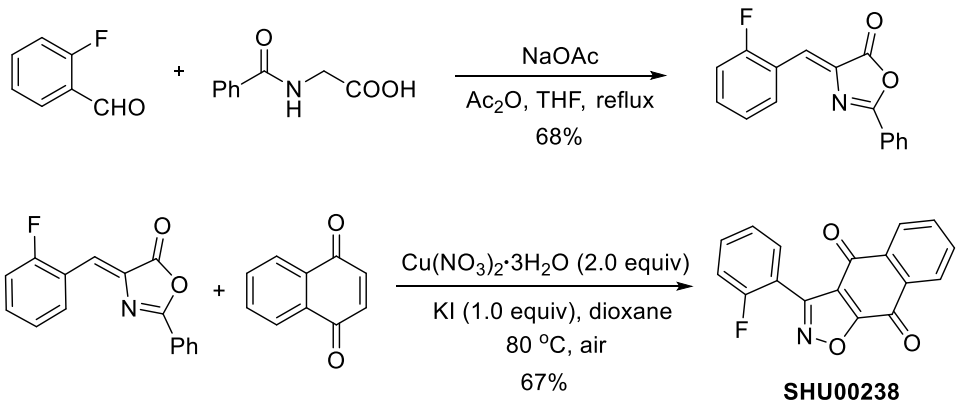
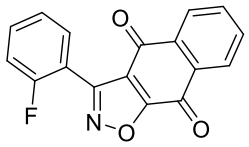
Supplementary materials

Preparation of Isoxazole Derivative SHU00238

Isoxazole derivative SHU00238 was prepared according to the reported method [1]. The melting point was measured on a WRS-1A Digital Melting Point Apparatus without correction. Infrared spectrum was obtained using an AVATAR 370 FT-IR spectrometer. ^{1}H, ^{13}C and ^{19}F-NMR spectra were recorded on a Bruker AV-500 spectrometer. Mass spectrum was measured on an Agilent 5975C using an electron impact technique.



Scheme 1. Synthesis of isoxazole derivative SHU00238.



SHU00238

3-(2-Fluorophenyl)naphtho[2,3-*d*]isoxazole-4,9-dione (SHU00238) [1]**:** M.p. 192-194 °C; IR (KBr, cm^{-1}): 3077, 1686, 1584, 1514, 1465, 1336, 1197, 918, 758, 716; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.31-8.29 (m, 1H), 8.23-8.21 (m, 1H), 7.87-7.82 (m, 2H), 7.70 (td, J = 7.4, 1.8 Hz, 1H), 7.62-7.57 (m, 1H), 7.35-7.27 (m, 2H); ^{19}F NMR ($CDCl_3$, 470 MHz): δ -111.2 (m, Ar-F); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 178.1, 173.2, 165.5, 160.6 (d, $^{1}J_{C\text{-}F}$ = 252.8 Hz), 156.4, 135.3, 134.4, 133.6, 133.1 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 132.0, 131.2 (d, $^{4}J_{C\text{-}F}$ = 1.2 Hz), 127.5 (d, $^{3}J_{C\text{-}F}$ = 9.1 Hz), 124.4 (d, $^{4}J_{C\text{-}F}$ = 3.6 Hz), 120.6, 116.2 (d, $^{2}J_{C\text{-}F}$ = 21.0 Hz), 114.7 (d, $^{2}J_{C\text{-}F}$ = 14.4 Hz); EI-MS m/z: 293 [M^{+}].

Reference

1. Lin, Y.; Zhang, K.; Gao, M.; Jiang, Z.; Liu, J.; Ma, Y.; Wang, H.; Tan, Q.; Xiao, J.; Xu, B. Copper nitrate-mediated synthesis of 3-aryl isoxazolines and isoxazoles from olefinic azlactones. *Org. Biomol. Chem.* **2019**, *17*, 5509-5513.