

Product Name: BAY 6035

Catalog No.: 6561

Batch No.: 1

CAS Number: 2247890-13-5

IUPAC Name: (2*S*)-1-(3-Azabicyclo[3.1.0]hex-3-ylcarbonyl)-*N*-(2-cyclopropylethyl)-2,3,4,5-tetrahydro-2-methyl-4-oxo-1*H*-1,5-benzodiazepine-7-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₈N₄O₃·½H₂O

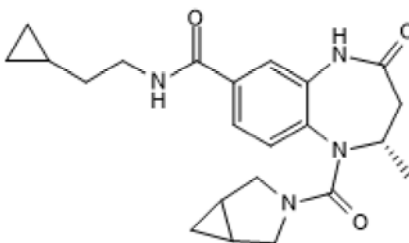
Batch Molecular Weight: 405.49

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.47 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.7% purity

Chiral HPLC: Shows >99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.17	7.21	13.82
Found	65.21	7.14	13.72

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Description:

Potent SMYD3 inhibitor (IC₅₀ = 70 nM for inhibition of MEKK2 methylation in cells). Exhibits >100-fold selectivity for SMTD3 over other histone methyltransferases.

Physical and Chemical Properties:

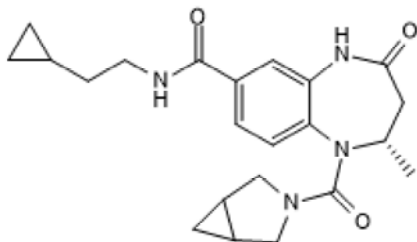
Batch Molecular Formula: C₂₂H₂₈N₄O₃·½H₂O

Batch Molecular Weight: 405.49

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY-6035 probe summary on the SGC website.

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