

Short Note

## 3-(1-Phenyl-1*H*-pyrazol-4-yl)-1,2-benzisoxazole 2-oxide

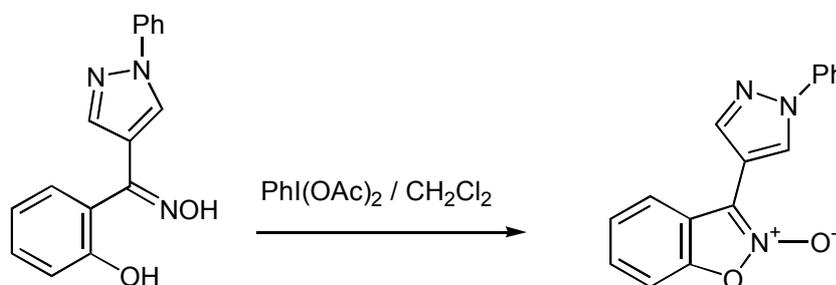
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It is well known that both isoxazole ring as well as pyrazole ring possess various biological activities and they both show interesting antimicrobial activity [1-3]. Therefore, it is not unreasonable to believe that a molecule bearing both moieties would possible show combined activity. Having this in mind we designed the synthesis of 3-(1-phenyl-1*H*-pyrazol-4-yl)-1,2-benzisoxazole 2-oxide as shown below. Nitrogen derivatives of *o*-hydroxyaryl ketones have been proved valuable starting materials in organic synthesis[4]. Thus, we synthesised (2-hydroxyphenyl)(1-phenyl-1*H*-pyrazol-4-yl)methanone oxime and we subsequently oxidized it with diacetoxy iodobenzene (DIB). The reaction led to the formation of the oxidative cyclisation product, giving the desired 3-(1-phenyl-1*H*-pyrazol-4-yl)-1,2-benzisoxazole 2-oxide, in 61% yield.



(2-Hydroxyphenyl)(1-phenyl-1*H*-pyrazol-4-yl)methanone oxime was prepared according to the literature methods by refluxing (2-hydroxyphenyl)(1-phenyl-1*H*-pyrazol-4-yl)methanone and

hydrochloric hydroxylamine in ethanol in the presence of pyridine whereas commercially available diacetoxy iodobenzene were supplied by Aldrich.

### Oxidation of (2-hydroxyphenyl)(1-phenyl-1*H*-pyrazol-4-yl)methanone oxime

0.58 g (1.79 mmol) of DIB are added to a suspension of 0.5 g (1.79 mmol) of (2-hydroxyphenyl)(1-phenyl-1*H*-pyrazol-4-yl)methanone oxime in 20 ml CH<sub>2</sub>Cl<sub>2</sub> in an ice-bath. The mixture was then magnetically stirred for 3 hrs. Evaporation of the solvent gave an oil which was then subjected to column chromatography (silica gel 70-230 mesh). Elution with a mixture of petroleum ether / ethylacetate 3:1 afforded the desired 3-(1-phenyl-1*H*-pyrazol-4-yl)-1,2-benzisoxazole 2-oxide as white crystals (0.30 g, 61 %). The product was identified by its <sup>1</sup>H NMR, <sup>13</sup>C NMR and MS and elemental analysis.

M.p. 179-180 °C.

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): 7.44-7.52 (m, 3H), 7.58-7.70 (m, 3H), 8.04-8.07(m, 2H), 8.32-8.34(d, *J*=8.0Hz, 1H), 8.67(s, 1H), 9.36(s, 1H).

<sup>13</sup>C NMR (100 MHz, DMSO-d<sub>6</sub>): 107.7, 109.5, 118.9, 119.9, 120.1, 121.6, 125.1, 127.3, 127.7, 128.1, 129.6, 130.2, 139.5, 139.7, 149.1, 150.5.

MS *m/z* (ES<sup>+</sup>): 300 [M+Na]<sup>+</sup>, 277 [M]<sup>+</sup>, 261, 247.

Anal. Calc. for C<sub>16</sub>H<sub>11</sub>N<sub>3</sub>O<sub>2</sub>: C 69.31, H 4.00, N 15.15; found: C 69.22, H 3.88, N, 15.10

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