Supporting Information

One-Pot Synthesis of Isoquinolin-1(2H)-ones by a Sequential Ugi 4CC/Wittig Process

Zhuan Duan, Yun Gao, Ding Yuan, Ming-Wu Ding*
Key Laboratory of Pesticide and Chemical Biology of Ministry of Education, Central China Normal University, Wuhan 430079, People’s Republic of China
E-mail: mwding@mail.ccnu.edu.cn

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**General Methods:**
All reactions were performed in round-bottom flasks under an atmosphere of air. Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. Toluene was distilled from Na, and stored over 4Å molecular sieves. Column chromatography purifications were performed under “flash” conditions using 400-630 mesh silica gel. Analytical thin-layer chromatography (TLC) was carried out on silica gel 60 F254 plates, which were visualized by exposure to ultraviolet light. Melting points were uncorrected. MS were measured on Finnigan Trace MS spectrometer or determined using API 2000 liquid chromatography-tandem mass spectrometer. \(^1\)H NMR were recorded in CDCl\(_3\) on a Varian Mercury 400 or 600 spectrometer and resonances relative to TMS. Data are reported as follows: chemical shift, multiplicity (s = single, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. \(^13\)C NMR spectra were recorded on Varian Mercury 400/600 (100/150 MHz) with complete proton decoupling spectrometers (CDCl\(_3\): 77.0 ppm). Elementary analyses were taken on a Vario EL III elementary analysis instrument. The X-ray diffraction data were collected on a Bruker SMART AXS CCD diffract meter, MoK\(_\alpha\), 2\(\theta\) = 1.86-27.50\(^{\circ}\).

**One-pot Preparation of 2, 3-disubstituted isoquinolin-1(2\(H\))-ones 6:**

Aldehyde 2 (1 mmol), (2-carboxyphenyl)triphenylphosphonium bromide 1 (0.48 g, 1 mmol), and isocyanide 4 (1 mmol) were added sequentially to a solution of secondary amine 3 (1 mmol) in anhydrous methylene dichloride (5 mL) at room temperature. Molecular sieves (4 Å, 1 g) were added and the reaction was stirred at ambient temperature for 12-24 h. After molecular sieves was filtered off, the solvent was removed off under reduced pressure. Then anhydrous toluene (5 ml) and potassium carbonate (0.27 g, 2 mmol) was added. After the reaction mixture was stirred for 1-2 h at 70-80 \(^{\circ}\)C, the solid was filtered and the solvent was removed off under reduced pressure. The residue was purified by chromatography eluting with Et\(_2\)O/petroleum ether (1:2) to give isoquinolin-1(2\(H\))-ones 6.

**2-cyclohexyl-3-(morpholino(phenyl)methyl)isoquinolin-1(2\(H\))-one (6a):**

White solid (yield 0.318 g, 79%), mp 165-166 \(^{\circ}\)C; \(^1\)H NMR (CDCl\(_3\), 600 MHz) \(\delta\) (ppm) 8.31 (d, \(J = 7.8\) Hz, 1H, Ar-H), 7.62-7.26 (m, 8H, Ar-H), 6.66 (s, 0.5H, =CH), 4.82 (s, 0.5H, =CH), 4.42-3.77 (m, 6H, 2CH and 2OCH\(_2\)), 2.82-2.62 (m, 4H, 2NCH\(_2\)), 2.28-0.53 (m, 10H, 5CH\(_2\)); \(^13\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\) (ppm) 163.8, 142.4, 137.1, 135.8, 131.9, 129.6, 129.4, 128.5, 127.4, 126.4, 126.3, 125.6, 105.1, 71.6, 67.0, 58.9, 53.2, 28.6, 27.7, 26.4, 25.1; MS (EI, 70 eV) m/z (%) 402 (M\(^+\), 19), 319 (60), 317 (33), 315 (39), 272 (25), 259 (22), 235 (52), 176 (100), 91 (18). Anal. Caled for C\(_{26}\)H\(_{30}\)N\(_2\)O\(_2\): C, 77.58; H, 7.51; N, 6.96. Found: C, 77.69; H, 7.70; N, 7.25.

