## a biotechne brand

## Print Date: Jan 14th 2020

## **Certificate of Analysis**

## www.tocris.com

## Product Name: CYM 50358 hydrochloride

Catalog No.: 4679 Bat

Batch No.: 2

CAS Number: IUPAC Name: 1781750-72-8

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

Storage: Batch Molecular Structure: C<sub>20</sub>H<sub>18</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>.HCl.½H<sub>2</sub>O 434.75 Off White solid water to 100 mM DMSO to 100 mM Store at -20°C

NH2 .HCI

## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.1% purity Consistent with structure Consistent with structure

	Carbon Hydrogen Nitroge				
Theoretical	55.25	4.64	6.44		
Found	55.33	4.65	6.5		

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

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### **Description:**

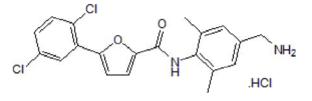
Potent S1P<sub>4</sub> antagonist (IC<sub>50</sub> = 25 nM). Displays selectivity for S1P<sub>4</sub> against S1P<sub>1</sub>, S1P<sub>2</sub>, S1P<sub>3</sub> and S1P<sub>5</sub> receptors.

#### **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{20}H_{18}Cl_2N_2O_2$ .HCl.½H<sub>2</sub>O Batch Molecular Weight: 434.75 Physical Appearance: Off White solid

#### Minimum Purity: ≥97%

#### **Batch Molecular Structure:**



Storage: Store at -20°C

Solubility & Usage Info: water to 100 mM DMSO 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  $45-60^{\circ}C$  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:**

**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.

**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.

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