

SUPPLEMENTARY MATERIAL TO

Improved synthesis of quinocetone and its two desoxymetabolites

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ANALYTIC AND SPECTRAL DATA

3-methyl-2-cinnamoyl-quinoxaline-1,4-dioxide(3): Anal. Calcd. for C₁₈H₁₄N₂O₃: C:70.58, H: 4.61, N: 9.15. Found: C: 70.71, H: 4.82, N: 8.97. ¹HNMR (400MHz, CDCl₃): δ = 2.57 (3H, s, -CH₃), 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* = 8.4Hz, Ar-H), 8.66 (1H, d, *J* = 8.0Hz, Ar-H). ¹³CNMR (100MHz, CDCl₃): δ= 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.

3-methyl-2-cinnamoyl-quinoxaline-4-oxide (4): Anal. Calcd. for C₁₈H₁₄N₂O₂: C: 74.47, H: 4.86, N: 9.65. Found: C: 74.31, H: 4.84, N: 9.57. ¹HNMR (500MHz, CDCl₃): δ = 2.85(3H, s, -CH₃), 7.43-7.84(9H, m, Ar-H and -CH=CH-), 8.20(1H, t, *J* = 4.0 Hz, Ar-H), 8.63 (1H, t, *J* = 4.0 Hz, Ar-H). ¹³CNMR(CDCl₃, 100MHz): δ=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.

3-methyl-2-cinnamoyl-quinoxaline (5): Anal. Calcd. for C₁₈H₁₄N₂O: C:78.81, H:5.14, N:10.21. Found: C:78.57, H: 5.09,N: 9.98. ¹HNMR (500MHz, CDCl₃): δ = 2.94(3H, s, -CH₃), 7.43-7.87(9H, m, Ar-H and -CH=CH-), 8.01-8.18(2H, m, Ar-H). ¹³CNMR(CDCl₃, 100MHz): δ= 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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