EST73502 monohydrochloride

Cat. No.: HY-134189A

CAS No.: 2535970-65-9

Molecular Formula: $C_{19}H_{27}ClF_2N_2O_2$

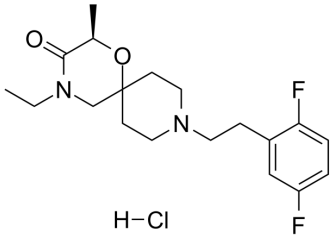
Molecular Weight: 388.88

Target: Sigma Receptor; Opioid Receptor

Pathway: Neuronal Signaling; GPCR/G Protein

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (128.57 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5715 mL	12.8574 mL	25.7149 mL
	5 mM	0.5143 mL	2.5715 mL	5.1430 mL
	10 mM	0.2571 mL	1.2857 mL	2.5715 mL

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 (6.43 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.43 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.43 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

EST73502 monohydrochloride is a selective, orally active and blood-brain barrier (BBB) penetrant dual μ-opioid receptor (MOR) agonist and σ1 receptor (σ1R) antagonist, with K_is of 64 nM and 118 nM for MOR and σ1R, respectively. EST73502 monohydrochloride has antinociceptive activity[1].

IC_{50} & Target

Ki: 64 nM (MOR), 118 nM (σ1R)[1]

In Vivo

EST73502 monohydrochloride (10-40 mg/kg; p.o.) shows a dose-response analgesic effect reaching a maximum of 64% and an EC_{50} of 14 mg/kg in the paw pressure test in CD1 male mice[1].

EST73502 monohydrochloride (5 mg/kg; i.p.; twice a day; for 10 days) attenuates partial sciatic nerve ligation (PSNL)-

induced mechanical allodynia in male CD1 mice[1].

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

Animal Model:	Male CD1 mice, PSNL model[1]
Dosage:	5 mg/kg
Administration:	Intraperitoneal injection, twice a day, for 10 days
Result:	Attenuated the expression of mechanical allodynia induced by PSNL, reaching a maximal effect of 56%.

REFERENCES

[1]. Mónica García, et al. Discovery of EST73502, a Dual μ-Opioid Receptor Agonist and σ 1 Receptor Antagonist Clinical Candidate for the Treatment of Pain. J Med Chem. 2020 Oct 16.

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