

Product Name: GSK 591 dihydrochloride

Catalog No.: 5777

Batch No.: 1

CAS Number: 2320953-89-5

IUPAC Name: 2-(Cyclobutylamino)-N-[(2S)-3-(3,4-dihydro-2(1H)-isoquinolinyl)-2-hydropropyl]-4-pyridinecarboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₈N₄O₂·2HCl·H₂O

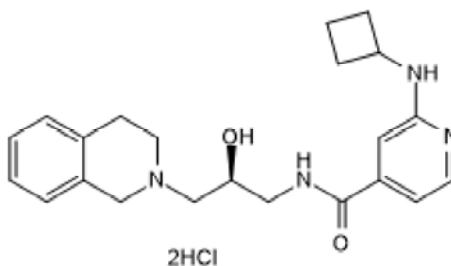
Batch Molecular Weight: 471.43

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.26 (Ethyl acetate)

HPLC: Shows 98.8% purity

Chiral HPLC: Shows 97.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +27.2 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.05	6.84	11.88
Found	55.68	6.81	11.8

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Description:

Potent and selective PRMT5 inhibitor ($IC_{50} = 4 \text{ nM}$). Selective for PRMT5 over a panel of other PRMTs and lysine methyltransferases. Inhibits proliferation of mantle cell lymphoma (MCL) in vitro. To request the negative control for GSK 591, please fill out the SGC 2096 request form on the SGC website.

Physical and Chemical Properties:

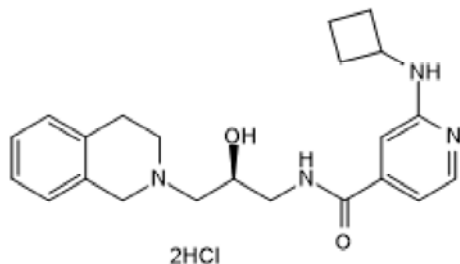
Batch Molecular Formula: $C_{22}H_{28}N_4O_2 \cdot 2HCl \cdot H_2O$

Batch Molecular Weight: 471.43

Physical Appearance: White solid

Minimum Purity: $\geq 97\%$

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM

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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the GSK591 probe summary on the SGC website.

References:

Scheer *et al* (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. *Nat. Commun.* **10** 19. PMID: 30604761.

Duncan *et al* (2015) Structure and property guided design in the identification of PRMT5 tool compound EPZ015666. *ACS. Med. Chem. Lett.* **7** 162. PMID: 26985292.

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