

Product Name: SB 431542

Catalog No.: 1614

Batch No.: 7

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: C₂₂H₁₆N₄O₃·1¼H₂O

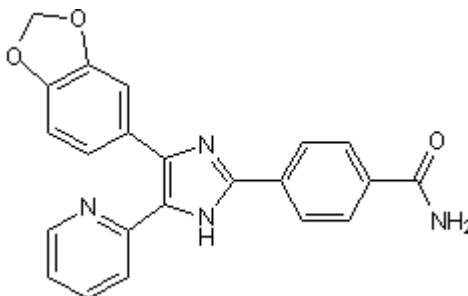
Batch Molecular Weight: 415.91

Physical Appearance: Yellow solid

Solubility: ethanol to 10 mM
DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol:Ammonia soln. [95:5:0.1])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 63.53 4.73 13.47

Found 63.24 4.75 13.51

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

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

Description:

Potent and selective inhibitor of the transforming growth factor- β (TGF- β) type I receptor activin receptor-like kinase ALK5 (IC_{50} = 94 nM), and its relatives ALK4 and ALK7. Suppresses TGF- β -induced proliferation of human osteosarcoma cells. Stimulates proliferation, differentiation and sheet formation of ESC-derived endothelial cells.

Physical and Chemical Properties:

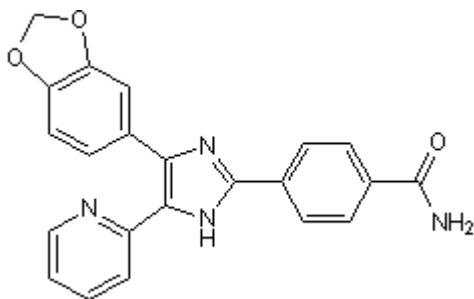
Batch Molecular Formula: $C_{22}H_{16}N_4O_3 \cdot 1\frac{3}{4}H_2O$

Batch Molecular Weight: 415.91

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

ethanol to 10 mM

DMSO 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.

References:

Inman et al (2002) SB-431542 is a potent and specific inhibitor of transforming growth factor- β superfamily type I activin receptor-like kinase (ALK) receptors ALK4, ALK5, and ALK7. *Mol.Pharmacol.* **62** 65. PMID: 12065756.

Laping et al (2002) Inhibition of transforming growth factor (TGF)- β 1-induced extracellular matrix with a novel inhibitor of the TGF- β type I receptor kinase activity: SB-431542. *Mol.Pharmacol.* **62** 58. PMID: 12065755.

Matsuyama et al (2003) SB-431542 and Gleevec 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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