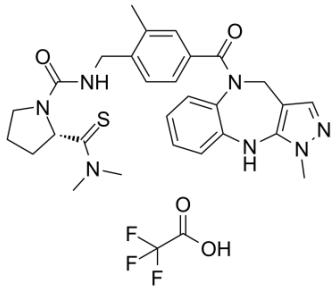
LIT-001

Cat. No.:	HY-124733A
CAS No.:	2245072-21-1
Molecular Formula:	$C_{30}H_{34}F_3N_7O_4S$
Molecular Weight:	645.7
Target:	Oxytocin Receptor
Pathway:	GPCR/G Protein
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (387.18 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5487 mL	7.7435 mL	15.4871 mL
	5 mM	0.3097 mL	1.5487 mL	3.0974 mL
	10 mM	0.1549 mL	0.7744 mL	1.5487 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: ≥ 2.17 mg/mL (3.36 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.17 mg/mL (3.36 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.17 mg/mL (3.36 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

LIT-001 is the first nonpeptide oxytocin receptor (OT-R) agonist (EC_{50}=55 nM; K_i=226 nM). LIT-001 improves social interaction in a mouse model of autism[1].

IC_{50} & Target

EC50: 55 nM (OT-R)[1]
Ki: 226 nM (OT-R)[1]

In Vitro

In vitro signaling experiments, LIT-001 is a nonbiased OT-R agonist on the two main signaling pathways of this receptor, with

	minor antagonist effect on V1a and agonist effect on V1b receptors, observed at high concentrations only[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	LIT-001 (10-20 mg/kg; i.p.) alleviates core symptoms in the context of autism spectrum disorders (ASD)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Oprm1$^{-/-}$ mice (bred in house on a 50% 129SVPas–50% C57BL/6J hybrid background)[1]
Dosage:	10, 20 mg/kg
Administration:	i.p.
Result:	Alleviated core symptoms in the context of ASD.

REFERENCES

[1]. Frantz MC, et al. LIT-001, the First Nonpeptide Oxytocin Receptor Agonist that Improves Social Interaction in a Mouse Model of Autism. J Med Chem. 2018 Oct 11;61(19):8670-8692.

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