Crisaborole

Cat. No.: HY-10978

CAS No.: 906673-24-3

Molecular Formula: $C_{14}H_{10}BNO_3$

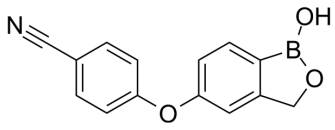
Molecular Weight: 251.05

Target: Phosphodiesterase (PDE)

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (398.33 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (9.96 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (9.96 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (9.96 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Crisaborole (AN-2728) is a potent inhibitor of PDE4 and cytokine release; inhibit PDE4 with an IC_{50} of 0.49 μM.

IC_{50} & Target

PDE4

In Vitro

Crisaborole (AN-2728) inhibits PDE4, TNF-α, IL-2, IFN-γ, IL-5 and IL-10 with IC_{50} values of 0.49, 0.54, 0.61, 0.83, 2.4 and 5.3 μM. Crisaborole (AN-2728) shows the most potent activity against PDE4 catalytic domain, but it also shows inhibition against

	PDE1A3, PDE3Cat, and PDE7A1. Crisaborole (AN-2728) inhibits PDE isozymes PDE1A3, PDE3Cat , PDE4Cat and PDE7A1 with IC_{50} values of 6.1, 6.4, 0.11 and 0.73 μM[1]. 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[2]. Crisaborole (AN-2728) is a topically administered, boron-containing, anti-inflammatory compound that inhibits PDE4 activity and thereby suppresses the release of TNFalpha, IL-12, IL-23 and other cytokines[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Crisaborole (AN-2728) shows significant inhibition against the ear edema caused by phorbol ester after dosing at 1 mg/ear×2 (78% and 68%, respectively). The efficacy is comparable to that of dexamethasone, suggesting that Crisaborole (AN-2728) has good anti-inflammatory activity as well as skin penetration[1]. Crisaborole (AN-2728) is reported to be well tolerated and to demonstrate significant effects on markers of efficacy, with results that are comparable to positive controls in clinical trials[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Int J Pharm. 2022 Feb 21;121610.
- Front Pharmacol. 22 June 2022.
- Eur J Pharmacol. 2021 Jun 14;174258.

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REFERENCES

[1]. 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.

[2]. 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.

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