SUPPORTING INFORMATION

Copper catalysed [3+2] cycloaddition with concomitant annulation: Formation of 2,4-diaryl-1,4-oxazepan-7-ones *via* ketenimine route

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Experimental Section

General

Nuclear Magnetic Resonance (^{1}H and ^{13}C NMR) spectra were recorded on a Bruker 300 MHz NMR spectrometer in $CDCl_3$ using TMS as internal standard. Chemical shifts are reported in parts per million (δ), coupling constants (J values) are reported in Hertz (Hz). ^{13}C NMR spectra were routinely run with broadband decoupling. Melting points were determined on a melting point apparatus equipped with a thermometer and were uncorrected. Silica gel-G plates (Merck) were used for TLC analysis with a mixture of petroleum ether (60–80 ^{o}) and ethyl acetate as eluent. Elemental analyses were performed on a Perkin Elmer 2400 Series II Elemental CHNS analyzer.

General procedure for the preparation of compound 3: A mixture of reduced monophenacyl aniline (1 mmol) and potassium carbonate (1 mmol) in DMF (3 mL) was stirred well for 10 mins. Then propargyl bromide (2 mmol) was added and stirred for 2 h. After completion of the reaction (TLC), the mixture was poured into ice, extracted with ethyl acetate, concentrated under vacuum and the viscous liquid obtained was subjected for purification through column chromatography using petroleum ether/ethyl acetate mixture (9:1; v/v) as eluent to get the pure product.

General procedure for the preparation of compound 6: A mixture of alkyne 3 (1 mmol) and tosyl azide (1.2 mmol), copper (I) salt (10 mol %) and triethylamine (2 mmol) in dichloromethane (10 mL) at room temperature was vigorously stirred for 15-30 mins. After completion of the reaction (monitored by TLC), the mixture was washed with water (2 x 20 mL) and dried over sodium sulphate and concentrated under vacuum. Then the crude residue was subjected for purification through column chromatography using petroleum ether/ ethyl acetate mixture (9:1; v/v) as eluent to get the pure product.

Analytical Data

1-Phenyl-2-(phenyl(prop-2-ynyl)amino)ethanol (3a)

Isolated as viscous liquid ; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.25 (t, 1H, *J* = 2.4 Hz, CH), 2.69 (s, 1H, OH), 3.44 (dd, 1H, *J* = 15.0, 9.3 Hz, CH_2), 3.65 (dd, 1H, *J* = 15.0, 3.6 Hz, CH_2), 4.00 - 4.16 (m, 2H, CH_2), 5.01 - 5.03 (m, 1H, CH), 6.87 (t, 1H, *J* = 7.5 Hz, Ar-H), 6.98 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.27 - 7.35 (m, 2H, Ar-H), 7.37 - 7.47 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 40.7, 59.5, 71.3, 72.2, 79.7, 114.2, 118.4, 125.6, 127.5, 128.2, 128.9, 141.5, 147.9. Anal. Calcd for $C_{17}H_{17}NO$: C, 81.24; H, 6.82; N, 5.57. Found C, 81.17; H, 6.74; N, 5.49%.

1-Phenyl-2-(prop-2-ynyl(p-tolyl)amino)ethanol (3b)

Isolated as viscous liquid ; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.23 (t, 1H, *J* = 2.4 Hz, CH); 2.28 (s, 3H, CH_3), 2.82 (s, 1H, OH), 3.34 (dd, 1H, *J* = 14.7, 9.6 Hz, CH_2), 3.59 (dd, 1H, *J* = 14.7, 3.3 Hz, CH_2), 3.96 - 4.09 (m, 2H, CH_2), 4.95 (dd, 1H, *J* = 9.6, 3.3 Hz, CH_2), 6.91 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.10 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.29 - 7.45 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 20.3, 41.5, 60.2, 71.3, 72.5, 79.7, 115.6, 125.8, 127.6, 128.4, 128.6, 129.7, 141.6, 146.1. Anal. Calcd for $C_{18}H_{19}NO$: C, 81.47; H, 7.22; N, 5.28. Found C, 81.59; H, 7.11; N, 5.19%.

2-((4-Methoxyphenyl)(prop-2-ynyl)amino)-1-phenylethanol (3c)

Isolated as viscous liquid ; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.26-2.27 (m, 1H, CH); 3.16 (s, 1H, OH), 3.23 (dd, 1H, *J* = 14.1, 9.9 Hz, CH_2), 3.57 (dd, 1H, *J* = 14.1, 3.3 Hz, CH_2), 3.80 (s, 3H, OCH_3), 4.01 (m, 2H, CH_2), 4.89 (dd, 1H, *J* = 9.6, 2.7 Hz, CH_2), 6.89 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.04 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.28 - 7.46 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.9, 55.2, 60.3, 70.6, 72.4, 79.4, 114.2, 117.7, 125.6, 127.2, 128.0, 141.8, 142.5, 153.2 Anal. Calcd for $C_{18}H_{19}NO_2$: C, 76.84; H, 6.81; N, 4.98. Found C, 76.72; H, 6.72; N, 4.93%.

2-((4-Fluorophenyl)(prop-2-ynyl)amino)-1-phenylethanol (3d)

Isolated as viscous liquid ; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.23 (t, 1H, *J* = 2.4 Hz, CH), 2.90 (s, 1H, OH), 3.36 (dd, 1H, *J* = 14.4, 9.3 Hz, CH_2), 3.53 (dd, 1H, *J* = 3.6, 14.4 Hz, CH_2), 3.90 - 4.03 (m, 2H, CH_2), 4.87 - 4.90 (m, 1H, CH_2), 6.88 - 6.99 (m, 4H, Ar-H), 7.27 - 7.41 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 42.0, 60.46, 71.3, 72.9, 79.3, 115.6, 117.3, 125.8, 127.9, 128.5, 141.4, 145.1, 157.0. Anal. Calcd for $C_{17}H_{16}FNO$: C, 75.82; H, 5.99; N, 5.20; Found C, 75.75; H, 6.08; N, 5.13%.

2-((4-Bromophenyl)(prop-2-ynyl)amino)-1-phenylethanol (3e)

Isolated as viscous liquid ; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.70 (t, 1H, J = 2.1 Hz, CH); 2.82 (s, 1H, OH), 3.47 (dd, 1H, J = 15.0, 8.7 Hz, CH_2), 3.60 (dd, 1H, J = 15.0, 3.9 Hz, CH_2), 3.96 - 4.06 (m, 2H, CH_2), 4.97 - 5.01 (m, 1H, CH_2), 6.83 (d, 2H, J = 9.0 Hz, Ar-H), 7.34 - 7.46 (m, 7H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 40.5, 59.3, 71.3, 72.2, 79.2, 115.2, 125.6, 127.4, 128.1*, 131.4, 141.8, 146.9. Anal. Calcd for $C_{17}H_{16}BrNO$: C, 61.83; H, 4.88, N, 4.24;. Found C, 61.874; H, 4.81; N, 4.20%.

1-(4-Chlorophenyl)-2-((4-chlorophenyl)(prop-2-ynyl)amino)ethanol (3f)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.08 (t, 1H, J = 2.4 Hz, CH); 2.62 (s, 1H, OH), 3.20 (dd, 1H, J = 14.7, 9.0 Hz, CH_2), 3.38 (dd, 1H, J = 15.0, 3.6 Hz, CH_2), 3.77 - 3.92 (m, 2H, CH_2), 4.75 - 4.80 (m, 1H, CH_2), 6.68 (d, 2H, J = 9.3 Hz, Ar-H), 7.03 - 7.08 (m, 2H, Ar-H), 7.12 - 7.18 (m, 4H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.3, 59.9, 70.9, 72.8, 79.2, 115.8, 123.9, 127.2, 128.6, 129.0, 133.5, 140.0, 146.7 Anal. Calcd for $C_{17}H_{15}Cl_2NO$: C, 63.76; H, 4.72; N, 4.37. Found C, 63.60; H, 4.66; N, 4.28%.

2-(Phenyl(prop-2-ynyl)amino)-1-*p*-tolylethanol (3g)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.19 (m, 1H, CH); 2.32 (s, 3H, CH_3), 2.82 (s, 1H, OH), 3.38 (dd, 1H, J = 14.7, 9.3 Hz, CH_2), 3.57 (dd, 1H, J = 15.0, 9.3 Hz, CH_2), 3.99 - 4.13 (m, 2H, CH_2), 4.92 (dd, 1H, J = 9.3, 3.3 Hz, CH_2), 6.82 (t, 1H, J = 7.5 Hz, Ar-H), 6.93 (d, 2H, J = 8.4 Hz, Ar-H), 7.14 - 7.30 (m, 6H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 21.0, 41.0, 59.9, 71.4, 72.3, 79.7, 114.4, 118.6, 125.7, 126.7, 129.1, 137.3, 138.6, 148.1. Anal. Calcd for $C_{18}H_{19}NO$: C, 81.47; H, 7.22; N, 5.28. Found C, 81.42; H, 7.32; N, 5.12%.

2-((4-Chlorophenyl)(prop-2-ynyl)amino)-1-*p*-tolylethanol (3h)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.26 (t, 1H, J = 2.4 Hz, CH); 2.38 (s, 3H, CH_3), 2.52 (s, 1H, OH), 3.44 (dd, 1H, J = 15.0, 9.00 Hz, CH_2), 3.58 (dd, 1H, J = 14.7, 3.6 Hz, CH_2), 3.97 - 4.12 (m, 2H, CH_2), 4.96 (dd, 1H, J = 9.0, 3.6 Hz, CH_2), 6.88 (d, 2H, J = 8.7 Hz, Ar-H), 7.20 - 7.27 (m, 4H, Ar-H), 7.33 (d, 2H, J = 8.1 Hz, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 20.9, 40.7, 59.5, 71.3, 72.4, 79.3, 115.1, 122.9, 125.6, 128.7, 128.9, 137.2, 138.5, 146.6. Anal. Calcd for $C_{18}H_{18}ClNO$: C, 72.11; H, 6.05; N, 4.67. Found C, 71.94; H, 6.13; N, 4.60%.

1-(Biphenyl-4-yl)-2-(phenyl(prop-2-ynyl)amino)ethanol (3i)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.18 (m, 1H, CH), 2.80 (s, 1H, OH), 3.31 (dd, 1H, J = 14.7, 9.9 Hz, CH_2), 3.58 (dd, 1H, J = 14.4, 2.7 Hz, CH_2), 4.0 (m, 2H, CH_2), 4.93-4.96 (m, 1H, CH_2), 6.87 (d, 1H, J = 8.1 Hz, Ar-H), 7.06 (d, 2H, J = 8.4 Hz, Ar-

H), 7.29 (d, 2H, J = 6.9 Hz, Ar-H), 7.35 - 7.46 (m, 4H, Ar-H), 7.50 - 7.56 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.8, 60.3, 71.1, 72.7, 79.7, 115.9, 125.9, 126.3, 127.0, 127.2*, 128.7*, 129.0, 140.6, 140.7, 146.2. Anal. Calcd for $C_{23}H_{21}NO$ C, 84.37; H, 6.46; N, 4.28. Found C, 84.23; H, 6.55; N, 4.16%. (* Two carbons merged together)

1-(Biphenyl-4-yl)-2-(prop-2-ynyl(*p*-tolyl)amino)ethanol (3j)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.25 (m, 1H, CH); 2.29 (s, 3H, CH_3), 3.38 (dd, 1H, J = 14.7, 9.6 Hz, CH_2), 3.65 (dd, 1H, J = 14.4, 3.3 Hz, CH_2), 3.98-4.07 (m, 2H, CH_2), 5.01 (dd, 1H, J = 9.6, 3.0 Hz, CH_2), 6.94 (d, 2H, J = 8.4 Hz, Ar-H), 7.12 (d, 2H, J = 8.4 Hz, Ar-H), 7.36 (d, 2H, J = 7.5 Hz, Ar-H), 7.42 - 7.50 (m, 3H, Ar-H), 7.51 (d, 2H, J = 8.4 Hz, Ar-H), 7.57 - 7.63 (m, 3H, Ar-H); ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 20.3, 41.7, 60.2, 71.1, 72.6, 79.7, 115.7, 126.3, 127.0, 127.1, 127.2*, 128.7, 128.9, 129.7, 140.6, 140.7, 146.1. Anal. Calcd for $C_{24}H_{23}NO$: C, 84.42; H, 6.79; N, 4.10. Found C, 84.25; H, 6.71; N, 4.03%.

2-((4-Chlorophenyl)(prop-2-ynyl)amino)-1-(naphthalen-2-yl)ethanol (3k)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.24-2.25 (m, 1H, CH), 3.51 (dd, 1H, J = 15.0, 9.0 Hz, CH_2), 3.67 (dd, 1H, J = 14.7, 3.6 Hz, CH_2), 4.02-4.10 (m, 2H, CH_2), 5.13-5.16 (m, 1H, CH_2), 6.90 (d, 2H, J = 8.4 Hz, Ar-H), 7.48-7.57 (m, 3H, Ar-H), 7.80 - 7.88 (m, 5H, Ar-H), 7.98 (s, 1H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.1, 59.8, 71.7, 72.4, 79.3, 115.4, 123.3, 123.8, 124.7, 125.8, 126.1, 127.6, 127.8, 128.2, 128.9, 132.9, 133.1, 139.2, 147.7. Anal. Calcd for $C_{21}H_{18}ClNO$: C, 75.11; H, 5.40; N, 4.17. Found C, 75.26; H, 5.23; N, 4.04%.

1-(4-Nitrophenyl)-2-(phenyl(prop-2-ynyl)amino)ethanol (3l)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.23 (s, 1H, CH), 3.19 (s, 1H, OH), 3.28-2.36 (m, 1H, CH_2), 3.58-3.63 (m, 1H, CH_2), 3.94-4.09 (m, 2H, CH_2), 4.93-5.06 (m, 1H, CH_2), 6.84 - 6.92 (m, 2H, Ar-H), 7.22 - 7.24 (m, 2H, Ar-H), 7.46 -7.58 (m, 3H, Ar-H), 8.15 (t, 2H, J = 8.1 Hz, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.3, 59.6, 70.6, 72.6, 79.4, 114.8, 119.1, 123.4, 126.0, 129.1, 147.2, 147.9, 153.5. Anal. Calcd for $C_{17}H_{16}N_2O_3$: C, 68.91; H, 5.44; N, 9.45. Found C, 68.75; H, 5.36; N, 9.30%.

2,4-Diphenyl-1,4-oxazepan-7-one (6a)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.92 (dd, 1H, J = 14.7, 5.7 Hz, CH_2), 3.20 (t, 1H, J = 14.1 Hz, CH_2), 3.47 (dd, 1H, J = 14.7, 5.4 Hz, CH_2), 3.57 (dd, 1H, J = 15.3, 8.4 Hz, CH_2), 3.97 (d, 2H, J = 15.0 Hz, CH_2), 5.54 (d, 1H, J = 8.1 Hz, CH), 6.90 (t, 2H, J = 8.7 Hz, Ar-H), 7.28 - 7.43 (m, 8H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 36.3, 46.4, 60.0, 80.6, 116.3, 125.9*, 128.6, 128.8, 129.7, 137.9, 148.7, 173.0. Anal. Calcd for

$C_{17}H_{17}NO_2$: C, 76.38; H, 6.41; N, 5.24. Found C, 76.47; H, 6.47; N, 5.12%.* Two carbons merged together.

2-Phenyl-4-*p*-tolyl-1,4-oxazepan-7-one (6b)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, CDCl$_3$) δ_H: 2.29 (s, 3H, CH$_3$), 2.90 (dd, 1H, *J* = 14.7, 6.0 Hz, CH$_2$), 3.22 (t, 1H, *J* = 14.4 Hz, CH$_2$), 3.44 (dd, 1H, *J* = 14.4, 11.1 Hz, CH$_2$), 3.54 (dd, 1H, *J* = 15.3,8.4 Hz, CH$_2$), 3.91 (d, 2H, *J* = 14.7 Hz, CH), 5.55 (d, 1H, *J* = 8.4 Hz, CH), 6.81 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.12 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.35 - 7.43 (m, 5H, Ar-H).^{13}C NMR (75 MHz, CDCl$_3$) δ_C: 20.4, 36.1, 46.8, 60.3, 80.6, 116.7, 125.9, 128.6, 128.8, 129.8, 130.2, 138.0, 146.4, 173.4. Anal. Calcd for $C_{18}H_{19}NO_2$: C, 76.84; H, 6.81; N, 4.98. Found C, 76.90; H, 6.92; N, 5.05 %.

