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Print Date: Aug 19th 2024

Certificate of Analysis

www.tocris.com

Product Name: SB 590885

Catalog No.: 2650 Batch No.: 4

CAS Number: IUPAC Name: 405554-55-4

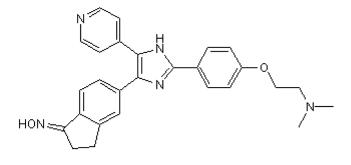
5-[2-[4-[2-(Dimethylamino)ethoxy]phenyl]-5-(4-pyridinyl)-1H-imidazol-4-yl]-2,3-dihydro-1H-inden-1-one oxime

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

 $C_{27}H_{27}N_5O_2.14H_2O$ 458.04 Off White solid DMSO to 10 mM ethanol to 5 mM with gentle warming Store at -20°C

Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.8% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitrogen				
Theoretical	70.8	6.05	15.29		
Found	69.75	6.02	14.98		

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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5-[2-[4-[2-(Dimethylamino)ethoxy]phenyl]-5-(4-pyridinyl)-1H-imidazol-4-yl]-2,3-dihydro-1H-inden-1-one oxime

Description:

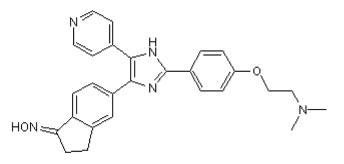
SB 590885 is a potent B-Raf inhibitor (K_d = 0.3 nM). Selective for B-Raf against 46 other kinases (K_{i app} values are 0.16 and 1.72 nM for B-Raf and c-Raf respectively). Decreases anchorage-independent growth of melanoma cell lines. Inhibits ERK phosphorylation and proliferation in tumor cells expressing B-Raf^{V600E}. The compound can be used in protocols for the chemical reprogramming of somatic cells to iPSCs.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{27}H_{27}N_5O_2$.¹/₄H₂O Batch Molecular Weight: 458.04 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 2650

Solubility & Usage Info:

DMSO to 10 mM ethanol to 5 mM with gentle warming

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Guan et al (2022) Chemical reprogramming of human somatic cells to pluripotent stem cells. Nature 605 325. PMID: 35418683.

King et al (2006) Demonstration of a genetic therapeutic index for tumors expressing oncogenic BRAF by the kinase inhibitor SB-590885. Cancer Res. 66 11100. PMID: 17145850.

Takle *et al* (2006) The identification of potent and selective imidazole-based inhibitors of B-Raf kinase. Bioorg.Med.Chem.Lett. **16** 378. PMID: 16260133.

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