

**Product Name:** RWJ 56110

**Catalog No.:** 2614

**Batch No.:** 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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>41</sub>H<sub>43</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>7</sub>O<sub>3</sub>·2HCl·1½H<sub>2</sub>O

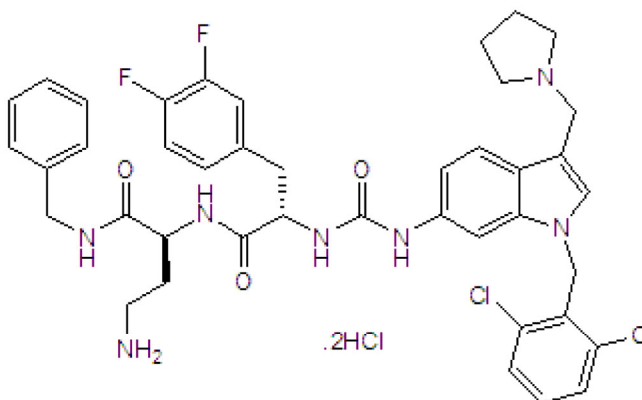
**Batch Molecular Weight:** 890.67

**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<sub>f</sub> = 0.19 (Chloroform:Methanol:Ammonia soln. [9:1:0.1])

**HPLC:** Shows 98.1% purity

**<sup>1</sup>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

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**Description:**

RWJ 56110 is a selective protease-activated receptor-1 (PAR<sub>1</sub>) antagonist; displays no activity at PAR<sub>2</sub>, PAR<sub>3</sub>, or PAR<sub>4</sub> 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:**

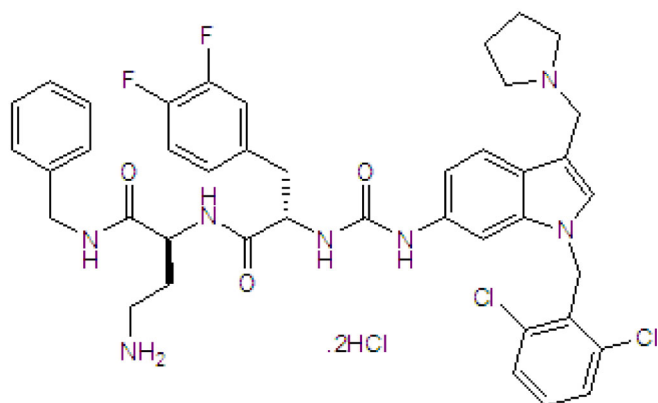
Batch Molecular Formula: C<sub>41</sub>H<sub>43</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>7</sub>O<sub>3</sub>·2HCl·1½H<sub>2</sub>O

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 in lyophilized form. It may appear as a solid, gel or film and 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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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.

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