**2-cyclohexyl-3-((4-fluorophenyl)(morpholino)methyl)isoquinolin-1(2\(H\))-one (6b):**

White solid (yield 0.365 g, 87%), mp 177-178 \(^{\circ}\)C; \(^1\)H NMR (CDCl\(_3\), 600 MHz) \(\delta\) (ppm) 8.31 (d, \(J = 8.4\) Hz, 1H, Ar-H), 7.64-7.02 (m, 7H, Ar-H), 6.62 (s, 0.5H, =CH), 4.75 (s, 0.5H, =CH), 4.39-3.76 (m, 6H, 2CH and 2OCH\(_2\)), 2.83-0.59 (m, 14H, 2NCH\(_2\) and 5CH\(_2\)\)); \(^13\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\) (ppm) 163.5, 142.0, 135.6, 132.8, 131.8, 131.1, 129.6, 127.2, 126.3, 125.5, 115.3, 109.8, 104.9, 70.5, 66.8, 58.5, 52.8, 28.4, 27.4, 26.3, 24.9; MS (EI, 70 eV) m/z (%) 420 (M\(^+\), 19), 319 (60), 317 (33), 315 (39), 272 (25), 259 (22), 235 (52), 176 (100), 91 (18). Anal. Caled for C\(_{26}\)H\(_{29}\)FN\(_2\)O\(_2\): C, 77.58; H, 7.51; N, 6.96. Found: C, 77.69; H, 7.70; N, 7.25.

**3-((4-chlorophenyl)(morpholino)methyl)-2-cyclohexylisoquinolin-1(2\(H\))-one (6c):**

White solid (yield 0.372 g, 85%), mp 160-161 \(^{\circ}\)C; \(^1\)H NMR (CDCl\(_3\), 400 MHz) \(\delta\) (ppm) 8.31 (d, \(J = 8.0\) Hz, 1H, Ar-H), 7.63-7.26 (m, 7H, Ar-H), 6.63 (s, 0.5H, =CH), 4.74 (s, 0.5H, =CH), 4.39-3.76 (m, 6H, 2CH and 2OCH\(_2\)), 2.82-2.48 (m, 4H, 2NCH\(_2\)), 2.25-0.62 (m, 10H, 5CH\(_2\)\)); \(^13\)C NMR (CDCl\(_3\), 100 MHz) \(\delta\) (ppm) 163.7, 141.9,
3-((4-bromophenyl)(morpholino)methyl)-2-cyclohexylisoquinolin-1(2H)-one (6d): white solid (yield 0.385 g, 80%), mp 171-172 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.31 (d, J = 7.8 Hz, 1H, Ar-H), 7.63-7.27 (m, 7H, Ar-H), 6.63 (s, 0.5H, =CH), 4.73 (s, 0.5H, =CH), 4.42-3.79 (m, 6H, 2CH and 2OCH₂), 2.84-2.48 (m, 4H, 2NCH₂), 2.28-0.16 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.5, 141.8, 141.4, 136.3, 135.5, 131.8, 131.0, 129.6, 127.3, 126.4, 125.6, 122.2, 120.9, 109.9, 105.0, 70.7, 66.8, 58.8, 53.0, 28.5, 27.7, 26.4, 24.9; MS (EI, 70 eV) m/z (%) 480 (M⁺, 12), 399 (63), 397 (96), 352 (20), 338 (30), 314 (64), 256 (100), 233 (81), 169 (29). Anal. Calcd for C₂₆H₂₉BrN₂O₂: C, 64.87; H, 6.07; N, 5.82. Found: C, 64.69; H, 5.98; N, 5.62.

