

**Product Name:** Ceralifimod

**Catalog No.:** 6690

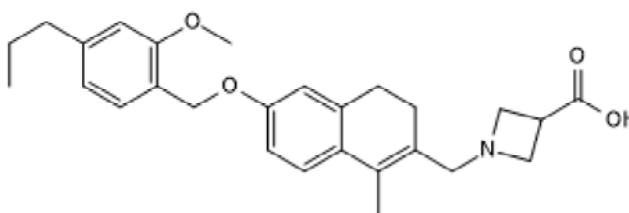
**Batch No.:** 1

CAS Number: 891859-12-4

IUPAC Name: 1-[[[3,4-Dihydro-6-[(2-methoxy-4-propylphenyl)methoxy]-1-methyl-2-naphthalenyl]methyl]-3-azetidinecarboxylic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>33</sub>NO<sub>4</sub>·<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O  
**Batch Molecular Weight:** 449.07  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 10 mM with gentle warming  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 96% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	72.22	7.74	3.12
Found	72.37	7.56	3.4

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

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**Description:**

Highly potent and selective S1P<sub>1</sub> and S1P<sub>5</sub> agonist (EC<sub>50</sub> values are 0.027 and 0.33 nM, respectively, in a cAMP assay). K<sub>i</sub> values are 0.574, 0.626, 28.7 >5450 and >5630 nM for S1P<sub>5</sub>, S1P<sub>1</sub>, S1P<sub>4</sub>, S1P<sub>2</sub>, S1P<sub>3</sub>, respectively. Reduces peripheral lymphocyte count in a mouse EAE model. Orally bioavailable.

**Physical and Chemical Properties:**

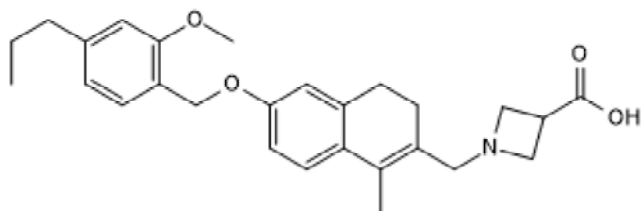
Batch Molecular Formula: C<sub>27</sub>H<sub>33</sub>NO<sub>4</sub>·¾H<sub>2</sub>O

Batch Molecular Weight: 449.07

Physical Appearance: Off White solid

**Minimum Purity:** >95%

**Batch Molecular Structure:**



**References:**

**Kurata et al** (2017) Discovery of a 1-methyl-3,4-dihydro-2-naphthalene-based sphingosine-1-phosphate (S1P) receptor agonist ceralifimod (ONO-4641). A S1P<sub>1</sub> and S1P<sub>5</sub> selective agonist for the treatment of autoimmune diseases. *J.Med.Chem.* **60** 9508. PMID: 29120624.

**Storage:** Store at -20°C. This product is packaged under an inert atmosphere.

**Solubility & Usage Info:**

DMSO to 10 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.

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