

Certificate of Analysis

Product Name: NVP 231

Catalog No.: 3960

Batch No.: 1

CAS Number: 362003-83-6

IUPAC Name: *N*-[2-(Benzoylamino)-6-benzothiazolyl]tricyclo[3.3.1.1^{3,7}]decane-1-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₅N₃O₂S·½H₂O

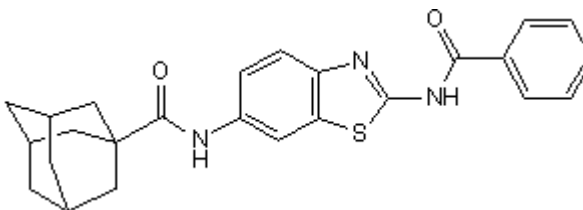
Batch Molecular Weight: 440.56

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
ethanol to 5 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.27 (Chloroform:Methanol [97:3])

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.16	5.95	9.54
Found	68.31	5.83	9.54

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Description:

Potent, selective and reversible ceramide kinase (CerK) inhibitor (IC₅₀ = 12 nM in vitro). Displays selectivity for CerK over sphingosine kinases (IC₅₀ ≥100 μM) and other lipid kinases.

Physical and Chemical Properties:

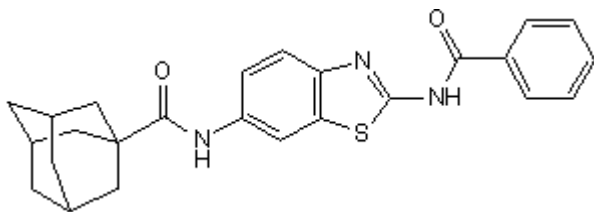
Batch Molecular Formula: C₂₅H₂₅N₃O₂S.½H₂O

Batch Molecular Weight: 440.56

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 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:

Graf et al (2009) A secondary assay for ceramide kinase inhibitors based on cell growth inhibition by short-chain ceramides. *Anal.Biochem.* **384** 166. PMID: 18831956.

Niwa et al (2009) Ceramide kinase deficiency impairs microendothelial cell angiogenesis in vitro. *Microvasc.Res.* **77** 389. PMID: 19323974.

Graf et al (2009) Targeting ceramide metabolism with a potent and specific ceramide kinase inhibitor. *Mol.Pharmacol.* **74** 925.

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