3-((2-chlorophenyl)(morpholino)methyl)-2-cyclohexylisoquinolin-1(2H)-one (6e): white solid (yield 0.309 g, 71%), mp 170-171 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.33 (d, J = 7.8 Hz, 1H, Ar-H), 7.63-7.21 (m, 8H, Ar-H), 5.06 (s, 1H, CH), 3.76-3.73 (m, 5H, NCH and 2OCH₂), 2.84-2.57 (m, 4H, 2NCH₂), 2.40-0.40 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.4, 142.3, 135.5, 134.4, 131.5, 130.6, 129.5, 129.3, 127.0, 125.9, 125.4, 105.3, 66.8, 58.2, 51.5, 28.1, 27.2, 25.9, 25.7, 24.8; MS (EI, 70 eV) m/z (%) 436 (M⁺, 14), 353 (88), 351 (30), 314 (34), 270 (66), 234 (50), 232 (66), 210 (100), 125 (29). Anal. Calcd for C₂₆H₂₉ClN₂O₂: C, 71.46; H, 6.69; N, 6.41. Found: C, 71.52; H, 6.71; N, 6.52.

3-((3-chlorophenyl)(morpholino)methyl)-2-cyclohexylisoquinolin-1(2H)-one (6f): white solid (yield 0.336 g, 77%), mp 171-172 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.31 (d, J = 6.6 Hz, 1H, Ar-H), 7.64-7.27 (m, 7H, Ar-H), 6.64 (s, 0.5H, =CH), 4.75 (s, 0.5H, =CH), 4.46-3.79 (m, 6H, 2CH and 2OCH₂), 2.86-2.47 (m, 4H, 2NCH₂), 2.28-0.16 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.5, 149.4, 139.4, 135.5, 134.3, 131.8, 129.6, 128.3, 127.8, 127.2, 126.4, 125.5, 110.1, 105.2, 70.8, 66.7, 58.8, 53.2, 28.3, 27.7, 26.4, 25.0; MS (EI, 70 eV) m/z (%) 436 (M⁺, 13), 353 (66), 351 (46), 306 (23), 270 (82), 233 (38), 212 (35), 210 (100), 125 (23). Anal. Calcd for C₂₆H₂₉ClN₂O₂: C, 71.46; H, 6.69; N, 6.41. Found: C, 71.36; H, 6.61; N, 6.23.

2-cyclohexyl-3-(morpholino(4-(trifluoromethyl)phenyl)methyl)isoquinolin-1(2H)-one (6g): white solid (yield 0.424 g, 90%), mp 151-152 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.30 (d, J = 6.6 Hz, 1H, Ar-H), 7.64-7.44 (m, 7H, Ar-H), 6.67 (s, 0.5H, =CH), 4.72 (s, 0.5H, =CH), 4.53-3.79 (m, 6H, 2CH and 2OCH₂), 2.86-2.50 (m, 4H, 2NCH₂), 2.27-0.14 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.5, 141.4, 139.4, 135.5, 134.3, 131.8, 129.6, 128.3, 127.8, 127.2, 126.4, 125.5, 110.1, 105.2, 70.8, 66.7, 58.8, 53.2, 28.3, 27.7, 26.4, 25.0; MS (EI, 70 eV) m/z (%) 436 (M⁺, 13), 353 (66), 351 (46), 306 (23), 270 (82), 233 (38), 212 (35), 210 (100), 125 (23). Anal. Calcd for C₂₇H₂₉F₃N₂O₂: C, 68.92; H, 6.21; N, 5.95. Found: C, 69.05; H, 6.46; N, 6.02.

3-((4-(tert-butyl)phenyl)(morpholino)methyl)-2-cyclohexylisoquinolin-1(2H)-one (6h): white solid (yield 0.315 g, 69%), mp 179-180 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.30 (d, J = 7.8 Hz, 1H, Ar-H), 7.62-7.26 (m, 7H, Ar-H), 6.64 (s, 0.5H, =CH), 4.80 (s, 0.5H, =CH), 4.44-3.78 (m, 6H, 2CH and 2OCH₂), 2.85-2.63 (m, 4H, 2NCH₂), 2.31-0.48 (m, 19H, 5CH₂ and 3CH₃); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.6, 151.3, 150.2, 142.7, 135.8, 133.9, 131.7, 129.4, 127.5, 127.2, 126.0, 125.2, 106.9, 104.7, 71.1, 66.9,
58.5, 52.9, 34.2, 31.0, 28.5, 27.3, 26.5, 25.0; MS (EI, 70 eV) m/z (%) 458 (M⁺, 13), 375 (46), 371 (47), 328 (20), 314 (25), 291 (29), 232 (100), 158 (20). Anal. Calcd for C₃₀H₃₈N₂O₂: C, 78.56; H, 8.35; N, 6.11. Found: C, 78.77; H, 8.21; N, 6.12.

