

## Certificate of Analysis

**Product Name:** CYM 50358 hydrochloride

**Catalog No.:** 4679

**Batch No.:** 1

**IUPAC Name:** *N*-[4-(Aminomethyl)-2,6-dimethylphenyl]-5-(2,5-dichlorophenyl)-2-furancarboxamide hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>18</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>.HCl.¼H<sub>2</sub>O

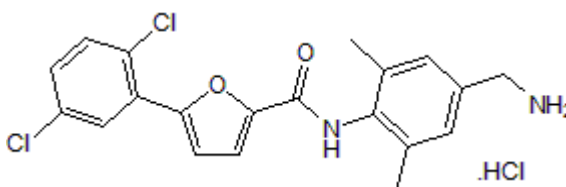
**Batch Molecular Weight:** 430.24

**Physical Appearance:** Off-white solid

**Solubility:** water to 100 mM  
DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.15 (Chloroform:Methanol [9:1])

**HPLC:** Shows >98% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	55.83	4.57	6.51
Found	55.91	4.6	6.49

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**Description:**

Potent S1P<sub>4</sub> antagonist (IC<sub>50</sub> = 25 nM). Displays selectivity for S1P<sub>4</sub> against S1P<sub>1</sub>, S1P<sub>2</sub>, S1P<sub>3</sub> and S1P<sub>5</sub> receptors.

**Physical and Chemical Properties:**

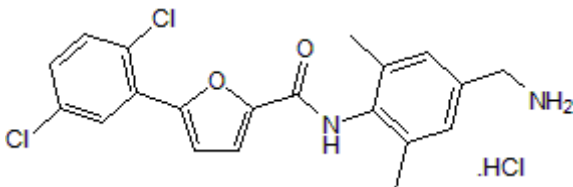
Batch Molecular Formula: C<sub>20</sub>H<sub>18</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>.HCl.¼H<sub>2</sub>O

Batch Molecular Weight: 430.24

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

water to 100 mM  
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:**

**Guerrero *et al*** (2011) Discovery, design and synthesis of the first reported potent and selective sphingosine-1-phosphate 4 (S1P<sub>4</sub>) receptor antagonists. *Bioorg.Med.Chem.Lett.* **21** 3632. PMID: 21570287.

**Cencetti *et al*** (2013) TGFβ1 evokes myoblast apoptotic response via a novel signaling pathway involving S1P4 transactivation upstream of Rho-kinase-2 activation. *FASEB J.* **27** 4532. PMID: 23913862.

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