4-(4-Methoxyphenyl)-2-phenyl-1,4-oxazepan-7-one (6c)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, CDCl$_3$) δ_H: 2.73 (dd, 1H, *J* = 14.1, 6.3 Hz, CH$_2$), 3.01-3.10 (m, 1H, CH$_2$), 3.14-3.20 (m, 1H, CH$_2$), 3.30 (dd, 1H, *J* = 15.0,8.4 Hz, CH$_2$), 3.50-3.60 (m, 5H, CH$_2$), 5.40 (d, 1H, *J* = 8.4 Hz, CH), 6.70 (s, 4H, Ar-H), 7.16 - 7.28 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, CDCl$_3$) δ_C: 36.5, 48.2, 55.6, 61.6, 80.8, 114.8, 119.6, 125.9, 128.5, 128.8, 138.0, 143.6, 154.3, 173.4. Anal. Calcd for $C_{18}H_{19}NO_3$: C ,72.71; H, 6.44; N, 4.71. Found C, 72.61; H, 6.38; N, 4.78%.

4-(4-Fluorophenyl)-2-phenyl-1,4-oxazepan-7-one (6d)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, CDCl$_3$) δ_H: 2.82 (dd, 1H, *J* = 14.7, 6.3 Hz, CH$_2$), 3.06-3.18 (m, 1H, CH$_2$), 3.25-3.33 (m 1H, CH$_2$), 3.40 (dd, 1H, *J* = 15.3,8.7 Hz, CH$_2$), 3.69 (d, 2H, *J* = 14.7 Hz, CH$_2$), 5.44 (d, 1H, *J* = 8.4 Hz, CH), 6.73 - 6.77 (m, 2H, Ar-H), 6.87-6.93 (m, 2H, Ar-H), 7.31 - 7.36 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, CDCl$_3$) δ_C: 36.2, 47.5, 60.9, 80.5, 116.0, 118.6, 125.8, 128.4, 128.5, 137.8, 145.8, 157.3, 173.0. Anal. Calcd for $C_{17}H_{16}FNO_2$: C, 71.56; H, 5.65; N, 4.91. Found C, 71.47; H, 5.75; N, 4.83%.

4-(4-Bromophenyl)-2-phenyl-1,4-oxazepan-7-one (6e)

Isolated as colorless solid; m.p. 124 ^{o}C. ^{1}H NMR (300 MHz, CDCl$_3$) δ_H: 2.80 (dd, 1H, *J* = 15.0, 5.7 Hz, CH$_2$), 3.05 (dd, 1H, *J* = 13.8 Hz, CH$_2$), 3.31 - 3.49 (m, 2H, CH$_2$), 3.77 - 3.82 (m, 2H, CH$_2$), 5.39 (d, 1H, *J* = 8.1 Hz, CH), 6.64 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.29 - 7.32 (m, 7H, Ar-H). ^{13}C NMR (75 MHz, CDCl$_3$) δ_C: 35.84, 45.9, 59.5, 80.2, 112.0, 117.6, 125.7, 128.7, 128.8, 132.4, 137.5, 147.4, 172.8. Anal. Calcd for $C_{17}H_{16}BrNO_2$: C, 58.97; H, 4.66; N, 4.05. Found C, 59.02; H, 4.59; N, 4.11%.

2,4-Bis(4-chlorophenyl)-1,4-oxazepan-7-one (6f)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.85 (dd, 1H, *J* = 14.7, 5.7 Hz, CH_2), 3.10 (t, 1H, *J* = 15.0 Hz, CH_2), 3.25 - 3.48 (m, 2H, CH_2), 3.75 - 3.85 (m, 2H, CH_2), 5.41 (d, 1H, *J* = 8.4 Hz, CH), 6.71 (d, 2H, *J* = 9.0 Hz, Ar-H), 7.18 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.26 - 7.33 (m, 4H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 35.8, 46.2, 59.7, 79.6, 117.4, 125.0, 127.1, 129.0, 129.5, 134.4, 136.0, 147.0, 172.7. Anal. Calcd for $C_{17}H_{15}Cl_2NO_2$: C, 60.73; H, 4.50; N, 4.17. Found C, 60.66; H, 4.58; N, 4.11%.

4-Phenyl-2-*p*-tolyl-1,4-oxazepan-7-one (6g)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.34 (s, 3H, CH_3), 2.77 (dd, 1H, *J* = 14.4, 5.1 Hz, CH_2), 3.14 (t, 1H, *J* = 14.8 Hz, CH_2), 3.38 - 3.47 (m, 1H, CH_2), 3.53 (dd, 1H, *J* = 15.3,8.4 Hz, CH_2), 3.92 (d, 2H, *J* = 14.7 Hz, CH_2), 5.48 (d, 1H, *J* = 8.4 Hz, CH), 6.84 - 6.90 (m, 2H, Ar-H), 7.17 - 7.22 (m, 3H, Ar-H), 7.29 - 7.32 (m, 4H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 21.3, 36.1, 46.1, 59.7, 80.4, 116.1, 119.9, 125.7, 129.1, 129.4, 129.6, 134.9, 138.4, 173.3. Anal. Calcd for $C_{18}H_{19}NO_2$: C, 76.84; H, 6.81; N, 4.98. Found C, 76.90; H, 6.73; N, 4.86%.

4-(4-Chlorophenyl)-2-(4-methylphenyl)-1,4-oxazepan-7-one (6h)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.36 (s, 3H, CH_3), 2.91 (dd, 1H, *J* = 15.0, 6.0 Hz, CH_2), 3.11 - 3.21 (m, 1H, CH_2), 3.41-3.49 (m, 2H, CH_2), 3.85 - 3.93 (m, 2H, CH_2), 5.47 (d, 1H, *J* = 8.4 Hz, CH), 6.78 (d, 2H, *J* = 9.3 Hz, Ar-H), 7.22 - 7.31 (m, 6H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 21.2, 36.0, 46.3, 59.8, 80.4, 117.5, 124.9, 125.8, 129.3, 129.6, 134.7, 138.6, 147.2, 173.1 . Anal. Calcd for $C_{18}H_{18}ClNO_2$: C, 68.46; H, 5.75; N, 4.44.Found C, 68.57; H, 5.66; N, 4.49%.

2-(Biphenyl-4-yl)-4-phenyl-1,4-oxazepan-7-one (6i)

Isolated as viscous liquid;^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.86 (dd, 1H, *J* = 14.7, 5.7 Hz, CH_2), 3.17 (t, 1H, *J* = 14.6 Hz, CH_2), 3.40 (dd, 1H, *J* = 14.4, 11.1 Hz, CH_2), 3.53 (dd, 1H, *J* = 15.3, 8.4 Hz, CH_2), 3.85 - 3.94 (m, 2H, CH_2), 5.55 (d, 1H, *J* = 8.4 Hz, CH), 6.79 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.11 (d, 2H, *J* = 8.4 Hz, Ar-H), 7.31 - 7.36 (m, 1H, Ar-H), 7.40 - 7.48 (m, 5H, Ar-H), 7.54 - 7.61 (m, 4H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 36.0, 46.6, 60.1, 80.2, 116.6, 126.2, 127.0, 127.4, 127.5, 128.7, 129.6, 130.1, 136.8, 140.3, 141.4, 146.3, 173.2. Anal. Calcd for $C_{23}H_{21}NO_2$: C, 80.44; H, 6.16; N, 4.08. Found C, 80.34; H, 6.09; N, 4.19%.

2-(Biphenyl-4-yl)-4-*p*-tolyl-1,4-oxazepan-7-one (6j)

Isolated as colourless liquid; m.p. 105 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.29 (s, 3H, CH_3), 2.91 (dd, 1H, *J* = 14.4, 5.4 Hz, CH_2), 3.22 (t, 1H, *J* = 14.4 Hz, CH_2), 3.40-3.49 (m, 1H, CH_2), 3.57 (dd, 1H, *J* = 15.3, 8.4 Hz, CH_2), 3.96 (d, 2H, *J* = 15.0 Hz, CH_2), 5.59 (d, 1H, *J* = 8.1 Hz, CH), 6.82 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.12 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.38 (d, 2H, *J* = 7.2 Hz, Ar-H), 7.44 (d, 2H, *J* = 7.5 Hz, Ar-H), 7.50 (d, 2H, *J* = 8.4 Hz, Ar-H), 7.58 - 7.64 (m, 3H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 20.3, 36.1, 46.8, 60.3, 80.4, 116.7, 126.3, 127.1, 127.5*, 128.8, 129.8, 130.2, 136.9, 140.4, 141.5, 146.4, 173.4. Anal. Calcd for $C_{24}H_{23}NO_2$: C, 80.64; H, 6.49; N, 3.92. Found C, 80.73; H, 6.60; N, 4.08%. (*Two carbons merged together)

4-(4-Chlorophenyl)-2-(naphthalen-2-yl)-1,4-oxazepan-7-one (6k)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.98 (dd, 1H, *J* = 15.3, 6.3 Hz, CH_2), 3.25 (t, 1H, *J* = 12.6 Hz, CH_2), 3.51 (t, 1H, *J* = 12.6 Hz, CH_2), 3.64 (dd, 1H, *J* = 15.0, 7.5 Hz, CH_2), 3.97 - 4.02 (m, 2H, CH_2), 5.69 (d, 1H, *J* = 8.1 Hz, CH), 6.84 (d, 2H, *J* = 8.4 Hz, Ar-H), 7.48 - 7.55 (m, 4H, Ar-H), 7.87 - 7.96 (m, 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 36.0, 46.4, 60.0, 80.5, 117.5, 123.3, 125.0, 125.1, 126.5, 126.6, 127.7, 128.1, 128.9, 129.6, 133.1, 133.2, 134.8, 147.2, 173.0. Anal. Calcd for $C_{21}H_{18}ClNO_2$: C, 71.69; H, 5.16; N, 3.98. Found C, 71.80; H, 5.05; N, 3.85%.

2-(4-Nitrophenyl)-4-phenyl-1,4-oxazepan-7-one (6l)

Isolated as viscous liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.90 (dd, 1H, *J* = 14.7, 5.4 Hz, CH_2), 3.17-3.26 (m, 1H, CH_2), 3.39-3.48 (m, 1H, CH_2), 3.53 (dd, 1H, *J* = 15.3,8.4 Hz, CH_2), 3.89 - 3.96 (m, 2H, CH_2), 5.55 (d, 1H, *J* = 8.4 Hz, CH), 6.81 (d, 2H, *J* = 8.4 Hz, Ar-H), 7.13 (d, 2H, *J* = 8.4 Hz, Ar-H), 7.33 - 7.45 (m, 5H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 36.1, 46.8, 60.3, 80.5, 116.6, 125.8, 128.5, 128.8, 129.7, 130.2, 137.9, 146.4, 173.3. Anal. Calcd for $C_{17}H_{16}N_2O_4$: C, 65.38; H, 5.16; N, 8.97. Found C, 65.50; H, 5.09; N, 8.88%.

