NCT-501

Cat. No.: HY-18768
CAS No.: 1802088-50-1
Molecular Formula: C₂₁H₃₂N₆O₃
Molecular Weight: 416.52
Target: Aldehyde Dehydrogenase (ALDH)
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 : ≥ 28 mg/mL (67.22 mM)
* "≥" means soluble, but saturation unknown.

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 mM</td>
<td></td>
<td>2.4008 mL</td>
<td>12.0042 mL</td>
<td>24.0085 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td></td>
<td>0.4802 mL</td>
<td>2.4008 mL</td>
<td>4.8017 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td></td>
<td>0.2401 mL</td>
<td>1.2004 mL</td>
<td>2.4008 mL</td>
</tr>
</tbody>
</table>

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
NCT-501 is a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1), inhibits hALDH1A1 with IC₅₀ of 40 nM, typically shows better selectivity over other ALDH isozymes and other dehydrogenases (hALDH1B1, hALDH3A1, and hALDH2, IC₅₀ >57 μM).

IC₅₀ & Target
IC₅₀: 40 nM (hALDH1A1)[2]

In Vitro
NCT-501 shows a 16% decrease in the Cal-27 CisR cell line at 20 nM concentration, though the difference was not statistically significant[1].
In Vivo

NCT-501 (100 µg/animal; i.t.; every alternate day for 20 days) shows a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts[1].

<table>
<thead>
<tr>
<th>Animal Model:</th>
<th>5-6 weeks old male Hsd: Athymic Nude-Foxn1nu (immuno-deficient-mice bearing Cal-27 CisR cells)[1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dosage:</td>
<td>100 µg/animal</td>
</tr>
<tr>
<td>Administration:</td>
<td>Intra-tumorally (i.t); every alternate day for 20 days</td>
</tr>
<tr>
<td>Result:</td>
<td>Showed a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts.</td>
</tr>
</tbody>
</table>

CUSTOMER VALIDATION

- Mol Cancer Ther. 2019 Sep 18. pii: molcanther.0242.2019

See more customer validations on www.MedChemExpress.com

REFERENCES
