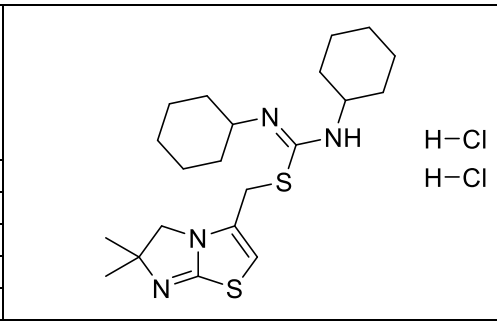
Product data sheet

MedKoo Cat#: 522450 Name: IT1t dihydrochloride CAS: 1092776-63-0 (HCl salt) Chemical Formula: $C_{21}H_{36}Cl_2N_4S_2$ Molecular Weight: 479.567	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

IT1t is a potent and selective CXCR4 antagonist (IC50 = 1.1 nM in calcium mobilization assays). IT1t may be potential useful as anti-HIV agent. The CXC chemokine receptor 4 (CXCR4) is an alpha G-protein coupled chemokine receptor that is widely expressed on most hematopoietic cells, predominantly leukocytes including neutrophils, monocytes, and macrophages.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	17.4	36.28
Water	48.98	102.13

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.09 mL	10.43 mL	20.85 mL
5 mM	0.42 mL	2.09 mL	4.17 mL
10 mM	0.21 mL	1.04 mL	2.09 mL
50 mM	0.04 mL	0.21 mL	0.42 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Ward RJ, Pediani JD, Marsango S, Jolly R, Stoneman MR, Biener G, Handel TM, Raicu V, Milligan G. Chemokine receptor CXCR4 oligomerization is disrupted selectively by the antagonist ligand IT1t. J Biol Chem. 2021 Jan-Jun;296:100139. doi: 10.1074/jbc.RA120.016612. Epub 2020 Dec 6. PMID: 33268380; PMCID: PMC7949023.
2. Smith N, Rodero MP, Bekaddour N, Bondet V, Ruiz-Blanco YB, Harms M, Mayer B, Bader-Meunier B, Quartier P, Bodemer C, Baudouin V, Dieudonné Y, Kirchhoff F, Sanchez Garcia E, Charbit B, Leboulanger N, Jahrsdörfer B, Richard Y, Korganow AS, Münch J, Nisole S, Duffy D, Herbeuval JP. Control of TLR7-mediated type I IFN signaling in pDCs through CXCR4 engagement-A new target for lupus treatment. Sci Adv. 2019 Jul 10;5(7):eaav9019. doi: 10.1126/sciadv.aav9019. PMID: 31309143; PMCID: PMC6620093.

In vivo study

1. Tulotta C, Stefanescu C, Beletkaia E, Bussmann J, Tarbashevich K, Schmidt T, Snaar-Jagalska BE. 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. 2016 Feb;9(2):141-53. doi: 10.1242/dmm.023275. Epub 2016 Jan 7. PMID: 26744352; PMCID: PMC4770151.

7. Bioactivity

Product data sheet

Biological target:

IT1t dihydrochloride is a potent CXCR4 antagonist; inhibits CXCL12/CXCR4 interaction with an IC50 of 2.1 nM.

In vitro activity

Additionally, binding of the CXCR4 antagonist IT1t-a small drug-like isothiourea derivative-rapidly destabilizes the oligomeric structure, whereas AMD3100, another well-characterized CXCR4 antagonist, does not. Although a mutation that regulates constitutive activity of CXCR4 also results in monomerization of the receptor, binding of IT1t to this variant promotes receptor dimerization.

Reference: J Biol Chem. 2021 Jan-Jun;296:100139. https://pubmed.ncbi.nlm.nih.gov/33268380/

In vivo activity

Tumor cell invasion at the metastatic site was effectively reduced upon CXCR4 silencing (Fig. 7B), similar to the antagonist IT1t (Fig. 7C). Therefore, using chemical and genetic approaches, this study demonstrates that CXCR4 signaling inhibition reduces the formation of TNBC early metastases in zebrafish xenograft models and describe IT1t as a potential therapeutic for metastatic TNBC.

Reference: Dis Model Mech. 2016 Feb;9(2):141-53. https://pubmed.ncbi.nlm.nih.gov/26744352/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.