2-cyclohexyl-3-((4-methoxyphenyl)(morpholino)methyl)isoquinolin-1(2H)-one (6i): white solid (yield 0.281 g, 65%), mp 179-180 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.31 (d, J = 6.0 Hz, 1H, Ar-H), 7.63-7.27 (m, 5H, Ar-H), 6.86 (d, J = 8.4 Hz, 2H, Ar-H), 6.62 (s, 0.5H, =CH), 4.86 (s, 0.5H, =CH), 4.45-3.75 (m, 9H, 2CH, OCH₃ and 2OCH₂), 2.84-2.63 (m, 4H, 2NCH₂), 2.43-0.19 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.6, 159.2, 142.7, 135.9, 131.7, 130.6, 128.8, 127.2, 126.0, 125.6, 113.7, 104.6, 70.7, 66.8, 58.3, 54.9, 52.9, 28.5, 27.3, 26.3, 25.0; MS (EI, 70 eV) m/z (%) 432 (M⁺, 10), 349 (26), 302 (23), 289 (31), 264 (48), 206 (100), 158 (31), 121 (21). Anal. Calcd for C₂₇H₃₂N₂O₃: C, 74.97; H, 7.46; N, 6.48. Found: C, 74.85; H, 7.53; N, 6.42.

2-cyclohexyl-3-(phenyl(pyrrrolidin-1-yl)methyl)isoquinolin-1(2H)-one (6j): light yellow solid (yield 0.221 g, 57%), mp 154-155 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.31 (d, J = 7.8 Hz, 1H, Ar-H), 7.62-7.25 (m, 9H, Ar-H), 4.35-4.15 (m, 2H, 2CH), 2.70-2.67 (m, 4H, 2NCH₂), 2.24-0.49 (m, 14H, 2NCH₂ and 5CH₂); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.8, 143.6, 139.4, 136.1, 131.8, 128.8, 128.3, 127.7, 127.4, 126.3, 126.1, 125.6, 105.7, 71.4, 58.6, 53.9, 28.3, 27.8, 26.4, 25.2, 23.3; MS (EI, 70 eV) m/z (%) 386 (M⁺, 9), 303 (64), 272 (19), 257 (16), 236 (34), 160 (100), 91 (29). Anal. Calcd for C₂₆H₃₀N₂O: C, 80.79; H, 7.82; N, 7.25. Found: C, 80.75; H, 7.73; N, 7.02.

2-butyl-3-((2-chlorophenyl)(morpholino)methyl)isoquinolin-1(2H)-one (6k): white solid (yield 0.267 g, 65%), mp 133-134 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.37 (d, J = 7.8 Hz, 1H, Ar-H), 7.66-7.18 (m, 8H, Ar-H), 4.36 (s, 1H, CH), 4.32-3.72 (m, 6H, NCH₂ and 2OCH₂), 2.64-2.31 (m, 4H, 2NCH₂), 1.54-0.96 (m, 7H, CH₂CH₂CH₃); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 162.8, 141.6, 139.4, 135.9, 134.6, 131.9, 129.9, 129.0, 128.4, 127.7, 127.5, 126.3, 125.9, 124.7, 105.2, 70.6, 66.7, 52.7, 43.0, 30.9, 20.0, 13.6; MS (EI, 70 eV) m/z (%) 410 (M⁺, 16), 325 (77), 294 (30), 269 (22), 210 (100), 200 (72), 125 (20). Anal. Calcd for C₂₄H₂₇ClN₂O₂: C, 70.15; H, 6.62; N, 6.82. Found: C, 70.06; H, 6.53; N, 6.65.

