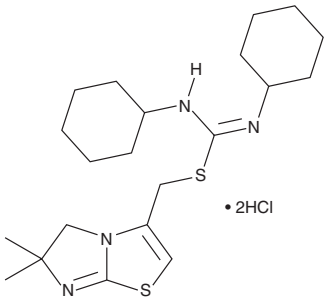
PRODUCT INFORMATION

IT1t (hydrochloride)

Item No. 28434

CAS Registry No.:	1092776-63-0
Formal Name:	N,N′-dicyclohexyl-carbamimidothioic acid, (5,6-dihydro-6,6-dimethylimidazo[2,1-b] thiazol-3-yl)methyl ester, dihydrochloride
MF:	$C_{21}H_{34}N_4S_2$ • 2HCl
FW:	479.6
Purity:	≥95%
UV/Vis.:	λ_{max}: 233 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

IT1t (hydrochloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the IT1t (hydrochloride) in the solvent of choice, which should be purged with an inert gas. IT1t (hydrochloride) is soluble in the organic solvent DMSO.

Description

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 µM) reduces tumor growth in an MDA-MB-231-B zebrafish xenograft model.[3]

References

1. Thoma, G., Streiff, M.B., Kovarik, J., *et al.* Orally bioavailable isothioureas block function of the chemokine receptor CXCR4 in vitro and in vivo. *J. 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 inhibitors. *PLoS One* **12(4)**, e0176057 (2017).
3. Tulotta, C., Stefanescu, C., Beletkaia, E., *et al.* Inhibition of 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 model. *Dis. Model Mech.* **9(2)**, 141-153 (2016).

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