

**Certificate of Analysis** 

www.tocris.com

Print Date: Jan 14th 2016

Product Name: NQDI 1 Catalog No.: 4429 Batch No.: 1

CAS Number: 175026-96-7

IUPAC Name: 2,7-Dihydro-2,7-dioxo-3*H*-naphtho[1,2,3-de]quinoline-1-carboxylic acid ethyl ester

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{13}NO_4$ Batch Molecular Weight:319.31Physical Appearance:Yellow solidSolubility:DMSO to 10 mMStorage:Store at +4°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

HPLC: Shows 100% purity

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

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen
Theoretical 71.47 4.1 4.39
Found 71.43 4.09 4.45



## **Product Information**

Print Date: Jan 14<sup>th</sup> 2016

www.tocris.com

Product Name: NQDI 1 Catalog No.: 4429 Batch No.: 1

CAS Number: 175026-96-7

IUPAC Name: 2,7-Dihydro-2,7-dioxo-3*H*-naphtho[1,2,3-*de*]quinoline-1-carboxylic acid ethyl ester

**Description:** 

Selective inhibitor of apoptosis signal-regulating kinase 1 (ASK1, MAP3K5) ( $IC_{50}$  = 3  $\mu$ M,  $K_i$  = 500 nM).

**Physical and Chemical Properties:** 

Batch Molecular Formula: C<sub>19</sub>H<sub>13</sub>NO<sub>4</sub> Batch Molecular Weight: 319.31 Physical Appearance: Yellow solid

**Minimum Purity: >99%** 

**Batch Molecular Structure:** 

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 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:

**Bu** et al (2001) Synthesis and cytotoxic activity of 7-oxo-7*H*-dibenz[f,ij]isoquinoline and 7-oxo-7*H*-benzo[e]perimidine derivatives. J.Med.Chem. **44** (12) 2004. PMID: 11384245.

**Volynets** *et al* (2011) Identification of 3*H*-naphtho[1,2,3-*de*]quinoline-2,7-diones as inhibitors of apoptosis signal-regulating kinase 1 (ASK1). J.Med.Chem. *54* (8) 2680. PMID: 21449566.

e.com Tel: +44 (0)1235 529449