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 (¹H and ¹³C NMR) spectra were recorded on a Bruker 300 MHz NMR spectrometer in CDCl₃ using TMS as internal standard. Chemical shifts are reported in parts per million (δ), coupling constants (J values) are reported in Hertz (Hz). ¹³C 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 °) 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$_3$) $\delta_H$: 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$_3$) $\delta_C$: 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$_3$) $\delta_H$: 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$_3$) $\delta_C$: 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$_3$) $\delta_H$: 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$_3$) $\delta_C$: 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$_3$) $\delta_H$: 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$_3$) $\delta_C$: 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\(_3\)) \(\delta\): 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), 6.83 (d, 2H, \(J = 9.0\) Hz, Ar-H), 7.34 - 7.46 (m, 7H, Ar-H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\): 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\(_3\)) \(\delta\): 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), 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\(_3\)) \(\delta\): 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\(_2\)NO: 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\(_3\)) \(\delta\): 2.19 (m, 1H, CH); 2.32 (s, 3H, CH\(_3\)), 2.82 (s, 1H, OH), 3.20 (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\(_2\)), 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\(_3\)) \(\delta\): 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\(_3\)) \(\delta\): 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\(_3\)) \(\delta\): 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\(_3\)) \(\delta\): 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). 13C NMR (75 MHz, CDCl3) δC: 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 C23H21NO 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; 1H NMR (300 MHz, CDCl3) δH: 2.25 (m, 1H, CH); 2.29 (s, 3H, CH3), 3.38 (dd, 1H, J = 14.7, 9.6 Hz, CH2), 3.65 (dd, 1H, J = 14.4, 3.3 Hz, CH2), 3.98-4.07 (m, 2H, CH2), 5.01 (dd, 1H, J = 9.6, 3.0 Hz, CH2), 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); 13C NMR (75 MHz, CDCl3) δC: 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 C24H23NO: 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; 1H NMR (300 MHz, CDCl3) δH: 2.24-2.25 (m, 1H, CH), 3.51 (dd, 1H, J = 15.0, 9.0 Hz, CH2), 3.67 (dd, 1H, J = 14.7, 3.6 Hz, CH2), 4.02-4.10 (m, 2H, CH2), 5.13-5.16 (m, 1H, CH2), 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). 13C NMR (75 MHz, CDCl3) δC: 41.1, 59.8, 71.7, 72.4, 79.3, 115.4, 123.3, 123.8, 124.7, 125.8, 126.1, 127.6, 128.2, 128.9, 132.9, 133.1, 139.2, 147.7. Anal. Calcd for C21H18ClNO: 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; 1H NMR (300 MHz, CDCl3) δH: 2.23 (s, 1H, CH), 3.19 (s, 1H, OH), 3.28-2.36 (m, 1H, CH2), 3.58-3.63 (m, 1H, CH2), 3.94-4.09 (m, 2H, CH2), 4.93-5.06 (m, 1H, CH2), 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). 13C NMR (75 MHz, CDCl3) δC: 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 C17H16N2O3: 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; 1H NMR (300 MHz, CDCl3) δH: 2.92 (dd, 1H, J = 14.7, 5.7 Hz, CH2), 3.20 (t, 1H, J = 14.1 Hz, CH2), 3.47 (dd, 1H, J = 14.7, 5.4 Hz, CH2), 3.57 (dd, 1H, J = 15.3, 8.4 Hz, CH2), 3.97 (d, 2H, J = 15.0 Hz, CH2), 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). 13C NMR (75 MHz, CDCl3) δC: 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; ^1H 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). ^13C 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; ^1H 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). ^13C 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; ^1H 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). ^13C 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 °C. ^1H 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). ^13C 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$_3$) $\delta_{H}$: 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$_3$) $\delta_{C}$: 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$_2$NO$_2$: 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$_3$) $\delta_{H}$: 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$_3$) $\delta_{C}$: 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$_3$) $\delta_{H}$: 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$_3$) $\delta_{C}$: 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$_3$) $\delta_{H}$: 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$_3$) $\delta_{C}$: 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 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta_{H}$: 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).

13C NMR (75 MHz, CDCl3) 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 C24H23NO2: 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; 1H NMR (300 MHz, CDCl3) δ H: 2.98 (dd, 1H, J = 15.3, 6.3 Hz, CH2), 3.25 (t, 1H, J = 12.6 Hz, CH2), 3.51 (t, 1H, J = 12.6 Hz, CH2), 3.64 (dd, 1H, J = 15.0, 7.5 Hz, CH2), 3.97 - 4.02 (m, 2H, CH2), 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). 13C NMR (75 MHz, CDCl3) 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 C21H18ClNO2: 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; 1H NMR (300 MHz, CDCl3) δ H: 2.90 (dd, 1H, J = 14.7, 5.4 Hz, CH2), 3.17-3.26 (m, 1H, CH2), 3.39-3.48 (m, 1H, CH2), 3.53 (dd, 1H, J = 15.3,8.4 Hz, CH2), 3.89 - 3.96 (m, 2H, CH2), 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). 13C NMR (75 MHz, CDCl3) 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 C17H16N2O4: 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. $^{1}H$ NMR spectrum of 6e

Figure 24. $^{13}C$ 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 61

Figure 38. $^{13}$C NMR spectrum of 61