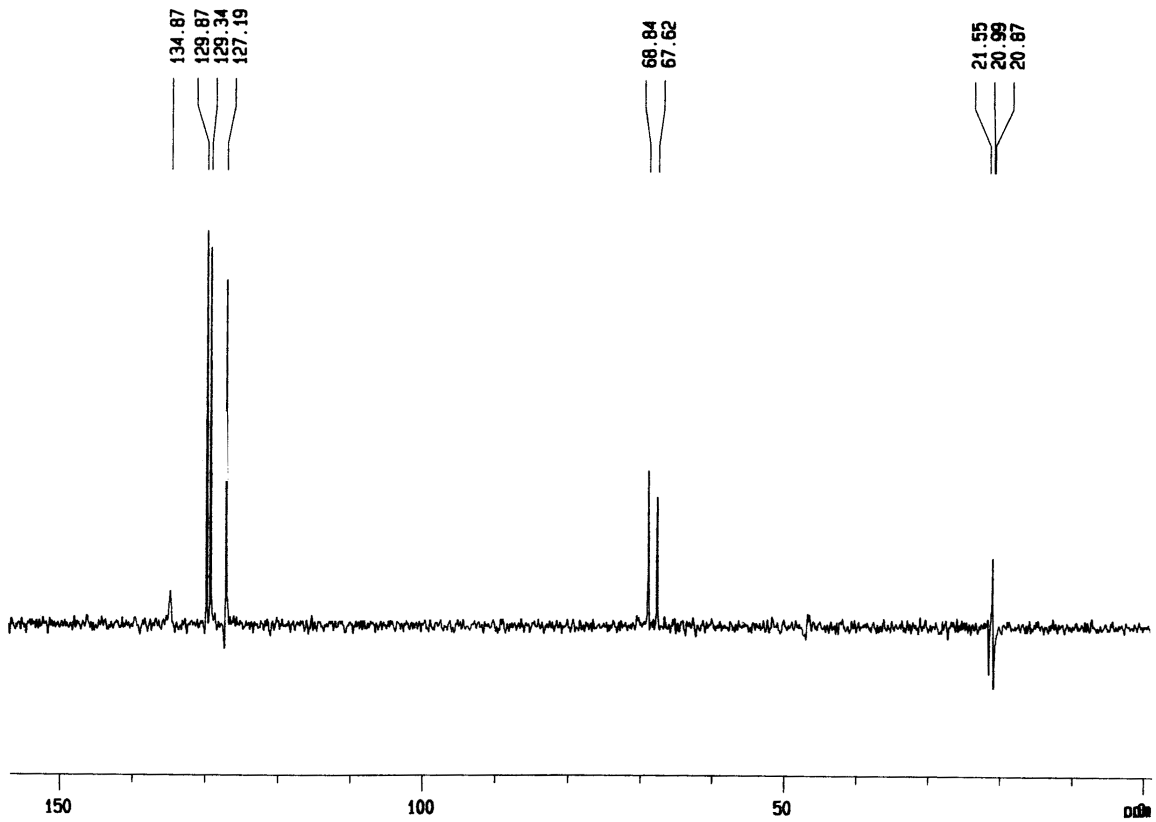
^{1}H NMR – $CDCl_3$ (300 MHz)

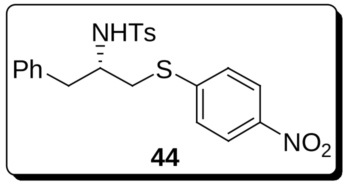


^{13}C NMR – $CDCl_3$ (75 MHz)

