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SUPPLEMENTARY MATERIAL TO

Improved synthesis of quinocetone and its two deoxy metabolites

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PHYSICAL, ANALYTICAL AND SPECTRAL DATA

1-(3-methyl-1,4-dioxide-2-quinoxalinyl)-3-phenyl-2-propen-1-one ***(3)***. Yield: 95 %; yellow crystals; m.p.: 188.4–189 °C (lit: 187–189 °C[1]); Anal. Calcd. for $C_{18}H_{14}N_2O_3$: C, 70.58; H, 4.61; N, 9.15 %. Found: C, 70.71; H, 4.82; N, 8.97 %; ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.57 (3H, *s*, CH_3), 7.16 (1H, *d*, *J* = 16.4 Hz, CH=CH), 7.38–7.46 (3H, *m*, Ar-H), 7.57–7.59 (2H, *m*, Ar-H), 7.60 (1H, *d*, *J* = = 16.0 Hz, CH=CH), 7.84–7.93 (2H, *m*, Ar-H), 8.59 (1H, *d*, *J* = 8.4 Hz, Ar-H), 8.66 (1H, *d*, *J* = 8.0 Hz, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 14.17, 120.23, 120.26, 124.73, 129.01, 129.08, 131.45, 131.71, 132.54, 133.63, 137.00, 137.95, 139.08, 139.87, 147.41, 185.88.

1-(3-methyl-4-oxido-2-quinoxalinyl)-3-phenyl-2-propen-1-one ***(4)***. Yield: 88.5 %; yellow crystals; m.p.: 156–157 °C (lit: 155–156.3 °C[2]); Anal. Calcd. for $C_{18}H_{14}N_2O_2$: C, 74.47; H, 4.86; N, 9.65 %. Found: C, 74.31; H, 4.84; N, 9.57 %; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 2.85 (3H, *s*, CH_3), 7.43–7.84 (9H, *m*, Ar-H & CH=CH), 8.20 (1H, *t*, *J* = 4.0 Hz, Ar-H), 8.63 (1H, *t*, *J* = 4.0 Hz, Ar-H); ^{13}C-NMR (125 MHz, $CDCl_3$, δ / ppm): 13.94, 118.95, 123.28, 128.88, 128.99, 130.55, 131.06, 131.12, 131.59, 134.48, 137.01, 140.44, 142.12, 146.68, 151.67, 189.97.

1-(3-methyl-2-quinoxalinyl)-3-phenyl-2-propen-1-one ***(5)***. Yield: 92 %, yellow crystals; m.p.: 144.9–145.5 °C (lit: 44.6–147.0 °C[2]); Anal. Calcd. for $C_{18}H_{14}N_2O$: C, 78.81, H, 5.14; N, 10.21 %. Found: C, 78.57; H, 5.09; N, 9.98 %; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 2.94 (3H, *s*, CH_3), 7.43–7.87 (9H, *m*, Ar-H & CH=CH), 8.01–8.18 (2H, *m,* Ar-H); ^{13}C-NMR (125 MHz, $CDCl_3$, δ / ppm): 24.06, 123.35, 128.05, 128.37, 128.52, 128.82, 128.95, 129.60, 129.75, 130.82, 131.77, 134.80, 139.72, 145.61, 153.57, 191.09.

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