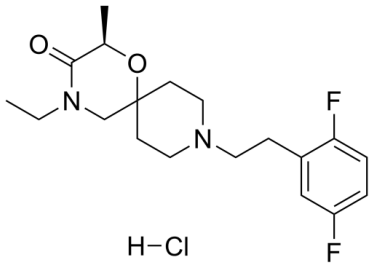
Data Sheet

Product Name:	EST73502 (monohydrochloride)
Cat. No.:	CS-0143090
CAS No.:	2535970-65-9
Molecular Formula:	$C_{19}H_{27}ClF_2N_2O_2$
Molecular Weight:	388.88
Target:	Opioid Receptor; Sigma Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : 50 mg/mL (128.57 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

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].

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.

CAIndexNames:

1-Oxa-4,9-diazaspiro[5.5]undecan-3-one, 9-[2-(2,5-difluorophenyl)ethyl]-4-ethyl-2-methyl-, hydrochloride (1:1), (2R)-

SMILES:

FC1=CC=C(F)C=C1CCN(CC2)CCC2(O[C@@H]3C)CN(CC)C3=O.[H]Cl

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

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