



SUPPLEMENTARY MATERIAL TO  
**N-Methylimidazole-mediated synthesis of aryl alkyl ethers under microwave irradiation and solvent free conditions**

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE COMPOUNDS **4a-k**

*4-Methoxy-2H-chromen-2-one (4-methoxycoumarin, **4a**)*. [20280-81-3]

Yield: 0.33 g (95 %); pale yellow crystals; m.p.: 121–123 °C [lit.: 123–125 °C<sup>1</sup>]; IR (KBr, cm<sup>-1</sup>): 1705 (–C=O stretching of –COOR group), 1238 and 1030 (–C–O stretching of –C–O group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 4.02 (3H, s, CH<sub>3</sub>), 5.72 (1H, s, vinyl), 7.28–7.35 (2H, m, aromatic), 7.57 (1H, dt, J = 7.2 Hz, J = 1.6 Hz, aromatic), 7.84 (1H, dd, J = 6.4 Hz, J = 1.6 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 56.4 (OCH<sub>3</sub>), 90.1 (CH=), 115.6 (CH=), 116.8 (CH=), 123.0 (CH=), 123.9 (CH=), 132.4 (C), 153.3 (C–O), 162.9 (C=O), 166.5 (C–O).

*4-Ethoxy-2H-chromen-2-one (4-ethoxycoumarin, **4b**)*. Yield: 0.34 g (90 %); yellow crystals; m.p.: 135–137 °C; IR (KBr, cm<sup>-1</sup>): 1721 (–C=O stretching of –COOR group), 1238 and 1027 (–C–O stretching of –C–O group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 1.57 (3H, t, J = 7.2 Hz, CH<sub>3</sub>), 4.23 (2H, q, J = 7.2 Hz, OCH<sub>2</sub>), 5.69 (1H, s, vinyl), 7.29–7.35 (2H, m, aromatic), 7.57 (1H, dt, J = 7.2 Hz, J = 1.6 Hz, aromatic), 7.86 (1H, dd, J = 6.4 Hz, J = 1.6 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 14.1 (CH<sub>3</sub>), 65.2 (OCH<sub>2</sub>), 90.4 (CH=), 115.8 (CH=), 116.9 (CH=), 123.1 (CH=), 123.8 (CH=), 132.3 (C), 153.4 (C–O), 163.1 (C = O), 165.7 (C–O).

*7-Methoxy-2H-chromen-2-one (7-methoxycoumarin, **4d**)*. [531-59-9] Yield: 0.34 g (98 %), pale yellow crystals; m.p.: 119–121 [lit. 117–121 °C<sup>1</sup>]; IR (KBr, cm<sup>-1</sup>): 1702 (–C=O stretching of –COOR group), 1230 (–C–O stretching of –C–O group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 3.91 (3H, s, OCH<sub>3</sub>), 6.29 (1H, d, J = 9.5 Hz, aromatic), 6.85–6.89 (1H, m, aromatic), 7.40 (1H, d, J = 8.5 Hz,

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aromatic), 7.67 (1H, *d*, *J* = 9.5 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 55.8 (OCH<sub>3</sub>), 101.0 (CH=), 112.6 (C), 112.7 (CH=), 113.2 (CH=), 128.8 (CH=), 143.8 (CH=), 156.0 (C–O), 161.3 (C=O), 163.0 (C–O).

*7-Ethoxy-2H-chromen-2-one (7-ethoxycoumarin, 4e).* [31005-02-4] Yield: 0.36 g (95 %); golden yellow crystals; m.p.: 84–86 °C [lit. 89–90 °C<sup>1</sup>]. IR (KBr, cm<sup>-1</sup>): 1734 (–C=O stretching of –COOR group), 1231 and 1044 (–C–O, stretching of –C–O group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 1.46 (3H, *t*, *J* = 6.8 Hz, CH<sub>3</sub>), 4.08 (2H, *q*, *J* = 6.8 Hz, OCH<sub>2</sub>), 6.24 (1H, *d*, *J* = 9.2 Hz, aromatic), 6.79–6.85 (2H, *m*, aromatic), 7.37 (1H, *d*, *J* = 8.8 Hz, aromatic), 7.64 (1H, *d*, *J* = 9.6 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 14.6 (CH<sub>3</sub>), 64.2 (OCH<sub>2</sub>), 101.3 (CH=), 112.4 (C), 112.9 (CH=), 112.9 (CH=), 128.7 (CH=), 143.5 (CH=), 155.9 (C–O), 161.3 (C=O), 162.2 (C–O).

