Supporting information

Synthesis of fused oxazole containing coumarin derivatives via oxidative cross coupling reaction using a combination of CuCl₂ and TBHP

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Experimental General: Melting points were determined on a Büchi melting point apparatus. IR spectra were recorded on Perkin-Elmer 281 IR spectrophotometer. \(^1\)H NMR spectra were recorded on Brucker 600 MHz and Varian 400 MHz spectrometer with TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). \(^1\)H NMR Spectra are reported in the order: multiplicity, coupling constant (J value) in hertz (Hz) and no. of protons, signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet), and dd (doublet of double). HRMS spectra were recorded using WATERS MS system, Q-TOF premier and data analyzed using Mass Lynx 4.1. The X-ray crystal structures were determined with a Siemen P-4 diffractometer. Complete crystallographic data of 2a (CCDC 1405370) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (\(\lambda = 0.71073\) Å) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Compound 2a empirical formula C\(_{16}\)H\(_{9}\)NO\(_3\), pale yellow crystal, formula wt 263.24, Monoclinic, P2(1)/n, \(a = 7.1596(4)\) Å, \(b = 13.3572(7)\) Å, \(c = 13.0999(6)\) Å, \(V = 1239.47(11)\) Å\(^3\), \(Z = 4\), \(F(0 0 0) = 544\), GOF(S) = 0.976. Final indices \(R_{obs} = 0.0501\), \(wR_{obs} = 0.1013\) with \(I > 2\sigma(I)\); \(R_{all} = 0.1039\), \(wR_{all} = 0.1238\) for all data.

![Ortep diagram of 2a](image)

Figure 1. Ortep diagram of 2a (CCDC number 1405370)
General procedure for the synthesis of various derivatives of 3-(benzylamino)-2H-chromen-2-one (1a-u):

\[
\begin{align*}
\text{Into a 25 mL round bottom flask was taken a mixture of 3-aminocomarin (1 mmol), benzyl bromide (1 mmol) and K}_2\text{CO}_3 (1.2 mmol) in 3 mL of DMF. The reaction mixture was heated at 100 °C for 2-8 h and after completion of the reaction, the reaction mixture was worked-up with ethyl acetate. The crude product obtained after evaporation of the solvent in rotary evaporator was treated with ethanol to remove impurities. Finally a solid pure product (1a-u) was obtained in 75-85 %.}
\end{align*}
\]

General procedure for the synthesis of various derivatives of 2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2a-u):

\[
\begin{align*}
\text{Into a 10 mL round bottom flask 0.3 mmol of 1 was taken and then 3 mL of DCM was added into it. Then after adding 20 mol % of CuCl}_2\text{ and 3 equivalent of TBHP, the reaction mixture was stirred at room temperature 18-24 h. The progress of the reaction was checked by TLC. After completion of the reaction, the reaction mixture was worked up with DCM and the crude product obtained after rotary evaporator was purified with column chromatography eluting with hexane and ethylacetate mixture (9:1). The pure product obtained after column chromatography was characterized by H}^1\text{ NMR, } ^{13}\text{C NMR and HRMS.}
\end{align*}
\]

