

Product Name: GSK 2250665A

Catalog No.: 5401

Batch No.: 1

CAS Number: 1246030-96-5

IUPAC Name: *trans*-4-[[4-[(6-Ethyl-2-benzothiazolyl)amino]-6-(phenylmethyl)-2-pyrimidinyl]amino]cyclohexanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₉N₅OS.½H₂O

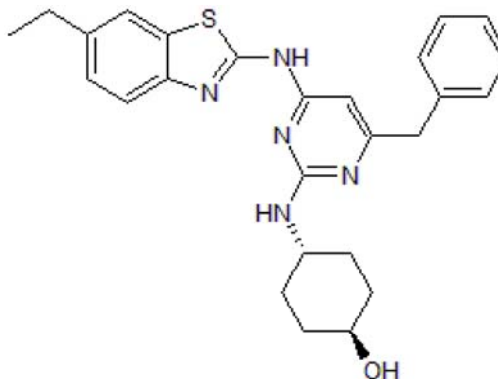
Batch Molecular Weight: 468.62

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
1eq. HCl to 20 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (2% Methanol in Ethyl acetate)

HPLC: Shows 97.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.64	6.45	14.94
Found	66.42	6.28	14.82

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Description:

Itk inhibitor ($pK_i = 9.2$). Exhibits selectivity for Itk over Aurora B kinase and Btk (pIC_{50} values are 6.4 and 6.5, respectively) and a panel of other kinases. Inhibits IFN γ production in PBMCs.

Physical and Chemical Properties:

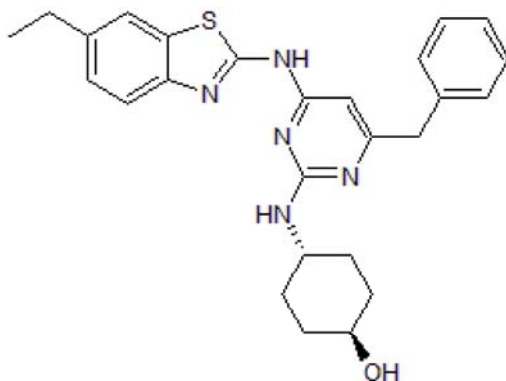
Batch Molecular Formula: C₂₆H₂₉N₅OS.½H₂O

Batch Molecular Weight: 468.62

Physical Appearance: Off White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. HCl to 20 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:

Sold for research purposes under agreement from GlaxoSmithKline

References:

Alder *et al* (2013) Identification of a novel and selective series of Itk inhibitors via a template-hopping strategy. ACS Med.Chem.Lett. **12** 948. PMID: 24900590.

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