Spectral copies

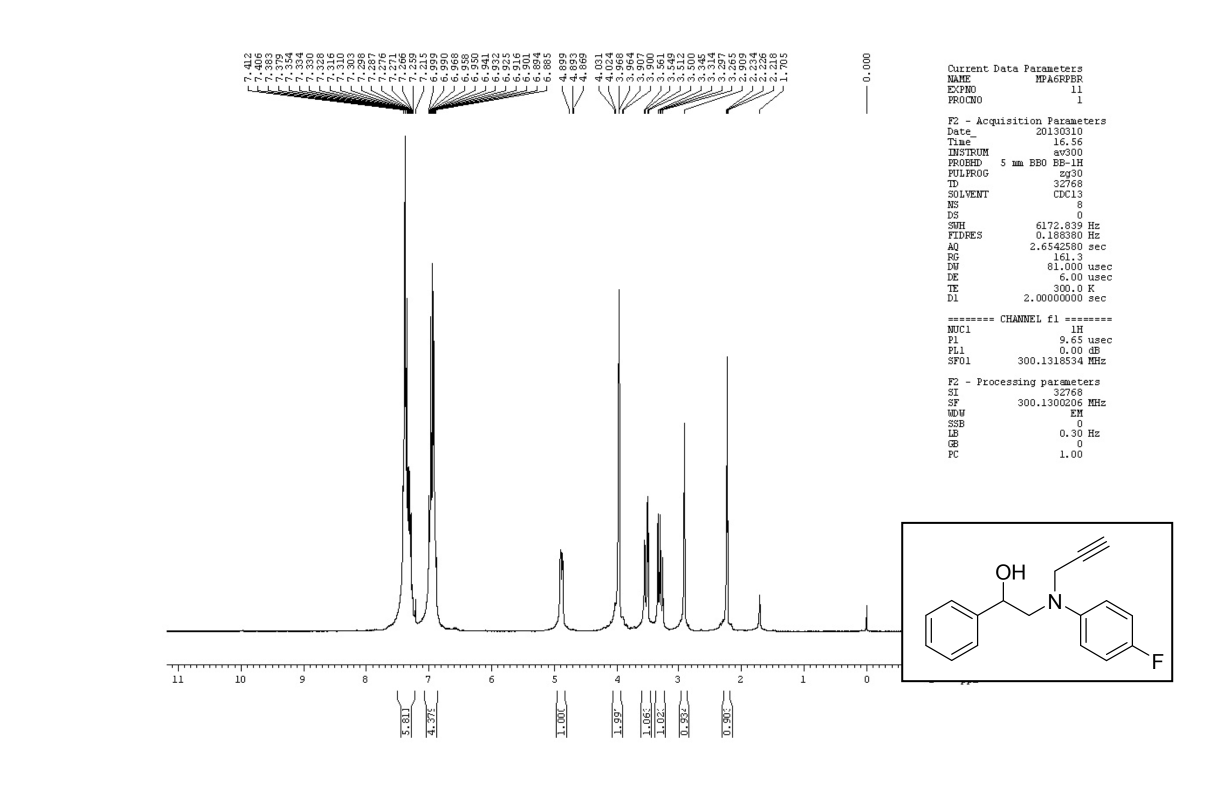


Figure 1. ^{1}H NMR spectrum of **3d**

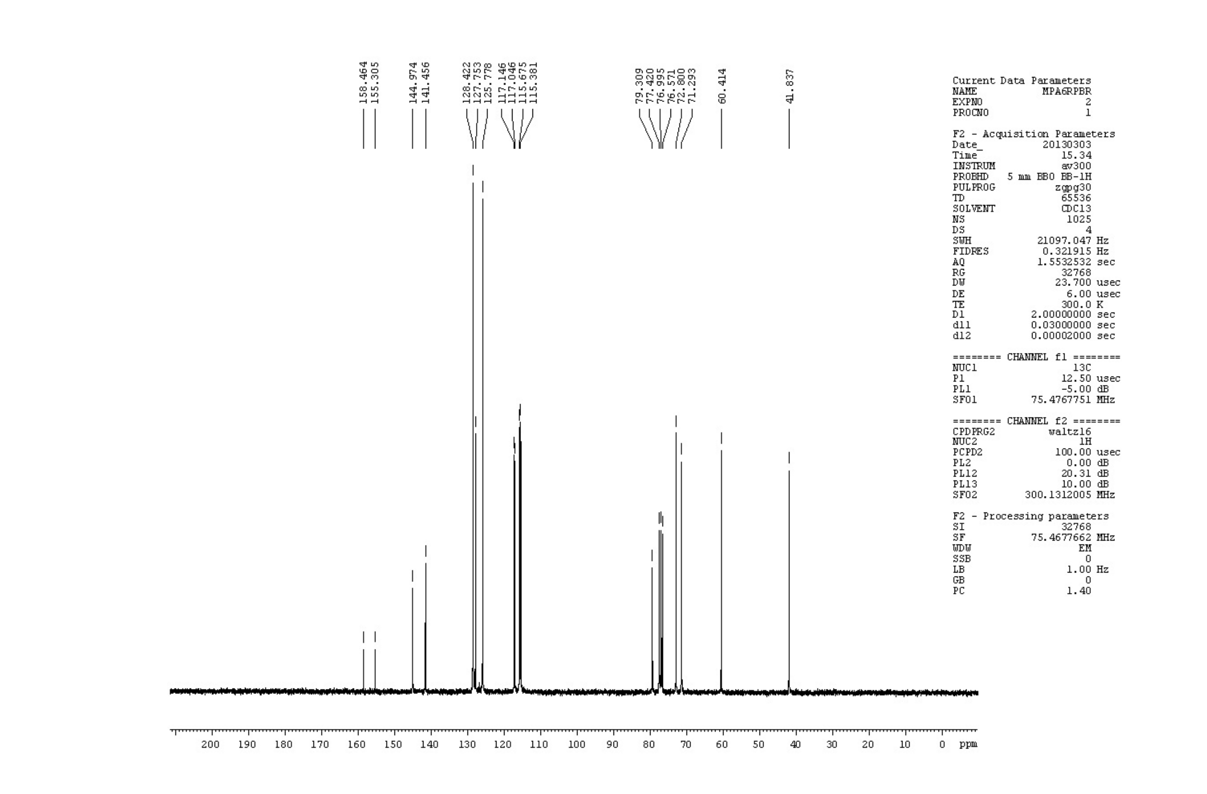


Figure 2. ^{13}C NMR spectrum of **3d**

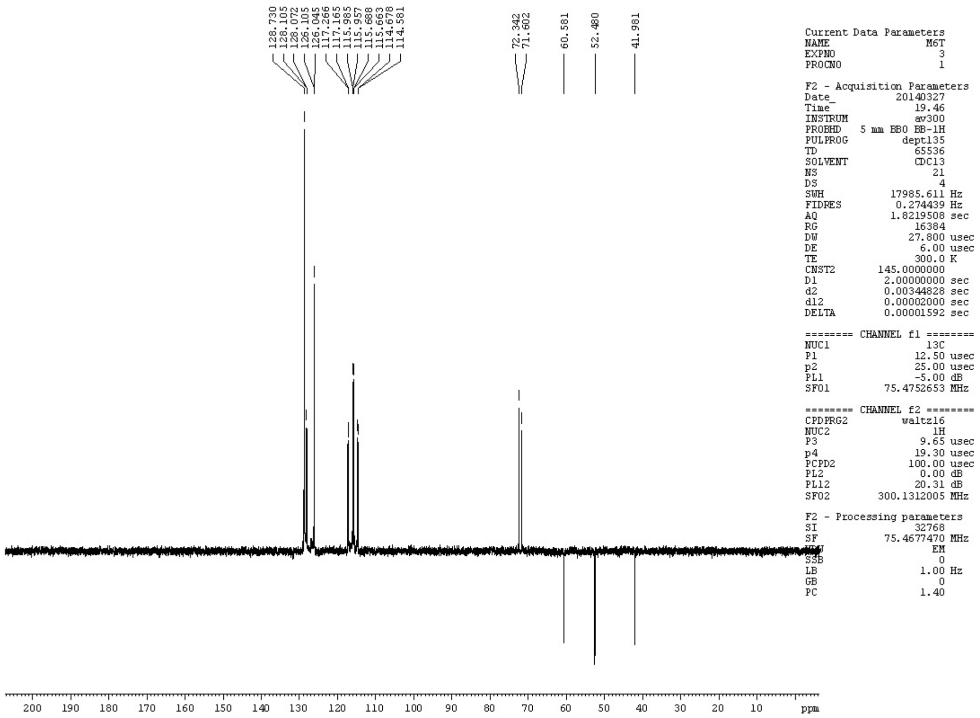


Figure 3. DEPT-135 spectrum of **3d**

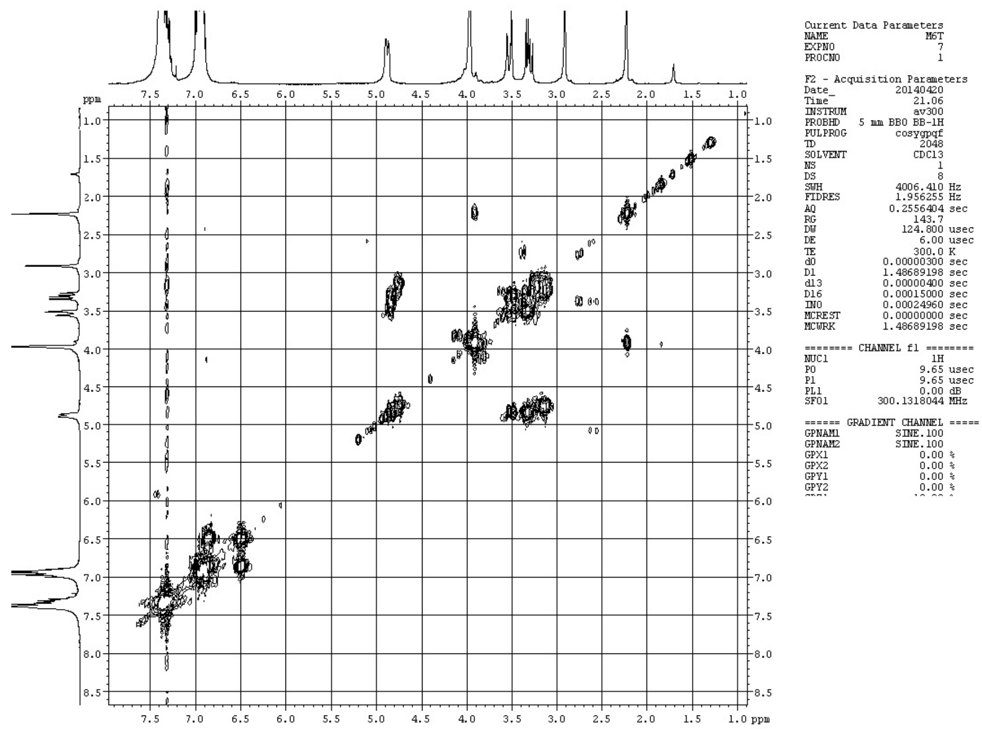


Figure 4. H,H-COSY spectrum of **3d**

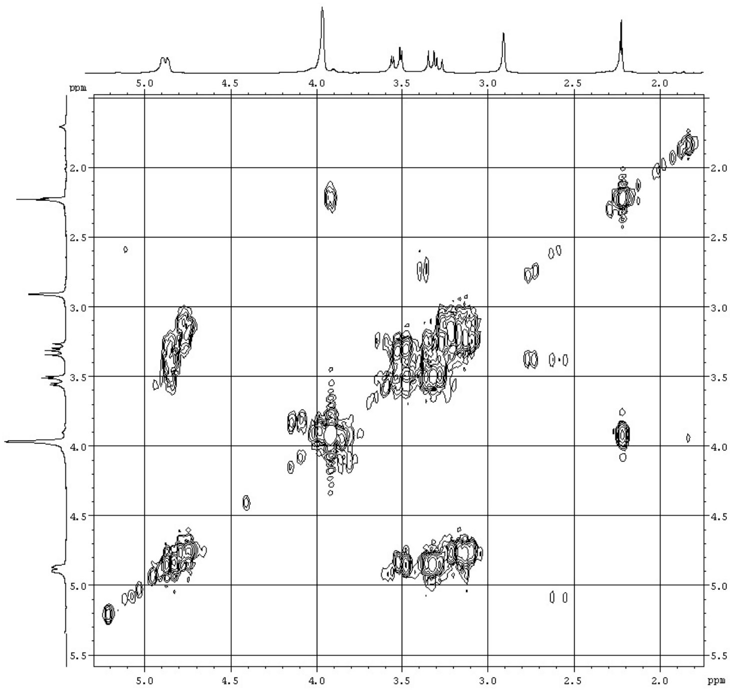


Figure 5. H,H-COSY spectrum of **3d** (expanded)

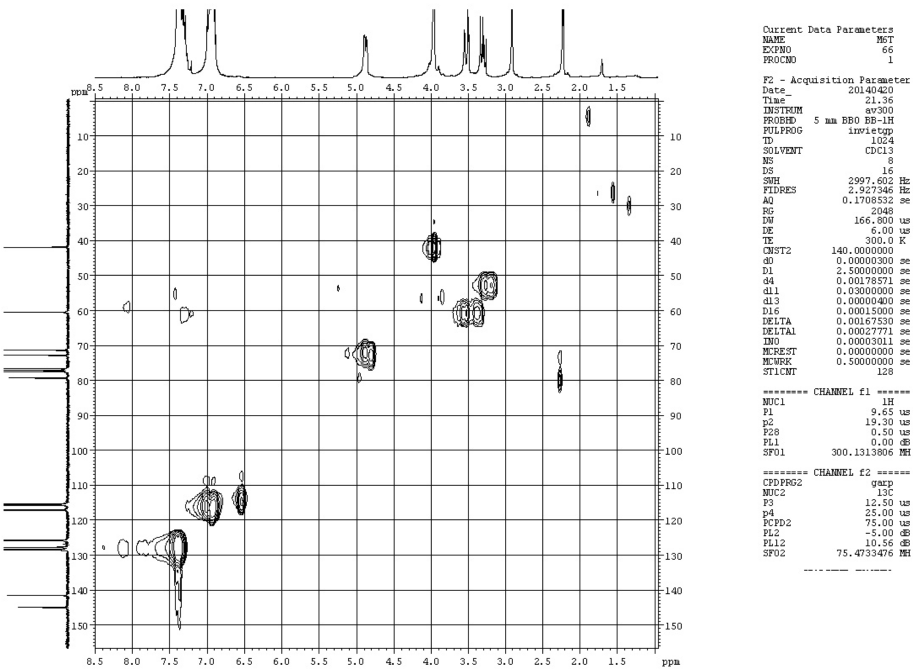


Figure 6. C,H-COSY spectrum of **3d**

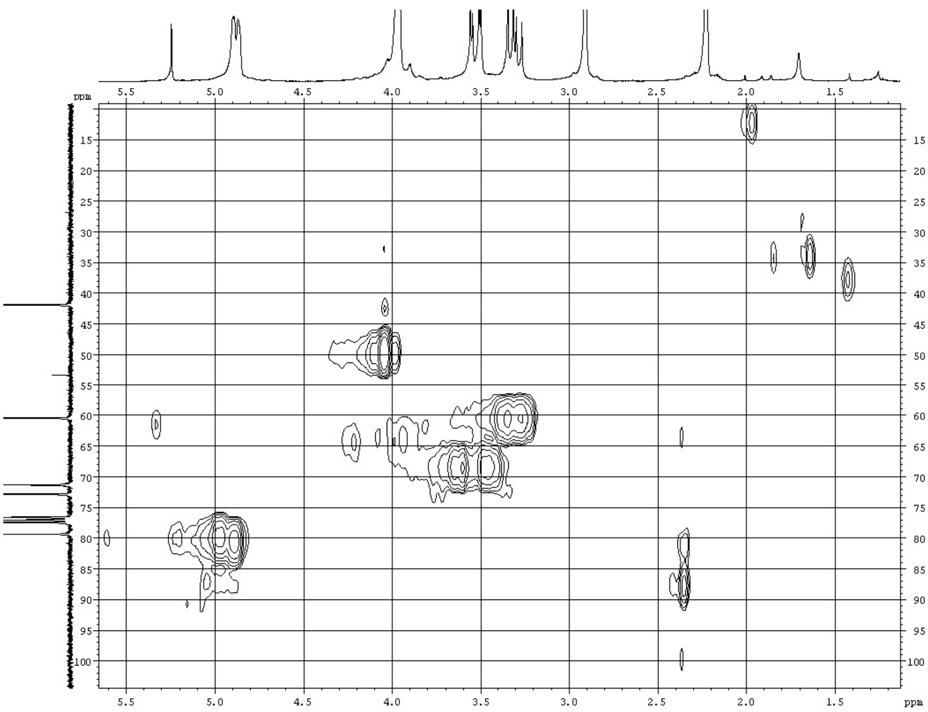


Figure 7. C,H-COSY spectrum of **3d** (expanded)