2-butyl-3-((3-chlorophenyl)(morpholino)methyl)isoquinolin-1(2H)-one (6l): white solid (yield 0.294 g, 72%), mp 134-135 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.38 (d, J = 7.8 Hz, 1H, Ar-H), 7.67-7.18 (m, 8H, Ar-H), 5.12 (s, 1H, CH), 4.30-4.26 (m, 1H, NCH), 3.75-3.69 (m, 4H, 2OCH₂), 3.49-3.45 (m, 1H, NCH), 2.85-2.35 (m, 4H, 2NCH₂), 1.63-1.37 (m, 4H, CH₂CH₂CH₃), 0.93 (t, J = 6.6 Hz, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 163.1, 142.3, 136.1, 135.1, 134.4, 132.1, 130.9, 129.9, 129.6, 127.7, 127.6, 126.4, 126.0, 105.6, 67.2, 64.9, 51.7, 43.4, 31.3, 20.3, 13.9; MS (EI, 70 eV) m/z (%) 410 (M⁺, 12), 325 (61), 294 (30), 269 (16), 234 (24), 210 (100), 200 (72), 125 (20). Anal. Calcd for C₂₄H₂₇ClN₂O₂: C, 70.15; H, 6.62; N, 6.82. Found: C, 70.16; H, 6.76; N, 6.99.

2-butyl-3-((4-chlorophenyl)(morpholino)methyl)isoquinolin-1(2H)-one (6m): white solid (yield 0.311 g, 76%), mp 162-163 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.36 (d, J = 7.8 Hz, 1H, Ar-H), 7.66-7.20 (m, 8H, Ar-H), 4.35 (s, 1H, CH), 4.34-3.70 (m, 6H, NCH₂ and 2OCH₂), 2.64-2.29 (m, 4H, 2NCH₂), 1.57-0.96 (m, 7H, CH₂CH₂CH₃); ¹³C NMR (CDCl₃, 100 MHz) δ (ppm) 162.9, 141.9, 136.0, 135.7, 134.1, 132.0, 130.6, 128.9, 127.6, 126.4, 125.9, 124.7, 105.0, 70.3, 66.8, 52.8, 42.8, 31.1, 20.2, 13.7; MS (EI, 70 eV) m/z (%) 410 (M⁺, 11), 325 (76), 294 (28), 288 (18), 210 (100), 200 (51), 125 (18). Anal. Calcd for C₂₄H₂₇ClN₂O₂: C, 70.15; H, 6.62; N, 6.82. Found: C, 70.37; H, 6.71; N, 6.67.
2-butyl-3-(morpholino(phenyl)methyl)isoquinolin-1(2H)-one (6n): white solid (yield 0.267 g, 71%), mp 99-101 °C; 1H NMR (CDCl3, 600 MHz) δ (ppm) 8.37 (d, J = 8.4 Hz, 1H, Ar-H), 7.65-7.18 (m, 9H, Ar-H), 4.45-4.32 (m, 2H, CH and NCH), 3.76-3.71 (m, 4H, 2OCH2), 3.61-3.59 (m, 1H, NCH), 2.65-2.25 (m, 4H, 2NCH2), 1.55-0.83 (m, 7H, CH2CH2CH3); 13C NMR (CDCl3, 100 MHz) δ (ppm) 162.7, 142.2, 137.0, 136.0, 131.7, 129.1, 128.5, 128.1, 127.4, 126.0, 125.7, 124.5, 104.9, 71.2, 66.7, 52.7, 42.8, 30.8, 20.0, 13.6; MS (EI, 70 eV) m/z (%) 376 (M+, 12), 291 (75), 260 (32), 246 (21), 200 (41), 176 (100), 91 (18). Anal. Calcd for C24H28N2O2: C, 76.56; H, 7.50; N, 7.44. Found: C, 76.46; H, 7.71; N, 7.73.