2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2a). Pale yellow solid; Yield = 72% (57 mg); MP = 188-190 °C; IR(KBr) \(\nu_{\text{max}} = 2958.00, 2923.26, 1756.03, 1606.03, 1261.51, 1156.54, 1103.31, 1064.16 \text{ cm}^{-1}\); H\(^1\) NMR (400 MHz, CDCl\(_3\)) \(\delta = 8.26 (d, J = 7.2 \text{ Hz}, 2 \text{ H}), 7.94 (d, J = 7.6 \text{ Hz}, 1 \text{ H}), 7.52 (m, 5 \text{ H}), 7.44 (t, J = 7.6 \text{ Hz}, 1 \text{ H}) \text{ ppm.} ^{13}\text{C NMR (100 MHz, CDCl}_3\text{)} \(\delta = 163.6, 156.4, 155.5, 153.2, 132.3, 131.9, 129.5, 128.4, 127.3, 119.2, 118.7, 118.1, 117.9, 117.5, 117.3, 116.8, 116.5, 115.8, 115.3, 114.9, 114.5, 113.3, 112.7, 112.3, 111.9, 111.6, 111.2, 110.8, 110.5, 106.5 \text{ ppm.}
\]
2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2b). Pale yellow solid; Yield = 68% (56 mg); MP = 246 °C; IR(KBr) \(\nu_{max}\) = 3062.59, 2920.20, 1756.65, 1639.88, 1261.33, 1155.35, 1110.03, 1065.66 cm\(^{-1}\); H\(^1\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.13 (d, \(J = 8\) Hz, 2 H), 7.92 (d, \(J = 7.6\) Hz, 1 H), 7.70 (t, \(J = 7.6\) Hz, 1 H), 7.50 (d, \(J = 8\) Hz, 1 H), 7.42 (t, \(J = 4.8\) Hz, 1 H), 7.34 (d, \(J = 8\) Hz, 2 H), 2.44 (s, 3 H) ppm. \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 163.8, 156.4, 155.2, 153.1, 143.0, 131.7, 130.1, 127.6, 126.1, 125.1, 123.2, 121.6, 117.9, 111.8, 21.9. HRMS [ESI+] m/z: calecd for C\(_{16}\)H\(_{15}\)NO\(_3\) [M+H]\(^+\) = 278.0812 (found 278.0813)

2-(4-fluorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (2c). Pale yellow solid; Yield = 64% (54 mg); MP = 233 °C; IR(KBr) \(\nu_{max}\) = 2924.10, 2853.13, 1737.29, 1634.64, 1229.50, 1097.64, 1068.25, 1027.01 cm\(^{-1}\); H\(^1\) NMR (600 MHz, CDCl\(_3\)) \(\delta\) 8.27 (t, \(J = 7.6\) Hz, 2 H), 7.93 (d, \(J = 7.6\) Hz, 1 H), 7.62 (t, \(J = 7.8\) Hz, 1 H), 7.53 (d, \(J = 8.4\) Hz, 1 H), 7.44 (t, \(J = 7.8\) Hz, 1 H), 7.25 (t, \(J = 8.4\) Hz, 2 H) ppm. \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 166.6, 164.0, 162.7, 156.3, 155.5, 153.2, 132.0, 130.0, 129.95, 125.2, 122.3, 121.6, 118.0, 116.8, 116.6, 111.7 ppm; HRMS [ESI+] m/z: calecd for C\(_{16}\)H\(_{15}\)FNO\(_3\) [M+H]\(^+\) = 282.0561 (found 282.0567)

2-(4-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (2d). Pale yellow solid; Yield = 60% (54 mg); MP = 226-229 °C; IR(KBr) \(\nu_{max}\) = 2963.49, 2925.09, 2845.34, 1760.06, 1604.80, 1261.57, 1093.47, 1020.06 cm\(^{-1}\); H\(^1\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.18 (d, \(J = 8.4\) Hz, 2 H), 7.92 (d, \(J = 8\) Hz, 1 H), 7.61 (t, \(J = 7.6\) Hz, 1 H), 7.51 (t, \(J = 7.6\) Hz, 3 H), 7.43 (t, \(J = 7.6\) Hz, 1 H) ppm. \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 163.7, 155.4, 153.2, 139.2, 133.1, 131.8, 129.2, 128.2, 125.8, 125.1, 124.8, 121.6, 117.8, 111.5 ppm; HRMS [ESI+] m/z: calecd for C\(_{16}\)H\(_{14}\)CINO\(_3\) [M+H]\(^+\) = 298.0265 (found 298.0278)