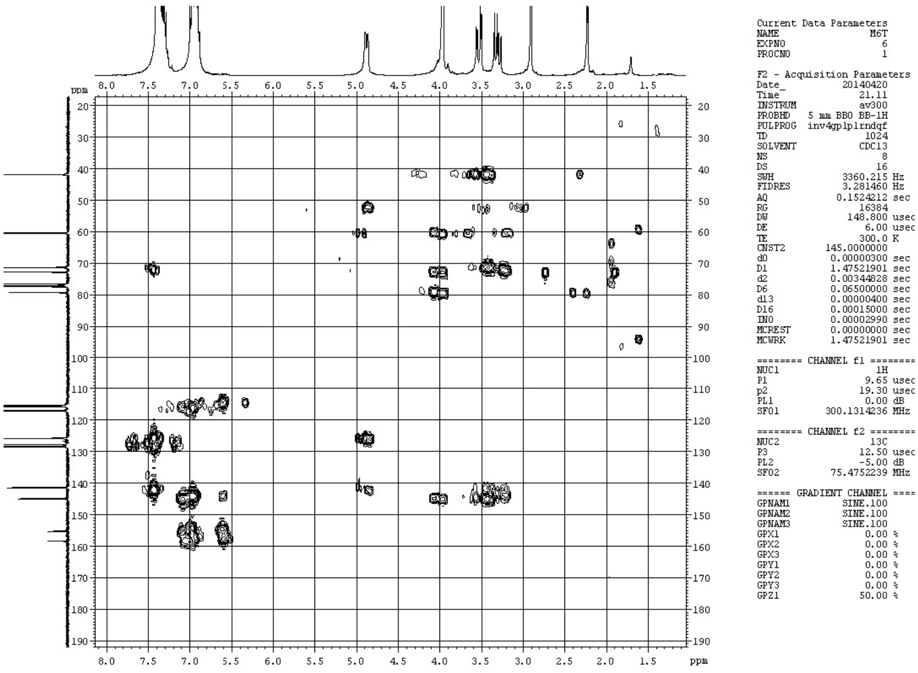


Figure 8. HMBC spectrum of **3d**

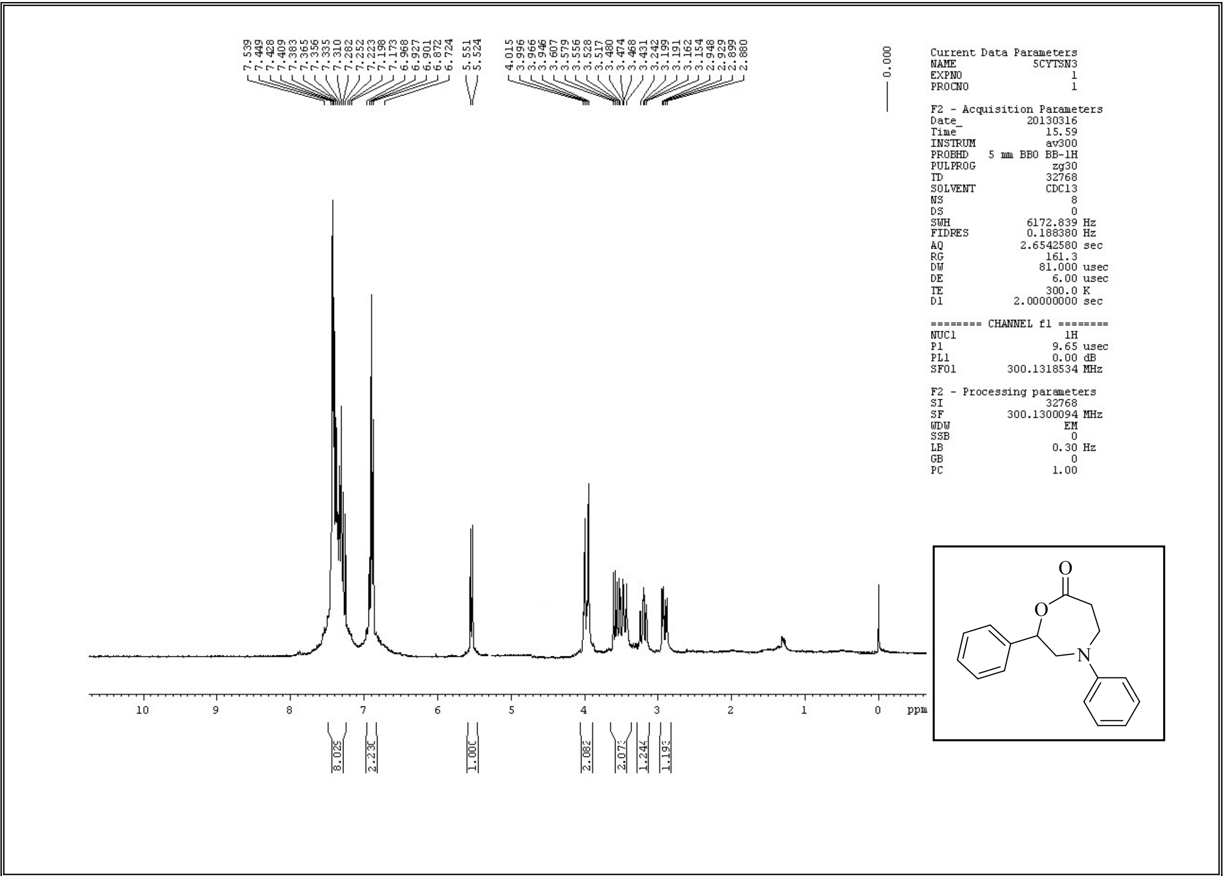


Figure 9. ^{1}H NMR spectrum of **6a**

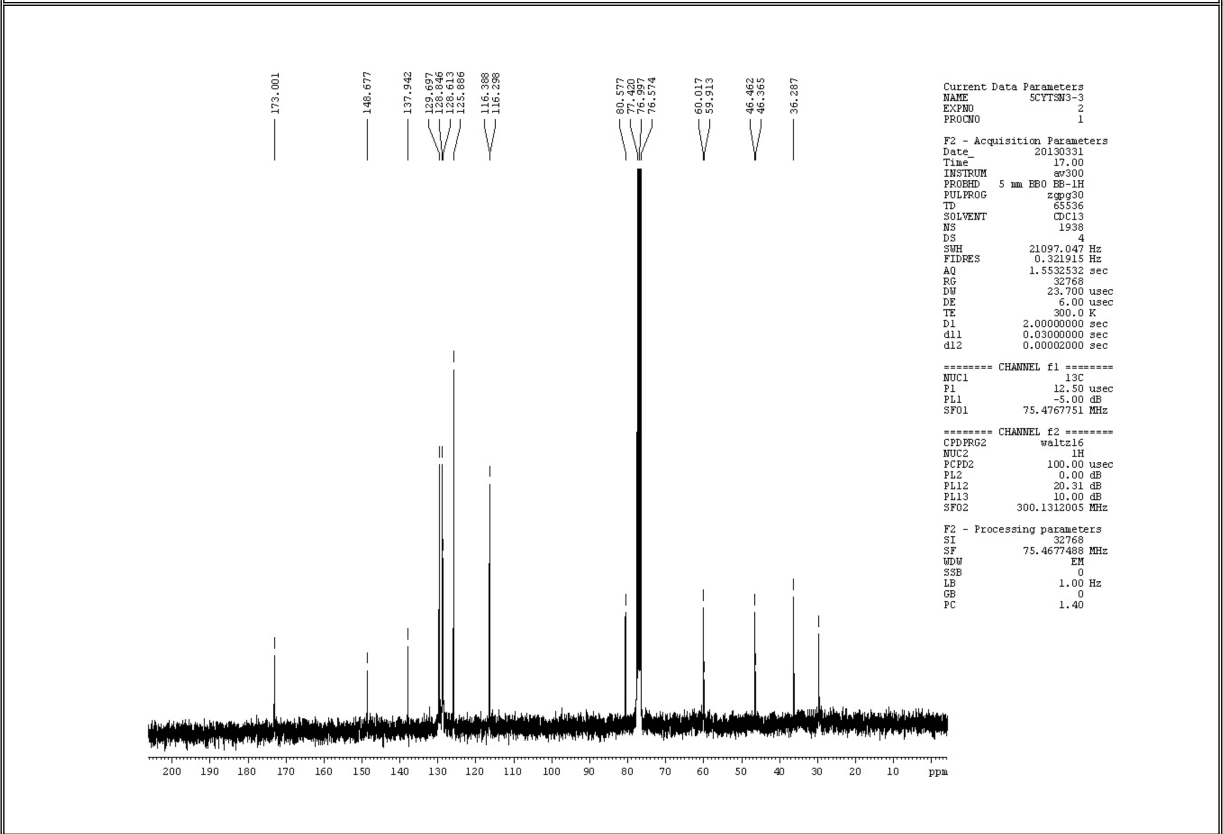


Figure 10. ^{13}C NMR spectrum of **6a**

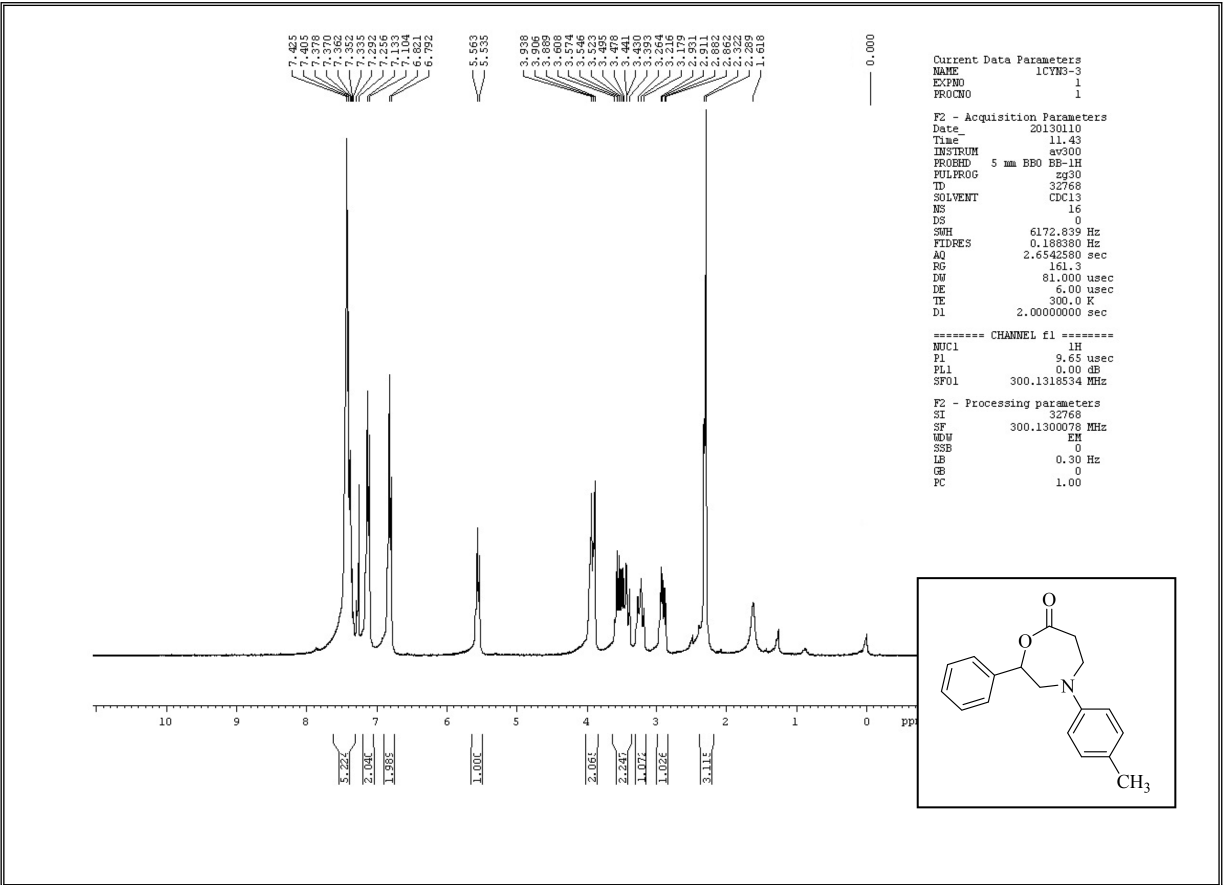


Figure 11. ^{1}H NMR spectrum of **6b**

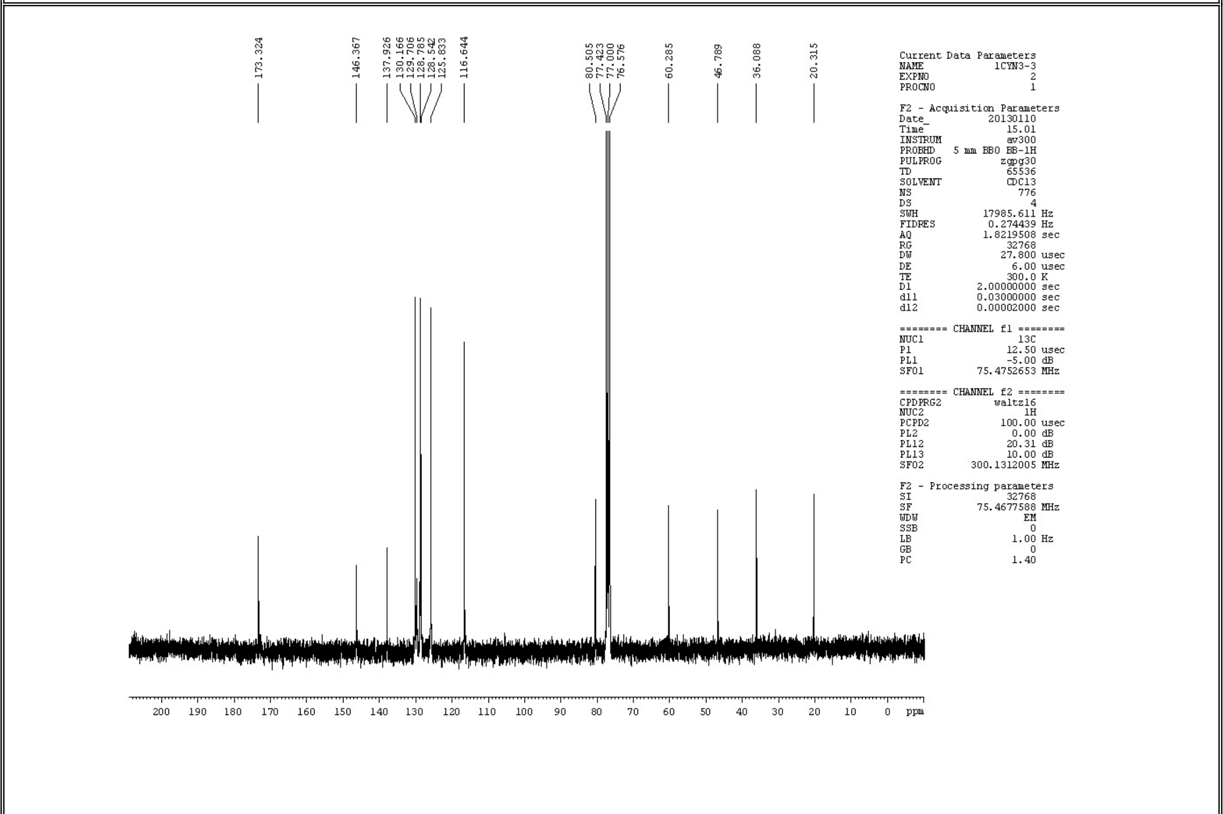


Figure 12. ^{13}C NMR spectrum of **6b**

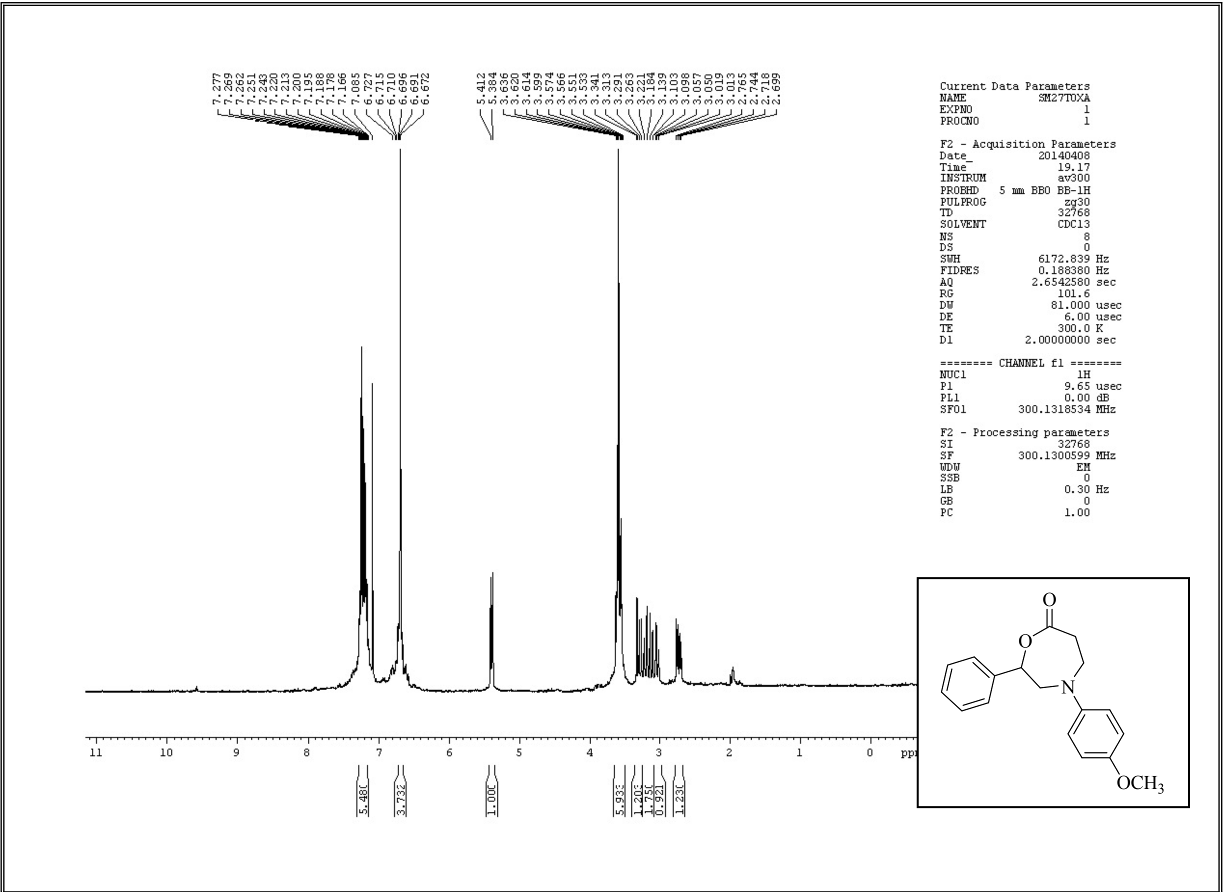


Figure 13. ^{1}H NMR spectrum of **6c**

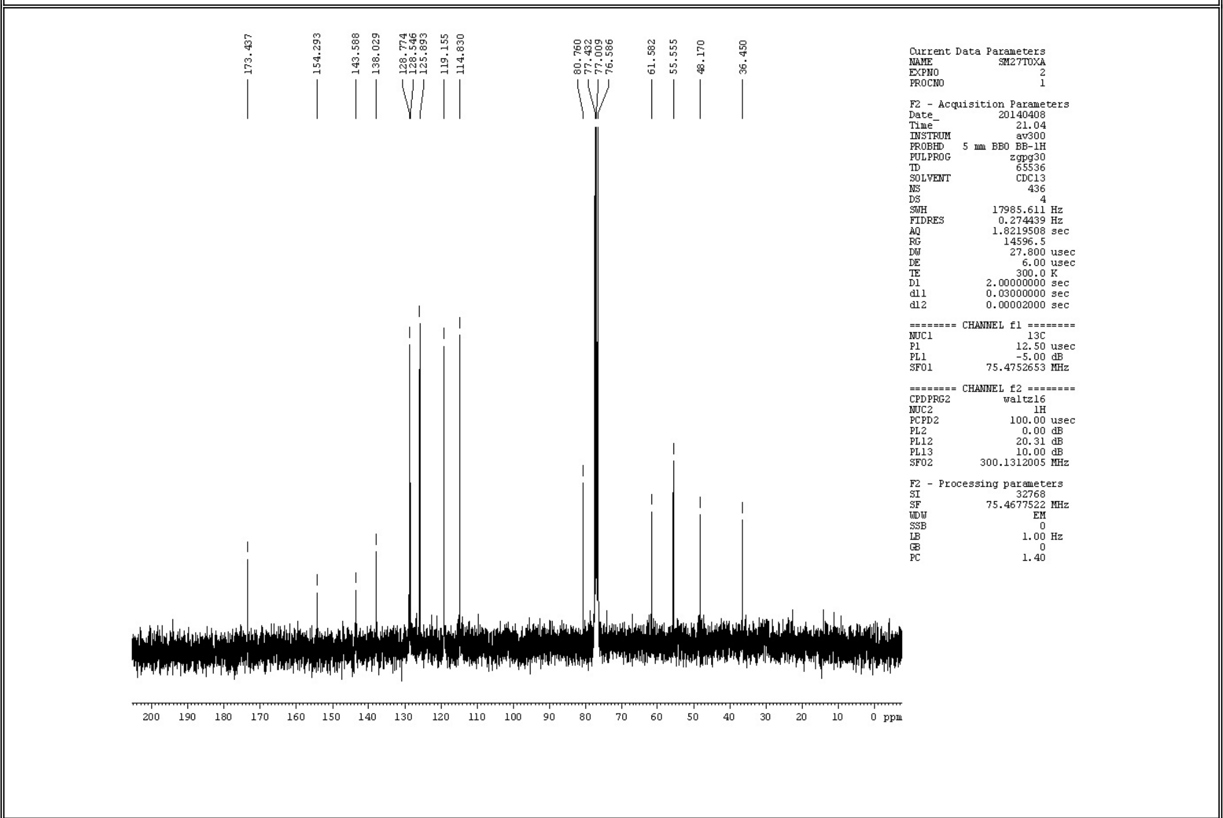


