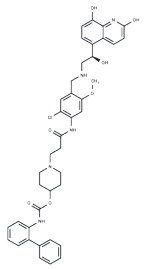
Data Sheet (Cat.No.T7079)

TargetMol

Batefenterol

Chemical Properties



CAS No. : 743461-65-6

Formula: C40H42ClN5O7

Molecular Weight: 740.24

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	Batefenterol (TD-5959) (GSK961081, TD-5959) is a muscarinic receptor antagonist and β2-adrenoceptor agonist. It displays high affinity for hM2, hM3 muscarinic and hβ2-adrenoceptor (Ki:1.4/1.3/3.7 nM).
Targets(IC50)	Adrenergic Receptor,AChR
In vitro	In competition radioligand binding studies at human recombinant receptors, Batefenterol displays high affinity for hM2 (Ki; 1.4 nM), hM3 muscarinic receptors (Ki: 1.3 nM) and hβ2-adrenoceptors (Ki: 3.7 nM). Batefenterol behaves as a potent hβ2-adrenoceptor agonist (EC50: 0.29 nM for stimulation of cAMP levels) with 440- and 320-fold functional selectivity over hβ1- and hβ3-adrenoceptors, respectively [1].
In vivo	In the guinea pig broncho-protection assay, inhaled Batefenterol produces potent, dose-dependent inhibition of bronchoconstrictor responses via MA (ED50: 33.9 μg/mL), BA (ED50: 14.1 μg/mL), and MABA (ED50: 6.4 μg/mL) mechanisms. Significant bronchoprotective effects of Batefenterol are evident in guinea pigs via MA, BA, and MABA mechanisms for up to 7 days after dosing[1]. In guinea pig isolated trachea expressing native muscarinic M3 and β2, Batefenterol produces smooth muscle relaxation through a dual mechanism involving competitive antagonism of the M3 receptor (EC50: 50 nM) and agonism of the β2 receptor (EC50: 25 nM). The combined effect on both muscarinic receptors and β2 receptors is more potent than either function working alone (EC50: 10 nM) [2].

Solubility Information

Solubility	DMSO: 28.82 mg/mL (38.93 mM),Sonication is recommended. H2O: < 0.1 mg/mL (insoluble), (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (5.4 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.3509 mL	6.7546 mL	13.5091 mL
5 mM	0.2702 mL	1.3509 mL	2.7018 mL
10 mM	0.1351 mL	0.6755 mL	1.3509 mL
50 mM	0.027 mL	0.1351 mL	0.2702 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

Hegde SS, et al. Pharmacologic characterization of GSK-961081 (TD-5959), a first-in-class inhaled bifunctional bronchodilator possessing muscarinic receptor antagonist and β2-adrenoceptor agonist properties. J Pharmacol Exp Ther. 2014 Oct;351(1):190-9.

Machine learning-enabled virtual screening indicates the anti-tuberculosis activity of aldoxorubicin and quarfloxin with verification by molecular docking, molecular dynamics simulations, and biological evaluations

Hughes AD, et al. Discovery of (R)-1-(3-((2-chloro-4-(((2-hydroxy-2-(8-hydroxy-2-oxo-1,2-dihydroquinolin-5-yl) ethyl)amino)methyl)-5-methoxyphenyl)amino)-3-oxopropyl)piperidin-4-yl [1,1'-biphenyl]-2-ylcarbamate (TD-5959, GSK961081, batefenterol): first-in-class dual pharmacology multivalent muscarinic antagonist and β_2 agonist (MABA) for the treatment of chronic obstructive pulmonary disease (COPD). J Med Chem. 2015 Mar 26;58 (6):2609-22.