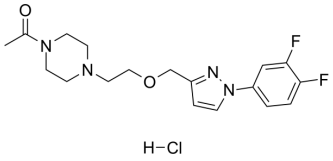
EST64454 hydrochloride

Cat. No.:	HY-131914A
CAS No.:	1950569-11-5
Molecular Formula:	$C_{18}H_{23}ClF_2N_4O_2$
Molecular Weight:	400.85
Target:	Sigma Receptor
Pathway:	Neuronal Signaling
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

H_2O : ≥ 100 mg/mL (249.47 mM)
DMSO : 100 mg/mL (249.47 mM; Need ultrasonic)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.4947 mL	12.4735 mL	24.9470 mL
5 mM	0.4989 mL	2.4947 mL	4.9894 mL
10 mM	0.2495 mL	1.2473 mL	2.4947 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 (6.24 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_{max}, $t_{1/2}$, $AUC_{0-\infty}$, 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_{max}, $t_{1/2}$, $AUC_{0-\infty}$, 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.

Animal Model:	Male Wistar rats (250-300 g)[1]
Dosage:	10 mg/kg
Administration:	P.o. (Pharmacokinetic Analysis)
Result:	The C_{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.

REFERENCES

[1]. Díaz JL, et al. EST64454: a Highly Soluble σ1 Receptor Antagonist Clinical Candidate for Pain Management. J Med Chem. 2020;63(23):14979-14988.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA