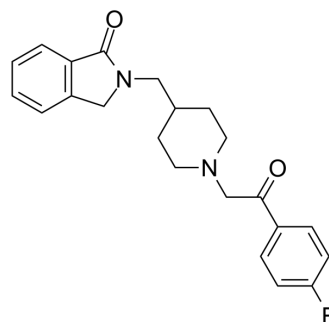


Roluperidone

Cat. No.:	HY-19469	
CAS No.:	359625-79-9	
Molecular Formula:	C ₂₂ H ₂₃ N ₂ O ₂	
Molecular Weight:	366.43	
Target:	5-HT Receptor; Sigma Receptor	
Pathway:	GPCR/G Protein; Neuronal Signaling	
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 : 33.33 mg/mL (90.96 mM; Need ultrasonic)																					
	<table border="1"> <thead> <tr> <th rowspan="2">Solvent</th> <th rowspan="2">Mass</th> <th colspan="3">Concentration</th> </tr> <tr> <th>1 mg</th> <th>5 mg</th> <th>10 mg</th> </tr> </thead> <tbody> <tr> <td rowspan="3">Preparing Stock Solutions</td> <td>1 mM</td> <td>2.7290 mL</td> <td>13.6452 mL</td> <td>27.2903 mL</td> </tr> <tr> <td>5 mM</td> <td>0.5458 mL</td> <td>2.7290 mL</td> <td>5.4581 mL</td> </tr> <tr> <td>10 mM</td> <td>0.2729 mL</td> <td>1.3645 mL</td> <td>2.7290 mL</td> </tr> </tbody> </table>	Solvent	Mass	Concentration			1 mg	5 mg	10 mg	Preparing Stock Solutions	1 mM	2.7290 mL	13.6452 mL	27.2903 mL	5 mM	0.5458 mL	2.7290 mL	5.4581 mL	10 mM	0.2729 mL	1.3645 mL	2.7290 mL
Solvent	Mass			Concentration																		
		1 mg	5 mg	10 mg																		
Preparing Stock Solutions	1 mM	2.7290 mL	13.6452 mL	27.2903 mL																		
	5 mM	0.5458 mL	2.7290 mL	5.4581 mL																		
	10 mM	0.2729 mL	1.3645 mL	2.7290 mL																		
	Please refer to the solubility information to select the appropriate solvent.																					
In Vivo	<ol style="list-style-type: none"> Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 3 mg/mL (8.19 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 3 mg/mL (8.19 mM); Clear solution Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (6.82 mM); Clear solution 																					

BIOLOGICAL ACTIVITY

Description	Roluperidone (CYR-101) is a novel cyclic amide derivative that has high equipotent affinities for 5-HT _{2A} and sigma-2 receptors (K _i of 7.53 nM and 8.19 nM for 5-HT _{2A} and sigma-2, respectively).	
IC₅₀ & Target	5-HT _{2A} Receptor 7.53 nM (K _i)	Sigma-2 Receptor 8.19 nM (K _i)
In Vitro	Roluperidone (CYR-101) also shows binding affinity for α ₁ -adrenergic receptors but low or no affinity for muscarinic,	

cholinergic, and histaminergic receptors. Although Risperidone (RIS-101) has no affinities for pre- or postsynaptic dopaminergic receptors, it is probable that sigma-2 receptors are implicated in the modulation of dopamine and glutamatergic pathways, as well as in calcium neuronal modulation^[1].

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

REFERENCES

[1]. Davidson M, et al. Efficacy and Safety of MIN-101: A 12-Week Randomized, Double-Blind, Placebo-Controlled Trial of a New Drug in Development for the Treatment of Negative Symptoms in Schizophrenia. Am J Psychiatry. 2017 Jul 28;appiajp201717010122.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA