Print Date: Sep 5th 2013

Certificate of Analysis

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Product Name: PF 429242 **Catalog No.: 3354** **Batch No.: 1**

CAS Number: 947303-87-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{35}N_3O_2 \cdot 1\frac{1}{2}H_2O$

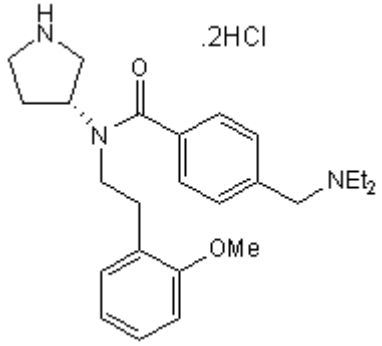
Batch Molecular Weight: 509.51

Physical Appearance: White solid

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

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol:Ammonia soln. [90:10:0.5])

HPLC: Shows 97.2% purity

Chiral HPLC: Shows 98% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -3.3 (Concentration = 1, Solvent = Ethanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.93	7.91	8.25
Found	59.09	7.59	8.35

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Description:

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

Physical and Chemical Properties:

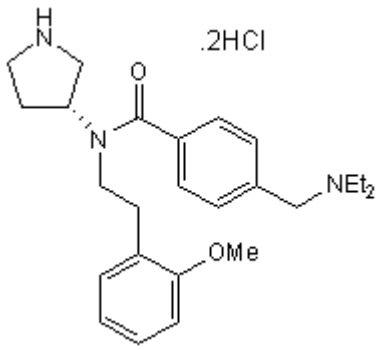
Batch Molecular Formula: $C_{25}H_{35}N_3O_2.1½H_2O$

Batch Molecular Weight: 509.51

Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at +4°C

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.

References:

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

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.

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.

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.