Figure 14. ^{13}C NMR spectrum of **6c**

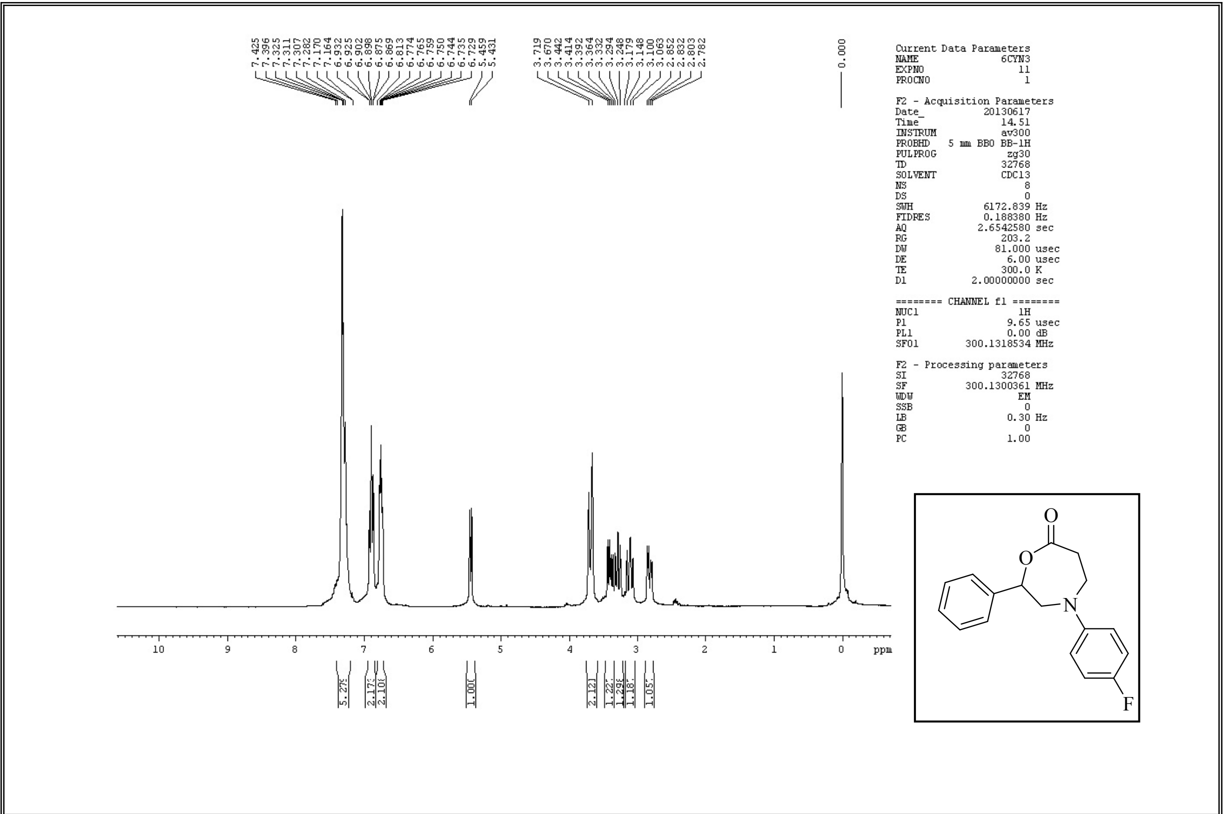


Figure 15. ^{1}H NMR spectrum of **6d**

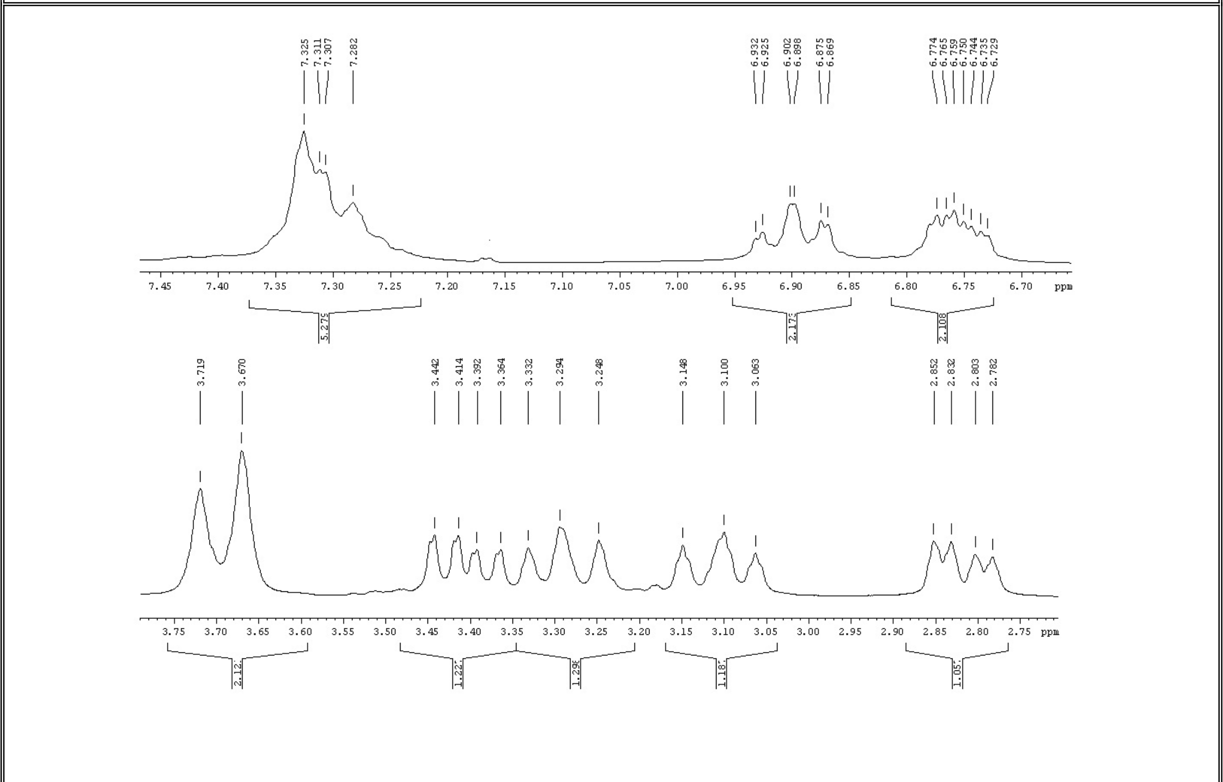


Figure 16. ^{1}H NMR spectrum of **6d** (expanded)

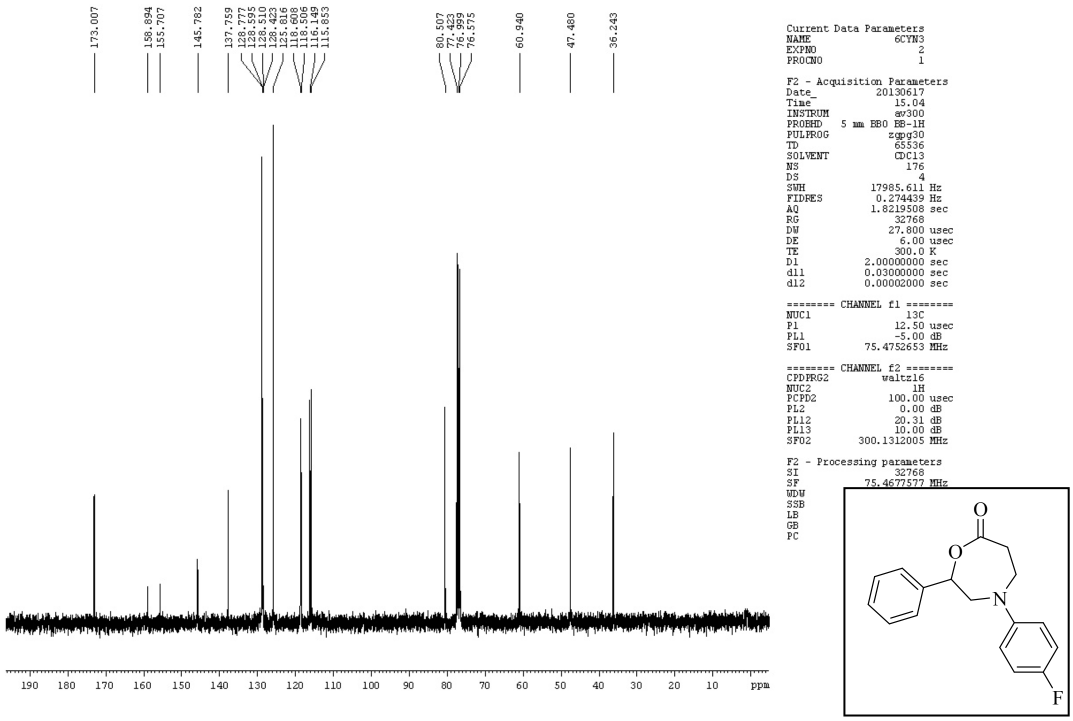


Figure 17. ^{13}C NMR spectrum of **6d**

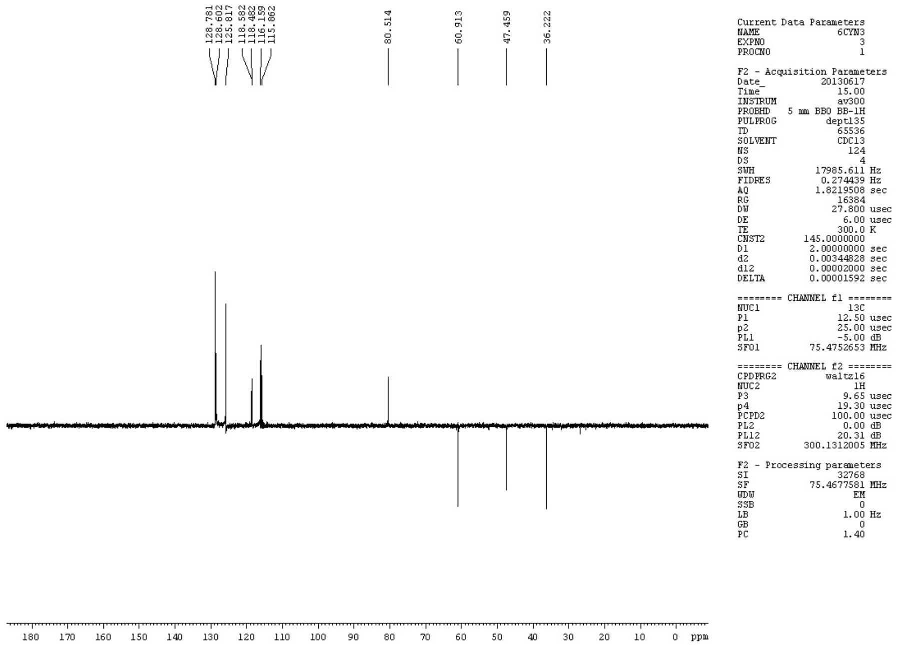


Figure 18. DEPT-135 spectrum of **6d**

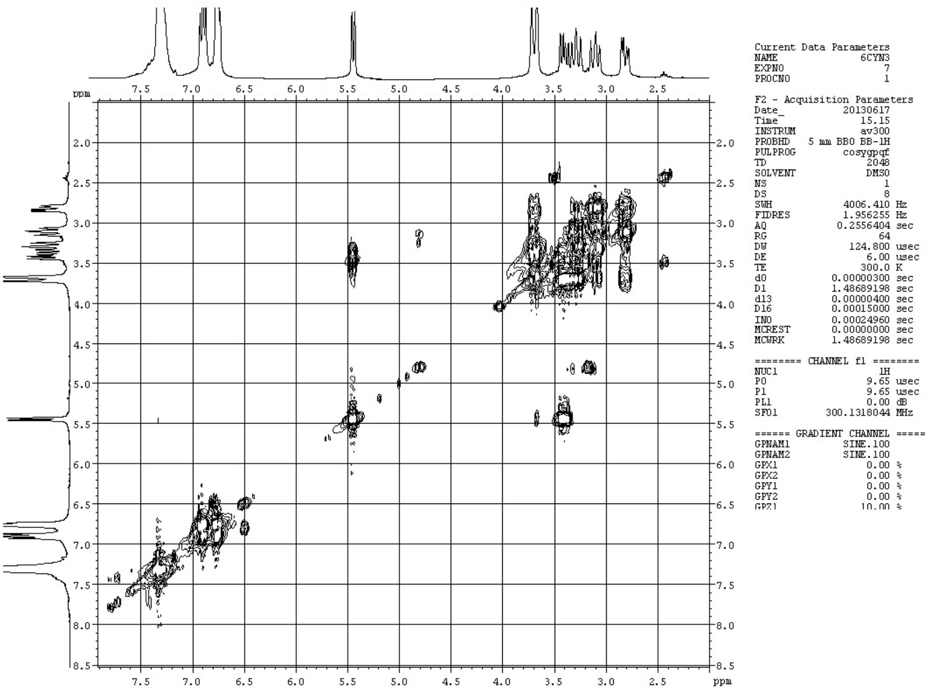


Figure 19. H,H-COSY spectrum of **6d**

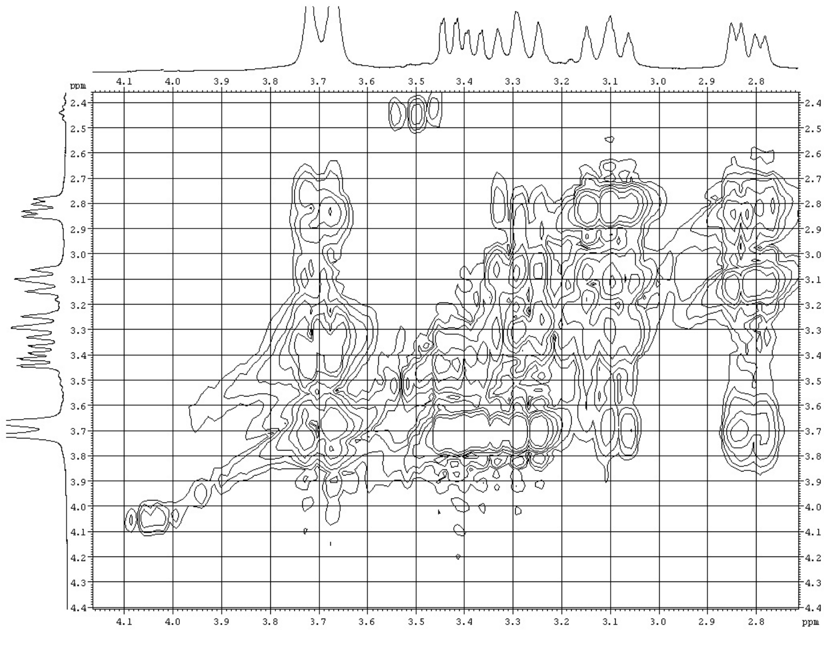


Figure 20. H,H-COSY spectrum of **6d** (expanded)

