

Product Name: SLM 6031434 hydrochloride

Catalog No.: 6281

Batch No.: 1

CAS Number: 1897379-34-8

IUPAC Name: (2S)-2-[3-[4-(Octyloxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-5-yl]-1-pyrrolidinecarboximidamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₃₀F₃N₅O₂.HCl.¼H₂O

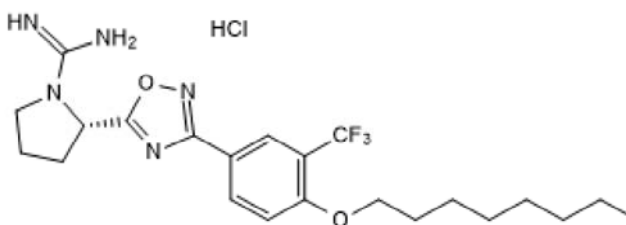
Batch Molecular Weight: 494.46

Physical Appearance: White solid

Solubility: water to 20 mM
DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	53.44	6.42	14.16
Found	53.36	6.45	14.24

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Sphk2 inhibitor ($K_i = 0.4 \mu\text{M}$ for mouse Sphk2). Exhibits 40-fold selectivity for Sphk2 over Sphk1. Decreases levels of sphingosine-1-phosphate (S1P) in U937 cells in vitro and increases blood levels of S1P in wild-type mice .

Physical and Chemical Properties:

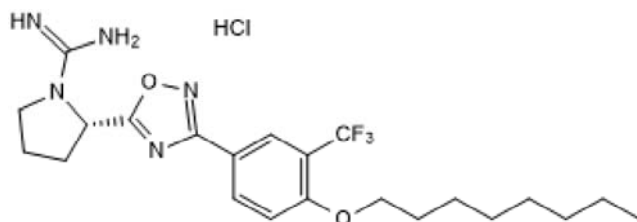
Batch Molecular Formula: $\text{C}_{22}\text{H}_{30}\text{F}_3\text{N}_5\text{O}_2 \cdot \text{HCl} \cdot \frac{1}{4}\text{H}_2\text{O}$

Batch Molecular Weight: 494.46

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 20 mM
DMSO to 100 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 with the permission of the University of Virginia Patent Foundation

References:

Kharel *et al* (2015) Sphingosine kinase 2 inhibition and blood sphingosine 1-phosphate levels. *J.Pharmacol.Exp.Ther.* **355** 23. PMID: 26243740.

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