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SUPPLEMENTARY MATERIAL TO

An efficient and facile synthesis of flavanones catalyzed by *N*-methylimidazole

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ANALYTIC AND SPECTRAL DATA FOR THE SYNTHESIZED FLAVANONES

*2-Phenylchroman-4-one (**2a**)*. Yield: 90 %; m.p.: 77–78 °C; Anal. Calcd. for $C_{15}H_{12}O_2$: C, 80.34; H, 5.39 %. Found: C, 80.03, H 5.62 %; IR (KBr, cm^{-1}): 1688 (s). ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.75–3.15 (2H, *m*, *J* = 13.2 Hz), 5.51 (1H, *dd*, *J* = 13.2 and 3.0 Hz), 7.04–7.93 (9H, *m*, *J* = 3.0 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 192.5, 162.1, 139.0, 136.6, 129.3, 129.2, 127.4, 126.6, 122.2, 121.3, 118.5, 80.1, 45.0; EI-MS 224 (M^+, 100), 223 (93), 147 (54), 120 (83), 92 (44), 77 (11).

*6-Methyl-2-phenylchroman-4-one (**2b**)*. Yield: 87 %; m.p.: 104–105 °C (lit. 104 °C[1]); Anal. Calcd. for $C_{16}H_{14}O_2$: C, 80.65; H, 5.92 %. Found: C, 80.90; H, 6.17 %; IR (KBr, cm^{-1}): 1700 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.46 (3H, *s*), 2.90 (2H, *dd*, *J* = 13.2 and 3.0 Hz), 5.41 (1H, *dd*, *J* = 13.2 and 3.0 Hz), 7.04–7.90 (8H, *m*); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 192.4, 159.8, 137.1, 135.3, 131.0, 128.9, 128.7, 127.8, 127.5, 120.7, 117.6, 71.3, 52.5, 20.5. EI-MS (*m*/*z* (relative abundance, %)): 238 (M^+, 100), 104 (23).

*6-Methyl-2-(p-tolyl)chroman-4-one (**2c**)*. Yield: 76 % m.p.: 90–91 °C (lit. 89–90 °C[2]). Anal. Calcd. for $C_{17}H_{16}O_2$: C, 80.93; H, 6.39 %. Found: C, 80.67; H, 6.51 %. IR (KBr, cm^{-1}): 1690 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.33 (3H, *s*), 2.38 (3H, *s*), 2.96 (2H, *dd*, *J* = 13.2 and 2.7 Hz), 5.42 (1H, *dd*, *J* = 13.2 and 2.7 Hz), 6.94–7.72 (7H, *m*); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 190.4, 159.8, 138.5, 137.3, 135.9, 130.9, 129.5, 126.6, 126.2, 120.7, 117.9, 79.2, 44.1, 21.5, 20.3. EI-MS (*m*/*z* (relative abundance, %)): 252 (M^+, 100), 237 (18), 134 (12), 104 (13).

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*6-Methoxy-2-phenylchroman-4-one (**2d**)*. Yield: 89 %; m.p.: 134–135 °C (lit. 136 °C[1]); Anal. Calcd. for $C_{16}H_{14}O_3$: C, 75.57; H, 5.55 %. Found: C, 75.90; H, 5.72 %; IR (KBr, cm^{-1}): 1676 (s). ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.87 (2H, *dd*, *J* = 13.3 and 3.0 Hz), 3.75 (3H, *s*), 5.37 (1H, *dd*, *J* = 13.3 and 3.0 Hz), 6.95–7.50 (8H, *m*); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 192.5, 156.8, 154.6, 139.1, 129.2, 129.1, 126.6, 125.8, 121.2, 119.9, 107.7, 80.1, 56.2, 45.1; EI-MS (*m*/*z* (relative abundance, %)): 254 (M^+, 81), 177 (19), 150 (100), 107 (18).