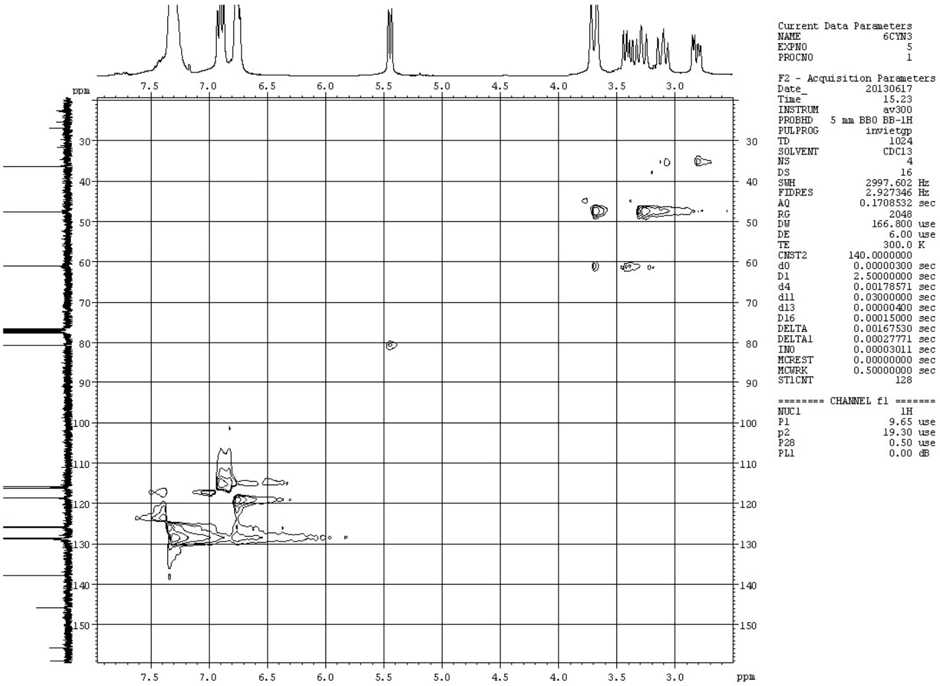


Figure 21. C,H-COSY spectrum of **3d**

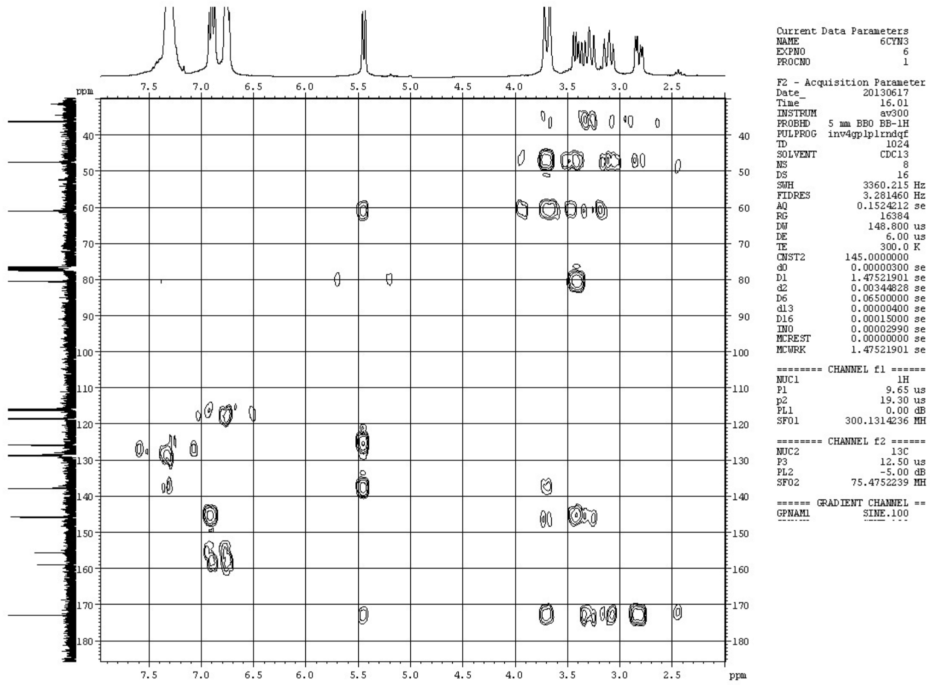


Figure 22. HMBC spectrum of **6d**

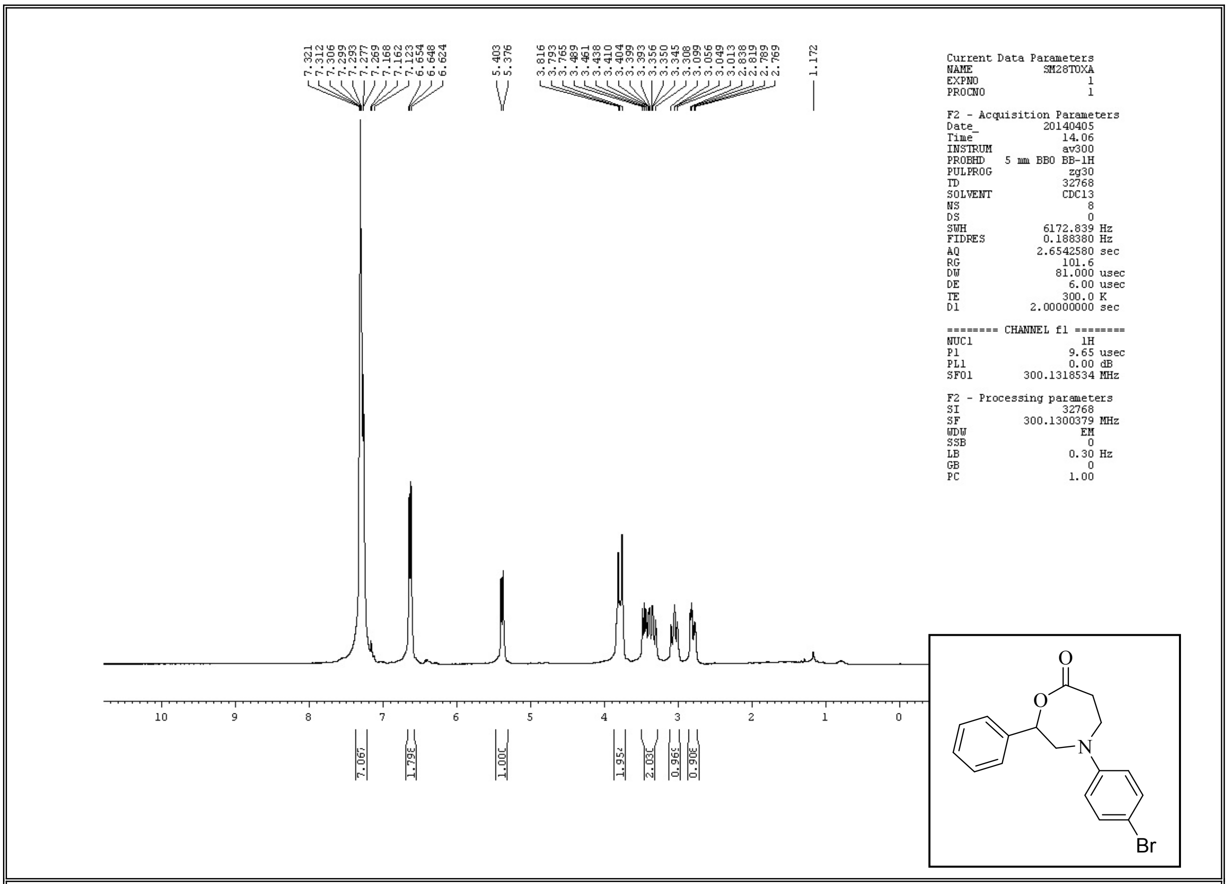


Figure 23. ¹H NMR spectrum of **6e**

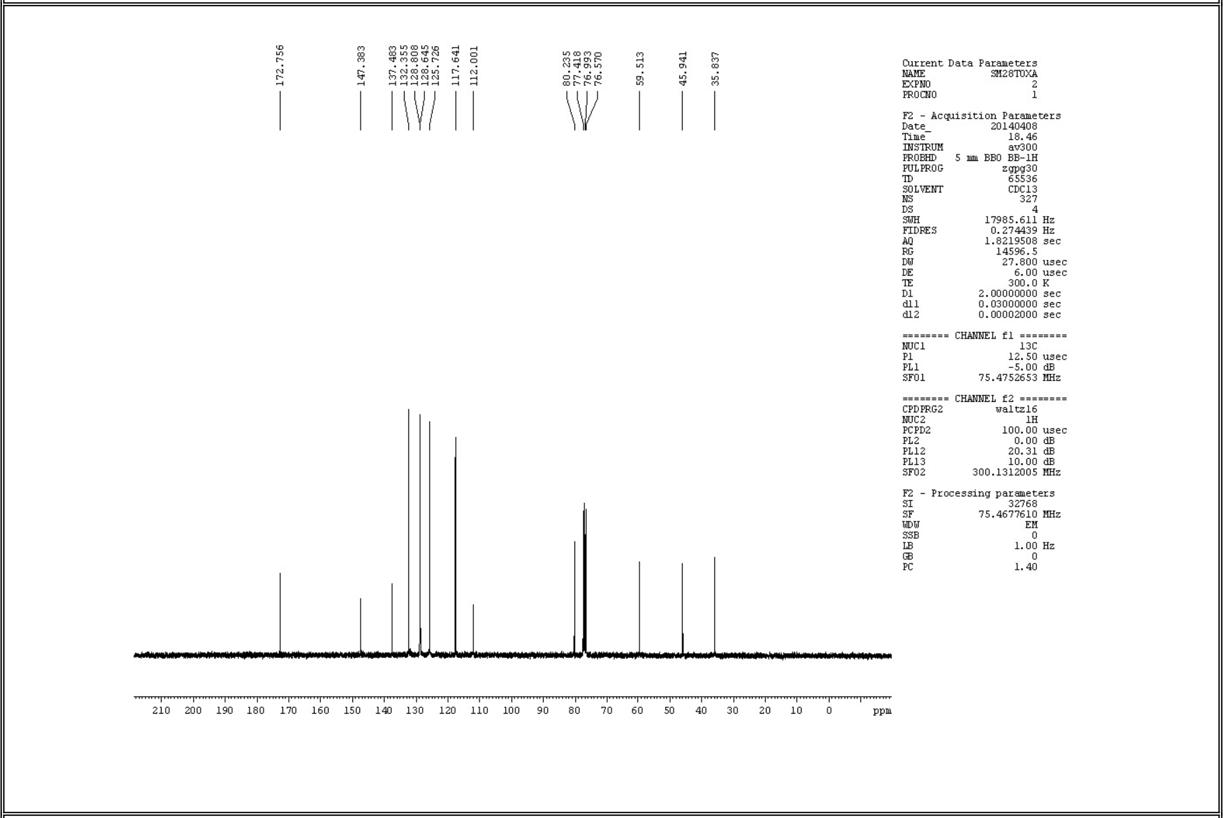
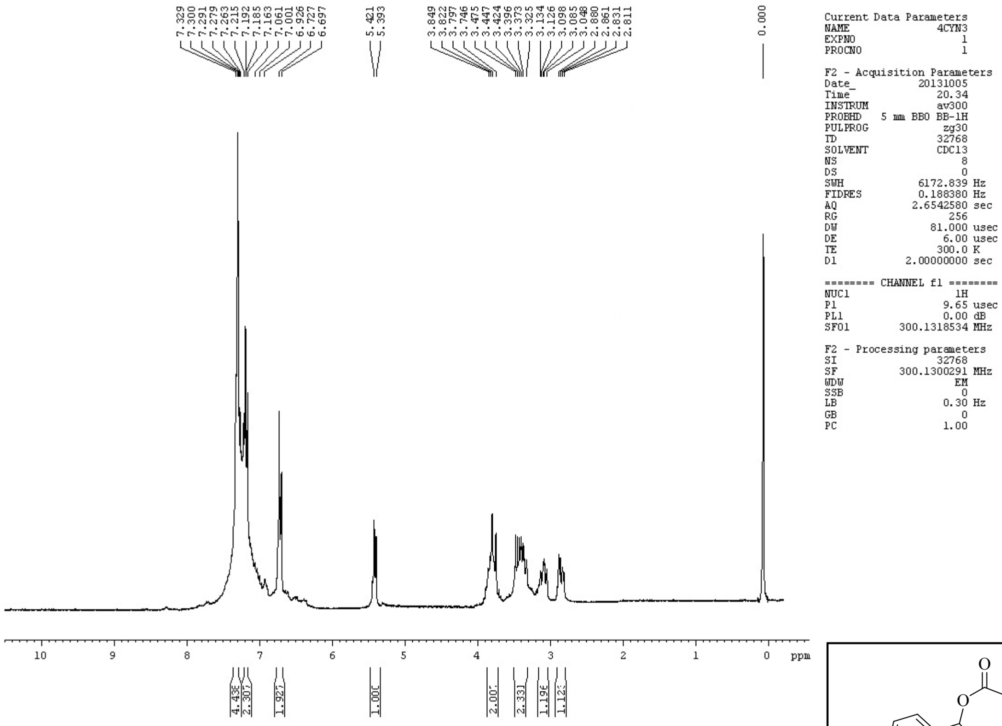


