

Certificate of Analysis

Print Date: Sep 14th 2021

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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: C₂₇H₃₃NO₄.³/₄H₂O

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 95.9% purity

¹H 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

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Product Information

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Description:

Ceralifimod is a highly potent and selective $S1P_1$ and $S1P_5$ agonist (EC $_{50}$ values are 0.027 and 0.33 nM, respectively, in a cAMP assay). K_i values are 0.574, 0.626, 28.7 >5450 and >5630 nM for $S1P_5$, $S1P_1$, $S1P_4$, $S1P_2$, $S1P_3$, respectively. Reduces peripheral lymphocyte count in a mouse EAE model. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₇H₃₃NO₄.3/4H₂O

Batch Molecular Weight: 449.07 Physical Appearance: Off White solid

Minimum Purity: ≥95%

Batch Molecular Structure:

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.

References:

Kurata *et al* (2017) Discovery of a 1-methyl-3,4-dihydronaphthalene-based sphingosine-1-phosphate (S1P) receptor agonist ceralifimod (ONO-4641). A S1P₁ and S1P₅ selective agonist for the treatment of autoimmune diseases. J.Med.Chem. *60* 9508. PMID: 29120624.

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