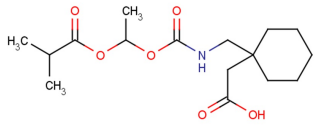
Data Sheet (Cat.No.T15366)

TargetMol
A DRUG SCREENING EXPERT

Gabapentin enacarbil

Chemical Properties



CAS No.:	478296-72-9
Formula:	C16H27NO6
Molecular Weight:	329.39
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	Gabapentin enacarbil (XP-13512) is a prodrug for the anticonvulsant and analgesic drug gabapentin.
Targets(IC_{50})	Others: None
In vitro	Gabapentin enacarbil demonstrated active apical to basolateral transport across Caco-2 cell monolayers and pH-dependent passive permeability across artificial membranes. Gabapentin enacarbil inhibited uptake of (14)C-lactate by human embryonic kidney cells expressing monocarboxylate transporter type-1, and direct uptake of prodrug by these cells was confirmed using liquid chromatography-tandem mass spectrometry. Gabapentin enacarbil inhibited uptake of (3)H-biotin into Chinese hamster ovary cells overexpressing human sodium-dependent multivitamin transporter (SMVT) [1].
In vivo	In 4 studies of healthy volunteers (136 subjects total), the pharmacokinetics of XP13512 immediate- and extended-release formulations were compared with those of oral gabapentin. XP13512 immediate-release (up to 2800 mg single dose and 2100 mg twice daily) was well absorbed (>68%, based on urinary recovery of gabapentin), converted rapidly to gabapentin, and provided dose-proportional exposure, whereas absorption of oral gabapentin declined with increasing doses to <27% at 1200 mg. Compared with 600 mg gabapentin, an equimolar XP13512 extended-release dose provided extended gabapentin exposure (time to maximum concentration, 8.4 vs 2.7 hours) and superior bioavailability (74.5% vs 36.6%) [2].

Solubility Information

Solubility	DMSO: 100 mg/mL (303.59 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.036 mL	15.18 mL	30.359 mL
5 mM	0.607 mL	3.036 mL	6.072 mL
10 mM	0.304 mL	1.518 mL	3.036 mL
50 mM	0.061 mL	0.304 mL	0.607 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. Cundy KC, et al. XP13512 [(+/-)-1-([(alpha-isobutanoyloxyethoxy)carbonyl] aminomethyl)-1-cyclohexane acetic acid], a novel gabapentin prodrug: I. Design, synthesis, enzymatic conversion to gabapentin, and transport by intestinal solute transporters. J Pha
2. Cundy KC, et al. Clinical pharmacokinetics of XP13512, a novel transported prodrug of gabapentin. J Clin Pharmacol. 2008 Dec;48(12):1378-88.

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