

Crisaborole

Chemical Properties

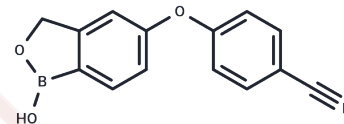
CAS No. : 906673-24-3

Formula: C₁₄H₁₀BN₃O

Molecular Weight: 251.05

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	Crisaborole (AN-2728) is a phosphodiesterase 4 inhibitor.
Targets(IC50)	PDE
In vitro	AN-2728 inhibits PDE isozymes PDE1A3, PDE3Cat, PDE4Cat and PDE7A1 with IC50 values of 6.1, 6.4, 0.11 and 0.73 μM. AN-2728 inhibits PDE4, TNF-α, IL-2, IFN-γ, IL-5 and IL-10 with IC50 values of 0.49, 0.54, 0.61, 0.83, 2.4 and 5.3 μM. AN-2728 shows the most potent activity against PDE4 catalytic domain, but it also shows inhibition against PDE1A3, PDE3Cat, and PDE7A1. Crystallography reveals that interaction of benzoxaboroles with the hydrophobic pocket in the PDE4 catalytic domain increase their affinity for PDE4. These benzoxaboroles strongly suppresses the secretion of cytokines associated with Ps and AD.
In vivo	AN-2728 is well tolerated and significantly impacts efficacy markers, showing comparable results to positive controls in clinical trials. It effectively inhibits ear edema induced by phorbol ester with a dosing of 1 mg/earx2 (78% and 68%, respectively), mirroring the efficacy of dexamethasone. This suggests AN-2728 possesses notable anti-inflammatory properties and skin penetration capabilities.

Solubility Information

Solubility	DMSO: 250 mg/mL (995.82 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 (7.97 mM),Sonication is recommended. <i>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.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.9833 mL	19.9164 mL	39.8327 mL
5 mM	0.7967 mL	3.9833 mL	7.9665 mL
10 mM	0.3983 mL	1.9916 mL	3.9833 mL
50 mM	0.0797 mL	0.3983 mL	0.7967 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

Akama T, et al. Discovery and structure-activity study of a novel benzoxaborole anti-inflammatory agent (AN2728) for the potential topical treatment of psoriasis and atopic dermatitis. *Bioorg Med Chem Lett*. 2009 Apr 15;19(8): 2129-32.

Nazarian R, et al. AN-2728, a PDE4 inhibitor for the potential topical treatment of psoriasis and atopic dermatitis. *Curr Opin Investig Drugs*. 2009 Nov;10(11):1236-42.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

This product is for Research Use Only · Not for Human or Veterinary or Therapeutic Use

Tel:781-999-4286 E_mail:info@targetmol.com Address:34 Washington Street,Wellesley Hills,MA 02481