*7-Methoxy-2-phenylchroman-4-one (**2e**)*. Yield: 90 %; m.p.: 90–91 °C (lit. 90–91 °C[3]); Anal. Calcd. for $C_{16}H_{14}O_3$: C, 75.57; H, 5.55 %. Found: C, 75.82; H, 5.80 %; IR (KBr, cm^{-1}): 1679 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.83 (1H, *dd*, *J* = 16.9 and 3.1 Hz), 3.05 (1H, *dd*, *J* = 16.9 and 13.2 Hz), 3.84 (3H, *s*), 5.45 (1H, *dd*, *J* = 13.2 and 3.0 Hz), 6.51 (2H, *d*, *J* = 2.4 Hz), 6.63 (1H, *dd*, *J* = 8.8 and 2.4 Hz), 7.37–7.51 (4H, *m*), 7.89 (1H, *d*, *J* = 8.8 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 191.0, 166.7, 164.0, 139.2, 129.3, 129.2, 126.7, 115.2, 110.8, 101.3, 80.4, 56.0, 44.7; EI-MS (*m*/*z* (relative abundance, %)): 252 (M^+, 100), 253 (65), 177 (62), 150 (65).

*7-Methoxy-2-(4-methoxyphenyl)chroman-4-one (**2f**)*. Yield: 79 %; m.p.: 94––95 °C (lit. 94–95 °C[3]); Anal. Calcd. for $C_{17}H_{16}O_4$: C, 71.82; H, 5.67 %. Found: C, 71.69; H, 5.84 %; IR (KBr, cm^{-1}): 1679 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / / ppm): 2.80 (1H, *dd*, *J* = 16.9 and 2.9 Hz), 3.06 (1H, *dd*, *J* = 16.9 and 13.2 Hz), 3.84 (6H, *s*), 5.43 (1H, *dd*, *J* = 13.2 and 2.9 Hz), 6.48 (1H, *d*, *J* = 2.4 Hz), 6.62 (1H, *dd*, *J* = 8.8 and 2.4 Hz), 6.96 (2H, *d*, *J* = 6.7 Hz), 7.40 (2H, *d*, *J* = 6.7 Hz), 7.87 (1H, d, *J* = 8.8 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / pm): 191.2, 166.7, 163.9, 160.4, 131.2, 129.1, 128.0, 115.2, 114.6, 110.7, 101.3, 80.2, 56.1, 55.8, 44.5; EI-MS 284 (M^+, 100), 283 (57), 177 (30), 134 (98), 121 (45).

*2-(3-Nitrophenyl)chroman-4-one (**2g**)*. Yield: 86 %; m.p.: 143–145 °C (lit. 142 °C[4]); Anal. Calcd. for $C_{15}H_{11}NO_4$: C, 66.91; H, 4.12; N, 5.20 %. Found: C, 66.52; H, 4.33; N, 5.43 %; IR (KBr, cm^{-1}): 1693 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.96 (1H, *dd*, *J* = 16.8 and 3.2 Hz), 3.09 (1H, *dd*, *J* = 16.8 and 12.8 Hz), 5.61 (1H, *dd*, *J* = 12.8 and 3.2 Hz), 7.12 (2H, *m*), 7.56–7.64 (2H, *m*, *J* = = 8.0 and 1.6 Hz), 7.81 (1H, *m*), 7.95 (1H, *dd*, *J* = 8.0 and 1.6 Hz), 8.26 (1H, *m*), 8.42 (1H, *t*, *J* = 2.0 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$. δ / ppm): 190.8, 160.9, 148.6, 141.0, 136.4, 131.9, 130.0, 127.2, 123.6, 122.3, 121.2, 120.7, 118.0, 78.2, 44.5; EI-MS (*m*/*z* (relative abundance, %)): 269 (M^+, 35), 268 (40), 147 (100), 121 (33), 120 (66), 92 (99).

