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 for 3 years
  - 4°C for 2 years
- **In solvent**
  - -80°C for 6 months
  - -20°C for 1 month

**SOLVENT & SOLUBILITY**

**In Vitro**

DMSO : 125 mg/mL (246.36 mM; Need ultrasonic)

<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>1.9709 mL</td>
<td>9.8544 mL</td>
<td>19.7087 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td></td>
<td>0.3942 mL</td>
<td>1.9709 mL</td>
<td>3.9417 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td></td>
<td>0.1971 mL</td>
<td>0.9854 mL</td>
<td>1.9709 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: ≥ 2.08 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 (IC₅₀=0.014 µM) with >100-fold selectivity against ABHD6 and >200-fold selectivity against PLA2G7. ABX-1431 inhibits human PC3 cells with an IC₅₀ of 0.0022 µM. In the cell-based assay, >100-fold
selectivity for MGLL over ABHD6 (IC\textsubscript{50}=0.253 µM) and PLA2G7 (IC\textsubscript{50}=494 µM) is maintained\textsuperscript{[1]}. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

| In Vivo | ABX-1431 inhibits MGLL activity in rodent brain (ED\textsubscript{50}=0.5-1.4 mg/kg), increases brain 2-AG concentrations, and suppresses pain behavior in the rat formalin pain model\textsuperscript{[1]}. MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

**PROTOCOL**

**Cell Assay**\textsuperscript{[1]}

Human prostate cancer PC3 cells are grown in F-12K medium supplemented with 10% fetal bovine serum at 37°C with 5% CO\textsubscript{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\textsuperscript{[1]}. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**Animal Administration**\textsuperscript{[1]}

Rats\textsuperscript{[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\textsuperscript{[1]}. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**REFERENCES**