

**Product Name:** SB 590885

**Catalog No.:** 2650

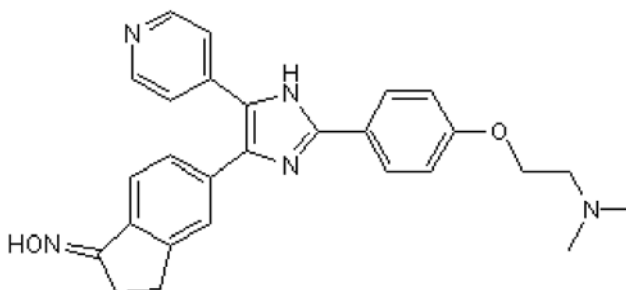
**Batch No.:** 3

CAS Number: 405554-55-4

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>27</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub> ·2H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	489.57
<b>Physical Appearance:</b>	Yellow solid
<b>Solubility:</b>	DMSO to 10 mM ethanol to 5 mM with gentle warming
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 98.1% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	66.24	6.38	14.31
Found	66.07	5.97	14.22

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

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**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<sup>V600E</sup>. The compound can be used in protocols for the chemical reprogramming of somatic cells to iPSCs.

**Physical and Chemical Properties:**

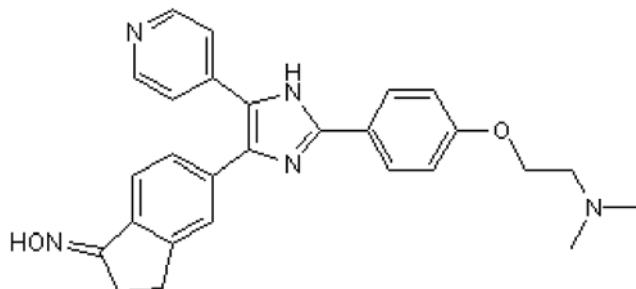
Batch Molecular Formula:  $C_{27}H_{27}N_5O_2 \cdot 2H_2O$

Batch Molecular Weight: 489.57

Physical Appearance: Yellow 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.

**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. 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:**

**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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