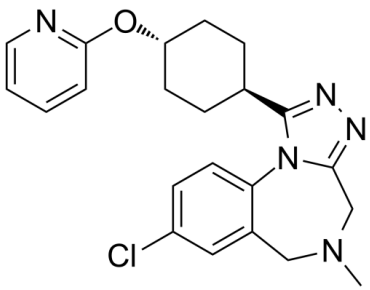
Data Sheet

Product Name:	Balovaptan
Cat. No.:	CS-0030526
CAS No.:	1228088-30-9
Molecular Formula:	$C_{22}H_{24}ClN_5O$
Molecular Weight:	409.91
Target:	Vasopressin Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : 62.5 mg/mL (152.47 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Balovaptan (RG7314) is an orally available, selective brain-penetrant **vasopressin 1a (hV1a) receptor** antagonist, with **K_i**s of 1 and 39 nM for human (hV1a) and mouse (mV1a) receptors, and is used for the research of autism. IC50 & 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].

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.

CAIndexNames:

4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-5,6-dihydro-5-methyl-1-[trans-4-(2-pyridinyloxy)cyclohexyl]-

SMILES:

CN1CC2=NN=C([C@H]3CC[C@H](OC4=NC=CC=C4)CC3)[N@]2[C@]5=CC=C(Cl)C=C5C1

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