

**Certificate of Analysis** 

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Print Date: Jan 14th 2016

Product Name: IQ 3 Catalog No.: 4550 Batch No.: 1

CAS Number: 312538-03-7

IUPAC Name: 11*H*-Indeno[1,2-*b*]quinoxalin-11-one O-(2-furanylcarbonyl)oxime

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{11}N_3O_3$ Batch Molecular Weight:341.32Physical Appearance:Yellow solidSolubility:DMSO to 20 mMStorage:Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.21$  (Ethyl acetate:Petroleum ether [1:2])

HPLC: Shows 99.2% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.38 3.25 12.31 Found 70.2 3.18 12.37



# **Product Information**

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## **Description:**

Selective JNK3 inhibitor ( $K_d$  values are 66, 240 and 290 nM for JNK3, JNK1 and JNK2 respectively). Inhibits NF- $\kappa$ B/AP1 transcriptional activity in THP1-Blue cells (IC<sub>50</sub> = 1.4  $\mu$ M). Also inhibits TNF- $\alpha$  and IL-6 production in vitro.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub> Batch Molecular Weight: 341.32 Physical Appearance: Yellow solid

Minimum Purity: >98%

## **Batch Molecular Structure:**

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

## Solubility & Usage Info:

DMSO to 20 mM

### Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

#### References:

Schepetkin et al (2012) Identification and characterization of a novel class of c-Jun N-terminal kinase inhibitors. Mol.Pharmacol. 81 832. PMID: 22434859.