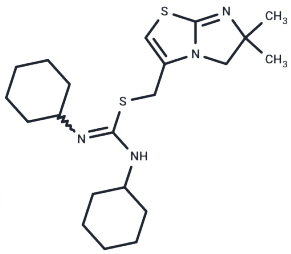
Data Sheet (Cat.No.T11693)

TargetMol

IT1t

Chemical Properties



CAS No. : 864677-55-4

Formula: C21H34N4S2

Molecular Weight: 406.65

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	IT1t inhibits CXCL12/CXCR4 interaction with an IC50 of 2.1 nM. is a potent CXCR4 antagonist.
Targets(IC50)	Others,HIV Protease,CXCR
In vitro	IT1t, a drug-like isothiourea derivative, exhibits potent, dose-dependent inhibition of the CXCL12/CXCR4 interaction, boasting an IC50 value of 2.1 nM, and similarly impedes calcium flux with an IC50 of 23.1 nM. Notably, IT1t demonstrates strong electron density within the binding cavity of the CXCR4 homodimer's both subunits. Its binding mode in CXCR4 dimers reveals interactions solely on the extracellular sides of helices V and VI, maintaining a minimal 4 Å gap between the intracellular regions, likely occupied by lipids. Both IT1t and the CVX15 peptide act as competitive inhibitors against CXCL12, sharing several crucial receptor-ligand contacts for CXCL12 binding, such as Asp187, Glu288 (7.39), and Asp972 (2.63), suggesting these areas as essential for binding. IT1t's interaction site indicates a significant anchor point within this domain. CXCR4 plays a critical role in chemotaxis, functions as a coreceptor for T-tropic HIV-1 entry, and is implicated in cancer metastasis.
In vivo	IT1t effectively diminishes the development of early metastases in triple-negative breast cancer (TNBC) within the zebrafish xenograft model. Similarly, targeting CXCR4 to silence its expression markedly reduces tumor cell invasion at the metastatic site, akin to the results observed with the antagonist IT1t.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4591 mL	12.2956 mL	24.5912 mL
5 mM	0.4918 mL	2.4591 mL	4.9182 mL
10 mM	0.2459 mL	1.2296 mL	2.4591 mL
50 mM	0.0492 mL	0.2459 mL	0.4918 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

Van Hout A, et al. Comparison of cell-based assays for the identification and evaluation of competitive CXCR4 inhibitors. PLoS One. 2017 Apr 14;12(4):e0176057.
Wu B, et al. Structures of the CXCR4 chemokine GPCR with small-molecule and cyclic peptide antagonists. Science. 2010 Nov 19;330(6007):1066-71.
Tulotta C, et al. Inhibition of signaling between human CXCR4 and zebrafish ligands by the small molecule IT1timpairs the formation of triple-negative breast cancer early metastases in a zebrafish xenograft model. Dis Model Mech. 2016 Feb;9(2):141-53.