



SUPPLEMENTARY MATERIAL TO
**Iodine-mediated one-pot synthesis of 3-cyanocoumarins and
3-cyano-4-methylcoumarins**

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SPECTRAL DATA FOR THE SYNTHESISED COUMARINS

3-Cyanocoumarin (3a). IR (KBr, λ_{\max} / cm^{-1}): 1725 (C=O), 2226 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.30–7.60 (2H, *m*), 7.68–8.0 (2H, *m*), 8.75 (1H, *s*); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 101.5, 113.6, 114.8, 119.7, 122.8, 126.1, 128.8, 131.8, 154.8, 161.2.

6-Bromo-3-cyanocoumarin (3b). IR (KBr, λ_{\max} / cm^{-1}): 1737 (C=O), 2235 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.35 (1H, *d*, *J* = 9.0 Hz), 7.83–7.85 (1H, *dd*, *J* = 9.0 Hz, *J* = 2.5 Hz), 7.90 (1H, *d*, *J* = 2.5 Hz), 8.55 (1H, *s*); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 101.2, 113.2, 117.8, 118.2, 118.5, 118.8, 130.9, 136.6, 154.2, 161.0.

6-Chloro-3-cyanocoumarin (3c). IR (KBr, λ_{\max} / cm^{-1}): 1726 (C=O), 2228 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 7.50 (1H, *d*, *J* = 9.0 Hz), 7.82–7.84 (1H, *dd*, *J* = 9.0 Hz, *J* = 2.5 Hz), 7.95 (1H, *d*, *J* = 2.5 Hz), 8.72 (1H, *s*); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 101.4, 113.4, 116.8, 120.6, 122.8, 130.2, 131.0, 132.6, 154.8, 161.5.

3-Cyano-6-methylcoumarin (3d). IR (KBr, λ_{\max} / cm^{-1}): 1725 (C=O), 2225 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.48 (3H, *s*, CH₃), 7.22–7.72 (3H, *m*), 8.22 (1H, *s*); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 21.6, 101.4, 113.7, 117.8, 118.5, 119.7, 128.6, 134.2, 137.4, 155.2, 162.1.

3-Cyano-7-methoxycoumarin (3e). IR (KBr, λ_{\max} / cm^{-1}): 1715 (C=O), 2215 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 3.45 (3H, *s*), 7.18 (1H, *d*, *J* = 2.5 Hz), 7.82–7.85 (2H, *m*), 8.92 (1H, *s*); ¹³C-NMR (100 MHz, CDCl₃, δ / ppm): 56.2, 101.8, 102.2, 111.4, 112.6, 113.4, 119.8, 132.6, 156.4, 159.8, 164.4.

3-Cyano-4-methylcoumarin (3f). IR (KBr, λ_{\max} / cm^{-1}): 1725 (C=O), 2230 (C≡N); ¹H-NMR (400 MHz, CDCl₃, δ / ppm): 2.72 (3H, *s*), 7.20–7.52 (4H, *m*);

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^{13}C -NMR (100 MHz, CDCl_3 , δ / ppm): 18.1, 96.2, 113.2, 120.4, 122.8, 124.6, 126.8, 129.8, 155.6, 157.4, 165.1.

3-Cyano-4,6-dimethylcoumarin (3g). IR (KBr, λ_{max} / cm^{-1}): 1735 (C=O), 2234 (C \equiv N); ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 2.45 (3H, s), 2.75 (3H, s), 7.32 (1H, d, J = 9.0 Hz), 7.45–7.70 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3 , δ / ppm): 17.8, 21.4, 96.4, 112.8, 118.2, 120.8, 129.8, 133.4, 136.4, 156.1, 157.2, 164.8.

6-Bromo-3-cyano-4-methylcoumarin (3h). IR (KBr, λ_{max} / cm^{-1}): 1738 (C=O), 2236 (C \equiv N); ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 2.72 (3H, s), 7.35 (1H, d, J = 9.0 Hz), 7.20–8.15 (2H, m); ^{13}C -NMR (100 MHz, CDCl_3 , δ / ppm): 18.2, 95.8, 113.1, 114.8, 118.8, 121.8, 132.6, 136.2, 152.6, 157.2, 164.1.

3-Cyano-7-methoxy-4-methylcoumarin (3i). IR (KBr, λ_{max} / cm^{-1}): 1720 (C=O), 2227 (C \equiv N); ^1H -NMR (400 MHz, CDCl_3 , δ / ppm): 2.70 (3H, s), 3.95 (3H, s), 6.85–7.05 (2H, m), 7.68 (1H, d, J = 9.0 Hz); ^{13}C -NMR (100 MHz, CDCl_3 , δ / ppm): 18.1, 21.4, 96.2, 105.2, 112.2, 112.8, 116.6, 125.4, 152.1, 157.1, 160.6, 164.2.