*2-(4-Chlorophenyl)chroman-4-one (**2h**)*. Yield: 87 % m.p.: 84–85 °C (lit. 84–85 °C[2]); Anal. Calcd. for $C_{15}H_{11}ClO_2$: C, 69.64; H, 4.29 %. Found: C, 69.37; H, 4.58 %; IR (KBr, cm^{-1}): 1692 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.87 (1H, *dd*, *J* = 17.2 and 3.2 Hz), 3.06 (1H, *dd*, *J* = 17.2 and 13.2 Hz), 5.48 (1H, *dd*, *J* = 13.2 and 3.2 Hz), 7.05 (2H, *m*), 7.45 (4H, *m*), 7.52 (1H, *m*), 7.93 (1H, *dd*, *J* = = 8.0 and 2.0 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 191.5, 161.2, 137.1,

136.3, 134.6, 128.9, 127.5, 127.1, 121.9, 120.9, 118.1, 78.9, 44.6; EI-MS (*m*/*z* (relative abundance, %)): 258 (M^+, 70), 257 (100), 223 (28), 147 (65), 120 (67), 92 (75).

*2-(4-Fluorophenyl)chroman-4-one (**2i**)*. Yield; 65 %; m.p.: 79–80 °C (lit. 78–79 °C[5]); Anal. Calcd. for $C_{15}H_{11}FO_2$: C, 74.37; H, 4.58 %. Found: C, 74.52; H, 4.85 %; IR (KBr, cm^{-1}): 1695 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.88 (1H, *dd*, *J* = 16.8 and 2.8 Hz), 3.08 (1H, *dd*, *J* = 16.8 and 13.2 Hz), 5.49 (1H, *dd*, *J* = 13.2 and 2.8 Hz), 7.10 (4H, *m*), 7.47 (2H, *m*), 7.52 (1H, *td*, *J* = 8.4 and 1.6 Hz), 7.93 (1H, *dd*, *J* = 8.0 and 2.0 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 191.8, 162.8, 161.4, 136.2, 134.6, 129.9, 127.2, 121.8, 120.9, 118.0, 115.8, 79.0, 44.6. EI-MS (*m*/*z* (relative abundance, %)): 242 (M^+, 56), 241 (86), 147 (43), 122 (40), 121 (36), 120 (68), 92 (100), 63 (23).

*2-(p-Tolyl)chroman-4-one (**2j**)*. Yield: 87 %; m.p.: 82–83 °C (lit. 82–84 °C[6]); Anal. Calcd. for $C_{16}H_{14}O_2$: C, 80.65; H, 5.92. Found: C, 80.79; H, 6.16 %; IR (KBr, cm^{-1}): 1696 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.38 (3H, *s*), 2.88–3.12 (2H, *m*), 5.43 (1H, *dd*, *J* = 13.8 and 2.0 Hz), 7.03–7.06 (2H, *m*), 7.23 (2H, d, *J* = 8.0 Hz), 7.36 (d, 2H, *J* = 8.0 Hz), 7.49 (m, 1H), 7.93 (dd, 1H, *J* = 8.5 and 2.0 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 192.3, 161.8, 138.9, 136.2, 135.6, 129.6, 127.2, 126, 3, 121.8, 120.9, 118.3, 77.5, 44.6, 21.3; EI-MS (*m*/*z* (relative abundance, %)): 238 (M^+, 100), 237 (86), 161 (56), 134 (32), 104 (23).

*2-(4-Methoxyphenyl)chroman-4-one (**2k**)*. Yield: 90 %; m.p.: 97–98 °C (lit. 98 °C[7]); Anal. Calcd. for $C_{16}H_{14}O_3$: C, 75.57; H, 5.55 %. Found: C, 75.72; H, 5.78 %; IR (KBr, cm^{-1}): 1690 (s); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 2.86 (1H, *dd*, *J* = 16.8 and 2.8 Hz), 3.10 (1H, *dd*, *J* = 16.8 and 13.3 Hz), 3.84 (3H, *s*), 5.43 (1H, *dd*, *J* = 13.3 and 2.8 Hz), 6.96 (2H, *d*, *J* = 8.7 Hz), 7.02–7.08 (2H, *m*), 7.41 (2H, *d*, *J* = 8.7 Hz), 7.46–7.53 (1H, *m*), 7.93 (1H, *dd*, *J* = 8.3 and 1.7 Hz); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 192.7, 162.1, 160.4, 136.5, 131.2, 128.2, 127.4, 122.0, 121.3, 118.5, 114.6, 79.8, 55.9, 44.9; EI-MS (*m*/*z* (relative abundance, %)): 254 (M^+, 65), 253 (48), 147 (16), 134 (100).

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