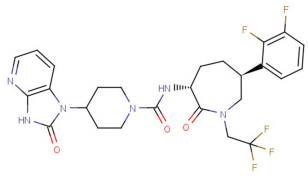
Data Sheet (Cat.No.T16093)

TargetMol
A DRUG SCREENING EXPERT

Telcagepant

Chemical Properties



CAS No.:	781649-09-0
Formula:	C26H27F5N6O3
Molecular Weight:	566.52
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Telcagepant is an orally active antagonist of calcitonin gene-related peptide (CGRP) receptor (Kis: 0.77 nM and 1.2 nM for human and rhesus CGRP receptors, respectively).
Targets(IC_{50})	human CGRP: (ki)0.77 nM rhesus CGRP: 1.2 nM(ki)
In vitro	Telcagepant shows affinity (Ki) for the canine and rat receptors, with values of 1204 nM and 1192 nM (n=10), respectively. Telcagepant displays saturable binding to SK-N-MC membranes with a KD of 1.9 nM and Bmax of 479 fmol/mg protein. Telcagepant effectively blocks human α-CGRP-stimulated cAMP responses in the human CGRP receptor-expressing HEK293 cells (IC50: 2.2 nM)[1]. Telcagepant also displays saturable binding to rhesus cerebellum homogenate (KD: 1.3 nM and Bmax of 20 fmol/mg)[2].
In vivo	The pharmacokinetics of Telcagepant (MK-0974) remains linear across 0.5-10 mg/kg intravenous dose in monkeys, but the oral area under the plasma concentration-time curve (AUC) enhances (5-30 mg/kg) is 15-fold over dose-proportional. Telcagepant (i.v. bolus, 1 mg/kg) demonstrates that the efficacy of this antagonist is time-dependent and correlated with plasma levels[1][3].

Solubility Information

Solubility	DMSO: 50 mg/mL (88.26 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.765 mL	8.826 mL	17.652 mL
5 mM	0.353 mL	1.765 mL	3.53 mL
10 mM	0.177 mL	0.883 mL	1.765 mL
50 mM	0.035 mL	0.177 mL	0.353 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Salvatore CA, et al. Pharmacological characterization of MK-0974 [N-[(3R,6S)-6-(2,3-difluorophenyl)-2-oxo-1-(2,2,2-trifluoroethyl)azepan-3-yl]-4-(2-oxo-2,3-dihydro-1H-imidazo[4,5-b]pyridin-1-yl)piperidine-1-carboxamide], a potent and orally active calcitonin gene-related peptide receptor antagonist for the treatment of migraine. J Pharmacol Exp Ther. 2008 Feb;324(2):416-21. Epub 2007 Nov 26.

2. Moore EL, et al. Examining the binding properties of MK-0974: a CGRP receptor antagonist for the acute treatment of migraine. Eur J Pharmacol. 2009 Jan 14;602(2-3):250-4.

3. Roller S, et al. Preclinical pharmacokinetics of MK-0974, an orally active calcitonin-gene related peptide (CGRP)-receptor antagonist, mechanism of dose dependency and species differences. Xenobiotica. 2009 Jan;39(1):33-45.

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