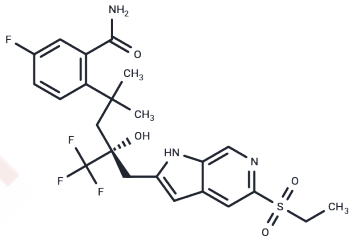
Data Sheet (Cat.No.T10535)

TargetMol

BI 653048

Chemical Properties



CAS No. : 1198784-72-3

Formula: C23H25F4N3O4S

Molecular Weight: 515.52

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	BI 653048 is a selective, orally active nonsteroidal glucocorticoid agonist (IC50: 55 nM) and an HCV NS3 protease inhibitor.
Targets(IC50)	Glucocorticoid Receptor,HCV Protease,Cytochromes P450
In vitro	BI 653048 exhibits improved drug-like properties, inhibits CP1A2, CYP2D6, CYP2C9, CYP2C19, and CYP3A4 (IC50s: 50 μM, 41 μM, 12 μM, 9 μM, and 8 μM). BI 653048 reduces affinity for the hERG ion channel with an IC50>30 μM in recombinant HEK293 cells expressing the human ERG potassium channel. BI 653048 inhibits TNF-stimulated IL-6 production in mouse RAW cells (IC50: 100 nM) [2].
In vivo	BI 653048 (p.o.; 3, 10, and 30 mg/kg) at 3 mg/kg has nonsignificant decreases for all measured histology parameters (ankle inflammation, cartilage damage, pannus formation, and bone resorption), Mid-dose (10 mg/kg) treatment significantly decreases pannus and bone resorption (33%) as well as summed scores (27%), while at high dose (30 mg/kg), all parameters are significantly decreased (87–96%). The ED50 value for the summed scores is 14 mg/kg [2].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.9398 mL	9.6989 mL	19.3979 mL
5 mM	0.388 mL	1.9398 mL	3.8796 mL
10 mM	0.194 mL	0.9699 mL	1.9398 mL
50 mM	0.0388 mL	0.194 mL	0.388 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Reeves JT, et al. Development of a large scale asymmetric synthesis of the glucocorticoid agonist BI 653048 BS H3PO4.J Org Chem. 2013 Apr 19;78(8):3616-35.
Harcken C, et al. Optimization of drug-like properties of nonsteroidal glucocorticoid mimetics and identification of a clinical candidate.ACS Med Chem Lett. 2014 Nov 20;5(12):1318-23.
Montse Llinas-Brunet, et al. Latest bibliographic data on file with the International Bureau

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481