

Product Name: NQDI 1

Catalog No.: 4429

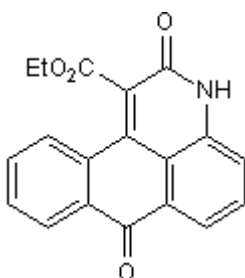
Batch No.: 1

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: C₁₉H₁₃NO₄
Batch Molecular Weight: 319.31
Physical Appearance: Yellow solid
Solubility: DMSO to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H 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

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Description:

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

Physical and Chemical Properties:

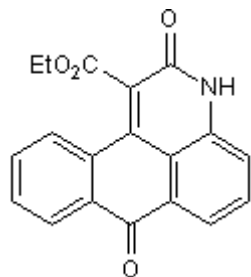
Batch Molecular Formula: $C_{19}H_{13}NO_4$

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

Volynets (2011) Identification of 3H-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.

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