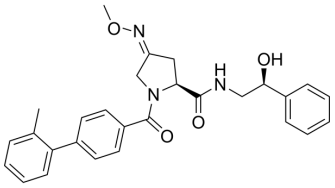
OT-R antagonist 1

Cat. No.:	HY-15015
CAS No.:	364071-17-0
Molecular Formula:	$C_{28}H_{29}N_3O_4$
Molecular Weight:	471.55
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 : 100 mg/mL (212.07 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1207 mL	10.6033 mL	21.2067 mL
	5 mM	0.4241 mL	2.1207 mL	4.2413 mL
	10 mM	0.2121 mL	1.0603 mL	2.1207 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 (5.30 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (5.30 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (5.30 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

OT-R antagonist 1 is a new potent and selective nonpeptide low molecular weight OT-R antagonist. OT-R antagonist 1 inhibits oxytocin-evoked intracellular Ca2+ mobilization (IC50 = 8 nM).IC50 value: 8 nMTarget: oxytocin receptorin vitro: OT-R antagonist 1 inhibitis IP3-Synthesis, rat OT-R (IC50=0.03 uM). [4] OT-R antagonist 1 inhibits phosphodiesterase IV with IC50 = 6.1 μM, a value about 300-fold higher than the affinity for OT-R. OT-R antagonist 1 shows a very clean selectivity profile with specific interaction with OT-R. OT-R antagonist 1 competitively inhibits binding of [3H]oxytocin and the peptide antagonist 125I-ornithine vasotocin analog to human and rat oxytocin receptor expressed in human embryonic kidney 293-EBNA or Chinese hamster ovary cells with nanomolar potency. Selectivity against vasopressin receptor subtypes is >6-fold

for V1a and >350-fold for V2 and V1b. [1]in vivo: Oxytocininduced contraction of isolated rat uterine strips is blocked by OT-R antagonist 1 (pA2 = 7.82). In anesthetized nonpregnant rats, single administration of OT-R antagonist 1 by i.v. or oral routes causes dose-dependent inhibition of contractions elicited by repeated injections of oxytocin with ED50 = 3.5 mg/kg i.v. and 89 mg/kg p.o., respectively. OT-R antagonist 1 significantly inhibits spontaneous uterine contractions in pregnant rats near term when administered intravenously or orally. [1]

REFERENCES

[1]. Serge Halazy, et al. Pharmaceutically active pyrrolidine derivatives as bax inhibitors. WO/2001072705/A1.

[2]. Cirillo R, et al. Pharmacology of (2S,4Z)-N-[(2S)-2-hydroxy-2-phenylethyl]-4-(methoxyimino) -1-[(2'-methyl[1,1'-biphenyl]-4-yl)carbonyl]-2-pyrrolidinecarboxamide, a new potent and selective nonpeptide antagonist of the oxytocin receptor. J Pharmacol Exp Ther. 2003 Jul;306(1):253-61.

[3]. William Nadler, et al. Method for preparing pyrrolidine oximes. WO/2005082848/A2.

[4]. Serge Halazy, et al. Pharmaceutically active pyrrolidine derivatives as bax inhibitors.WO/2001074769/A1.

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