

Product Name: PF 429242 dihydrochloride

Catalog No.: 3354

Batch No.: 3

CAS Number: 2248666-66-0

IUPAC Name: 4-[(Diethylamino)methyl]-N-[2-(2-methoxyphenyl)ethyl]-N-(3R)-3-pyrrolidinybenzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₃₅N₃O₂·2HCl·H₂O

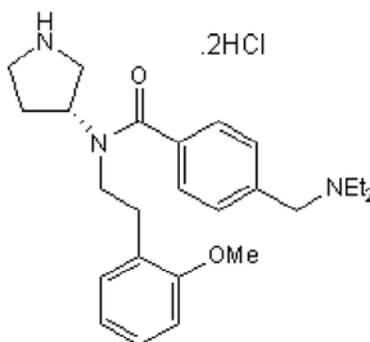
Batch Molecular Weight: 500.51

Physical Appearance: White solid

Solubility: water to 50 mM
DMSO to 50 mM
ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -5.7 (Concentration = 1, Solvent = Ethanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.99	7.85	8.4
Found	60.01	8	8.38

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Description:

Reversible, competitive inhibitor of sterol regulatory element-binding protein (SREBP) site 1 protease ($IC_{50} = 0.175 \mu M$). Selective for site 1 protease against a panel of serine proteases. Inhibits rate of cholesterol synthesis in CHO cells ($IC_{50} = 0.53 \mu M$). Also displays antiviral activity. Cell permeable.

Physical and Chemical Properties:

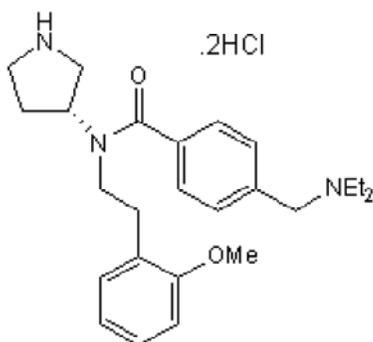
Batch Molecular Formula: $C_{25}H_{35}N_3O_2 \cdot 2HCl \cdot H_2O$

Batch Molecular Weight: 500.51

Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 50 mM
DMSO to 50 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Olmstead (2012) Human subtilase SKI-1/S1P is a master regulator of the HCV lifecycle and a potential host cell target for developing indirect-acting antiviral agents. *PLoS.Pathog.* **8** e1002468. PMID: 22241994.

Urata et al (2011) Antiviral activity of a small-molecule inhibitor of arenavirus glycoprotein processing by the cellular site 1 protease. *J.Virol.* **85** 795. PMID: 21068251.

Hawkins et al (2008) Pharmacologic inhibition of site 1 protease activity inhibits sterol regulatory element-binding protein processing and reduces lipogenic enzyme gene expression and lipid synthesis in cultured cells and experimental animals. *J.Pharmacol.Exp.Ther.* **326** 801. PMID: 18577702.

Hay et al (2007) Aminopyrrolidineamide inhibitors of site-1 protease. *Bioorg.Med.Chem.Lett.* **17** 4411. PMID: 17583500.

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bio-techne.com

info@bio-techne.com
techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors
Tel:+1 612 379 2956