Figure 24. ¹³C NMR spectrum of **6e**



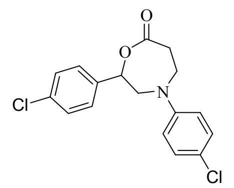


Figure 25. ^{1}H NMR spectrum of **6f**

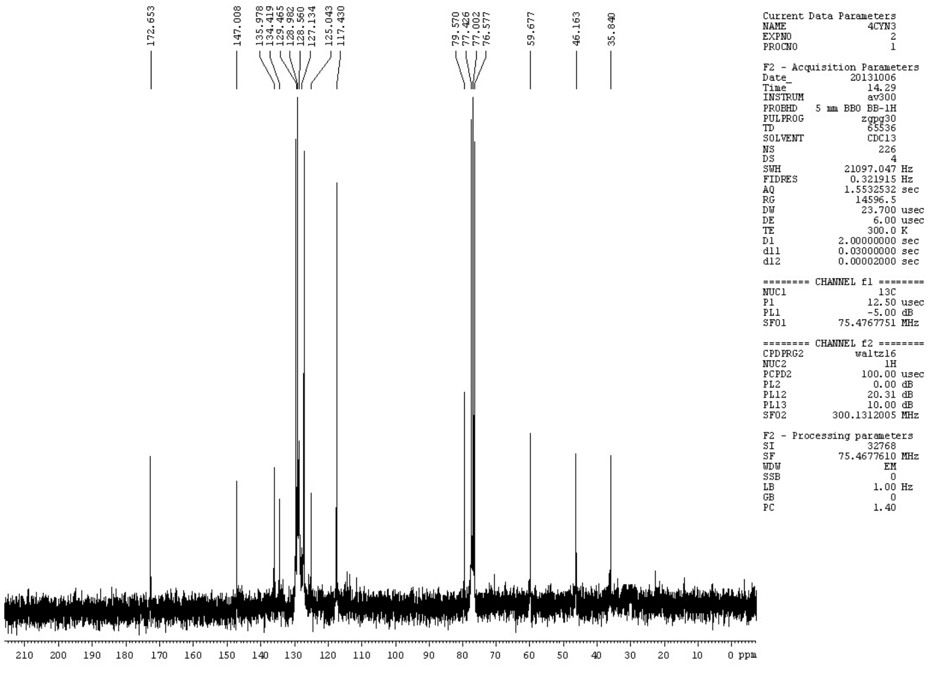


Figure 26. ^{13}C NMR spectrum of **6f**

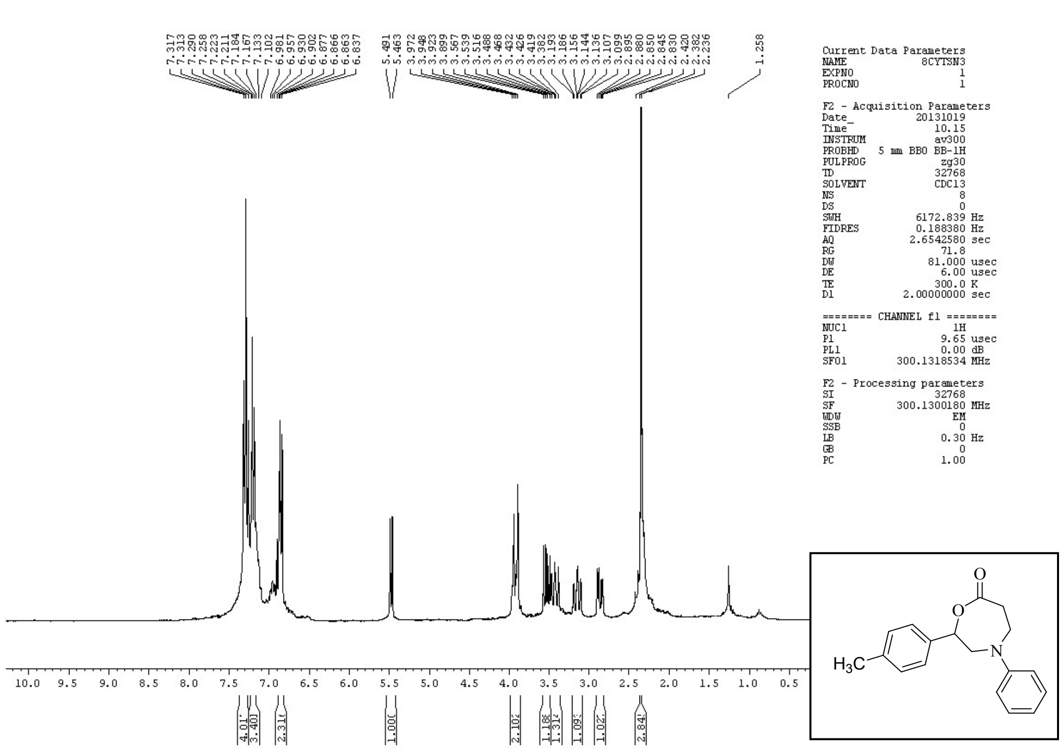


Figure 27. ^{1}H NMR spectrum of **6g**

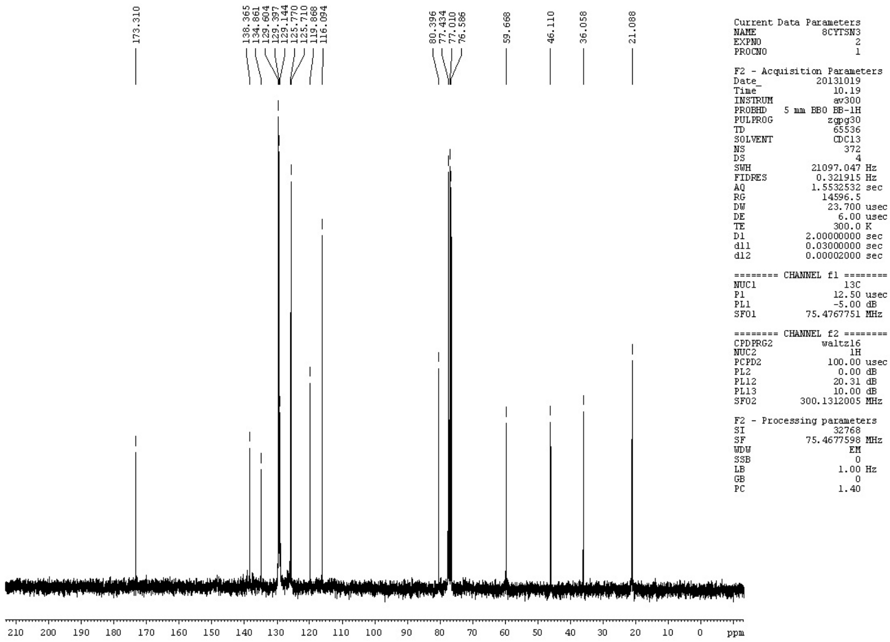


Figure 28. ^{13}C NMR spectrum of **6g**

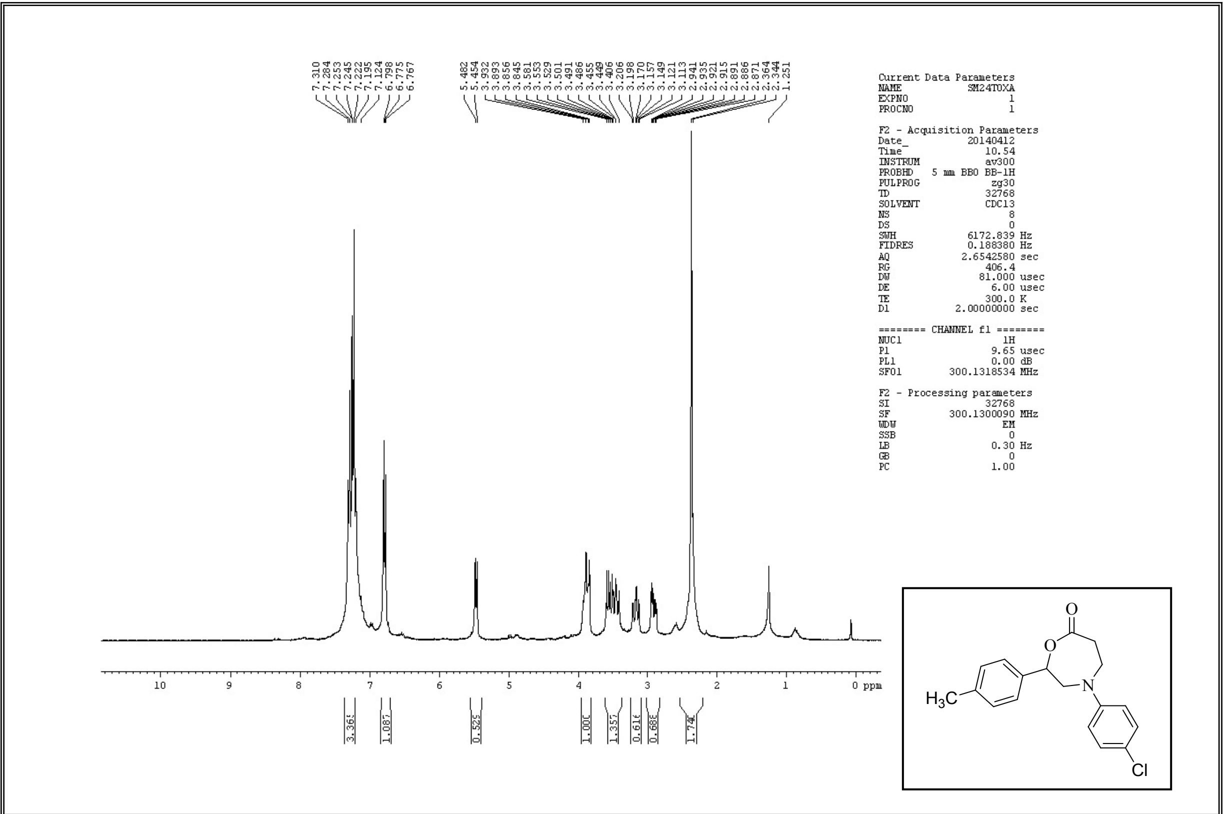


Figure 29. ^{1}H NMR spectrum of **6h**

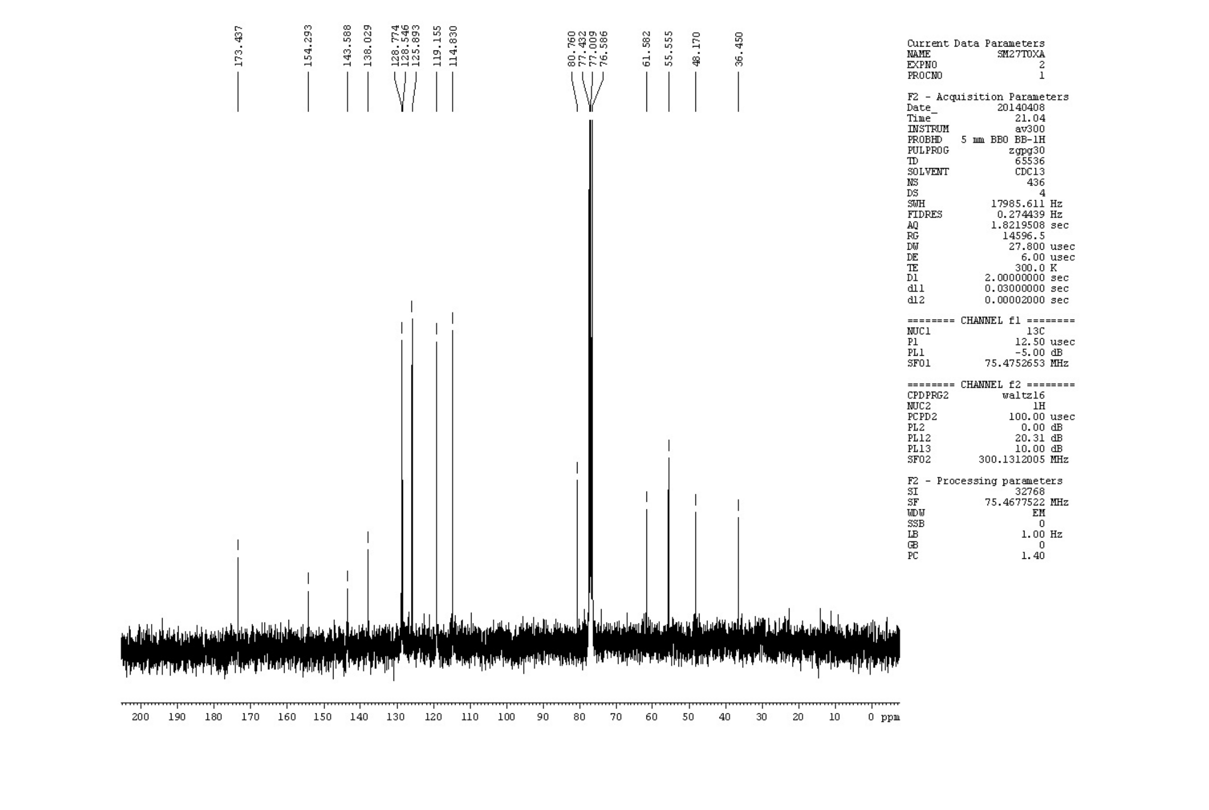


Figure 30. ^{13}C NMR spectrum of **6h**

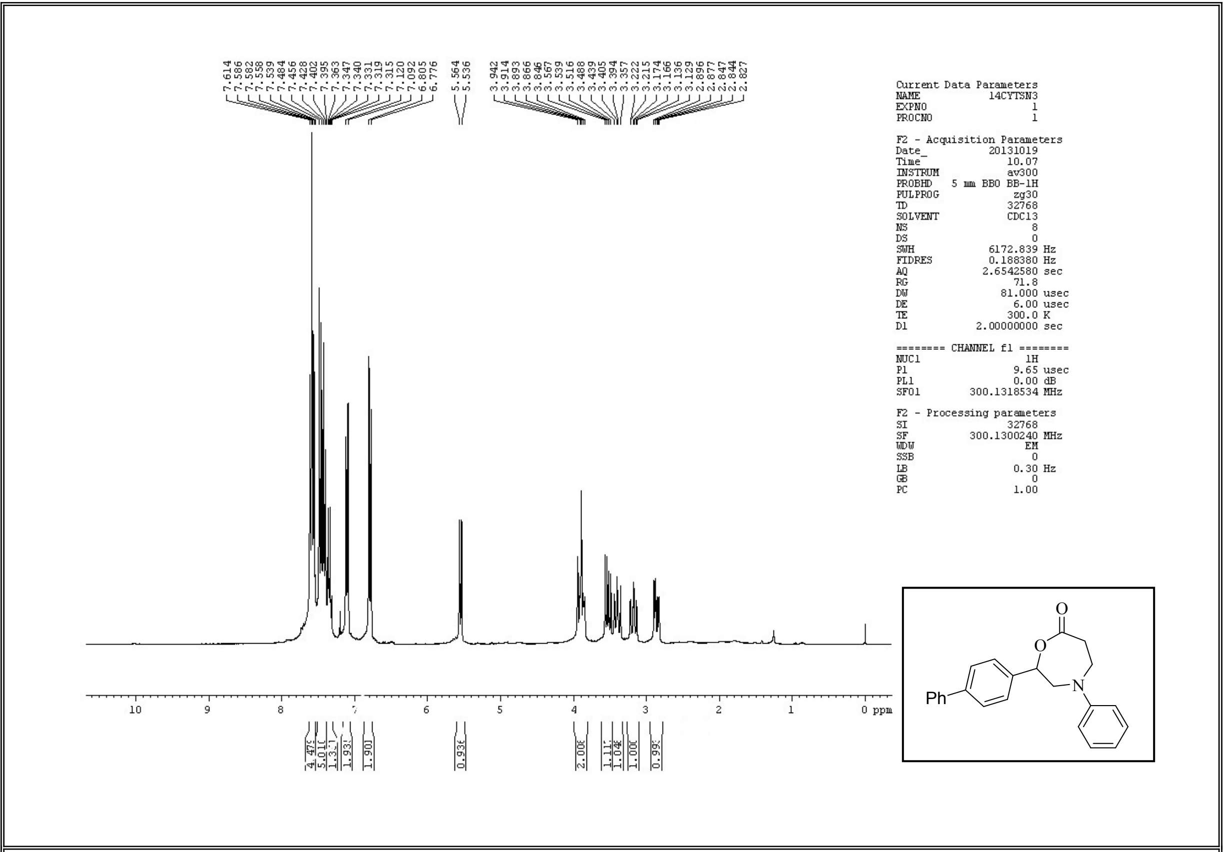