2-(m-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2e). Pale yellow solid; Yield = 62% (52 mg); MP = 188 °C; IR(KBr) \(\nu_{max}\) = 2956.72, 2918.40, 1753.81, 1639.30, 1102.98, 1060.65, 1031.94 cm\(^{-1}\); H\(^1\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 8.08 (s, 1 H), 8.04 (d, \(J = 6.8\) Hz, 1 H), 7.93 (d, \(J = 7.6\) Hz, 1 H), 7.60 (t, \(J = 7.2\) Hz, 1 H), 7.50 (d, \(J = 8.4\) Hz, 1 H), 7.42 (t, \(J = 7.6\) Hz, 2 H), 7.37 (d, \(J = 7.2\) Hz, 1 H), 2.45 (s, 3 H) ppm. \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 163.7, 155.4, 153.2, 139.2, 133.1, 131.8, 129.2, 128.2, 125.8, 125.1, 124.8, 121.6, 117.9, 111.8, 21.5 ppm; HRMS [ESI+] m/z: calecd for C\(_{16}\)H\(_{15}\)NO\(_3\) [M+H]\(^+\) = 278.0817 (found 278.0817)

2-(3-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (2f). Pale yellow solid; Yield = 56% (50 mg); MP = 232-234 °C; IR(KBr) \(\nu_{max}\) = 2923.34, 2852.57, 1755.61, 1638.29, 1286.06, 1096.19, 1052.92, 1029.17 cm\(^{-1}\); H\(^1\) NMR (600 MHz, CDCl\(_3\)) \(\delta\) 8.26 (t, \(J = 1.8\) Hz, 1 H), 8.16 (d, \(J = 7.8\) Hz, 1 H), 7.95 (dd, \(J = 7.8\), 1.8 Hz, 1 H), 7.64 (m, 1 H), 7.55 (d, \(J = 7.5\) Hz, 1 H), 7.53 (d, \(J = 8.4\) Hz, 1 H), 7.50 (t, \(J = 8.4\) Hz, 1 H), 7.45 (t, \(J = 7.2\) Hz, 1 H) ppm. \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 162.1, 156.2, 155.7, 153.3, 135.5, 132.3, 132.2, 130.7, 127.6, 127.5, 126.1, 125.7, 125.3, 121.7, 118.0, 111.6 ppm; HRMS [ESI+] m/z: calecd for C\(_{16}\)H\(_{14}\)ClNO\(_3\) [M+H]\(^+\) = 298.0265 (found 298.0271).
2-(2-chlorophenyl)-4H-chromeno[3,4-d]oxazol-4-one (2g). Pale yellow solid; Yield = 55% (49 mg); MP = 171-173 °C; IR(KBr) νmax = 2924.13, 2852.45, 1757.06, 1641.27, 1167.90, 1068.50, 1034.42; H1 NMR (400 MHz, CDCl3) δ = 8.23 (d, J = 8.4 Hz, 1 H), 7.95 (d, J = 7.6 Hz, 1 H), 7.63 (t, J = 8.8 Hz, 1 H), 7.59 (d, J = 8.4 Hz, 1 H), 7.53 (d, J = 8 Hz, 1 H), 7.49 (dd, J = 7.6, 1.6 Hz, 1 H), 7.46 (d, J = 3.6 Hz, 1 H), 7.45 (d, J = 3.2 Hz, 1 H) ppm; 13C NMR (100 MHz, CDCl3) 161.6, 156.2, 155.8, 153.4, 133.6, 132.8, 132.2, 131.8, 127.4, 125.8, 125.2, 125.0, 121.9, 118.0, 111.7 ppm. HRMS [APCI+] m/z: calcld for C16H15ClNO3 [M+H]+ = 298.0265 (found 298.0268).