*4-Methoxyquinoline (4g).* [607-31-8] Yield: 0.27 g (85 %); dark yellow oil; IR (KBr, cm<sup>-1</sup>): 1273 and 1073 (–C–O, stretching of –C–O group), 1618–1506 (C=C, stretching of –C=C aromatic group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 4.09 (3H, *s*, OCH<sub>3</sub>), 6.79 (1H, *d*, *J* = 5.6 Hz, aromatic), 7.55 (1H, *dt*, *J* = 6.8 Hz, *J* = 0.8 Hz, aromatic), 7.74 (1H, *dd*, *J* = 7.2 Hz, *J* = 1.6 Hz, aromatic), 8.1 (1H, *d*, *J* = 8.4 Hz, aromatic), 8.24 (1H, *dd*, *J* = 8.4 Hz, *J* = 1.2 Hz, aromatic), 8.80 (1H, *d*, *J* = 5.2 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 55.8 (OCH<sub>3</sub>), 100.1 (CH=), 121.4 (CH=), 121.9 (CH=), 125.9 (CH=), 128.4 (C), 130.1 (CH=), 148.5 (C), 151.0 (CN), 162.7 (C–O).

*6-Methoxyquinoline (4h).* [5263-87-6] Yield: 0.27 g (85 %); brown oil; m.p.: [lit. 18–20 °C<sup>1</sup>]; IR (KBr, cm<sup>-1</sup>): 1247 and 1037 (–C–O, stretching of –C–O group), 1600–1500 (C=C, stretching of –C=C aromatic group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 3.92 (3H, *s*, OCH<sub>3</sub>), 7.12 (1H, *d*, *J* = 2.8 Hz, aromatic), 7.41–7.44 (2H, *m*, aromatic), 8.08–8.15 (2H, *m*, aromatic), 8.8 (1H, *d*, *J* = 3.2 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 55.6 (OCH<sub>3</sub>), 105.1 (CH=), 121.4 (CH=), 121.7 (CH=), 122.8 (CH=), 129.5 (C), 130.3 (CH=), 135.5 (CH=), 147.3 (C–N), 158.0 (C–O).

*8-Methoxyquinoline (4i).* [938-33-0] Yield: 0.3 g (95 %); dark brown oil; IR (KBr, cm<sup>-1</sup>): 1258 and 1076 (–C–O, stretching of –C–O group), 1600–1500 (C=C, stretching of –C=C aromatic group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 4.1 (3H, *s*, OCH<sub>3</sub>), 7.04 (1H, *d*, *J* = 7.6 Hz, aromatic), 7.30–7.46 (3H, *m*, aromatic), 8.11 (1H, *dd*, *J* = 8.3 Hz, *J* = 1.6 Hz, aromatic), 8.92 (1H, *dd*, *J* = 4.2 Hz, *J* = 1.6 Hz, aromatic); <sup>13</sup>C-NMR (100.6 MHz, CDCl<sub>3</sub>, δ / ppm): 56.1 (OCH<sub>3</sub>), 108.0 (CH=), 119.9 (CH=), 122.1 (CH=), 127.1 (C), 129.7 (CH=), 136.4 (CH=), 140.4 (C), 149.5 (N–C), 155.7 (C–O).

*2-Methoxynaphthalene (4k).* [93-04-9] Yield: 0.28 g (90 %); gray solid; m.p.: 70–72 °C [lit. 70–73 °C<sup>1</sup>]; IR (KBr, cm<sup>-1</sup>): 1256 and 1027 (–C–O, stretching of –C–O group), 1593–1506 (C=C, stretching of –C=C aromatic group); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 3.96 (3H, *s*, OCH<sub>3</sub>), 7.17 (1H, *s*,

aromatic), 7.19 (1H, *d*, *J* = 2.4 Hz, aromatic), 7.38–7.47 (2H, *m*, aromatic), 7.76–7.81 (3H, *m*, aromatic);  $^{13}\text{C}$ -NMR (100.6 MHz,  $\text{CDCl}_3$ ,  $\delta$  / ppm): 55.3 ( $\text{OCH}_3$ ), 105.7 ( $\text{CH}=\text{}$ ), 118.7 ( $\text{CH}=\text{}$ ), 123.6 ( $\text{CH}=\text{}$ ), 126.4 ( $\text{CH}=\text{}$ ), 126.7 ( $\text{CH}=\text{}$ ), 127.7 ( $\text{CH}=\text{}$ ), 129.0 (C), 129.4 ( $\text{CH}=\text{}$ ), 134.5 (C), 157.6 (C=O).

#### REFERENCES

1. LookChem<sup>®</sup>, Look for Chemicals, [www.lookchem.com](http://www.lookchem.com) and [www.chemicalbook.com](http://www.chemicalbook.com) (accessed in Apr, 2015).