Supporting Information

Tandem Michael addition/intramolecular isocyanide [3 + 2] cycloaddition: highly diastereoselective one pot synthesis of fused oxazolines

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I. General information

All reagents were commercial and used without further purification, unless otherwise indicated. Chromatography was carried on flash silica gel (300−400 mesh). All reactions were monitored by TLC, which was performed on precoated aluminum sheets of silica gel 60 (F254). Melting points were uncorrected. The $^1$H NMR and $^{13}$C NMR spectra were determined at 25°C on a 500 MHz and 125 MHz, respectively, and TMS as internal standard. All shifts are given in ppm. IR spectra (KBr) were recorded on a Magna-560 FTIR spectrophotometer in the range of 400-4000 cm$^{-1}$. Mass spectra were obtained on Agilent 1100 LCMSD mass spectrometer using the ESI method. Elemental analyses were measured on a GmbH VarioEL analyzer (Elementar Analysensysteme). The compound 2a and 6b was glued on a glass fiber. Data were collected at 273K using graphite-monochromated Mo Kα radiation ($\lambda = 0.71073\text{Å}$) and Bruker APEX CCD area-detector in the range 1.70° < $\theta$ < 26.07°. Substrates 1 were prepared by the similar method as our previously reported papers$^1$.

II. Synthetic procedures/analytical data of compounds 2, 4, 6 and 8.

![Diagram](image)

**General procedure for the synthesis of 2, 4, 6 and 8 (taking 2a as an example):** To the mixture of 1a (352.5 mg, 1.0 mmol) and ethyl isocyanoacetate 2 (0.132 mL, 1.2 mmol) in THF (5 mL) was added NaOH (4.0 mg, 0.1 mmol) in one portion at room temperature. The reaction mixture was stirred at room temperature, and the reaction mixture was monitored by TLC. After the substrate 1a was consumed, the resulting mixture was poured into ice-water (30 mL) under stirring. The precipitated solid was collected by filtration, washed with water (3 × 10 mL), and dried in vacuo to afford the product 2a (428.4 mg, 92 %) as a white solid.

2a, ethyl 7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxo-4,7a-diphenylbenzo[d]oxazole-3a-carboxylate. White solid, m.p. 201-203°C. $^1$H NMR (CDCl$_3$, 500 Hz) $\delta$ 0.60 (t, $J = 7.0$ Hz, 3H), 2.76 (dd, $J = 17.0$, 3.5 Hz, 1H), 2.84-3.18 (m, 1H), 3.13-3.18 (m, 4H), 3.23-3.27 (m, 1H), 3.35-3.39 (m, 1H), 3.89 (dd, $J = 14.0$, 3.5 Hz, 1H), 7.19-7.25 (m, 4H), 7.27-7.34 (m, 3H), 7.43 (s, 1H), 7.52 (d, $J = 7.5$ Hz, 2H), 7.59 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 Hz) $\delta$ 12.8, 37.2, 37.5, 40.0, 41.1, 61.0, 84.1, 94.0, 122.4, 126.7, 127.1, 127.6, 127.8, 128.1, 128.8, 137.7, 139.8, 157.5, 168.3, 176.7, 190.8. IR (KBr, cm$^{-1}$) 3734, 3623, 2924, 1741, 1692, 1564, 1512, 1483, 1111, 676. ES-MS: m/z = 466.0 [M + H]$^+$. Anal. Calcd for C$_{25}$H$_{23}$NO$_4$S$_2$: C, 64.49; H, 4.98; N, 3.01; Found: C, 64.40; H, 5.03; N, 2.93.