2-(2-methoxyphenyl)-4H-chromeno[3,4-d]oxazol-4-one (2h). Pale yellow solid; Yield = 65% (57 mg); MP = 168-170 °C; IR 2956.26, 2924.46, 2853.39, 1751.49, 1652.71, 1265.42, 1166.69, 1069.43, 1021.09 cm-1; H1 NMR (400 MHz, CDCl3) δ = 8.16 (d, J = 7.2 Hz, 1 H), 7.93 (d, J = 8 Hz, 1 H), 7.59 (m, 1 H), 7.52 (t, J = 8.4 Hz, 2 H), 7.42 (t, J = 7.6 Hz, 1 H), 7.11 (m, 2 H), 4.02 (s, 3 H) ppm; 13C NMR (150 MHz, CDCl3) δ = 162.4, 158.6, 156.4, 155.2, 153.2, 138.5, 133.6, 131.7, 131.4, 125.0, 121.7, 121.0, 117.8, 115.0, 112.3, 119.9, 56.2 ppm. HRMS [ESI+] m/z: calcld for C17H15NO3 [M+H]+ = 294.0778 (found 294.0779).

2-(2-methoxyphenyl)-4H-chromeno[3,4-d]oxazol-4-one (2i). Pale yellow solid; Yield = 67% (64 mg); MP = 207-209 °C; IR 3066.92, 2949.93, 1684.67, 1285.19, 1167.19, 1063.56, 1041.90 cm-1; H1 NMR (400 MHz, CDCl3) δ = 8.19 (d, J = 8.4 Hz, 2 H), 7.94 (d, J = 7.6 Hz, 1 H), 7.61 (t, J = 7.4 Hz, 1 H), 7.56 (d, J = 8.4 Hz, 2 H), 7.51 (d, J = 8.8 Hz, 1 H), 7.43 (t, J = 7.2 Hz, 1 H), 1.38 (s, 9 H) ppm; 13C NMR (100 MHz, CDCl3) δ = 163.8, 156.6, 156.1, 155.3, 153.1, 131.8, 127.5, 126.3, 126.1, 125.1, 123.1, 121.6, 117.9, 111.8, 35.4, 31.3 ppm; HRMS [APCI+] m/z: calcld for C19H17NO3 [M+H]+ = 320.1281 (found 320.1280).

2-(thiophen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (2j). Pale yellow solid; Yield = 68% (55 mg); MP = 170-172 °C; IR 3095.65, 2924.28, 2853.43, 1752.86, 1634.11, 1210.78, 1101.71, 1068.24, 1032.66 cm-1; H1 NMR (400 MHz, CDCl3) δ = 7.95 (d, J = 3.2 Hz, 1 H), 7.90 (dd, J = 7.6, 1.2 Hz, 1 H), 7.60 (m, 2 H), 7.50 (d, J = 8 Hz, 1 H), 7.42 (t, J = 7.6 Hz, 1 H), 7.21 (t, J = 4.8 Hz, 1 H) ppm; 13C NMR (100 MHz, CDCl3) δ = 159.5, 156.2, 155.0, 153.1, 151.9, 151.3, 130.8, 128.6, 128.0, 126.0, 125.2, 121.6, 117.9, 111.5 ppm; HRMS [ESI+] m/z: calcld for C14H17NO3S [M+H]+ = 270.0219 (found 270.0240).

