

Product Data Sheet

Product Name: ITI214 free base

Cat. No.: GC30841

Chemical Properties

Cas. No. 1160521-50-5

SMILES O=C(C1=C(NC2=CC=CC=C2)N(CC3=CC=C(C4=NC(F)=CC=C4)C=C3)N=C1N56)N(C)C5=N[C@@]7([H])[C@]6([H])CCC7

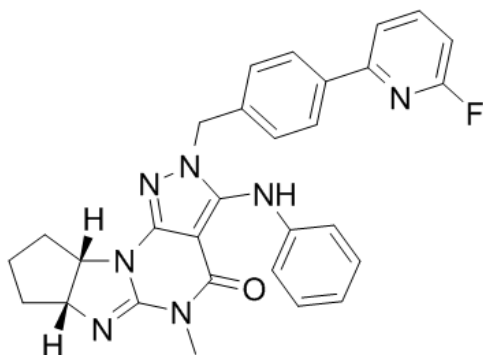
Formula $C_{29}H_{26}FN_7O$ M.Wt 507.56

Solubility Soluble in DMSO Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C 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



Background

ITI-214 (free base) is a picomolar PDE1 inhibitor with excellent selectivity against other PDE family

Caution: Product has not been fully validated for medical applications. For research use only.

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members and against a panel of enzymes, receptors, transporters, and ion channels, exhibits potent PDE1 inhibitory activity ($K_i = 58$ pM). IC₅₀ value: 58 pM (K_i) Target: PDE1 in vitro: ITI-214 exhibits picomolar inhibitory potency for PDE1, demonstrates excellent selectivity against all other PDE families. ITI214 exhibits excellent selectivity over other PDE family members. For instance, the K_i values of ITI214 against recombinant full-length human PDE1A, PDE1B, and PDE1C are 33 pM, 380 pM, and 35 pM, respectively. ITI214 is profiled in a panel of enzymes, receptors, transporters, and ion channels from Caliper at 10 μ M, which is over 170000 times higher than its K_i for PDE1, and demonstrates good selectivity. [1] in vivo: ITI214 possesses a good overall profile with balanced physicochemical properties, excellent potency and selectivity, and good pharmacokinetics. ITI214 is found to significantly enhance memory performance in the test with a minimum effective dose of 3 mg/kg. [1]

[1]. Li P, et al. Discovery of Potent and Selective Inhibitors of Phosphodiesterase 1 for the Treatment of Cognitive Impairment Associated with Neurodegenerative and Neuropsychiatric Diseases. J Med Chem. 2016 Feb 11;59(3):1149-64. [2]. Lawrence Wennogle. Novel uses. From PCT Int. Appl. (2014), WO 2014145617 A2 20140918. [3]. Peng Li, et al. Salt crystals. From PCT Int. Appl. (2013), WO 2013192556 A2 20131227. [4]. Allen A. Fienberg, et al. Organic compounds. From PCT Int. Appl. (2010), WO 2010132127 A1 20101118.

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