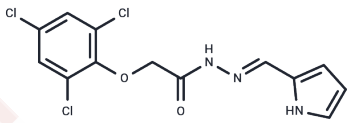
Data Sheet (Cat.No.T4399)

TargetMol

ML239

Chemical Properties



CAS No. : 1378872-36-6

Formula: C13H10Cl3N3O2

Molecular Weight: 346.6

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	ML239 (CID-49843203) is a potent and selective inhibitor of breast cancer stem cells, with an IC50 of 1.16 μM.
Targets(IC50)	Others
In vitro	ML239 (Compound 7j) serves as a powerful and selective inhibitor targeting breast cancer stem cells, exhibiting an IC50 value of 1.16 μM and demonstrating approximately 24-fold greater selectivity compared to the control cell line. It operates primarily by potentially activating fatty acid desaturase 2 (FADS2), thereby inhibiting the growth of breast cancer stem-like cells. Additionally, ML239 shows cytotoxic effects on NCIH661 cells. Interestingly, the reduction of FADS2 activity, either through direct knockdown or by using the FADS2 inhibitor SC-26196, diminishes the cytotoxicity of ML239 in cancer cell lines (CCLs), suggesting a critical role of FADS2 in ML239's mechanism of action.
Kinase Assay	ML239 is dissolved in DMSO.Cancer cell lines (CCLs) are plated at a density of 500 cells/well in white opaque tissue-culture-treated Aurora 1536-well MaKO plates in the provider-recommended growth media using a highly automated platform. Compounds (ML239) are added by acoustic transfer using a Labcyte Echo 555. 24 hours after plating. The effects of small molecules (ML239) are measured over a 16-point concentration range (two-fold dilution) in duplicate. DMSO is used at a constant concentration of 0.33%, including vehicle-only control wells. As a surrogate for viability, cellular ATP levels are assessed 72 hours after compound transfer by addition of CellTiterGlo followed by luminescence measurement using a ViewLux Microplate Imager. Duplicates are averaged and luminescence values normalized to vehicle (DMSO) treatment and background (media-only) wells

Solubility Information

Solubility	DMSO: 50 mg/mL (144.26 mM),Sonication is recommended. Ethanol: 50 mM,Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 2.5 mg/mL (7.21 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may*

In vivo Formulation	*vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.8852 mL	14.4259 mL	28.8517 mL
5 mM	0.577 mL	2.8852 mL	5.7703 mL
10 mM	0.2885 mL	1.4426 mL	2.8852 mL
50 mM	0.0577 mL	0.2885 mL	0.577 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Germain AR,etal.Identification of a selective small molecule inhibitor of breast cancer stem cells.Bioorg Med Chem Lett. 2012 May 15;22(10):3571-4.
Rees MG,etal.Correlating chemical sensitivity and basal gene expression reveals mechanism of action.Nat Chem Biol. 2016 Feb;12(2):109-16.