

Certificate of Analysis

Product Name: VPC 23019

Catalog No.: 4195

Batch No.: 3

CAS Number: 449173-19-7

IUPAC Name: 2-Amino-N-(3-octylphenyl)-3-(phosphonoxy)-propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₉N₂O₅P·¼H₂O

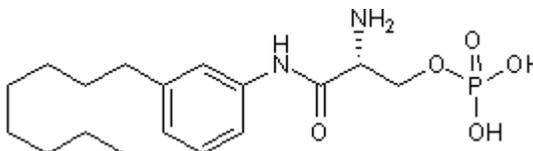
Batch Molecular Weight: 376.9

Physical Appearance: White solid

Solubility: Acidified DMSO (5% 1N HCl in DMSO) to 10 mM with gentle warming
2eq. NaOH to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.36 (Dichloromethane:Methanol [9:1])

HPLC: Shows 96.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.17	7.89	7.43
Found	54.4	7.84	7.59

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IUPAC Name: 2-Amino-N-(3-octylphenyl)-3-(phosphonoxy)-propanamide

Description:

Sphingosine-1-phosphate receptor antagonist; inhibits S1P₁ and S1P₃ receptors (pK_i values are 7.86 and 5.93 respectively).

Physical and Chemical Properties:

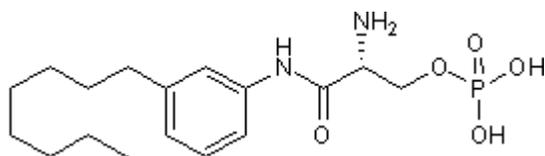
Batch Molecular Formula: C₁₇H₂₉N₂O₅P·¼H₂O

Batch Molecular Weight: 376.9

Physical Appearance: White solid

Minimum Purity: >95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

Acidified DMSO (5% 1N HCl in DMSO) to 10 mM with gentle warming
2eq. NaOH to 50 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.

References:

Davis et al (2005) Sphingosine-1-phosphate analogs as receptor antagonists. *J.Biol.Chem.* **280** 9833. PMID: 15590668.

Aoki et al (2007) The suppressive effect of sphingosine-1-phosphate on monocyte-endothelium adhesion may be mediated by the rearrangement of the endothelial integrins α₅β₁ and α_vβ₃. *J.Thromb.Haemost.* **5** 1292. PMID: 17403093.

Mihovilovic et al (2007) High-fat/cholesterol diet promotes a S1P receptor-mediated antiapoptotic activity for VLDL. *J.Lipid Res.* **48** 806. PMID: 17264352.

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