

Certificate of Analysis

Product Name: CID 2858522

Catalog No.: 4246

Batch No.: 1

CAS Number: 758679-97-9

IUPAC Name: 1-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-[2-[(3-hydroxypropyl)amino]-5,6-dimethyl-1*H*-benzimidazol-1-yl]ethanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{39}N_3O_3 \cdot \frac{1}{4}H_2O$

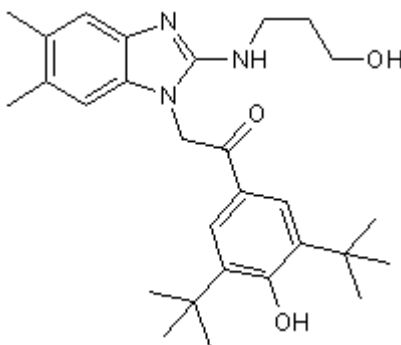
Batch Molecular Weight: 470.13

Physical Appearance: Pale yellow solid

Solubility: DMSO to 20 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.54	8.47	8.94
Found	71.24	8.29	9.06

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Description:

Selectively inhibits protein kinase C (PKC)-induced activation of the NF-κB pathway (IC₅₀ < 0.1 μM for PMA-stimulated IL-8 production). Inhibits antigen receptor-stimulated NF-κB activation in chronic lymphocytic leukemia (CLL) B cells. Does not inhibit other NF-κB pathways, including that activated by tumor necrosis factor (TNF).

Physical and Chemical Properties:

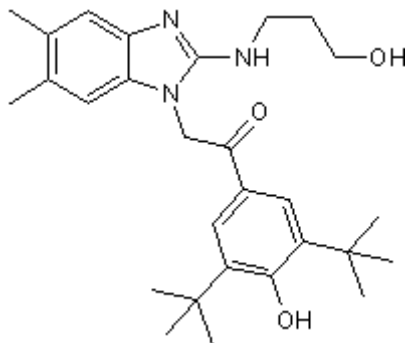
Batch Molecular Formula: C₂₈H₃₉N₃O₃·¼H₂O

Batch Molecular Weight: 470.13

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM
ethanol 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:

Peddibhotla et al (2010) Inhibition of protein kinase C-driven NF-κB activation: synthesis, SAR, and pharmacological profiling of pathway specific benzimidazole probe molecules. *J.Med.Chem.* **53** 4793. PMID: 20481485.

Shi et al (2010) Chemical biology strategy reveals pathway-selective inhibitor of NF-κB activation induced by protein kinase C and antigen receptors. *ACS Chem.Bio.* **5** 287.

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