

Certificate of Analysis

Product Name: TC-SP 14

Catalog No.: 4363

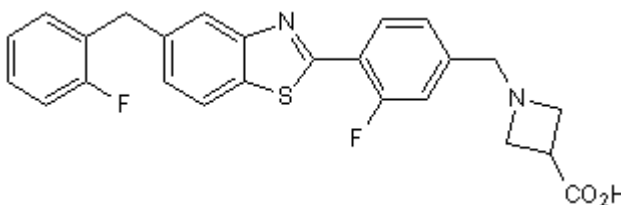
Batch No.: 2

CAS Number: 1257093-40-5

IUPAC Name: 1-[[3-Fluoro-4-[5-[(2-fluorophenyl)methyl]-2-benzothiazolyl]phenyl]methyl]-3-azetidincarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{20}F_2N_2O_2S \cdot 1\frac{1}{4}H_2O$
Batch Molecular Weight: 473.02
Physical Appearance: Off-white solid
Solubility: DMSO to 50 mM with gentle warming
Storage: Desiccate at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.13$ (Chloroform:Methanol [4:1])
HPLC: Shows 99.6% purity
 1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.48	4.79	5.92
Found	63.51	4.66	5.86

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

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Description:

Potent and selective S1P₁ agonist (EC₅₀ values are 0.042 and 3.47 μM for human S1P₁ and S1P₃ respectively). Attenuates immune response to antigen challenge and reduces circulating blood lymphocyte counts in a rodent model of delayed-type hypersensitivity. Orally bioavailable.

Physical and Chemical Properties:

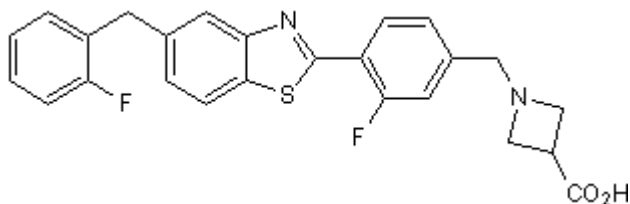
Batch Molecular Formula: C₂₅H₂₀F₂N₂O₂S.1¼H₂O

Batch Molecular Weight: 473.02

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 50 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:

Lanman et al (2011) Discovery of a potent, S1P₃-sparing benzothiazole agonist of sphingosine-1-phosphate receptor 1 (S1P₁). ACS Med.Chem.Lett. **2** 102.

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