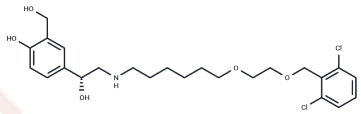
Data Sheet (Cat.No.T2645)

TargetMol

Vilanterol

Chemical Properties



CAS No. : 503068-34-6

Formula: C24H33Cl2NO5

Molecular Weight: 486.43

Storage: Keep away from moisture
Pure form: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Vilanterol is a selective long-acting beta2-adrenergic agonist (LABA) used in the treatment of COPD and asthma.
Targets(IC50)	Adrenergic Receptor
In vitro	The selectivity of Vilanterol for β2-AR over other β-AR receptor subtypes (β2 and β3) is demonstrated through its ability to elicit concentration-dependent increases in cAMP in CHO cells expressing human β1-, β2-, and β3-AR. Vilanterol shows high selectivity for β2-AR with at least a 1000-fold preference over β2- and β3-AR subtypes. This analysis yields a low-affinity pKD for [3H]Vilanterol of 9.44±0.07 (n=4) in the presence of Gpp(NH)p and a high-affinity pKD of 10.82±0.12 (n=4) and a low-affinity pKD of 9.47±0.17 (n=4) in the absence of Gpp(NH)p. Additionally, a low-affinity pKD of 9.52±0.24 (n=4) is observed for [3H]Vilanterol in the absence of Gpp(NH)p at 37°C. Vilanterol trifenatate is a novel inhaled long-acting β2-agonist with 24-hour activity in vitro, developed in combination with the inhaled corticosteroid fluticasone furoate for the treatment of both COPD and asthma. Vilanterol is a novel long-acting β2-agonist (LABA) with 24-hour activity, intended for once-daily clinical treatment of COPD and asthma in combination with the 24-hour active corticosteroid fluticasone furoate.
Kinase Assay	Saturation, association, and dissociation binding studies are performed for [3H] Vilanterol to determine receptor binding kinetics at the β2-AR (equilibrium dissociation constant (KD), total number of receptors (Bmax), association rate (kon), and dissociation rate (koff) are calculated). For saturation binding, membranes (in a volume of 1.4 mL to avoid ligand depletion) are incubated with increasing concentrations of [3H]Vilanterol (~0.01-1.3 nM) for 5 h before filtration. For association binding, membranes are incubated with different concentrations of [3H]Vilanterol (~0.1-1.9 nM) for varying incubation times up to 1 h before filtration. For dissociation binding, membranes are preincubated for 1 h with a fixed concentration of [3H]Vilanterol (~1.1 nM) before dissociation is initiated by a 1:20 dilution in binding buffer (containing 10 μM cold Vilanterol) and then incubated for varying times up to 8 h before filtration. Saturation binding is also completed for [3H]CGP12177 (increasing concentrations of ~0.01-2.8 nM) in the same format as described above for [3H]Vilanterol. To determine the affinity of β2-AR agonists and antagonists, competition binding displacement studies are completed in which membranes are incubated with a fixed concentration of [3H]

Kinase Assay	Vilanterol (~0.2 nM) and increasing concentrations of unlabeled agonist/antagonist for 5 h before filtration. All competition binding displacement studies are completed in the presence of 100 μM Gpp(NH)p to ensure that binding curves are monophasic[1].

Solubility Information

Solubility	DMSO: 50 mg/mL (102.79 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (4.11 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	2.0558 mL	10.279 mL	20.5579 mL
5 mM	0.4112 mL	2.0558 mL	4.1116 mL
10 mM	0.2056 mL	1.0279 mL	2.0558 mL
50 mM	0.0411 mL	0.2056 mL	0.4112 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

Kempsford R, et al. Vilanterol trifenatate, a novel inhaled long-acting beta2 adrenoceptor agonist, is well tolerated in healthy subjects and demonstrates prolonged bronchodilation in subjects with asthma and COPD. Pulm Pharmacol Ther. 2013 Apr;26(2):256-

Harrell A W , Siederer S K , Bal J , et al. Metabolism and Disposition of Vilanterol, a Long-Acting 2-Adrenoceptor Agonist for Inhalation Use in Humans[J]. Drug Metabolism and Disposition, 2013, 41(1):89-100.