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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **PF 431396** **Catalog No.: 4278** **Batch No.: 2**

CAS Number: 717906-29-1

IUPAC Name: *N*-Methyl-*N*-[2-[[[2-[(2,3-dihydro-2-oxo-1*H*-indol-5-yl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]methyl]phenyl] methanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{21}F_3N_6O_3S.½H_2O$

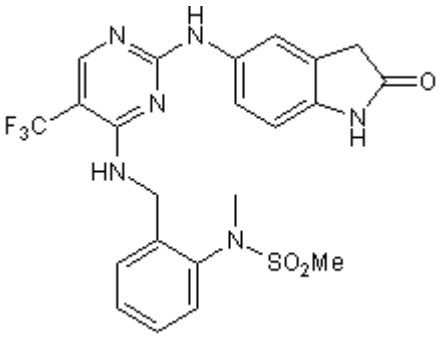
Batch Molecular Weight: 515.51

Physical Appearance: Beige solid

Solubility: DMSO to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.58 (Chloroform:Methanol [9:1])

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.26	4.3	16.3
Found	51.08	4.08	16.36

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Description:

Dual focal adhesion kinase (FAK) and proline-rich tyrosine kinase 2 (PYK2) inhibitor (IC_{50} values are 2 and 11 nM respectively). Promotes osteoblast recruitment and activity, and stimulates bone formation in ovariectomized rats.

Physical and Chemical Properties:

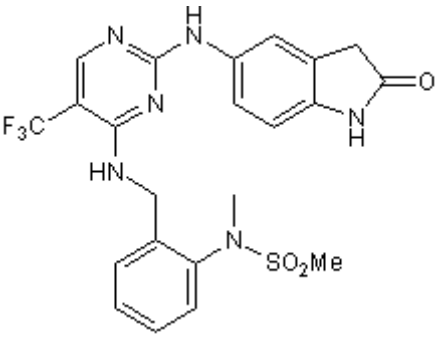
Batch Molecular Formula: $C_{22}H_{21}F_3N_6O_3S.½H_2O$

Batch Molecular Weight: 515.51

Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 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:

Buckbinder *et al* (2007) Proline-rich tyrosine kinase 2 regulates osteoprogenitor cells and bone formation, and offers an anabolic treatment approach for osteoporosis. Proc.Natl.Acad.Sci.USA ***104*** 10619. PMID: 17537919.

Han *et al* (2009) Structural characterization of proline-rich tyrosine kinase 2 (PYK2) reveals a unique (DFG-out) conformation and enables inhibitor design. J.Biol.Chem. ***284*** 13193. PMID: 19244237.

Allen *et al* (2010) Emerging targets in osteoporosis disease modification. J.Med.Chem. ***53*** 4332. PMID: 20218623.