2-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (2k). Pale yellow solid; Yield = 80% (75 mg); MP = 245°C; IR(KBr) νmax = 2925.03, 2852.61, 1755.81, 1605.26, 1101.74, 1067.46, 1029.24 cm-1; H1 NMR (400 MHz, CDCl3) δ = 8.77 (s, 1 H), 8.30 (d, J = 8.8 Hz, 1 H), 7.99 (d, J = 8 Hz, 3 H), 7.90 (d, J = 8.8 Hz, 1 H), 7.61 (m, 3 H), 7.53 (d, J = 8 Hz, 1 H), 7.46 (t, J = 7.6 Hz, 1 H) ppm; 13C NMR (100 MHz, CDCl3) δ = 163.8, 156.4, 155.5, 153.2, 153.1, 133.0, 131.9, 129.3, 129.2, 128.4, 128.36, 128.2, 127.4, 126.6, 125.2, 123.7, 123.2, 121.7, 118.0, 111.8 ppm; HRMS [ESI+] m/z: calcld for C20H18NO3 [M+H]+ = 314.0812 (found 314.0816).
6-methoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2n). Pale yellow solid; Yield = 66% (58 mg); MP = 220 °C; IR(KBr) \( \nu_{\text{max}} \) = 3063.33, 2997.68, 2928.07, 2844.55, 1759.97, 1640.76, 1277.78, 1075.41, 1043.28, 1002.19 cm\(^{-1}\); \( ^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.26 (d, \( J = 6 \text{ Hz, 2 H} \)), 7.56 (m, 3 H), 7.50 (d, \( J = 8 \text{ Hz, 1 H} \), 7.36 (t, \( J = 7.6 \text{ Hz, 1 H} \)), 7.14 (d, \( J = 8.4 \text{ Hz, 1 H} \)), 4.00 (s, 3 H) ppm; \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \( \delta \) 163.6, 155.8, 155.6, 148.2, 132.3, 129.3, 129.0, 127.5, 123.7, 123.4, 122.5, 113.6, 105.0, 101.9, 56.1, 21.9 ppm; HRMS [ESI+] m/z: calcd for C\(_{19}\)H\(_{15}\)NO\(_4\) [M+H]+ = 308.0917 (found 308.0931)

6-methoxy-2-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2o). Pale yellow solid; Yield = 66% (61 mg); MP = 228 °C; IR(KBr) \( \nu_{\text{max}} \) = 3063.33, 2997.68, 2928.07, 2844.55, 1759.97, 1640.76, 1277.78, 1075.41, 1043.28, 1002.19 cm\(^{-1}\); \( ^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.11 (d, \( J = 7.2 \text{ Hz, 2 H} \)), 7.62 (d, \( J = 8 \text{ Hz, 1 H} \)), 7.33 (t, \( J = 8 \text{ Hz, 3 H} \)), 7.11 (d, \( J = 7.6 \text{ Hz, 1 H} \)), 3.99 (s, 3 H), 2.43 (s, 3 H) ppm; \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \( \delta \) 163.8, 155.9, 155.3, 148.1, 143.0, 142.9, 130.0, 127.6, 126.2, 125.3, 123.2, 113.7, 112.9, 112.5, 56.6, 21.9 ppm; HRMS [ESI+] m/z: calcd for C\(_{18}\)H\(_{14}\)NO\(_4\) [M+H]+ = 308.0917 (found 308.0923)

2-(4-fluorophenyl)-6-methoxy-4H-chromeno[3,4-d]oxazol-4-one (2p). Pale yellow solid; Yield = 56% (52 mg); MP = 248 °C; IR(KBr) \( \nu_{\text{max}} \) = 3293.84, 2852.00, 1751.45, 1637.57, 1277.09, 1100.90, 1081.26, 1046.33 cm\(^{-1}\); \( ^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.26 (dd, \( J = 7.6, 5.2 \text{ Hz, 2 H} \)), 7.49 (d, \( J = 8 \text{ Hz, 1 H} \)), 7.36 (t, \( J = 8 \text{ Hz, 1 H} \)), 7.23 (d, \( J = 8.4 \text{ Hz, 2 H} \)), 7.15 (d, \( J = 8 \text{ Hz, 1 H} \)), 4.01 (s, 3 H) ppm; \(^{13}\)C NMR (50 MHz, CDCl\(_3\)) \( \delta \) 166.6, 164.0, 162.7, 155.8, 155.7, 148.2, 143.0, 130.0, 129.95, 126.2, 125.4, 122.3, 116.8, 116.6, 113.9, 112.9, 112.4, 56.6 ppm; HRMS [ESI+] m/z: calcd for C\(_{18}\)H\(_{16}\)NO\(_4\) [M+H]+ = 312.0667 (found 312.0682)

