

Product Name: CYM 5442 hydrochloride

Catalog No.: 3601

Batch No.: 3

CAS Number: 1783987-80-3

IUPAC Name: 2-(4-(5-(3,4-Diethoxyphenyl)-1,2,4-oxadiazol-3-yl)-2,3-dihydro-1H-inden-1-yl amino) ethanol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₇N₃O₄.HCl.½H₂O

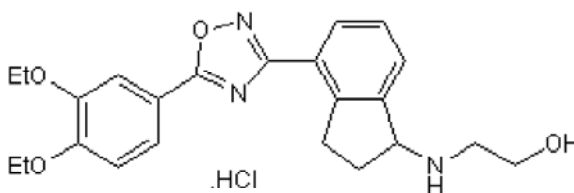
Batch Molecular Weight: 454.95

Physical Appearance: Off-white solid

Solubility: water to 10 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.72	6.42	9.24
Found	60.65	6.59	9.29

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Description:

Potent and selective S1P₁ agonist in vitro (EC₅₀ = 1.35 nM). Activates S1P₁-mediated p42/p44 MAPK phosphorylation in CHO-K1 cells transfected with S1P₁. Induces acute lymphopenia in mice. Brain penetrant.

Physical and Chemical Properties:

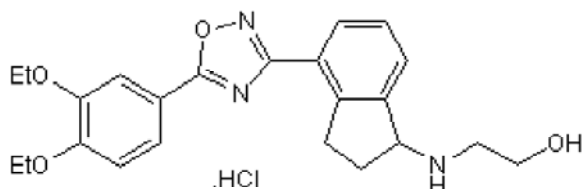
Batch Molecular Formula: C₂₃H₂₇N₃O₄.HCl.½H₂O

Batch Molecular Weight: 454.95

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 10 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°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:

Gonzalez-Cabrera et al (2008) Full pharmacological efficacy of a novel S1P1 agonist that does not require S1P-like headgroup interactions *Mol.Pharmacol.* **74** 1308. PMID: 18708635.

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