

Product Data Sheet

Product Name: BI 653048

Cat. No.: GC65345

Chemical Properties

Cas. No. 1198784-72-3

Formula C₂₃H₂₅F₄N₃O₄S

M.Wt 515.52

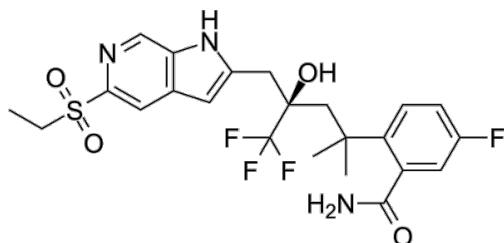
Solubility DMSO : 100 mg/mL (193.98 mM;
Need ultrasonic)

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



Protocol

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

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CYP1A2 CYP2D6 CYP2C9 CYP2C19 CYP3A4

50 μ M(IC₅₀) 41 μ M(IC₅₀) 12 μ M(IC₅₀) 9 μ M(IC₅₀) 8 μ M(IC₅₀)

Background

BI 653048 is a selective and orally active nonsteroidal glucocorticoid (GC) agonist with an IC₅₀ value of 55 nM[1]. BI 653048 inhibits CYP1A2, CYP2D6, CYP2C9, CYP2C19 and CYP3A4 isoforms' activity and reduces affinity for the hERG ion channel (IC₅₀>30 μ M)[2]. BI 653048 is extracted from patent WO2005028501A1 (Compound 103), is also a HCV NS3 protease inhibitor that can reduce viral loads infected with the hepatitis C virus[3].

BI 653048 exhibits an improved drug-like properties, inhibits CYP1A2, CYP2D6, CYP2C9, CYP2C19 and CYP3A4 with IC₅₀ values of 50 μ M, 41 μ M, 12 μ M, 9 μ M, and 8 μ M, respectively[2].

BI 653048 reduces affinity for the hERG ion channel with an IC₅₀>30 μ M in recombinant HEK293 cells expressing the human ERG potassium channel[2].

BI 653048 inhibits TNF-stimulated IL-6 production in mouse RAW cells with an IC₅₀ value of 100 nM[2].

BI 653048 (oral administration; 3, 10, and 30 mg/kg) at 3 mg/kg has nonsignificant decreases for all measured histology parameters (ankle inflammation, pannus formation, cartilage damage, 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].

[1]. 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.

[2]. 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.

[3]. Montse Llinas-Brunet, et al. Latest bibliographic data on file with the International Bureau

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