

# Certificate of Analysis

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**Product Name:** Ex 26

**Catalog No.:** 5833

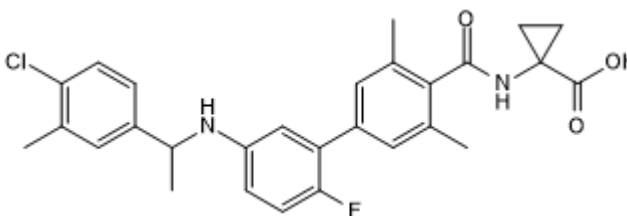
**Batch No.:** 1

CAS Number: 1233332-37-0

IUPAC Name: 1-[[[5'-[[1-(4-Chloro-3-methylphenyl)ethyl]amino]-2'-fluoro-3,5-dimethyl[1,1'-biphenyl]-4-yl]carbonyl]amino]-cyclopropanecarboxylic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>28</sub>ClFN<sub>2</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 494.98  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.75 (Ethyl acetate:Petroleum ether [3:7])  
**HPLC:** Shows >99.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	67.94	5.7	5.66
Found	67.72	5.73	5.96

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**Description:**

Potent and selective S1P<sub>1</sub> receptor antagonist (IC<sub>50</sub> = 0.93 nM). Exhibits > 3,000-fold selectivity for S1P<sub>1</sub> over S1P<sub>2</sub>, S1P<sub>3</sub>, S1P<sub>4</sub> and S1P<sub>5</sub>. Induces lymphocyte sequestration in peripheral lymph nodes and upregulates S1P<sub>1</sub> receptor expression. Reduces disease severity in mice with EAE. Increases IFN-α production in stimulated dendritic cells in vivo.

**Physical and Chemical Properties:**

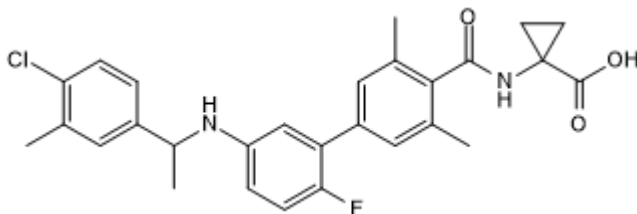
Batch Molecular Formula: C<sub>28</sub>H<sub>28</sub>ClFN<sub>2</sub>O<sub>3</sub>

Batch Molecular Weight: 494.98

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol to 100 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:**

**Tejaro et al** (2016) S1PR<sub>1</sub>-mediated IFNAR1 degradation modulates plasmacytoid dendritic cell interferon-α autoamplification. *Proc.Natl.Acad.Sci.U.S.A.* **113** 1351. PMID: 26787880.

**Cahalan et al** (2013) Sphingosine 1-phosphate receptor 1 (S1P<sub>1</sub>) upregulation and amelioration of experimental autoimmune encephalomyelitis by an S1P<sub>1</sub> antagonist. *Mol.Pharmacol.* **83** 316. PMID: 23204443.

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