EST64454 hydrochloride

Cat. No.: HY-131914A
CAS No.: 1950569-11-5
Molecular Formula: C₁₈H₂₃ClF₂N₄O₂
Molecular Weight: 400.85
Target: Sigma Receptor
Pathway: GPCR/G Protein; Neuronal Signaling
Storage: Please store the product under the recommended conditions in the Certificate of Analysis.

SOLVENT & SOLUBILITY

**In Vitro**
DMSO: 100 mg/mL (249.47 mM; Need ultrasonic)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<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>2.4947 mL</td>
<td>12.4735 mL</td>
<td>24.9470 mL</td>
<td></td>
</tr>
<tr>
<td>5 mM</td>
<td>0.4989 mL</td>
<td>2.4947 mL</td>
<td>4.9894 mL</td>
<td></td>
</tr>
<tr>
<td>10 mM</td>
<td>0.2495 mL</td>
<td>1.2473 mL</td>
<td>2.4947 mL</td>
<td></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 (6.24 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
Solubility: ≥ 2.5 mg/mL (6.24 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
Solubility: ≥ 2.5 mg/mL (6.24 mM); Clear solution

BIOLOGICAL ACTIVITY

**Description**
EST64454 hydrochloride is a selective and orally active sigma-1 receptor antagonist with a $K_i$ of 22 nM. EST64454 hydrochloride has the potential for the research of the pain[1].

**In Vivo**
EST64454 (10 mg/kg; p.o.; male Wistar rats) treatment shows the $C_{\text{max}}$, $t_{1/2}$, $\text{AUC}_0-\infty$, $V_{SS}$ and F% are 771 ng/mL, 3.4 hours, 1431 ng h/mL, 4.4 l/kg and 69%, respectively[1].
EST64454 (10 mg/kg; p.o.; male CD1 mice) treatment shows the $C_{\text{max}}$, $t_{1/2}$, $\text{AUC}_0-\infty$, $V_{SS}$ and F% were 1178 ng/mL, <1 hours, 2645 ng h/mL, 1.2 l/kg and 60%, respectively[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.
<table>
<thead>
<tr>
<th>Animal Model</th>
<th>Male Wistar rats (250-300 g)[1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dosage</td>
<td>10 mg/kg</td>
</tr>
<tr>
<td>Administration</td>
<td>P.o. (Pharmacokinetic Analysis)</td>
</tr>
<tr>
<td>Result</td>
<td>$C_{\text{max}}, t_{1/2}, AUC_{0-\infty}, V_{ss}$ and F% were 771 ng/mL, 3.4 hours, 1431 ng h/mL, 4.4 l/kg and 69%, respectively.</td>
</tr>
</tbody>
</table>

**REFERENCES**


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**Caution:** Product has not been fully validated for medical applications. For research use only.

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