

Product Name: SB 590885

Catalog No.: 2650

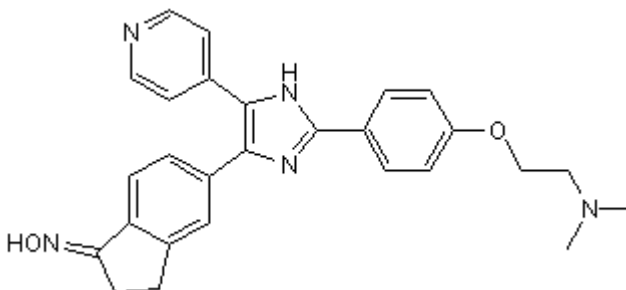
Batch No.: 3

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

Batch Molecular Formula: C₂₇H₂₇N₅O₂·2H₂O
Batch Molecular Weight: 489.57
Physical Appearance: Yellow solid
Solubility: DMSO to 10 mM
 ethanol to 5 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	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:

Potent B-Raf inhibitor ($K_d = 0.3$ nM). Selective for B-Raf against 46 other kinases ($K_{i\text{ app}}$ 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}.

Physical and Chemical Properties:

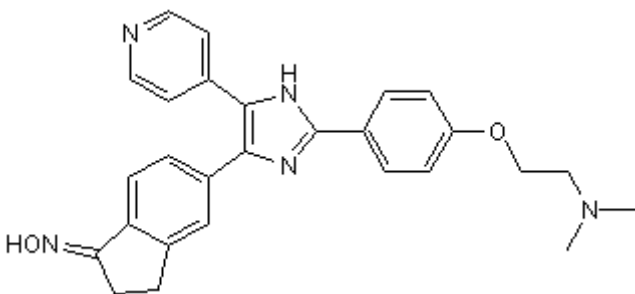
Batch Molecular Formula: C₂₇H₂₇N₅O₂·2H₂O

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.

References:

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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