2b, ethyl 4-(4-chlorophenyl)-7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxo-7a-phenylbenzo[d]oxazole-3a-carboxylate. White solid, m.p. 212-213 °C. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.64 (t, $J = 7.5$ Hz, 3H), 2.72 (dd, $J = 17.5$, 3.0 Hz, 1H), 3.00-3.17 (m, 5H), 3.18-3.26 (m, 1H), 3.36-3.41 (m, 1H), 3.85 (dd, $J = 11.0$, 3.0 Hz, 1H), 7.20-7.48 (m, 9H), 7.57 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 Hz) δ 12.9, 37.2, 37.5, 39.4, 40.9, 61.1, 83.9, 94.0, 122.2, 127.4, 127.7, 127.8, 128.0, 130.2, 132.5, 137.5, 157.7, 168.1, 177.0, 190.4. IR (KBr, cm$^{-1}$) 3064, 1728, 1611, 1129. ES-MS: m/z = 500.0 [M + H]$^+$. Anal. Calcd for C$_{25}$H$_{22}$ClNO$_4$S$_2$: C, 60.05; H, 4.43; N, 2.80; Found: C, 59.97; H, 4.47; N, 2.73.

2c, ethyl 7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-4-(4-methoxyphenyl)-6-oxo-7a-phenylbenzo[d]oxazole-3a-carboxylate. White solid, m.p. 213-214 °C. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.64 (t, $J = 7.0$ Hz, 3H), 2.72 (dd, $J = 17.5$, 3.5 Hz, 1H), 2.95-3.01 (m, 1H), 3.06-3.25 (m, 5H), 3.30-3.41 (m, 1H), 3.74 (s, 3H), 3.84 (dd, $J = 14.5$, 3.5 Hz, 1H), 6.77 (d, $J = 9.0$ Hz, 2H), 7.18-7.33 (m, 4H), 7.43 (d, $J = 9.0$ Hz, 2H), 7.40 (s, 1H), 7.57 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 Hz) δ 12.9, 37.2, 37.5, 39.2, 41.2, 54.8, 61.0, 84.3, 94.0, 113.1, 122.5, 126.3, 127.8, 128.0, 130.0, 131.8, 137.8, 157.4, 158.2, 168.4, 176.4, 191.0. IR (KBr, cm$^{-1}$) 3034, 1728, 1631, 1488, 1395, 1281, 1127, 1074. ES-MS: m/z = 496.0 [M + H]$^+$. Anal. Calcd for C$_{26}$H$_{25}$NO$_5$S$_2$: C, 63.01; H, 5.08; N, 2.83; Found: C, 62.96; H, 5.10; N, 2.79.

2d, ethyl 7-(1,3-dithiolan-2-ylidene)-4-(furan-2-yl)-3a,4,5,6,7,7a-hexahydro-6-oxo-7a-phenylbenzo[d]oxazole-3a-carboxylate. White solid, m.p. 189-190 °C. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.74 (t, $J = 7.5$ Hz, 3H), 2.91 (dd, $J = 17.0$, 4.0 Hz, 1H), 3.03-3.24 (m, 6H), 3.45-3.58 (m, 1H), 4.14 (dd, $J = 13.5$, 4.0 Hz, 1H), 6.26 (d, $J = 1.5$ Hz, 1H), 6.29 (d, $J = 2.5$ Hz, 1H), 7.29 (s, 1H), 7.33 (s, 3H), 7.39 (s, 1H), 7.58-7.62 (m, 1H). $^{13}$C NMR (CDCl$_3$, 125 Hz) δ 13.6, 35.0, 37.7, 38.0, 38.9, 61.7, 83.8, 94.2, 107.5, 110.5, 122.7, 127.5, 128.2, 128.7, 138.1, 141.5, 153.7, 158.2, 168.8, 177.4, 190.6. IR (KBr, cm$^{-1}$) 3044, 1729, 1625, 1395, 1249, 1118, 892, 691. ES-MS: m/z = 456.0 [M + H]$^+$. Anal. Calcd for C$_{23}$H$_{21}$NO$_5$S$_2$: C, 60.05; H, 4.43; N, 3.07; Found: C, 60.50; H, 4.58; N, 3.11.