6-ethoxy-2-phenyl-4H-chromeno[3,4-d]oxazol-4-one (2q). Pale yellow solid; Yield = 64% (59 mg); MP = 218 °C; IR(KBr) \( \nu_{\text{max}} \) = 2967.46, 2920.28, 2845.34, 1752.51, 1603.25, 1276.85, 1081.11, 1045.09, 1017.41 cm\(^{-1}\); \( ^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 8.26 (d, \( J = 6.4 \text{ Hz, 2 H} \)), 7.55 (m, 3 H), 7.49 (d, \( J = 7.6 \text{ Hz, 1 H} \)), 7.34 (t, \( J = 8.4 \text{ Hz, 1 H} \)), 7.14 (d, \( J = 8 \text{ Hz, 1 H} \)), 4.22 (q, \( J = 6.4 \text{ Hz, 2 H} \)), 1.54 (t, \( J = 7.6 \text{ Hz, 1 H} \))
= 6.8 Hz, 3 H) ppm; $^{13}$C NMR; (100 MHz, CDCl$_3$) $\delta$ 163.6, 156.1, 155.7, 147.6, 143.2, 132.3, 129.3, 127.7, 126.0, 125.4, 115.1, 112.9, 112.6, 65.4, 15.0 ppm. HRMS [ESI+] m/z: calcd for C$_{18}$H$_{13}$NO$_4$ [M+H]$^+$ = 308.0917 (found 308.0917).

**6-ethoxy-(p-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2r).** Pale yellow solid; Yield = 58% (56 mg); MP = 195-197 °C; IR(KBr) $\nu_{\text{max}}$ = 2959.14, 2923.05, 2844.49, 1752.97, 1637.36, 1276.51, 1262.41, 1081.73, 1102.88, 1017.50 cm$^{-1}$. $^{1}$H NMR (100 MHz, CDCl$_3$) $\delta$ 7.23 (m, 3 H), 7.04 (d, J = 7.6 Hz, 1 H), 4.14 (q, J = 6.4, 2 H), 2.37 (s, 3 H), 1.45 (t, J = 7.2, 3 H) ppm. $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.8, 156.1, 155.4, 147.5, 142.9, 130.0, 127.6, 126.1, 125.3, 123.2, 115.0, 112.8, 112.6, 65.4, 21.9, 15.0 ppm; HRMS [ESI+] m/z: calcd for C$_{19}$H$_{15}$NO$_4$ [M+H]$^+$ = 322.1074 (found 322.1077).

**6-ethoxy-(m-tolyl)-4H-chromeno[3,4-d]oxazol-4-one (2s).** Pale yellow solid; Yield = 59% (57 mg); MP = 189-190 °C; IR(KBr) $\nu_{\text{max}}$ = 2924.09, 2852.21, 1747.07, 1640.50, 1278.12, 1104.94, 1047.03, 1019.35 cm$^{-1}$; $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.08 (s, 1 H), 8.03 (d, J = 7.2 Hz, 1 H), 7.48 (d, J = 8 Hz, 1 H), 7.40 (t, J = 8 Hz, 1 H), 7.36 (t, J = 5.6 Hz, 1 H), 7.31 (d, J = 8 Hz, 1 H), 7.12 (d, J = 7.6 Hz, 1 H), 4.21 (q, J = 6.8 Hz, 2 H), 2.45 (s, 3 H), 1.52 (t, J = 7.2 Hz, 3 H) ppm. $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.7, 156.0, 155.6, 147.5, 139.3, 132.1, 129.2, 128.2, 125.8, 125.3, 124.8, 115.0, 112.8, 112.5, 65.4, 21.5, 15.0 ppm; HRMS [ESI+] m/z: calcd for C$_{19}$H$_{15}$NO$_4$ [M+H]$^+$ = 322.1074 (found 322.1079).

