

**Product Name:** PF 5274857 hydrochloride

**Catalog No.:** 5262

**Batch No.:** 1

CAS Number: 1613439-62-5

IUPAC Name: 1-[4-(5'-Chloro-3,5-dimethyl[2,4'-bipyridin]-2'-yl)-1-piperazinyl]-3-(methylsulfonyl)-1-propanone hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>25</sub>ClN<sub>4</sub>O<sub>3</sub>S.HCl.½H<sub>2</sub>O

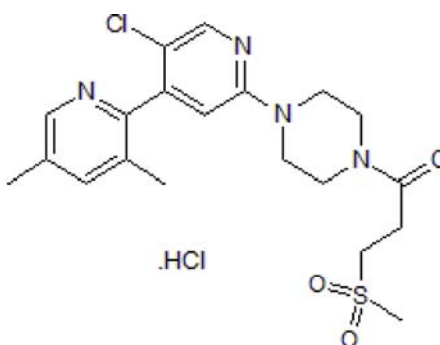
**Batch Molecular Weight:** 482.43

**Physical Appearance:** Pale yellow solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	49.79	5.64	11.61
Found	49.74	5.69	11.45

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**Description:**

High affinity and selective Smoothed (Smo) receptor antagonist ( $K_i = 4.6$  nM). Exhibits >1000-fold selectivity for Smo over a panel of other receptors, ion channels and enzymes. Inhibits Shh-induced Hedgehog signaling in MEF cells. Induces tumor regression in a medulloblastoma allograft mouse model. Orally available and brain penetrant.

**Physical and Chemical Properties:**

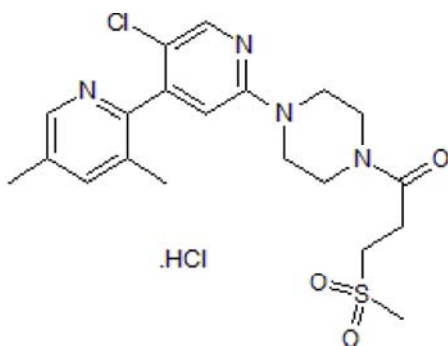
Batch Molecular Formula:  $C_{20}H_{25}ClN_4O_3S \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 482.43

Physical Appearance: Pale yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 100 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.

**Licensing Information:**

Sold for research purposes under agreement from Pfizer Inc.

**References:**

Rohner *et al* (2011) Effective targeting of Hedgehog signaling in a medulloblastoma model with PF-5274857, a potent and selective Smoothed antagonist that penetrates the blood-brain barrier. *Mol.Cancer Ther.* **11** 57. PMID: 22084163.

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