2e, ethyl 7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxo-7a-phenyl-4-(thiophen-2-yl)benzo[d]oxazole-3a-carboxylate. White solid, m.p. 200-202 °C. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.71 (t, $J = 7.0$ Hz, 3H), 2.86 (dd, $J = 17.5$, 4.0 Hz, 1H), 2.97-3.27 (m, 6H), 3.41-3.48 (m, 1H), 4.28 (dd, $J = 14.0$, 4.0 Hz, 1H), 6.87 (t, $J = 4.0$ Hz, 1H), 7.08 (d, $J = 3.0$ Hz, 1H), 7.13 (d, $J = 4.0$ Hz, 1H), 7.25 (s, 1H), 7.33 (s, 3H), 7.41 (s, 1H), 7.59 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 Hz) δ 12.9, 36.1, 37.2, 37.5, 42.0, 61.2, 84.2, 93.8, 122.2, 124.2, 125.9, 126.2, 126.5, 127.8, 128.1, 137.7, 141.9, 157.6, 168.1, 176.9, 189.9. IR (KBr, cm$^{-1}$) 3044, 1737, 1626, 1400, 1246, 1113, 678. ES-MS: m/z = 472.0 [M + H]$^+$. Anal. Calcd for C$_{23}$H$_{21}$NO$_4$S$_3$: C, 58.57; H, 4.49; N, 2.97; Found: C, 58.69; H, 4.53; N, 3.07.
2f. ethyl 7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxo-7a-phenyl-4-styrylbenzo[d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel. PE-Et2O, 1:1). Yellowish solid, m. p. 146-148 °C. 1H NMR (CDCl3, 500 Hz) δ 0.83 (t, J = 7.5 Hz, 3H), 2.68 (dd, J = 17.5, 4.5 Hz, 1H), 2.86 (dd, J = 17.5, 13.5 Hz, 1H), 3.08-3.23 (m, 5H), 3.56-3.61 (m, 1H), 6.29 (dd, J = 15.5, 8.5 Hz, 1H), 6.51 (d, J = 15.5 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.24-7.27 (m, 3H), 7.31-7.33 (m, 5H), 7.37 (s, 1H), 7.58 (s, 1H). 13C NMR (CDCl3, 125 Hz), δ 13.5, 37.5, 37.8, 38.8, 39.2, 61.5, 84.1, 93.8, 122.6, 126.3, 127.4, 127.5, 127.9, 128.3, 128.4, 133.2, 136.7, 138.1, 157.8, 168.8, 176.6, 190.9. ES-MS: m/z = 492.1 [M + H]+. Anal. Calcd for C27H25NO4S2: C, 65.96; H, 5.13; N, 2.85; Found: C, 65.81; H, 5.02; N, 2.97.

2h. ethyl 4-(4-chlorophenyl)-7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxo-7a-p-tolylbenzo[d]oxazole-3a-carboxylate. White solid, m. p. 210-212 °C. 1H NMR (CDCl3, 500 Hz) δ 0.66 (t, J = 7.5 Hz, 3H), 2.36 (s, 3H), 2.70 (dd, J = 17.5, 4.0 Hz, 1H), 3.03-3.17 (m, 5H), 3.21-3.27 (m, 1H), 3.35-3.41 (m, 1H), 3.85 (dd, J = 14.0, 4.0 Hz, 1H), 7.14 (d, J = 8.0 Hz, 3H), 7.21 (d, J = 8.5 Hz, 2H), 7.40 (s, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.47 (d, J = 8.5 Hz, 2H). 13C NMR (CDCl3, 125 Hz), δ 13.0, 21.0, 37.3, 37.6, 39.5, 41.0, 61.2, 83.9, 94.2, 122.3, 126.3, 127.1, 128.0, 128.4, 128.8, 130.3, 132.5, 134.5, 138.2, 138.6, 138.7, 157.9, 168.3, 177.1, 190.5. IR (KBr, cm−1) 3047, 1736, 1627, 1491, 1395, 1281, 1129, 1073, 874, 605. ES-MS: m/z = 514.0 [M + H]+. Anal. Calcd for C26H24ClNO4S2: C, 60.75; H, 4.71; N, 2.72; Found: C, 60.49; H, 4.69; N, 2.76.

