

BI 653048

Chemical Properties

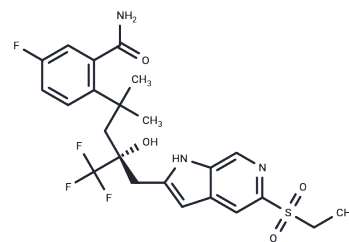
CAS No. : 1198784-72-3

Formula: C₂₃H₂₅F₄N₃O₄S

Molecular Weight: 515.52

Appearance: no data available

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year



Biological Description

Description	BI 653048 is a selective and orally active agonist of nonsteroidal glucocorticoid (IC ₅₀ : 55 nM). BI 653048 is also an HCV NS3 protease inhibitor.
Targets(IC ₅₀)	P450
In vitro	BI 653048 exhibits improved drug-like properties, inhibits CP1A2, CYP2D6, CYP2C9, CYP2C19, and CYP3A4 (IC ₅₀ s: 50 μM, 41 μM, 12 μM, 9 μM, and 8 μM). BI 653048 reduces affinity for the hERG ion channel with an IC ₅₀ >30 μM in recombinant HEK293 cells expressing the human ERG potassium channel. BI 653048 inhibits TNF-stimulated IL-6 production in mouse RAW cells (IC ₅₀ : 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 ED ₅₀ 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.

Reference

Reeves JT, et al. Development of a large scale asymmetric synthesis of the glucocorticoid agonist BI 653048 BS H3P04.J Org Chem. 2013 Apr 19;78(8):3616-35.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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