AN-2728

Cat. No.: HY-10978
CAS No.: 906673-24-3
Molecular Formula: $\text{C}_{14}\text{H}_{10}\text{BNO}_3$
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 6 months, -20°C 1 month

Solvent & Solubility

In Vitro

DMSO : ≥ 32 mg/mL (127.46 mM)
* “≥” means soluble, but saturation unknown.

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>Mass 1 mg</th>
<th>Mass 5 mg</th>
<th>Mass 10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td>3.9833 mL</td>
<td>19.9164 mL</td>
<td>39.8327 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.7967 mL</td>
<td>3.9833 mL</td>
<td>7.9665 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.3983 mL</td>
<td>1.9916 mL</td>
<td>3.9833 mL</td>
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Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description
AN-2728 is a potent inhibitor of PDE4 and cytokine release; inhibit PDE4 with an IC$_{50}$ of 0.49 μM.

IC$_{50}$ & Target
IC$_{50}$: 0.49 μM (PDE4)$[1]$

In Vitro
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. AN-2728 shows the most potent activity against PDE4 catalytic domain, but it also shows inhibition against PDE1A3, PDE3Cat, and PDE7A1. 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$[2]$. 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$[3]$. 

[1] Crystallography reveal 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] 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] 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. AN-2728 shows the most potent activity against PDE4 catalytic domain, but it also shows inhibition against PDE1A3, PDE3Cat, and PDE7A1. 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.
<table>
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<th>In Vivo</th>
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<tbody>
<tr>
<td>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 AN-2728 has good anti-inflammatory activity as well as skin penetration[1]. AN-2728 is reported to be well tolerated and to demonstrate significant effects on markers of efficacy, with results that were comparable to positive controls in clinical trials[3].</td>
</tr>
</tbody>
</table>

**REFERENCES**


**Caution: Product has not been fully validated for medical applications. For research use only.**

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