2i. ethyl 4-(4-chlorophenyl)-7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-7a-methyl-6-oxobenzo[d]oxazole-3a-carboxylate. White solid, m.p. 175-177 °C. 1H NMR (CDCl3, 500 Hz) δ 1.07 (t, J = 7.5 Hz, 3H), 1.92 (s, 3H), 2.59 (dd, J = 15.0, 5.0 Hz, 1H), 2.91 (dd, J = 19.0, 15.0 Hz, 1H), 3.14-3.19 (m, 1H), 3.30-3.38 (m, 2H), 3.44-3.47 (m, 1H), 3.73 (dd, J = 14.0, 3.5 Hz, 1H), 4.02 (m, 2H), 7.18 (s, 1H), 7.24 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H). 13C NMR (CDCl3, 125 Hz), δ 13.8, 20.2, 36.9, 37.4, 40.8, 41.4, 61.9, 81.9, 90.3, 123.3, 128.4, 130.5, 132.9, 138.4, 158.0, 169.5, 191.2. IR (KBr, cm−1) 3034, 1719, 1705, 1618, 1256, 1114. ES-MS: m/z = 438.0 [M + H]+. Anal. Calcd for C20H20ClNO4S2: C, 54.85; H, 4.60; N, 3.20; Found: C, 54.77; H, 4.53; N, 3.32.

2j. ethyl 7a-(4-chlorostyryl)-4-(4-chlorophenyl)-7-(1,3-dithiolan-2-ylidene)-3a,4,5,6,7,7a-hexahydro-6-oxobenzo[d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel. PE-Et2O, 3:1). Yellowish solid, m.p. 114-116 °C. m.p. 175-177 °C. 1H NMR (CDCl3, 500 Hz) δ 0.87 (t, J = 7.0 Hz, 3H), 2.64 (dd, J = 17.0, 3.5 Hz, 1H), 2.98 (dd, J = 17.0, 15.0 Hz, 1H), 3.22-3.33 (m, 4H), 3.65-3.68 (m, 1H), 3.75-3.79 (m, 1H), 3.88 (dd, J = 14.5, 3.0 Hz, 1H), 6.36 (d, J = 16.0 Hz, 1H), 6.70 (d, J = 16.0 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 7.32 (s, 5H), 7.45 (d, J = 8.0 Hz, 1H).
= 8.0 Hz, 2H). $^{13}$C NMR (CDCl$_3$, 125 Hz), δ 13.7, 37.7, 37.8, 40.6, 40.8, 61.8, 84.3, 91.4, 120.6, 126.5, 127.8, 128.3, 129.0, 130.5, 131.1, 133.0, 134.1, 157.5, 168.9, 176.3, 191.0. ES-MS: m/z = 560.0 [M + H]$^+$. Anal. Calcd for C$_{27}$H$_{23}$Cl$_2$NO$_4$S$_2$: C, 57.86; H, 4.14; N, 3.32; Found: C, 57.97; H, 4.00; N, 3.51.

4a. ethyl 3a,4,5,6,7,7a-hexahydro-7-cyclopropyl-6-oxo-7a-phenyl-4-p-tolylbenzo[d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel. PE-Et$_2$O, 9:1). Purified by flash chromatography (silica gel. PE-Et$_2$O, 9:1). Yellowish viscous liquid. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.60 (t, $J$ = 7.5 Hz, 3H), 0.62-0.65 (m, 1H), 1.12-1.16 (m, 1H), 1.19-1.25 (m, 1H), 1.57-1.61 (m, 1H), 2.29 (s, 3H), 2.65 (dd, $J$ = 18.0, 3.0 Hz, 1H), 2.92 (dd, $J$ = 18.0, 14.5 Hz, 1H), 3.31-3.35 (m, 1H), 3.38-3.43 (m, 1H), 3.51 (dd, $J$ = 14.5, 3.0 Hz, 1H), 7.09 (d, $J$ = 9.0 Hz, 2H), 7.24-7.33 (m, 3H), 7.37 (s, 2H), 7.39 (s, 1H), 7.41 (d, $J$ = 9.0 Hz, 2H). $^{13}$C NMR (CDCl$_3$, 125 Hz), δ 12.7, 13.1, 21.0, 21.3, 35.7, 42.2, 42.9, 61.3, 84.7, 94.3, 126.6, 127.4, 128.3, 128.8, 129.3, 135.7, 136.4, 136.6, 155.2, 168.9, 207.3. ES-MS: m/z = 404.2 [M + H]$^+$. Anal. Calcd for C$_{25}$H$_{25}$NO$_4$: C, 74.42; H, 6.25; N, 3.47; Found: C, 74.63; H, 6.12; N, 3.58.

