Balovaptan

Cat. No.: HY-109024

CAS No.: 1228088-30-9

Molecular Formula: $C_{22}H_{24}ClN_5O$

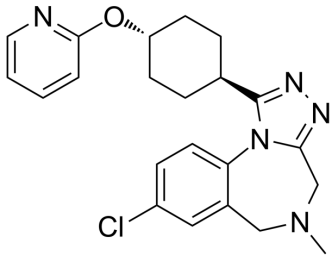
Molecular Weight: 409.91

Target: Vasopressin Receptor

Pathway: GPCR/G Protein

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (121.98 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4396 mL	12.1978 mL	24.3956 mL
	5 mM	0.4879 mL	2.4396 mL	4.8791 mL
	10 mM	0.2440 mL	1.2198 mL	2.4396 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 (6.10 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.10 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.10 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Balovaptan (RG7314) is an orally available, selective brain-penetrant vasopressin 1a (hV1a) receptor antagonist, with K_is of 1 and 39 nM for human (hV1a) and mouse (mV1a) receptors, and is used for the research of autism.

IC_{50} & Target

Ki: 1 nM (hV1a), 39 nM (mV1a)[1]

In Vitro

Balovaptan (RG7314) shows >30000-fold selectivity for hV1a over hV2 receptors, 9891-fold selectivity over hOTR (human oxytocin receptor)[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Ratni H, et al. Discovery of highly selective brain-penetrant vasopressin 1a antagonists for the potential treatment of autism via a chemogenomic and scaffold hopping approach. J Med Chem. 2015 Mar 12;58(5):2275-89.

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