

KRH-3955 hydrochloride Biochemical | KRH-3955 biochemical

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CATALOG #
AAA228276

PRODUCT SYNONYMS

KRH-3955 hydrochloride; KRH-3955 biochemical

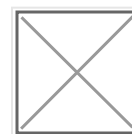
PRODUCT SPECIFICATIONS

Purity/Purification	98%
CAS	2253744-59-9
Targets&IC50	SDF-1alpha-CXCR4:0.61 nM (IC50), X4 HIV-1 NL4-3:0.3-1.0 nM (EC50)
Solubility	<1mg/ml refers to the product slightly soluble or insoluble
In vitro	KRH-3955 (10 mg/kg; a single p.o.) efficiently suppresses X4 HIV-1 infection in hu-PBL-SCID mice[1]. KRH-3955 (10 mg/kg; a single p.o.) exhibits moderate oral bioavailability (25.6%) and C max (86.3 ng/mL)[1]. KRH-3955 (10 mg/kg; a single i.v.) exhibits terminal elimination half-lives (99 h) due to high plasma clearance (3.9 liters/h/kg) combined with large volumes of distribution (374 liters/kg)[1]. Animal Model: C.B-17 SCID mice engrafted with human PBMCs and injected with infectious X4 HIV-1 (NL4-3)[1]. Dosage: 10 mg/kg. Administration: A single p.o. administration. Result: Four of five mock-treated mice were infected whereas only one of five mice treated with KRH-3955 was infected. Animal Model: Male Sprague-Dawley rats[1]. Dosage: 10 mg/kg (Pharmacokinetic Analysis). Administration: A single p.o. or i.v. administration. Result: Well absorbed and the absolute oral bioavailability in rats was calculated to be 25.6%. The half time (T 1/2) of 99.0+/-13.1 h. Stable in human hepatic microsomes, and no significant inhibition of CYP450 liver enzymes by this compound was observed.
Preparation and Storage	Powder: -20 degree C for 3 years In solvent: -80 degree C for 2 years

IMAGES



Structure
PDE2A-IN-1, CAS 2648290-28-0



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ADDITIONAL INFORMATION

Related Product Information for KRH-3955 biochemical	KRH-3955 hydrochloride is an orally bioavailable CXCR4 antagonist. KRH-3955 hydrochloride inhibits SDF-1alpha binding to CXCR4 with an IC 50 of 0.61 nM. KRH-3955 hydrochloride is also a highly potent and selective inhibitor of X4 HIV-1, with an EC 50 of 0.3 to 1.0 nM.
References	1. Tresadern G, et al. [1,2,4]Triazolo[1,5-a]pyrimidine Phosphodiesterase 2A Inhibitors: Structure and Free-Energy Perturbation-Guided Exploration. J Med Chem. 2020 Nov 12;63(21):12887-12910.

For Research Use Only. Not for use in diagnostic or therapeutic procedures. Small volumes of product may become entrapped in the seal of the vial during shipment and storage; if necessary, briefly centrifuge the vial on a tabletop centrifuge to dislodge any liquid in the cap.