Tubacin

Cat. No.: HY-13428
CAS No.: 537049-40-4
Molecular Formula: C₄₁H₄₃N₃O₇S
Molecular Weight: 721.86
Target: HDAC; Virus Protease
Pathway: Cell Cycle/DNA Damage; Epigenetics; Anti-infection
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: ≥ 100 mg/mL (138.53 mM)
H₂O: < 0.1 mg/mL (insoluble)
* “≥” means soluble, but saturation unknown.

Preparing Stock Solutions

<table>
<thead>
<tr>
<th>Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td>1.3853 mL</td>
<td>6.9266 mL</td>
<td>13.8531 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.2771 mL</td>
<td>1.3853 mL</td>
<td>2.7706 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.1385 mL</td>
<td>0.6927 mL</td>
<td>1.3853 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 >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: ≥ 2.5 mg/mL (3.46 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.5 mg/mL (3.46 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
Tubacin is a potent and selective inhibitor of HDAC6, with an IC₅₀ value of 4 nM and approximately 350-fold selectivity over HDAC1.

IC₅₀ & Target

<table>
<thead>
<tr>
<th>IC₅₀ &amp; Target</th>
<th>IC₅₀ &amp; Target</th>
<th>IC₅₀ &amp; Target</th>
<th>IC₅₀ &amp; Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>HDAC6</td>
<td>4 nM (IC₅₀)</td>
<td>HDAC3</td>
<td>1.27 μM (IC₅₀)</td>
</tr>
<tr>
<td>HDAC8</td>
<td>1.27 μM (IC₅₀)</td>
<td>HDAC1</td>
<td>1.40 μM (IC₅₀)</td>
</tr>
<tr>
<td>HDAC5</td>
<td>3.35 μM (IC₅₀)</td>
<td>HDAC10</td>
<td>3.71 μM (IC₅₀)</td>
</tr>
<tr>
<td>HDAC11</td>
<td>3.79 μM (IC₅₀)</td>
<td>HDAC9</td>
<td>4.31 μM (IC₅₀)</td>
</tr>
<tr>
<td>HDAC</td>
<td>IC$_{50}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>--------------</td>
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<td></td>
</tr>
<tr>
<td>HDAC2</td>
<td>6.27 µM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDAC7</td>
<td>9.70 µM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDAC4</td>
<td>17.30 µM</td>
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</tr>
</tbody>
</table>

**In Vitro**

Tubacin preferentially induces α-tubulin hyperacetylation at a concentration of 2.5 µM, and induces α-tubulin acetylation at 5 µM and protects prostate cancer (LNCaP) cells from hydrogen peroxide-induced death at 8 µM via peroxiredoxin acetylation[1]. Tubacin (2.5 and 5 µM) specifically induces acetylation of α-tubulin in MM cells. Tubacin significantly inhibits both drug-sensitive and drug-resistant MM cell growth, with IC$_{50}$ 5-20 µM at 72 h. Tubacin also induces apoptosis by activation of caspases. Moreover, Tubacin inhibits binding of HDAC6 with dynein, and it induces significant accumulation of polyubiquitinated proteins, when combined with bortezomib. Tubacin and bortezomib induce synergistic antitumor activity in MM cell lines, and inhibits paracrine MM Cell Growth. Tubacin (5 µM) synergistically enhances bortezomib-induced cytotoxicity in patient MM cells without cytotoxicity to PBMCs[2]. Tubacin can concentration-dependently inhibits JEV-induced cytopathic effect and apoptosis, as well as reduces virus yield in human cerebellar medulloblastoma cells. The IC$_{50}$ of virus yield is 0.26 µM for Tubacin. Tubacin also meaningfully blocks the production of intracellular infectious virus particles, with an IC$_{50}$ of 1.52 µM. Tubacin induces the hyperacetylation of a HDAC6 substrate Hsp90 and reduces the interaction of Hsp90 with JEV NS5 protein[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**PROTOCOL**

**Cell Assay**[3]

HDAC inhibitors TSA, VPA, tubacin, and TBSA are used in the assay. Cytotoxicity of HDACi to TE671 and BHK-21 cells is evaluated by MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay. 5 × 10$^4$ cells per well are seeded in 96-well plates and then treated with the indicated concentration of each HDACi. After 48-h of treatment, 25 µL of MTT solution (5 mg/mL) is added to each well and incubated at 37 °C with 5% CO2 for 3 h. After three washings with phosphate buffer saline (PBS), 100 µL DMSO is added into each well for dissolving formazan crystals. OD$_{570-630}$ is measured by micro-ELISA reader and survival rate are calculated to indicate suppressive effects of each HDACi on the survival of TE671 and BHK-21 cells. Survival rate (%) = ((Acontrol − Aexperiment)/Acontrol) × 100%. 50% cytotoxic concentration (CC$_{50}$) values are calculated by computer program[3].

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**REFERENCES**

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