

Certificate of Analysis

Product Name: NSC 687852

Catalog No.: 4566

Batch No.: 1

CAS Number: 1009817-63-3

IUPAC Name: 3,5-Bis[(4-nitrophenyl)methylene]-1-(1-oxo-2-propene-1-yl)-4-piperidone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{17}N_3O_6 \cdot \frac{1}{4}H_2O$

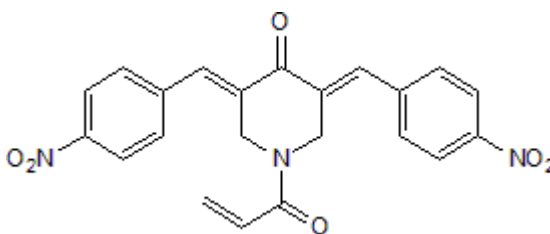
Batch Molecular Weight: 423.89

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows >97.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 62.34 | 4.16 | 9.91 |
| Found | 62.26 | 4.31 | 9.64 |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Inhibitor of 19S regulatory particle associated deubiquitinating enzymes (DUBs), UCHL5 and USP14. Shows minimal inhibition of UCHL-1, UCHL-3, USP2, USP7, USP, BAP1 and proteasome activity. Induces apoptosis by cathepsin D-dependent caspase-cleavage (IC₅₀ = 0.5 μM). Displays antitumor activity in vivo.

Physical and Chemical Properties:

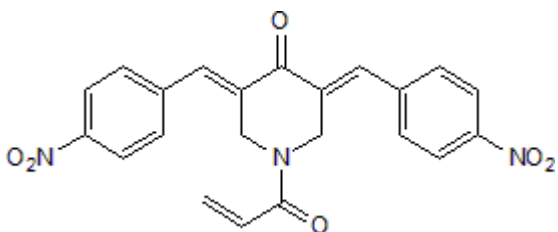
Batch Molecular Formula: C₂₂H₁₇N₃O₆. ¼H₂O

Batch Molecular Weight: 423.89

Physical Appearance: Yellow solid

Minimum Purity: >97%

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 100 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:

Berndtsson et al (2009) Induction of the lysosomal apoptosis pathway by inhibitors of the ubiquitin-proteasome system. *Int.J.Cancer* **124** 1463. PMID: 19089926.

D'Arcy et al (2011) Inhibition of proteasome deubiquitinating activity as a new cancer therapy. *Nat.Med.* **17** 1636. PMID: 22057347.

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