4b. ethyl 3a,4,5,6,7,7a-hexahydro-7-cyclopropyl-6-oxo-7a-phenyl-4-(4-chlorophenyl)benzo[d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel. PE-Et$_2$O, 9:1). Purified by flash chromatography (silica gel. PE-Et$_2$O, 9:1). Yellowish viscous liquid. $^1$H NMR (CDCl$_3$, 500 Hz) δ 0.60 (t, $J$ = 7.5 Hz, 3H), 0.62-0.64 (m, 1H), 1.12-1.16 (m, 1H), 1.21-1.25 (m, 1H), 1.55-1.61 (m, 1H), 2.65 (dd, $J$ = 18.0, 3.5 Hz, 1H), 2.92 (dd, $J$ = 18.0, 14.5 Hz, 1H), 3.31-3.35 (m, 1H), 3.38-3.43 (m, 1H), 4.27 (dd, $J$ = 14.5, 3.0 Hz, 1H), 7.09 (d, $J$ = 9.0 Hz, 2H), 7.24-7.33 (m, 3H), 7.37 (s, 2H), 7.39 (s, 1H), 7.41 (d, $J$ = 9.0 Hz, 2H). $^{13}$C NMR (CDCl$_3$, 125 Hz), δ 12.7, 13.1, 21.0, 21.3, 35.7, 42.2, 42.9, 61.3, 84.7, 94.3, 126.6, 127.4, 128.3, 128.8, 129.3, 135.7, 136.4, 136.6, 155.2, 168.9, 207.3. ES-MS: m/z = 424.1 [M + H]$^+$. Anal. Calcd for C$_{24}$H$_{22}$ClNO$_4$: C, 68.00; H, 5.23; N, 3.47; Found: C, 68.21; H, 5.11; N, 3.48.

6a. ethyl 4-(2-oxo-2-phenylethyl)-4,8b-dihydro-3aH-indeno[2,1-d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel. PE-Et$_2$O, 6:1). Yellowish solid, m.p. 131-133 °C. $^1$H NMR (CDCl$_3$, 500 Hz) δ 1.33 (t, $J$ = 7.5 Hz, 3H), 3.39 (dd, $J$ = 18.5, 6.0 Hz, 1H), 3.76 (dd, $J$ = 18.5, 8.0 Hz, 1H), 4.32-4.35 (m, 2H), 4.68 (dd, $J$ = 8.0, 6.0 Hz, 1H), 6.06 (s, 1H), 6.89 (s, 1H), 7.22 (d, $J$ = 8.0 Hz, 1H), 7.34-7.38 (m, 2H), 7.46 (t, $J$ = 8.0 Hz, 3H), 7.55 (t, $J$ = 8.0 Hz, 1H), 8.05 (d, $J$ = 8.0 Hz, 2H). $^{13}$C NMR (CDCl$_3$, 125 Hz), δ 14.1, 40.8, 47.5, 61.9, 83.9, 88.4, 124.3, 125.9, 128.1, 128.2, 128.5, 130.4, 133.1, 136.6, 137.6, 144.1, 155.1, 172.4, 198.3. ES-MS: m/z = 350.1 [M + H]$^+$. Anal. Calcd for C$_{21}$H$_{19}$NO$_4$: C, 72.19; H, 5.48; N, 4.01; Found: C, 72.32; H, 5.61; N, 4.26.
6b, ethyl 4-(2-methoxy-2-oxoethyl)-4,8b-dihydro-3aH-indeno[2,1-d]oxazole-3a-carboxylate. Purified by flash chromatography (silica gel, PE-Et2O, 9:1). White solid, m.p. 88-90 °C. 1H NMR (CDCl3, 500 Hz) $\delta$ 1.33 (t, $J = 7.0$ Hz, 3H), 2.79 (dd, $J = 17.0$, 6.0 Hz, 1H), 2.96 (dd, $J = 17.0$, 8.5 Hz, 1H), 3.76 (s, 3H), 4.31 (q, $J = 7.0$ Hz, 2H), 4.42 (dd, $J = 8.5$, 6.0 Hz, 1H), 5.98 (s, 1H), 6.90 (s, 1H), 7.22 (d, $J = 7.5$ Hz, 1H), 7.34 (t, $J = 7.5$ Hz, 1H), 7.38 (t, $J = 7.5$ Hz, 1H), 7.46 (d, $J = 7.5$ Hz, 1H), 7.46 (d, $J = 7.5$ Hz, 1H). $^{13}$C NMR (CDCl3, 125 Hz), $\delta$ 14.1, 35.7, 48.3, 51.8, 61.9, 83.7, 88.5, 124.0, 126.0, 130.4, 133.4, 135.3, 155.3, 172.2, 172.7. ES-MS: m/z = 304.1 [M + H]$^+$.

