Product Data Sheet

Product Name: Vilanterol
Cat. No.: GC13747

Chemical Properties

Cas. No.	503068-34-6		
Chemical Name	4-[(1R)-2-[6-[2-[(2,6-dichlorophenyl)methoxy]ethoxy]hexylamino]-1-hydroxyethyl]-2-(hydroxymethyl)phenol		
SMILES	C1=CC(=C(C(=C1)Cl)COCCOCCCCCCNCC(C2=CC(=C(C=C2)O)CO)O)Cl		
Formula	$C_{24}H_{33}Cl_2NO_5$	M.Wt	486.43
Solubility	DMF: 30 mg/ml,DMSO: 10 mg/ml,Ethanol: 30 mg/ml	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	Vilanterol		

Protocol

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Kinase experiment:

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]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].

References:

[1]. Slack RJ, et al. In vitro pharmacological characterization of vilanterol, a novel long-acting β2-

adrenoceptor agonist with 24-hour duration of action. J Pharmacol Exp Ther. 2013 Jan;344(1):218-30
[2]. Calzetta L, et al. Pharmacological characterization of the interaction between umeclidinium and vilanterol in human bronchi. Eur J Pharmacol. 2017 Jul 14. pii: S0014-2999(17)30470-3.
[3]. 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-
[4]. Harrell AW, et al. Metabolism and disposition of Vilanterol, a long-acting β(2)-adrenoceptor agonist for inhalation use in humans. Drug Metab Dispos. 2013 Jan;41(1):89-100.

Background

Vilanterol is a novel and selective agonist of β2-AR with a PEC50 value of 10.37±0.05 [1].

Vilanterol is a novel long-acting β2-AR agonist (LABA) with 24h activity in development for inhaled once daily treatment. In the radioligand binding studies, Vilanterol has shown the binding affinity in the one-affinity site model with pKD values of 9.44±0.07 and 10.82±0.12 in the presence Gpp(NH)p and absence Gpp(NH)p, respectively. In dissociation studies, Vilanterol has been reported to bind from the β2-AR with a dissociation t1/2 value of 3.5 min in the presence of Gpp(NH)p. Vilanterol has been

found to have a good selectivity for β2-AR over the other β-AR receptor subtypes(β1and β3) with pEC50 values of 10.37±0.05, 6.98±0.03 and 7.36±0.03, respectively. Vilanterol has exhibited at least 1000-fold selectivity over both β1-and β3-AR subtypes [1].

References:

[1] Slack RJ1, Barrett VJ, Morrison VS, Sturton RG, Emmons AJ, Ford AJ, Knowles RG.In vitro pharmacological characterization of vilanterol, a novel long-acting β2-adrenoceptor agonist with 24-hour duration of action.J Pharmacol Exp Ther. 2013 Jan; 344(1):218-30.