2-butyl-3-(1-(dipropylamino)butyl)isoquinolin-1(2H)-one (6o): light green oil (yield 0.138 g, 39%); 1H NMR (CDCl3, 600 MHz) δ (ppm) 8.41 (d, J = 8.4 Hz, 1H, Ar-H), 7.62-7.43 (m, 3H, Ar-H), 6.46 (s, 1H, =CH), 4.48-4.46 (m, 1H, 1/2NCH2), 4.32 (t, 1H, CH), 3.83-3.79 (m, 1H, 1/2NCH2), 2.63-2.36 (m, 4H, 2NCH2), 1.84-0.72 (m, 24H, 2CH2CH2CH3 and 2CH2CH3); 13C NMR (CDCl3, 100 MHz) δ (ppm) 163.2, 141.4, 135.6, 131.6, 127.4, 126.0, 125.5, 124.7, 105.4, 61.4, 52.7, 42.0, 31.6, 25.9, 22.0, 20.3, 19.9, 14.0, 13.7, 11.6; MS (EI, 70 eV) m/z (%) 356 (M+, 4), 313 (100), 256 (78), 200 (24), 156 (65), 100 (35). Anal. Calcd for C23H36N2O: C, 77.48; H, 10.18; N, 7.86. Found: C, 77.39; H, 10.20; N, 7.73.

3-((benzyl(methyl)amino)(4-chlorophenyl)methyl)-2-butylisoquinolin-1(2H)-one (6p): light yellow oil (yield 0.226 g, 51%); 1H NMR (CDCl3, 600 MHz) δ (ppm) 8.38 (d, J = 7.8 Hz, 1H, Ar-H), 7.65-7.19 (m, 13H, Ar-H), 4.63 (s, 1H, CH), 4.34-4.30 (m, 1H, 1/2NCH2), 2.17 (s, 3H, NCH3), 1.57-0.92 (m, 7H, CH2CH2CH3); 13C NMR (CDCl3, 100 MHz) δ (ppm) 162.8, 142.7, 138.5, 136.9, 136.0, 133.7, 131.9, 130.3, 128.7, 128.2, 127.6, 126.9, 126.2, 125.8, 124.7, 105.8, 69.0, 59.9, 43.0, 40.2, 30.9, 20.1, 13.6; MS (EI, 70 eV) m/z (%) 444 (M+, 3), 325 (25), 294 (12), 244 (21), 200 (19), 120 (32), 91 (100). Anal. Calcd for C28H29ClN2O: C, 75.57; H, 6.57; N, 6.30. Found: C, 75.71; H, 6.51; N, 6.06.
Crystal data and structure refinement for 6k.

Identification code: e:121122a_121122a_0m
Empirical formula: C_{24}H_{27}ClN_{2}O_{2}
Formula weight: 410.93
Temperature: 298(2) K
Wavelength: 0.71073 Å
Crystal system: Monoclinic
Space group: P2(1)/n
Unit cell dimensions:

\[ a = 12.626(9) \text{ Å}, \quad \alpha = 90^\circ \]
\[ b = 9.665(7) \text{ Å}, \quad \beta = 100.754(11)^\circ \]
\[ c = 18.180(13) \text{ Å}, \quad \gamma = 90^\circ \]

Volume: 2179(3) Å³

Z: 4
Density (calculated): 1.252 Mg/m³
Absorption coefficient: 0.197 mm⁻¹
F(000): 872
Crystal size: 0.12 x 0.10 x 0.10 mm³
Theta range for data collection: 1.82 to 30.00 °
Index ranges: -17 <= h <= 17, -6 <= k <= 13, -25 <= l <= 24
Reflections collected: 19027
Independent reflections: 6339 [R(int) = 0.0262]
Completeness to theta = 30.00: 99.7%
Absorption correction: None
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 6339 / 0 / 263
Goodness-of-fit on F²: 1.028
Final R indices [I>2σ(I)]: R1 = 0.0491, wR2 = 0.1429
R indices (all data): R1 = 0.0647, wR2 = 0.1631
Largest diff. peak and hole: 0.266 and -0.416 e.⁻³
$^1$H NMR and $^{13}$C NMR Spectrums for Compounds 6