

Product Name: JTE 013

Catalog No.: 2392

Batch No.: 6

CAS Number: 383150-41-2

IUPAC Name: 1-[1,3-Dimethyl-4-(2-methylethyl)-1*H*-pyrazolo[3,4-*b*]pyridin-6-yl]-4-(3,5-dichloro-4-pyridinyl)-semicarbazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₉N₇OCl₂·¼H₂O

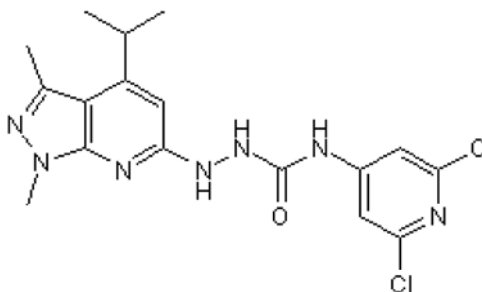
Batch Molecular Weight: 412.79

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Chloroform:Methanol [9:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.46	4.76	23.75
Found	49.71	4.95	23.22

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Description:

Sphingosine-1-phosphate (S1P) receptor antagonist, highly selective for S1P₂ (EDG-5). Inhibits S1P binding to human S1P₂ receptors with an IC₅₀ value of 17.6 nM. At concentrations up to 10 μM, displays 4.2% inhibition of S1P₃ and does not antagonize S1P₁. Enhances S1P-induced angiogenesis in vivo.

Physical and Chemical Properties:

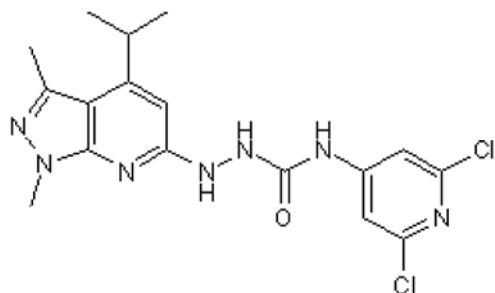
Batch Molecular Formula: C₁₇H₁₉N₇OCl₂·½H₂O

Batch Molecular Weight: 412.79

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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:

Inoki et al (2006) Negative regulation of endothelial morphogenesis and angiogenesis by S1P2 receptor. *Biochem.Biophys.Res.Comm.* **346** 293.

Parrill et al (2004) Sphingosine 1-phosphate and lysophosphatidic acid receptors: agonist and antagonist binding and progress toward development of receptor-specific ligands. *Semin.Cell.Dev.Biol.* **15** 467. PMID: 15271292.

Ohmori et al (2003) Spingosine 1-phosphate induces contraction of coronary artery smooth muscle cells via S1P2. *Cardiovasc.Res.* **58** 170. PMID: 12667959.

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