

## Certificate of Analysis

**Product Name:** CYM 5541

**Catalog No.:** 4897

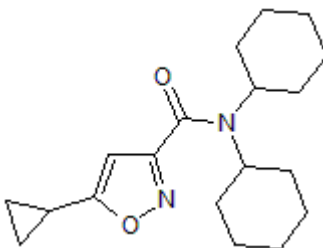
**Batch No.:** 1

CAS Number: 945128-26-7

IUPAC Name: *N,N*-Dicyclohexyl-5-cyclopropyl-3-isoxazolecarboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>19</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 316.44  
**Physical Appearance:** Off-white solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 50 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 97.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	72.12	8.92	8.85
Found	71.8	8.8	8.88

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

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**Description:**

Selective sphingosine-1-phosphate receptor 3 (S1P<sub>3</sub>) allosteric agonist (EC<sub>50</sub> = 72-132 nM). Occupies a different space within the ligand binding pocket of S1P<sub>3</sub> than S1P. Displays no activity at S1P<sub>1</sub>, S1P<sub>2</sub>, S1P<sub>4</sub> and S1P<sub>5</sub> receptors at concentrations up to 10 μM. Shows no significant activities in a profiling panel of 55 GPCRs, ion channels and transporters.

**Physical and Chemical Properties:**

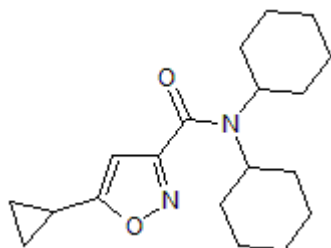
Batch Molecular Formula: C<sub>19</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>

Batch Molecular Weight: 316.44

Physical Appearance: Off-white solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**References:**

Jo *et al* (2012) Novel selective allosteric and bitopic ligands for the S1P<sub>3</sub> receptor. *ACS Chem.Biol.* **7** 1975. PMID: 22971058.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol 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.

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