Anal. Calcd for C16H17NO5: C, 63.36; H, 5.65; N, 4.62; Found: C, 63.21; H, 5.46; N, 4.83.

8, (E)-ethyl 2-(1-(1,3-dithiolan-2-ylidene)-2-oxo-4-(thiophen-2-yl)but-3-en-1-yl)furan-3-carboxylate. 1H NMR (CDCl3, 500 Hz) $\delta$ 1.25 (t, $J = 7.0$ Hz, 3H), 3.36 (t, $J = 6.5$ Hz, 2H), 3.51 (t, $J = 6.5$ Hz, 2H), 4.29 (q, $J = 7.0$ Hz, 2H), 6.24 (d, $J = 15.0$ Hz, 1H), 7.00 (t, $J = 5.0$ Hz, 1H), 7.21 (d, $J = 3.0$ Hz, 1H), 7.32 (d, $J = 5.0$ Hz, 1H), 7.83 (d, $J = 15.0$ Hz, 1H), 8.05 (s, 1H). $^{13}$C NMR (CDCl3, 125 Hz), $\delta$ 14.3, 36.3, 39.8, 61.6, 112.7, 121.4, 128.4, 128.8, 130.7, 131.7, 136.2, 140.5, 151.2, 153.3, 160.9, 174.8, 182.2. ES-MS: m/z = 394.1 [M + H]$^+$. Anal. Calcd for C17H15NO4S3: C, 51.89; H, 3.84; N, 3.56; Found: C, 51.97; H, 3.68; N, 3.72.

III. Crystal data and ORTEP drawing of compound 2a and 6b

2a: C100H92N4O16S8, M = 1862.26, orthorhombic, space group Fdd2, $a = 24.784(5)$, $b = 15.750(5)$, $c = 23.149(5)$ Å, $V = 9036(4)$ Å$^3$, $\alpha = 90.000(5)$, $\beta = 90.00(5)$, $\gamma = 90.00(5)$, $Z = 4$, $T = 273(2)$ K, F000 = 3904, 3965 reflections collected, 2710 unique, $R_1 = 0.0510$, $wR_2 = 0.0883$ ($I > 2\sigma(I)$).

6b: C16H17NO5, M = 303.31, orthorhombic, space group P212121, $a = 7.5750(8)$, $b = 12.0480(12)$, $c = 16.6840(17)$ Å, $V = 1522.6(3)$ Å$^3$, $\alpha = 90.00$, $\beta = 90.00$, $\gamma = 90.00$, $Z = 4$, $T = 273(2)$ K, F000 = 640, 3225 reflections collected, 2175 unique, $R_1 = 0.0523$, $wR_2 = 0.1323$ ($I > 2\sigma(I)$).
VI. Copies of $^1$H NMR and $^{13}$C NMR spectra of compounds 2, 4, 6 and 8

[Diagrams of NMR spectra for compounds 2a, 4, 6, and 8]
Supplementary Material (ESI) for Chemical Communications
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STANDARD PROTON PARAMETORS

Sample directory: /sample/directory
Sample name: compound

**Figure 1:**

STANDARD CARA蛏N PARAMETORS

Sample directory: /sample/directory
Sample name: compound

**Figure 2:**