ABX-1431

Cat. No.: HY-117632
CAS No.: 1446817-84-0
Molecular Formula: C₂₀H₂₂F₉N₃O₂
Molecular Weight: 507.39
Target: MAGL
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: 125 mg/mL (246.36 mM; Need ultrasonic)
H₂O: < 0.1 mg/mL (insoluble)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td></td>
<td>1.9709 mL</td>
<td>9.8544 mL</td>
<td>19.7087 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td>0.3942 mL</td>
<td>1.9709 mL</td>
<td>3.9417 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td>0.1971 mL</td>
<td>0.9854 mL</td>
<td>1.9709 mL</td>
</tr>
</tbody>
</table>

Preparation of Stock Solutions

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.10 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.10 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.10 mM); Clear solution

In Vivo
1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.10 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (4.10 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.10 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
ABX-1431 is a highly potent, selective, and orally available, CNS-penetrant monoacylglycerol lipase (MAGL) inhibitor with an IC₅₀ of 14 nM.

IC₅₀ & Target
IC₅₀: 14 nM (human MGLL)[1]
**In Vitro**

ABX-1431 is a potent human MGLL inhibitor (IC\(_{50}\)=0.014 µM) with >100-fold selectivity against ABHD6 and >200-fold selectivity against PLA2G7. ABX-1431 inhibits human PC3 cells with an IC\(_{50}\) of 0.0022 µM. In the cell-based assay, >100-fold selectivity for MGLL over ABHD6 (IC\(_{50}\)=0.253 µM) and PLA2G7 (IC\(_{50}\)=494 µM) is maintained\(^1\).

**In Vivo**

ABX-1431 inhibits MGLL activity in rodent brain (ED\(_{50}\)=0.5-1.4 mg/kg), increases brain 2-AG concentrations, and suppresses pain behavior in the rat formalin pain model\(^1\).

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**PROTOCOL**

**Cell Assay\(^1\)**

Human prostate cancer PC3 cells are grown in F-12K medium supplemented with 10% fetal bovine serum at 37°C with 5% CO\(_2\) to 80% confluency in 100 mm dishes. ABX-1431 is added to cells to give final concentration of 0.1-10 µM compound in serum free media. Cells are incubated for 30 min. Cells are washed, harvested, and lysed by probe sonication. Cell lysates (2mg/mL) are treated with JW912 (1µM) and analyzed by SDS-PAGE and in-gel fluorescence scanning\(^1\).

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

**Animal Administration\(^1\)**

**Rats\(^1\)**

ABX-1431 is administered in a volume of 5 mL/kg. Male ICR mice or male Sprague Dawley rats 6 to 12 weeks are administered single oral doses of ABX-1431 (0.5-32 mg/kg for mice and 0.03-10 mg/kg for rats). Four hours after ABX-1431 administration, animals are anesthetized. Following blood collection, animals are killed by decapitation and brains are removed, hemisected and frozen in liquid nitrogen for analysis\(^1\).

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

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**REFERENCES**