EPZ031686

Cat. No.: HY-19324
CAS No.: 2095161-11-6
Molecular Formula: C_{26}H_{34}ClF_3N_4O_4S
Molecular Weight: 591.09
Target: Histone Methyltransferase
Pathway: Epigenetics
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: 35 mg/mL (59.21 mM; ultrasonic and warming and heat to 60°C)

<table>
<thead>
<tr>
<th>Solvent Concentration</th>
<th>Mass 1 mg</th>
<th>Mass 5 mg</th>
<th>Mass 10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td>1.6918 mL</td>
<td>8.4589 mL</td>
<td>16.9179 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.3384 mL</td>
<td>1.6918 mL</td>
<td>3.3836 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.1692 mL</td>
<td>0.8459 mL</td>
<td>1.6918 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: 30% PEG300 >> 70% (20% SBE-β-CD in saline)
   Solubility: 10 mg/mL (16.92 mM); Suspended solution; Need ultrasonic and warming
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

EPZ031686 is an potent and orally active SMYD3 inhibitor and with an IC₅₀ value of 3 nM. EPZ031686 can be used for cancer research[1].

IC₅₀ & Target

SMYD3
3 nM (IC₅₀)
**In Vivo**

EPZ031686 (1-50 mg/mL; p.o. and i.v.; Male CD-1 mice) has good bioavailability following oral dosing in mice\(^1\).

**Pharmacokinetic Analysis in Male CD-1 mice\(^1\)**

<table>
<thead>
<tr>
<th>Route</th>
<th>Dose (mg/kg)</th>
<th>CL (mL/min/kg)</th>
<th>CL(_r) (mL/min/kg)</th>
<th>V(_s) (L/kg)</th>
<th>t(_{max}) (h)</th>
<th>t(_{max}) (h)</th>
<th>C(_{max}) (ng/mL)</th>
<th>AUC(_{last}) (ng·h/mL)</th>
<th>AUC(_{INF,obs}) (ng·h/mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>i.v.</td>
<td>1</td>
<td>27</td>
<td>5.3</td>
<td>2.3</td>
<td>1.7</td>
<td>/</td>
<td>/</td>
<td>603</td>
<td>616</td>
</tr>
<tr>
<td>p.o.</td>
<td>5</td>
<td>/</td>
<td>/</td>
<td>/</td>
<td>2.7/td&gt;</td>
<td>0.89</td>
<td>345</td>
<td>1281</td>
<td>1479</td>
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<tr>
<td>p.o.</td>
<td>50</td>
<td>/</td>
<td>/</td>
<td>/</td>
<td>2.2</td>
<td>1.3</td>
<td>4693</td>
<td>21158</td>
<td>21170</td>
</tr>
</tbody>
</table>

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

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**REFERENCES**