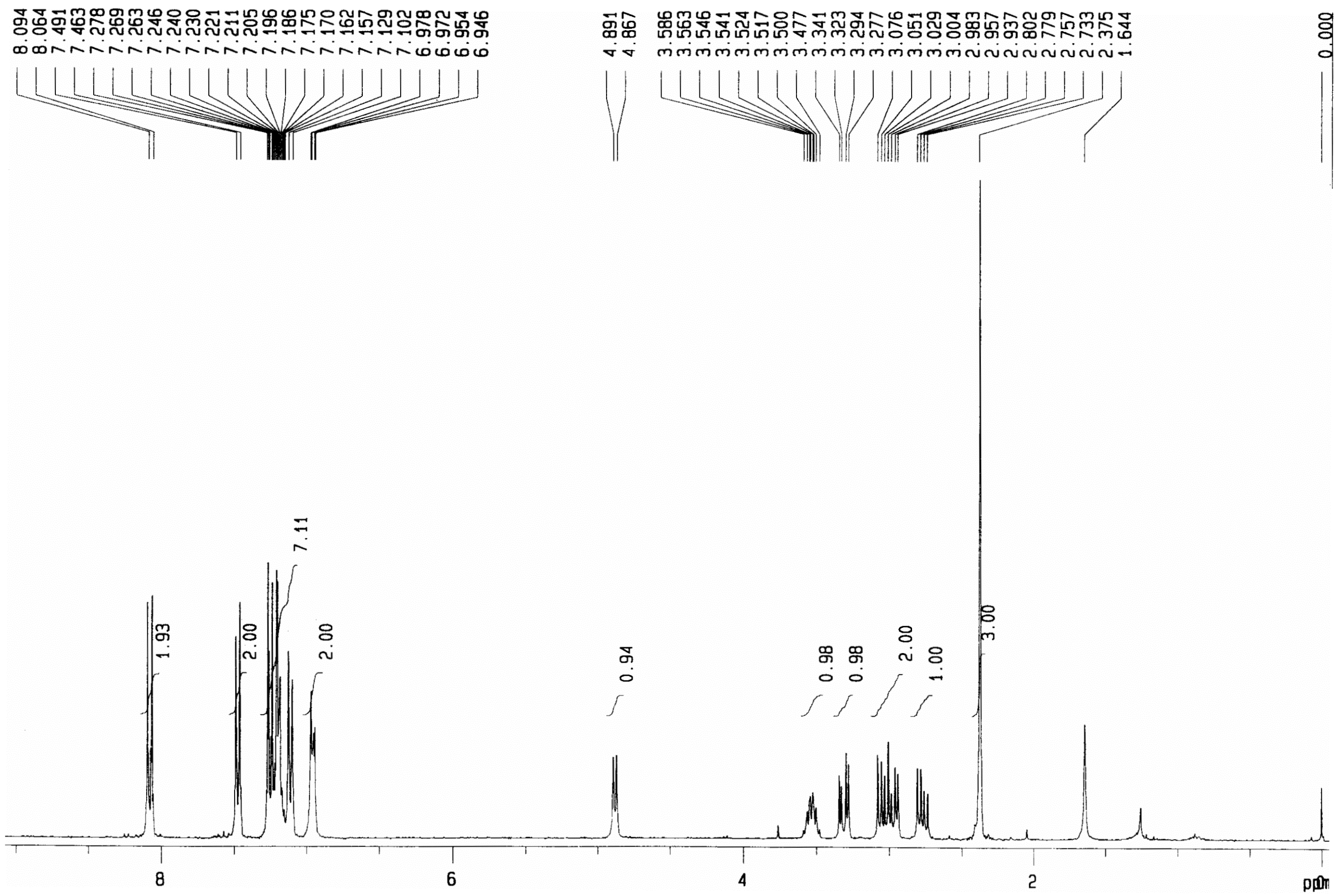


DEPT – $CDCl_3$ (75 MHz)

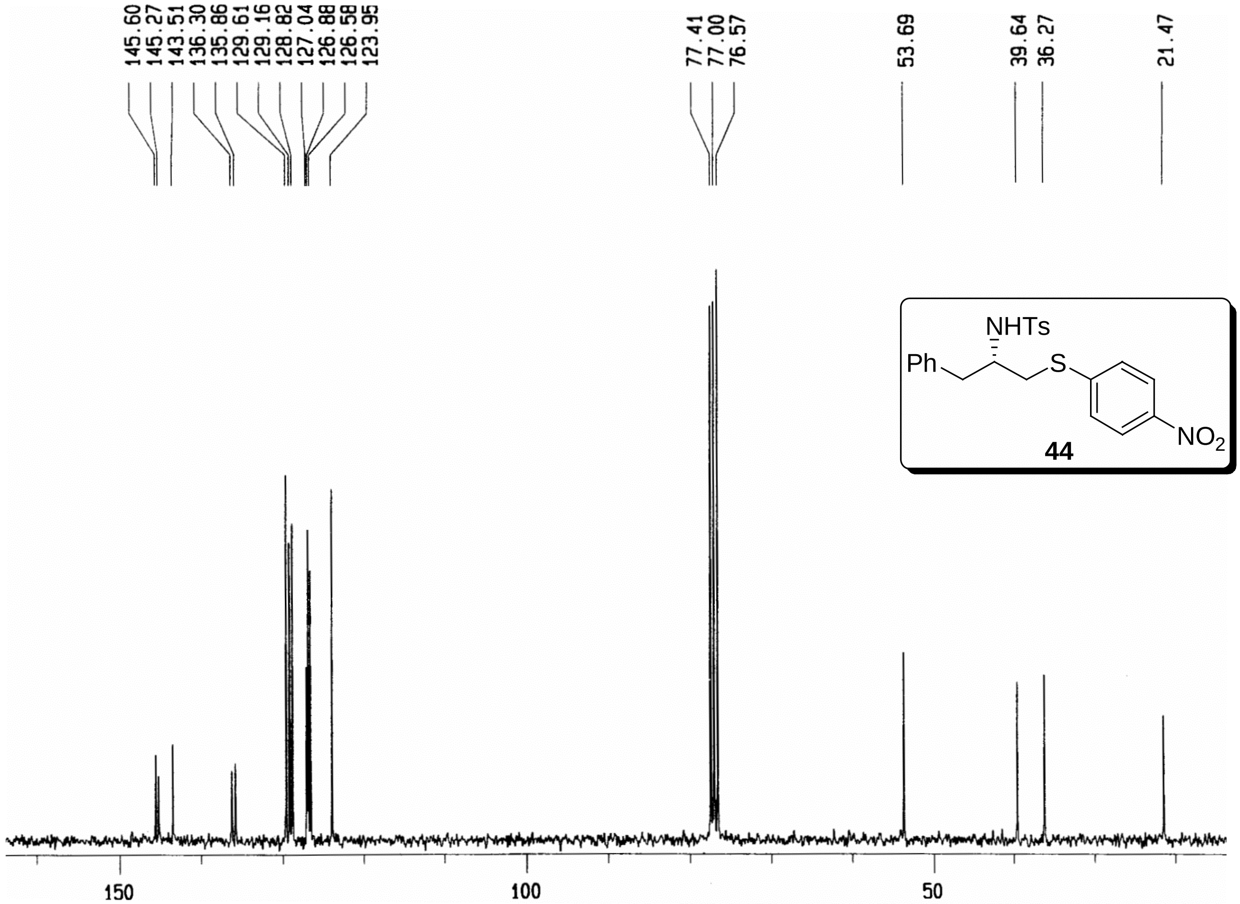




^1H NMR – $CDCl_3$ (300 MHz)



^{13}C NMR – $CDCl_3$ (75 MHz)



DEPT – $CDCl_3$ (75 MHz)