

Product Name: SM 16

Catalog No.: 6245

Batch No.: 1

CAS Number: 614749-78-9

IUPAC Name: 4-[4-(1,3-Benzodioxol-5-yl)-5-(6-methyl-2-pyridinyl)-1*H*-imidazol-2-yl]bicyclo[2.2.2]octane-1-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₆N₄O₃·¼H₂O

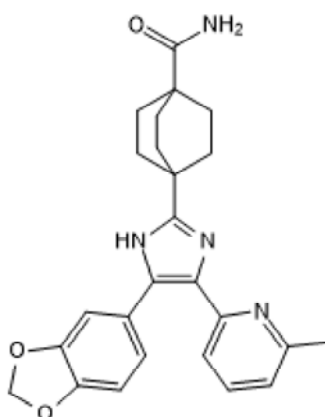
Batch Molecular Weight: 435

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Dichloromethane:Methanol [5:1])

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.03	6.14	12.88
Found	68.91	6.14	12.8

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Description:

Potent TGF- β receptor type 1 (TGF- β RI) inhibitor (IC_{50} = 64 nM in luciferase assay). Selective for TGF- β RI over other ALK family members. Decreases Smad phosphorylation and inhibits tumor growth in a mouse xenograft model. Attenuates increased TGF- β signaling in retinal vessels of diabetic rats. Also prevents intimal thickening and vascular remodeling in rat carotid balloon injury model. Orally bioavailable.

Physical and Chemical Properties:

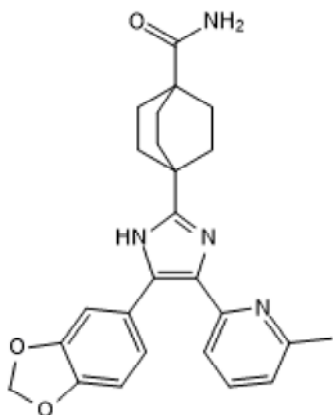
Batch Molecular Formula: $C_{25}H_{26}N_4O_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 435

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

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:

Dagher et al (2017) The increased transforming growth factor- β signaling induced by diabetes protects retinal vessels. *Am.J.Pathol.* **187** 627. PMID: 28162229.

Fu et al (2008) SM16, an orally active TGF- β type I receptor inhibitor prevents myofibroblast induction and vascular fibrosis in the rat carotid injury model. *Arterioscler.Thromb.Vasc.Biol.* **28** 665. PMID: 18202322.

Suzuki et al (2007) A novel small-molecule inhibitor of transforming growth factor β type I receptor kinase (SM16) inhibits murine mesothelioma tumor growth *in vivo* and prevents tumor recurrence after surgical resection. *Cancer Res.* **67** 2351. PMID: 17332368.

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