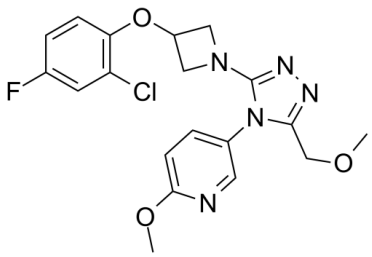
Data Sheet

Product Name:	Cligosiban
Cat. No.:	CS-5337
CAS No.:	900510-03-4
Molecular Formula:	$C_{19}H_{19}ClFN_5O_3$
Molecular Weight:	419.84
Target:	Oxytocin Receptor
Pathway:	GPCR/G Protein
Solubility:	DMSO : ≥ 50 mg/mL (119.09 mM)



BIOLOGICAL ACTIVITY:

Cligosiban (PF-3274167), a high oral bioavailability and good brain-penetrant non-peptide **oxytocin receptor** antagonist, shows a high-affinity (**K_i**=9.5 nM) and an excellent selectivity versus the vasopressin receptors with almost no affinity for the V_{1b} and V_{1a} subtypes. Cligosiban inhibits ejaculatory physiology in rodents[1][2]. IC50 & Target: Ki: 9.5 nM (oxytocin receptor)[2]

References:

[1]. Wayman C, et al. Cligosiban, A Novel Brain-Penetrant, Selective Oxytocin Receptor Antagonist, Inhibits Ejaculatory Physiology in Rodents. J Sex Med. 2018 Dec;15(12):1698-1706.

[2]. Karpenko IA, et al. Selective nonpeptidic fluorescent ligands for oxytocin receptor: design, synthesis, and application to time-resolved FRET binding assay. J Med Chem. 2015 Mar 12;58(5):2547-52.

CAIndexNames:

Pyridine, 5-[3-[3-(2-chloro-4-fluorophenoxy)-1-azetidinyl]-5-(methoxymethyl)-4H-1,2,4-triazol-4-yl]-2-methoxy-

SMILES:

FC1=CC(Cl)=C(OC2CN(C3=NN=C(COC)N3C4=CC=C(OC)N=C4)C2)C=C1

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