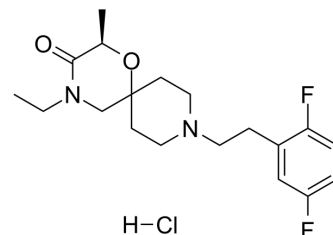


EST73502 monohydrochloride

Cat. No.:	HY-134189A
CAS No.:	2535970-65-9
Molecular Formula:	C ₁₉ H ₂₇ ClF ₂ N ₂ O 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)					
		Solvent Concentration	Mass	1 mg	5 mg	10 mg
	Preparing Stock Solutions	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	<ol style="list-style-type: none"> 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 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 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 _i s of 64 nM and 118 nM for MOR and σ1R, respectively. EST73502 monohydrochloride has antinociceptive activity ^[1] .
IC₅₀ & 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.

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

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