Product Data Sheet

Product Name: IT1t
Cat. No.: GC36350

Chemical Properties

Cas. No.	864677-55-4		
SMILES	CC1(C)CN2C(CS/C(NC3CCCCC3)=N\C4CCCCC4)=CSC2=N1		
Formula	$C_{21}H_{34}N_4S_2$	M.Wt	406.65
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	IT1t		

Background

IT1t is a chemokine (C-X-C motif) receptor 4 (CXCR4) antagonist (IC_{50}s = 8 and 11 nM for the human and rat receptors, respectively).[1] It is selective for CXCR4 over human ether-a-go-go-related gene potassium channels (hERG/K_V11.1; IC_{50} = 13,240 nM). IT1t inhibits calcium mobilization induced by chemokine (C-X-C-motif) ligand 12 (CXCL12) in CEM cells (IC_{50} = 1.1 nM) and decreases CXCL12-induced migration of Jurkat cells (IC_{50} = 79.1 nM).[1,2] It inhibits replication of the HIV-1 strain NL4-3 in MT-4 cells and isolated human peripheral blood mononuclear cells (PBMCs) stimulated with phytohemagglutinin (PHA; IC_{50}s = 14.2 and 19 nM, respectively).[2] IT1t (20 ?M) reduces tumor growth in an MDA-MB-231-B zebrafish xenograft model.[3]

1.Thoma, G., Streiff, M.B., Kovarik, J., et al.Orally bioavailable isothioureas block function of the chemokine receptor CXCR4 in vitro and in vivoJ. Med. Chem.51(24)7915-7920(2008) 2.Van Hout, A., D'huys, T., Oeyen, M., et al.Comparison of cell-based assays for the identification and evauation of competitive CXCR4 inhibitorsPLoS One12(4)e0176057(2017) 3.Tulotta, C., Stefanescu, C., Beletkaia, E., et al.Inhibition of

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signaling between human CXCR4 and zebrafish ligands by the small molecule IT1t impairs the formation of triple-negative breast cancer early metastases in a zebrafish xenograft modelDis. Model Mech.9(2)141-153(2016)

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