Certificate of Analysis

Product Name: **SB 431542** **Catalog No.: 1614** **Batch No.: 16**

CAS Number: 301836-41-9

IUPAC Name: 4-[4-(1,3-benzodioxol-5-yl)-5-(2-pyridinyl)-1*H*-imidazol-2-yl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{16}N_4O_3.2H_2O$

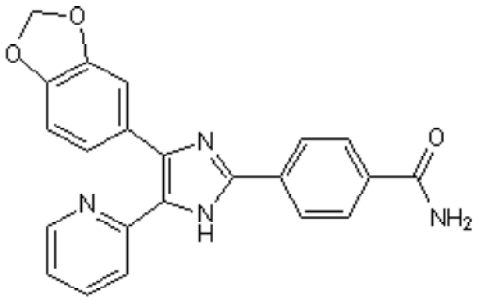
Batch Molecular Weight: 420.42

Physical Appearance: Pale yellow solid

Solubility: ethanol to 10 mM
DMSO to 100 mM with gentle warming

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.85	4.79	13.33
Found	62.75	4.77	13.36

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Product Information

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IUPAC Name: 4-[4-(1,3-benzodioxol-5-yl)-5-(2-pyridinyl)-1*H*-imidazol-2-yl]benzamide

Description:

SB 431542 is a potent and selective inhibitor of the transforming growth factor-β (TGF-β) type I receptor/ALK5 (IC_{50} = 94 nM), and its relatives ALK4 and ALK7. Suppresses TGF-β-induced proliferation of human osteosarcoma cells. Replaces SOX2 in reprogramming of fibroblasts into iPSCs. Stimulates proliferation, differentiation and sheet formation of ESC-derived endothelial cells. Inhibits TGF-β-induced EMT, migration, invasion and VEGF secretion in several human cancer cell lines. SB 431542 synthesized to cGMP guidelines also available. For more information about how SB 431542 may be used, see our protocols: 3D Culture ... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

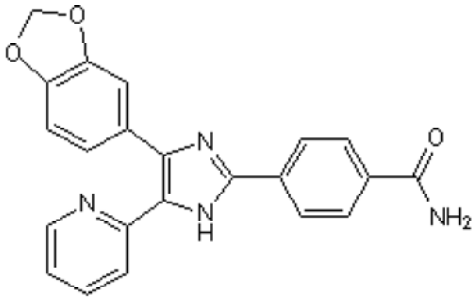
Batch Molecular Formula: $C_{22}H_{16}N_4O_3.2H_2O$

Batch Molecular Weight: 420.42

Physical Appearance: Pale yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

ethanol to 10 mM

DMSO to 100 mM with gentle warming

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Halder *et al* (2005) A specific inhibitor of TGF-beta receptor kinase, SB-431542, as a potent antitumor agent for human cancers. Neoplasia ***7*** 509. PMID: 15967103.

Matsuyama *et al* (2003) SB-431542 and Gle. inhibit transforming growth factor-β-induced proliferation of human osteosarcoma cells. Cancer Res. ***63*** 7791. PMID: 14633705.

Watabe *et al* (2003) TGF-beta receptor kinase inhibitor enhances growth and integrity of embryonic stem cell-derived endothelial cells. J.Cell Biol. ***163*** 163. PMID: 14676305.

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