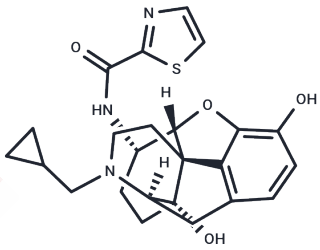
Data Sheet (Cat.No.T204644)

TargetMol

MOR modulator-1

Chemical Properties



CAS No. : 2976336-81-7

Formula: C24H27N3O4S

Molecular Weight: 453.554

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	MOR modulator-1 (compound 6) is a potent and selective modulator of the μ opioid receptor (MOR). Compared to NAT (6α-configuration), MOR modulator-1 demonstrates improved opioid receptor selectivity, enhanced antagonistic effects in vivo, and overall reduced withdrawal symptoms. It connects to the μ, δ, and γ receptors with carboxamide linkers, showing Ki values of 0.25, 41.1, and 1.30 nM respectively.
Targets(IC50)	Opioid Receptor
In vitro	MOR modulator-1 exhibits sub-nanomolar binding affinity at MOR and nanomolar binding affinity at KOR (kappa opioid receptor), with significantly lower binding affinity for DOR (delta opioid receptor), maintaining reasonable selectivity for MOR over DOR [1]. The compound shows the highest δ/μ selectivity, surpassing NAT by approximately 3-fold [1]. MOR modulator-1 connects carboxamide linker μ, δ, γ with Ki values of 0.25, 41.1, and 1.30 nM respectively [1]. It binds MOR [35S]GTPγS with an EC50 of 2.16 nM [1]. The EC50 for MOR modulator-1 binding to KOR [35S]GTPγS is 3.83 and 23.6 nM [1]. It has low efficacy with potencies ranging from nanomolar to sub-nanomolar and a %Emax value of 11.3 [1]. The compound significantly antagonizes DAMGO-induced increases in intracellular calcium in Gαqi5-transfected mMORCHO cells [1] and inhibits calcium ions with an IC50 of 5.64 nM [1].
In vivo	MOR modulator-1 (10 mg/kg, warm-water tail immersion, 20 min) is the most potent antagonist of morphine-mediated analgesia among this series of NAT analogs [1]. The AD 50 of MOR modulator-1 is 0.043 mg/kg, which is 10 times more potent than NAT [1]. Among MOR modulators based on epoxy morphinan molecules, MOR modulator-1 is the most active [1]. At all tested doses (0.05-10 mg/kg, s.c., 20 min), it showed less wet-dog shakes and paw tremors compared to 1 mg/kg naloxone (NLX), even at the highest doses of 5 mg/kg and 10 mg/kg [1]. The average values for wet-dog shakes, jumps, and paw tremors at 5 mg/kg, s.c., 20 min were 9.8, 36.8, and 30.2, respectively [1]. Following administration, brain concentrations of MOR modulator-1 were 0.187, 0.235, and 0.264 μg/g at 5, 10, and 30 minutes, respectively, indicating rapid brain penetration and prolonged retention [1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2048 mL	11.0241 mL	22.0483 mL
5 mM	0.441 mL	2.2048 mL	4.4097 mL
10 mM	0.2205 mL	1.1024 mL	2.2048 mL
50 mM	0.0441 mL	0.2205 mL	0.441 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.