

## Certificate of Analysis

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**Product Name:** CS 2100

**Catalog No.:** 4543

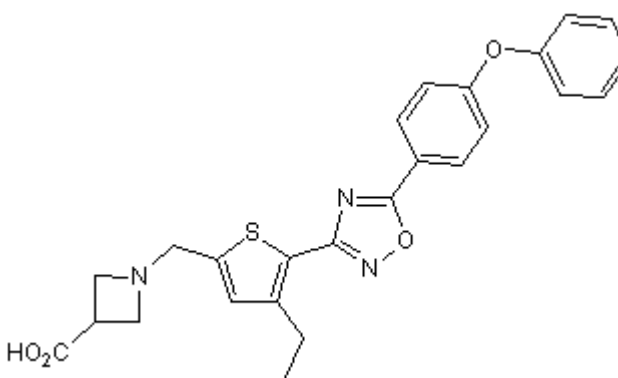
**Batch No.:** 1

CAS Number: 913827-99-3

IUPAC Name: 1-[[4-Ethyl-5-[5-(4-phenoxyphenyl)-1,2,4-oxadiazol-3-yl]-2-thienyl]methyl]-3-azetidinecarboxylic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>25</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub> S
<b>Batch Molecular Weight:</b>	461.53
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 5 mM with gentle warming
<b>Storage:</b>	Store at +4°C
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.1 (Dichloromethane:Methanol [9:1])
<b>HPLC:</b>	Shows 97.2% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	65.06	5.02	9.1
Found	64.97	5.01	8.93

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

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**Description:**

Sphingosine-1-phosphate receptor 1 (S1P<sub>1</sub>) agonist (EC<sub>50</sub> = 4.0 nM). Exhibits 5000-fold selectivity for human S1P<sub>1</sub> over S1P<sub>3</sub>. Displays efficacy in a rat adjuvant-induced arthritis model.

**Physical and Chemical Properties:**

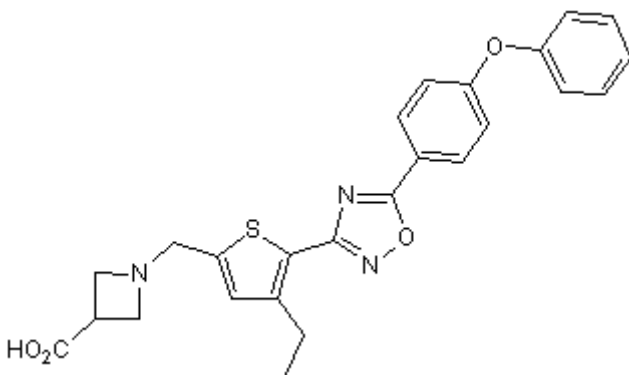
Batch Molecular Formula: C<sub>25</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>S

Batch Molecular Weight: 461.53

Physical Appearance: White solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 5 mM with gentle warming

**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:**

**Nakamura et al** (2012) Synthesis and evaluation of CS-2100, a potent, orally active and S1P<sub>3</sub>-sparing S1P<sub>1</sub> agonist. *Eur.J.Med.Chem.* **51** 92. PMID: 22405291.

**Nakamura et al** (2012) Discovery of CS-2100, a potent, orally active and S1P<sub>3</sub>-sparing S1P<sub>1</sub> agonist. *Bioorg.Med.Chem.Lett.* **22** 1788. PMID: 22264485.

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