**6-methoxy-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (2t).** Pale yellow solid; Yield = 78% (80 mg); MP = 270 °C; IR(KBr) $\nu_{\text{max}}$ = 2924.69, 2852.94, 1759.34, 1603.15, 1603.15, 1273.60, 1111.62, 1048.71 cm$^{-1}$; $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.76 (s, 1 H), 8.29 (d, J = 8.4 Hz, 1 H), 7.99 (d, J = 8 Hz, 2 H), 7.90 (d, J = 8.4, 1 H), 7.59 (t, J = 3.6 Hz, 2 H), 7.56 (d, J = 8 Hz, 1 H), 7.38 (t, J = 8 Hz, 1 H), 7.15 (d, J = 8 Hz, 1 H), 4.01 (s, 3 H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.8, 155.8, 155.7, 148.2, 135.1, 133.1, 129.3, 129.2, 128.4, 128.36, 128.2, 127.4, 126.4, 125.4, 123.8, 123.2, 113.9, 113.0, 112.5, 56.6 ppm; HRMS [ESI+] m/z: calcd for C$_{21}$H$_{13}$NO$_4$ [M+H]$^+$ = 344.0917 (found 344.0923).

**6-ethoxy-(naphthalen-2-yl)-4H-chromeno[3,4-d]oxazol-4-one (2u).** Pale yellow solid; Yield = 81% (87 mg); MP = 221°C; IR(KBr) $\nu_{\text{max}}$ = 2924.43, 2852.64, 1760.02, 1605.56, 1272.39, 2080.36, 1051.17, 1013.12 cm$^{-1}$; $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.76 (s, 1 H), 8.29 (d, J = 8.4 Hz, 1 H), 7.99 (d, J = 8 Hz, 2 H), 7.90 (d, J = 8.4, 1 H), 7.59 (t, J = 3.6 Hz, 2 H), 7.56 (d, J = 8 Hz, 1 H), 7.38 (t, J = 8 Hz, 1 H), 7.15 (d, J = 8 Hz, 1 H), 4.01 (s, 3 H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.8, 155.8, 155.7, 148.2, 135.1, 133.1, 129.3, 129.2, 128.4, 128.36, 128.2, 127.4, 126.4, 125.4, 123.8, 123.2, 113.9, 113.0, 112.5, 56.6 ppm; HRMS [ESI+] m/z: calcd for C$_{22}$H$_{15}$NO$_4$ [M+H]$^+$ = 358.1074 (found 358.1096).
H¹ NMR spectra of 2a
$^{13}$C NMR spectra of 2a
HRMS spectra of 2a
H\textsuperscript{1} NMR spectra of 2b
$^{13}$C NMR spectra of 2b
HRMS spectra of 2b

![HRMS Spectra](image)
H^1 NMR spectra of 2c
$^{13}$C NMR spectra of 2c
HRMS spectra of 2c
H¹ NMR spectra of 2d
$^{13}$C NMR spectra of 2d
HRMS spectra of 2d
H\textsuperscript{1} NMR spectra of 2e
13C NMR spectra of 2e
HRMS spectra of 2e

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+ESI Scan (20.5 sec) Frag=100.0V MB-B-17-14.d

278.0817

2e

![Chemical Structure](image)
H¹ NMR spectra of 2f
$^{13}$C NMR spectra of 2f
HRMS spectra of \(2f\)
H\textsuperscript{1} NMR spectra of 2g
$^{13}$C NMR spectra of 2g
HRMS spectra of 2g
H$^1$ NMR spectra of 2h
$^{13}$C NMR spectra of 2h
HRMS spectra of $2h$
H\textsuperscript{1} NMR spectra of 2i
$^{13}\text{C}$ NMR spectra of 2i
HRMS spectra of 2i
H\textsuperscript{1} NMR spectra of \textit{2j}
$^{13}$C NMR spectra of 2j
HRMS spectra of 2j
H\textsuperscript{1} NMR spectra of 2k
$^{13}$C NMR spectra of 2k
HRMS spectra of 2k

[Image of HRMS spectrum with chemical structure and data points]

