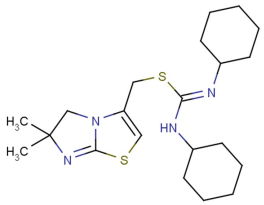
Data Sheet (Cat.No.T11693)

TargetMol
A DRUG SCREENING EXPERT

IT1t

Chemical Properties



CAS No.:	864677-55-4
Formula:	C21H34N4S2
Molecular Weight:	406.65
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	IT1t inhibits CXCL12/CXCR4 interaction with an IC50 of 2.1 nM. is a potent CXCR4 antagonist.
Targets(IC_{50})	CXCL12/CXCR4: 2.1 nM HIV-1 (X4): 19 nM (in PBMCs)
In vitro	IT1t is a small, drug-like, isothiourea derivative. IT1t shows very potent and dose-dependent inhibition of the CXCL12/CXCR4 interaction with an IC50 of 2.1 nM. This calcium flux is also inhibited by IT1t with an IC50 of 23.1. Strong electron density is observed for IT1t in the binding cavity of both subunits of the CXCR4 homodimer. In dimers of CXCR4 bound to IT1t, the monomers interact only at the extracellular side of helices V and VI, leaving at least a 4 Å gap between the intracellular regions, which is presumably filled by lipids. The IT1t compound and CVX15 peptide have both been characterized as competitive inhibitors of CXCL12, and many of the receptor-ligand contacts in the co-crystal structures presented are important for CXCL12 binding, including the acidic Asp187, Glu2887.39 and Asp972.63. The binding site of IT1t may point to the major anchor region for this domain. The CXCR4 is involved in chemotaxis and serves as a coreceptor for T-tropic HIV-1 viral entry and in cancer metastasis.
In vivo	IT1t reduces the formation of TNBC early metastases in the zebrafish xenograft model. Tumor cell invasion at the metastatic site is effectively reduced upon CXCR4 silencing , similar to the antagonist IT1t .

Solubility Information

Solubility	< 1 mg/ml refers to the product slightly soluble or insoluble

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.459 mL	12.296 mL	24.591 mL
5 mM	0.492 mL	2.459 mL	4.918 mL
10 mM	0.246 mL	1.23 mL	2.459 mL
50 mM	0.049 mL	0.246 mL	0.492 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. 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.

2. 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.

3. 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.

Inhibitors · Natural Compounds · Compound Libraries

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