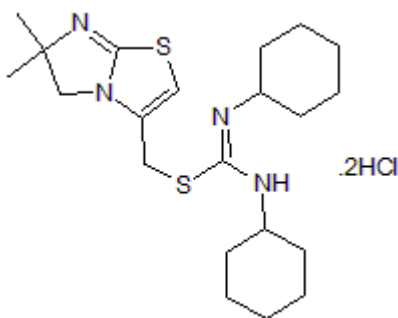


Product Name: IT1t **Catalog No.:** 4596 **Batch No.:** 1
CAS Number: 1092776-63-0
IUPAC Name: *N,N*-Dicyclohexylcarbamimidothioic acid (5,6-dihydro-6,6-dimethylimidazo[2,1-*b*]thiazol-3-yl)methyl ester dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{34}N_4S_2 \cdot 2HCl \cdot \frac{1}{2}H_2O$
Batch Molecular Weight: 488.58
Physical Appearance: Off-white solid
Solubility: DMSO to 10 mM
 ethanol to 100 mM
 water to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.63	7.63	11.47
Found	51.6	7.52	11.36

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

Product Name: IT1t **Catalog No.:** 4596 **Batch No.:** 1
CAS Number: 1092776-63-0
IUPAC Name: *N,N*-Dicyclohexylcarbamidodithioic acid (5,6-dihydro-6,6-dimethylimidazo[2,1-*b*]thiazol-3-yl)methyl ester dihydrochloride

Description:

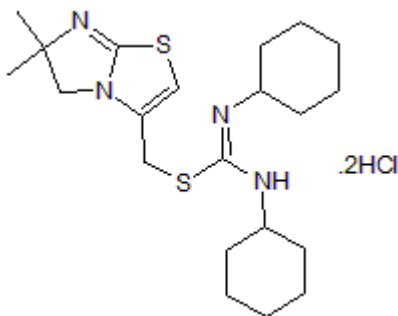
Potent CXCR4 antagonist (IC₅₀ = 1.1 nM in calcium mobilization assays). Orally available. Blocks interaction with the HIV envelope protein, gp120 (IC₅₀ = 7 nM, inhibition of X4-tropic HIV-1IIB attachment).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₃₄N₄S₂·2HCl·½H₂O
 Batch Molecular Weight: 488.58
 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Thoma et al (2008) Orally bioavailable isothioureas block function of the chemokine receptor CXCR4 *in vitro* and *in vivo*. *J.Med.Chem.* **51** 7915. PMID: 19053768.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 mM
 ethanol to 100 mM
 water to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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