Sample Name
Inj Vol
Data Filename

Position
Inj Position
ACQ Method

Instrument Name
Sample Type
Comment

User Name
IBM Calibration Status
Acquired Time

+ESI Scan (14.9 sec) Frag=100.0V MB-B-6-14.d
314.0816
H\textsuperscript{1} NMR spectra of 21

Pulse sequence
- Relax. delay 1.000 sec
- Pulse 45.0 degrees
- Acq. time 2.881 sec
- Width 4396.0 Hz
- 32 repetitions

Observe H1, 399.8509633

Data processing
- FT size 20788
- Total time 1 minutes

Note: 9:12-14-1H
- Solvent: cdcl3
- Temp. 29.5 C / 299.1 K
- Operator: chem
- Mercury: 600 "1H NMR"
$^{13}$C NMR spectra of 21
HRMS spectra of 2l

![HRMS Spectrum Image]

- **Sample Name**: MeO
- **Position**: InjPosition
- **Instrument Name**: ACQ Method
- **Comment**: ESI Scan (13.8 sec) Frag=135.0V M8-B-12-14.d
- **Acquired Time**: 294.0774
H¹ NMR spectra of 2m
$^{13}$C NMR spectra of $2m$
HRMS spectra of 2m

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- ESI Scan (20.8 sec) Frag=135.0V MB-B-13-14.d

308.0931

![Chemical Structure of 2m]
H¹ NMR spectra of 2n

![NMR spectrum of 2n](image)
$^{13}$C NMR spectra of 2n

![NMR Spectra Image]
HRMS spectra of 2n
H$^1$ NMR spectra of 2o
$^{13}$C NMR spectra of 2o

![NMR Spectrum](image)

**Pulse Sequence**
- Relax. delay: 1.000 sec
- Pulse: 45.0 degrees
- Acq. time: 1.104 sec
- Width: 2.123 Hz
- 2400 repetitions

**Observe**
- 100.8425824

**Decoupler**
- 399.6539999 Hz
- Power: 42 dB
- Continuously on
- WALTZ-16 modulated

**Data Processing**
- Line broadening: 6.0 Hz
- FT size: 65536
- Total time: 83 minutes

**Notes**
- Solvent: C6D6
- Temp: 25.0°C / 298.1 K
- Operator: chem
- Mercury-400 *VTXO-NMR*
HRMS spectra of **2o**

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![HRMS spectra graph with molecular structure](image)

**OMe**

**Me**
H$^1$ NMR spectra of 2p
$^{13}$C NMR spectra of 2p
HRMS spectra of 2p

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$312.0682$

*ESI Scan (15.9 sec) Frag=135.0V MB-B-14-14.d*
H\textsuperscript{1} NMR spectra of 2q
$^{13}$C NMR spectra of 2q
HRMS spectra of 2q
H\textsuperscript{1} NMR spectra of 2r
$\textsuperscript{13}$C NMR spectra of $2r$
HRMS spectra of 2r
H\textsuperscript{1} NMR spectra of 2s

MD-B-19-14-1H
Sample Name: MD-B-19-14-1H
Data Collected on: NMR-500 mercury600
Archive directory:
Sample directory:
File: MD-B-19-14-1H
Pulse Sequence: PROTON (2pul)
Solvent: dcd3
Data collected on: Nov 14 2014
Temp. 29.0 C / 308.1 K
Operator: chem
Balan. delay 1.000 sec
Pulse 45.0 degrees
Avg. time 3.561 sec
Width 0.090.6 Hz
32 repetitions
OBSERVE RL, 399.0596421 MHz
DATA PROCESSING
FT size 30728
Total time 2 min 12 sec
$^{13}$C NMR spectra of 2s
HRMS spectra of 2s
H¹ NMR spectra of 2t

![H¹ NMR spectra of 2t](image)
$^{13}$C NMR spectra of \(2t\)
HRMS spectra of 2t
H\textsuperscript{1} NMR spectra of 2u
$^{13}$C NMR spectra of 2u
HRMS spectra of 2u