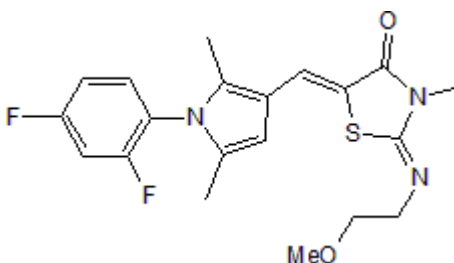


Product Name: CYM 50308 **Catalog No.:** 4678 **Batch No.:** 1
CAS Number: 1345858-76-5
IUPAC Name: (2Z,5Z)-5-[[1-(2,4-Difluorophenyl)-2,5-dimethyl-1*H*-pyrrol-3-yl]methylene]-2-[(2-methoxyethyl)imino]-3-methyl-4-thiazolidinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₁F₂N₃O₂S·½H₂O
Batch Molecular Weight: 409.96
Physical Appearance: Pale brown solid
Solubility: DMSO to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.52 (Ethyl acetate)
HPLC: Shows 98.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.6	5.29	10.25
Found	58.78	5.17	10.07

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

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Description:

Potent and selective sphingosine-1-phosphate receptor 4 (S1P₄) agonist (EC₅₀ values are 56 nM and 2100 nM for S1P₄ and S1P₅ receptors, respectively). Displays no activity at S1P₁, S1P₂ and S1P₃ receptors at concentrations up to 25 μM.

Physical and Chemical Properties:

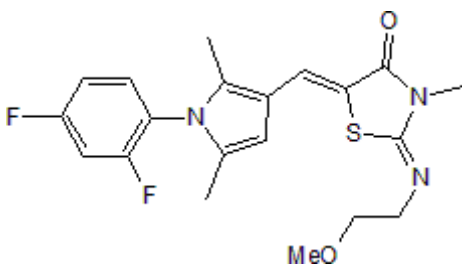
Batch Molecular Formula: C₂₀H₂₁F₂N₃O₂S. ¼H₂O

Batch Molecular Weight: 409.96

Physical Appearance: Pale brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 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:

Urbano *et al* (2011) Discovery, synthesis and SAR analysis of novel selective small molecule S1P₄-R agonists based on a (2Z,5Z)-5-((pyrrol-3-yl)methylene)-3-alkyl-2-(alkylimino)thiazolidin-4-one chemotype. *Bioorg.Med.Chem.Lett.* **21** 6739. PMID: 21982495.

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