Figure 31. ^{1}H NMR spectrum of **6i**

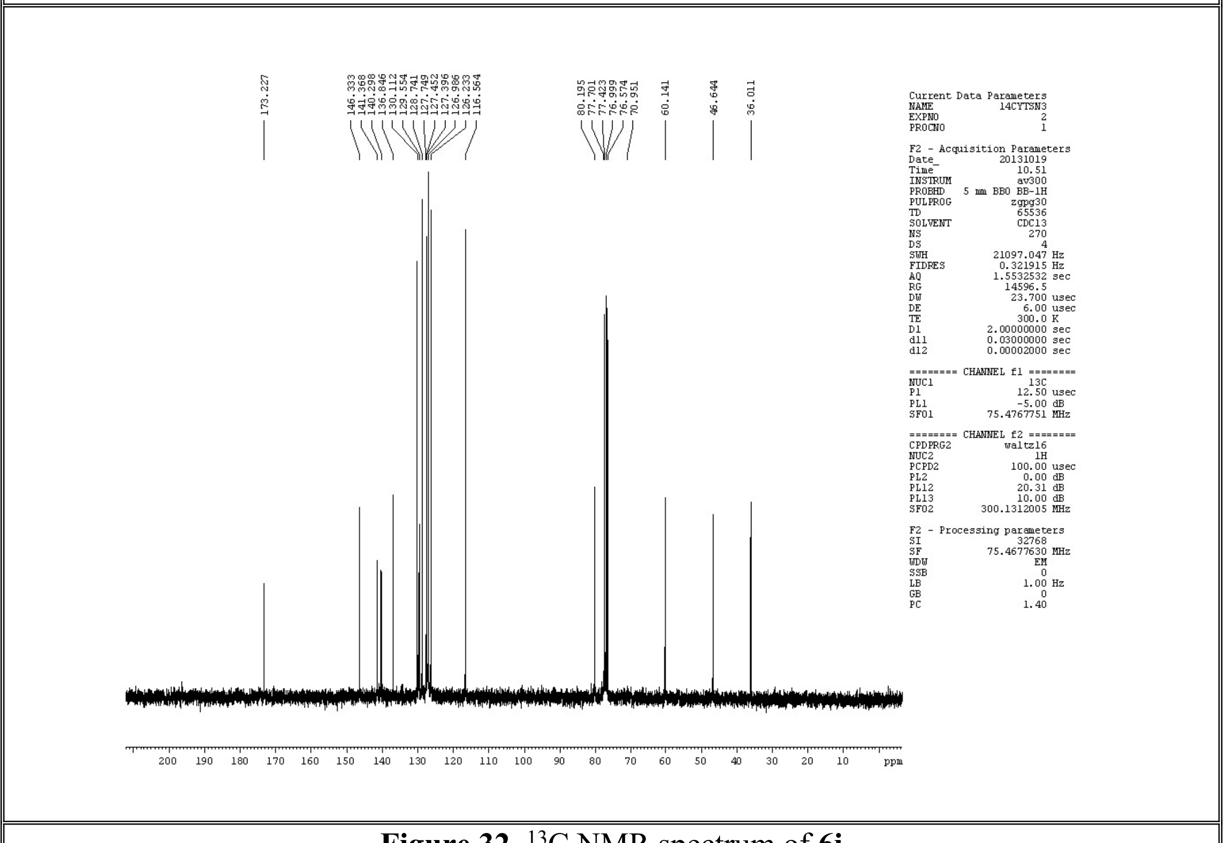


Figure 32. ^{13}C NMR spectrum of **6i**

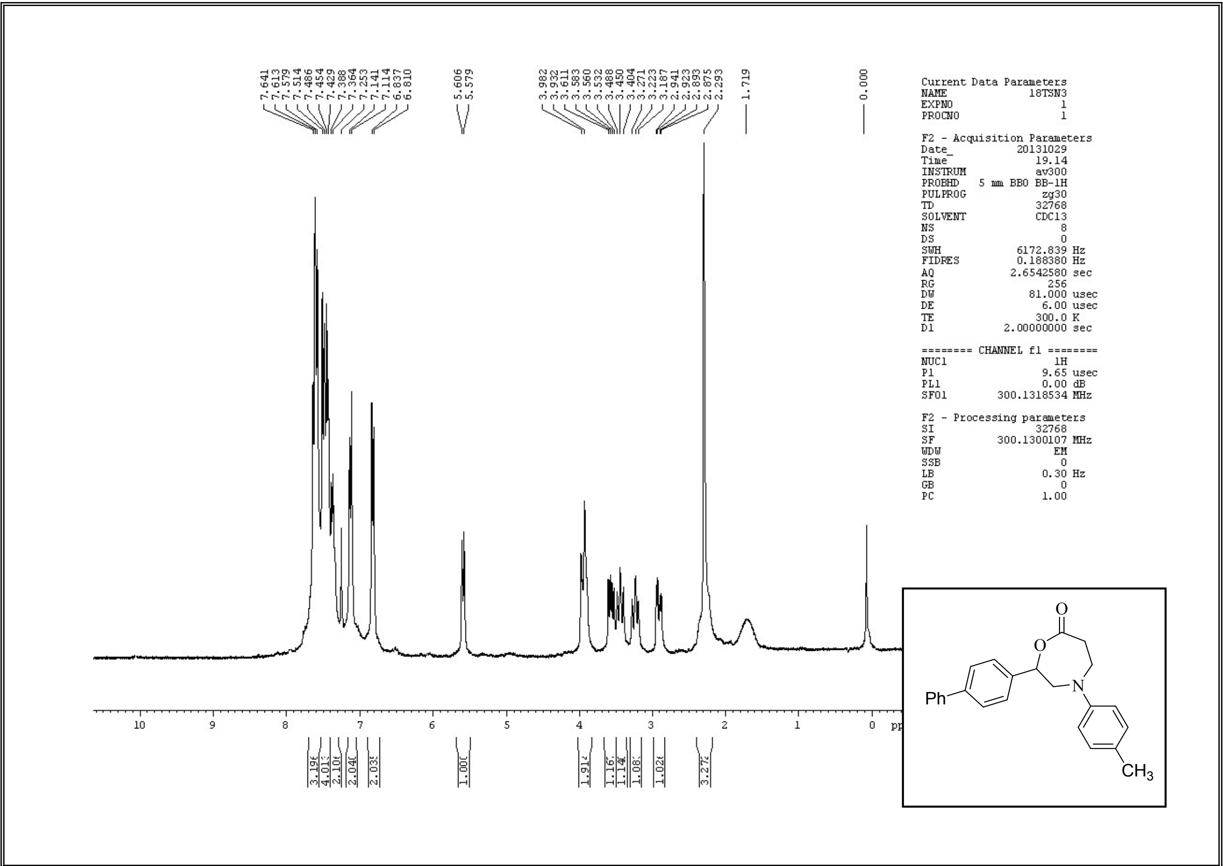


Figure 33. ^{1}H NMR spectrum of **6j**

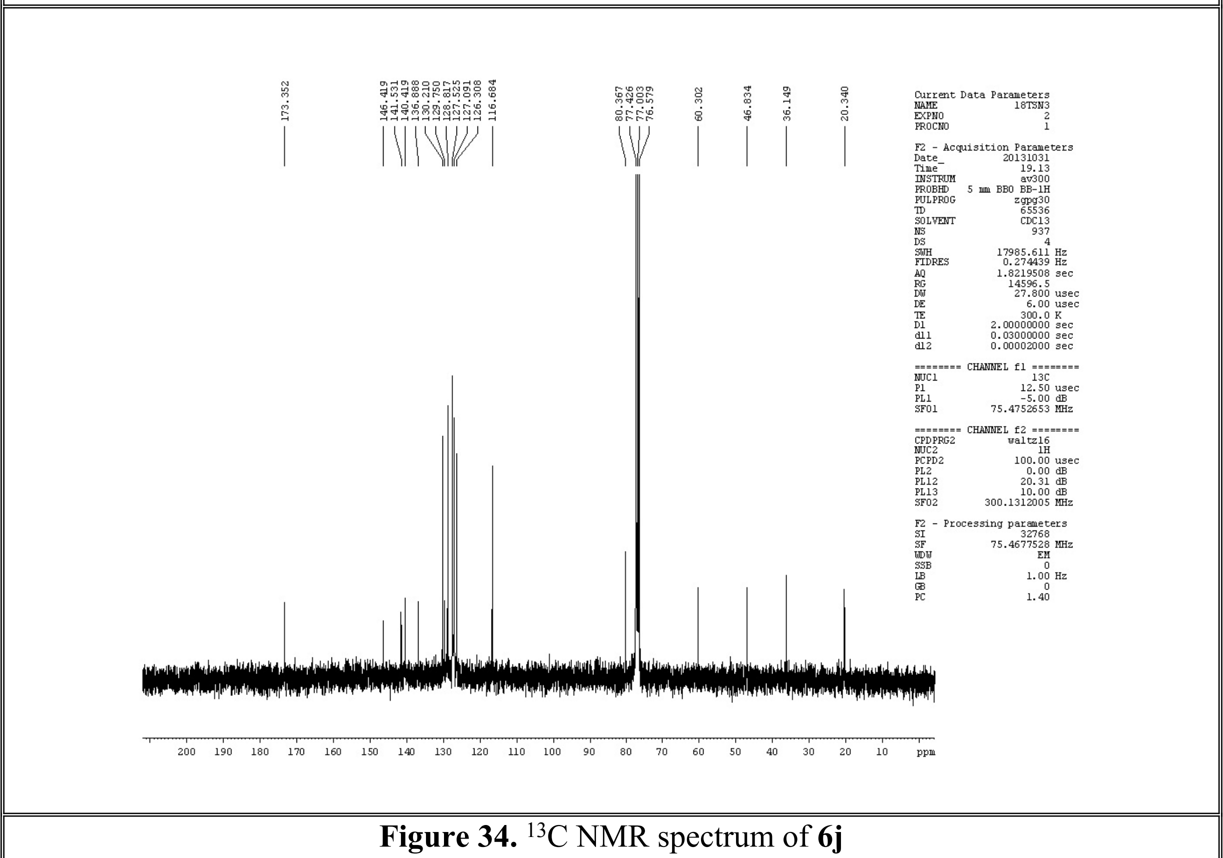


Figure 34. ^{13}C NMR spectrum of **6j**

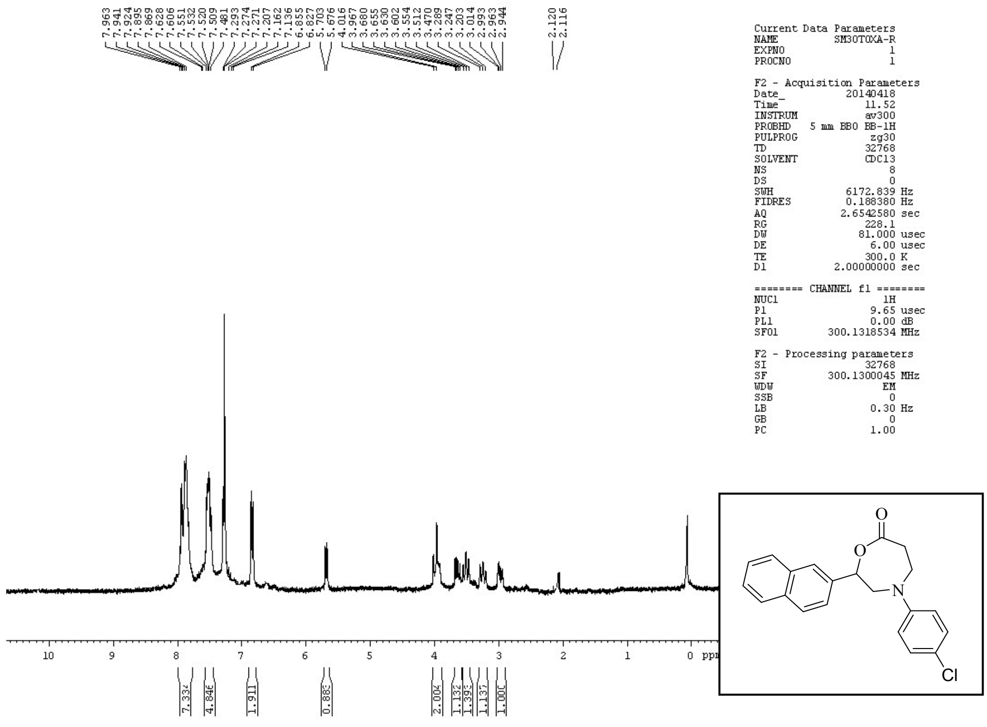


Figure 35. ^{1}H NMR spectrum of **6k**

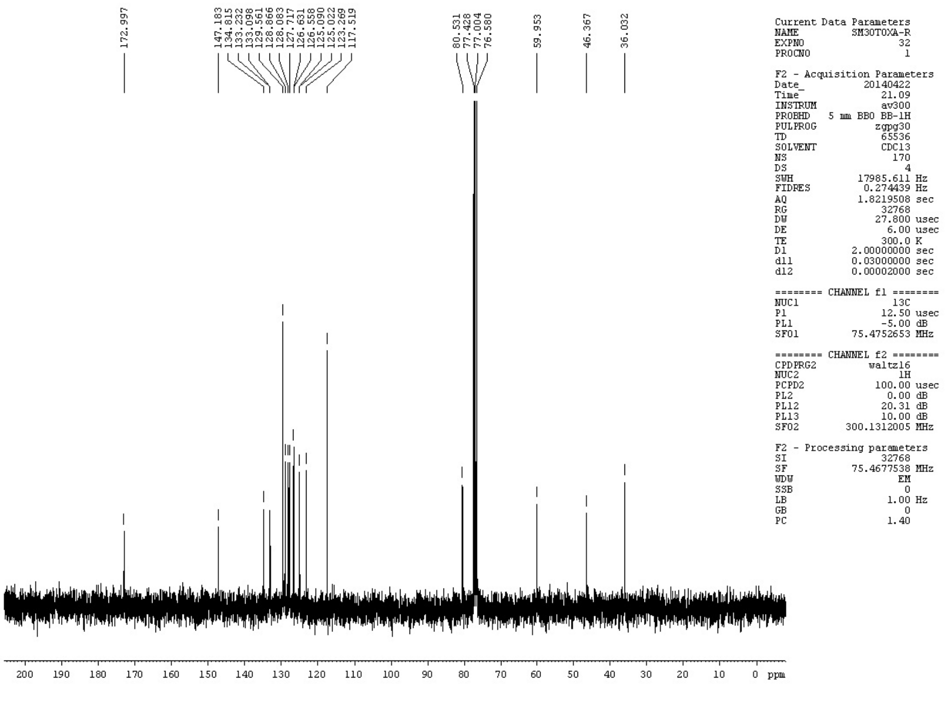


Figure 36. ^{13}C NMR spectrum of **6k**

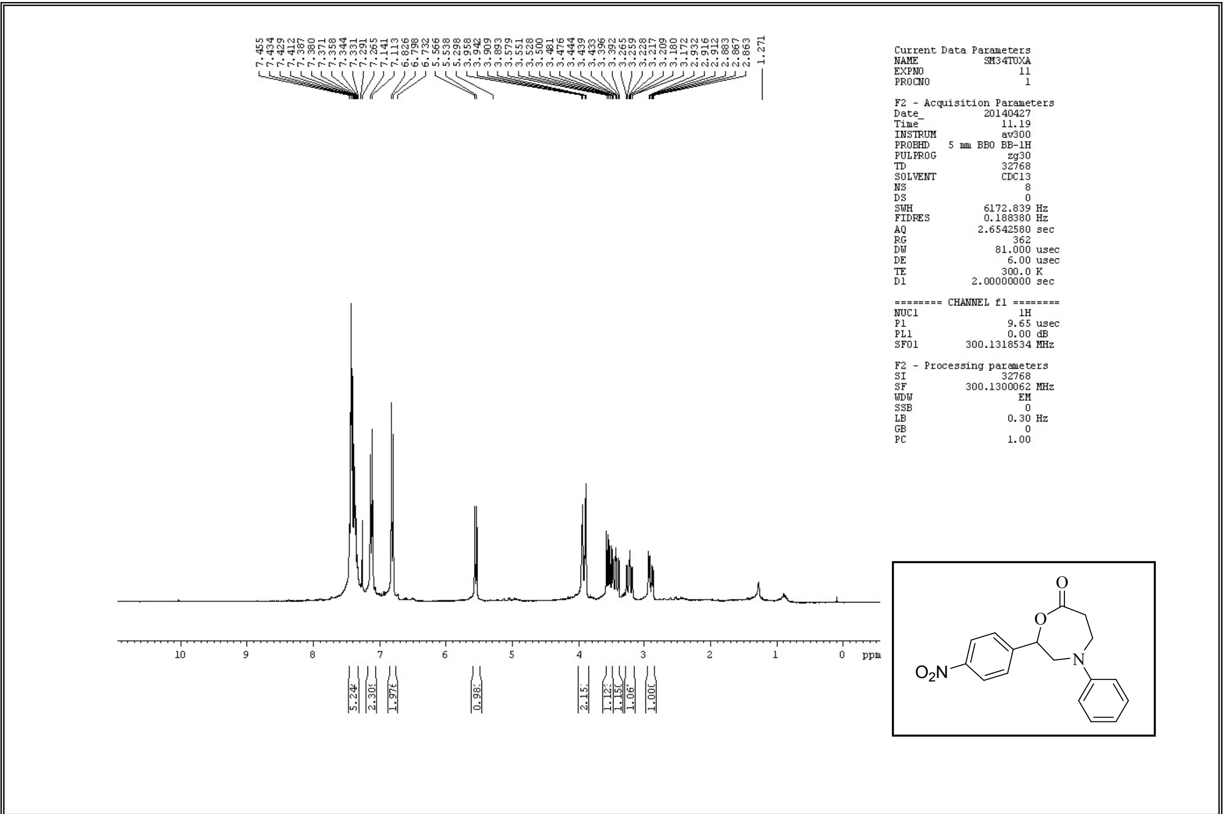


Figure 37. ^{1}H NMR spectrum of **6l**

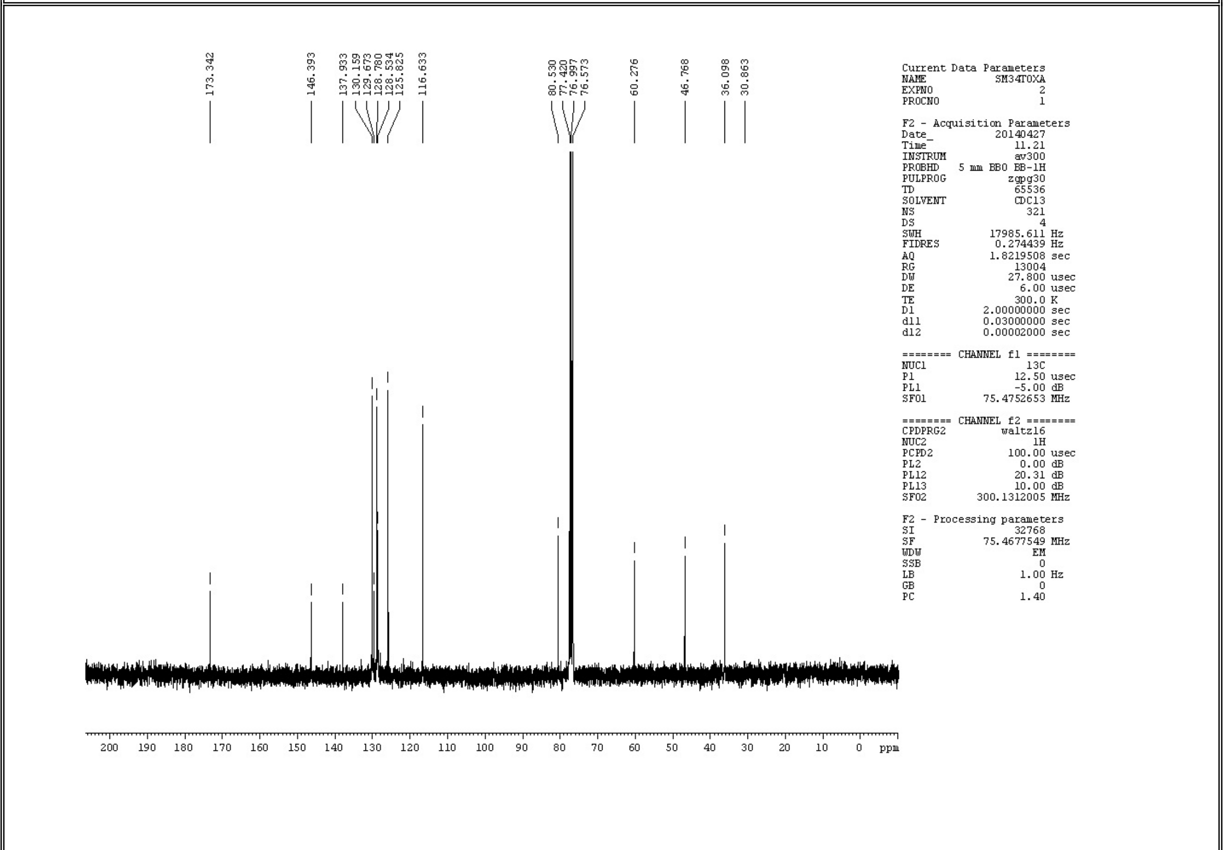


Figure 38. ^{13}C NMR spectrum of **6l**