Certificate of Analysis

Product Name: **RWJ 56110** **Catalog No.: 2614** **Batch No.: 2**

CAS Number: 2387505-58-8

IUPAC Name: (α*S*)-*N*-[(1*S*)-3-Amino-1-[[(phenylmethyl)amino]carbonyl]propyl]-α-[[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1*H*-indol-6-yl]amino]carbonyl]amino]-3,4-difluoro-benzenepropanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{41}H_{43}Cl_2F_2N_7O_3.2HCl.1½H_2O$

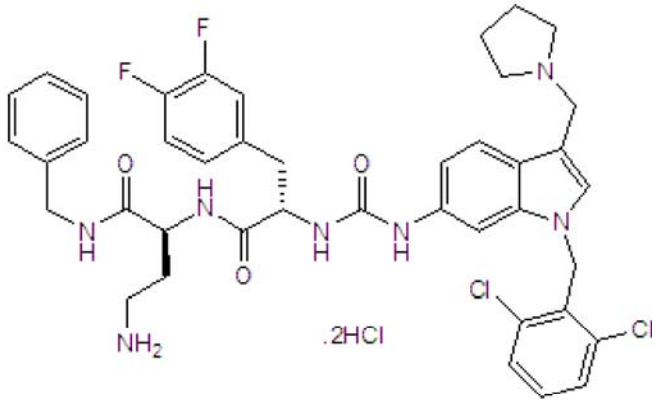
Batch Molecular Weight: 890.67

Physical Appearance: Grey solid

Solubility: water to 25 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.19 (Chloroform:Methanol:Ammonia soln. [9:1:0.1])

HPLC: Shows 98.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.29	5.43	11.01
Found	55.11	5.15	10.85

Product Name: **RWJ 56110** **Catalog No.: 2614** **2**

CAS Number: 2387505-58-8

IUPAC Name: (αS)-*N*-[(1*S*)-3-Amino-1-[[(phenylmethyl)amino]carbonyl]propyl]-α-[[[[1-[(2,6-dichlorophenyl)methyl]-3-(1-pyrrolidinylmethyl)-1*H*-indol-6-yl]amino]carbonyl]amino]-3,4-difluoro-benzenepropanamide

Description:

RWJ 56110 is a selective protease-activated receptor-1 (PAR_1) antagonist; displays no activity at PAR_2, PAR_3, or PAR_4 subtypes. Blocks thrombin-induced platelet aggregation and activation of MAPK in HUVECs. Also inhibits angiogenesis in a chick embryo angiogenesis model in vivo.

Physical and Chemical Properties:

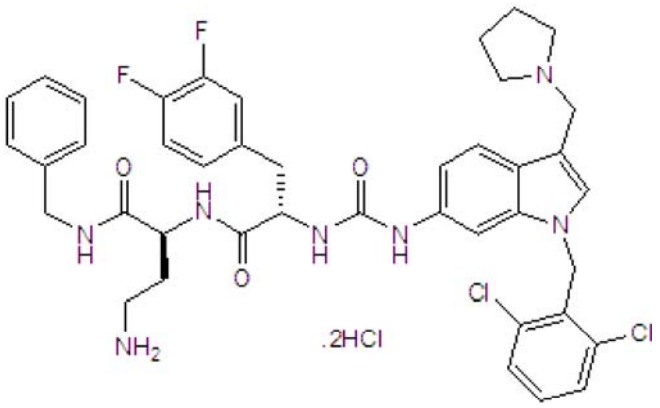
Batch Molecular Formula: $C_{41}H_{43}Cl_2F_2N_7O_3.2HCl.1½H_2O$

Batch Molecular Weight: 890.67

Physical Appearance: Grey solid

Minimum Purity: ≥96%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 25 mM
DMSO to 100 mM

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Zania *et al* (2006) Blockade of angiogenesis by small molecule antagonists to protease-activated receptor-1: association with endothelial cell growth suppression and induction of apoptosis. J.Pharmacol.Exp.Ther. ***318*** 246. PMID: 16595737.

Maryanoff *et al* (2003) Discovery of potent peptide-mimetic antagonists for the human thrombin receptor, protease-activated receptor-1 (PAR-1). Curr.Med.Chem.Cardiovasc.Hematol.Agents ***1*** 13. PMID: 15317288.

Andrade-Gordon *et al* (1999) Design, synthesis and biological characterization of a peptide-mimetic antagonist for a tethered-ligand receptor. Proc.Natl.Acad.Sci.USA ***96*** 12257. PMID: 10535908.