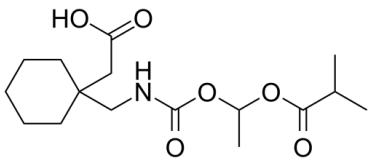
Data Sheet

Product Name:	Gabapentin enacarbil
Cat. No.:	CS-1698
CAS No.:	478296-72-9
Molecular Formula:	C16H27NO6
Molecular Weight:	329.39
Target:	Calcium Channel
Pathway:	Membrane Transporter/Ion Channel; Neuronal Signaling
Solubility:	H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

Gabapentin enacarbil (XP-13512) is a prodrug for the anticonvulsant and analgesic drug gabapentin. IC50 Value: Target: Calcium Channel Gabapentin enacarbil is an actively transported prodrug of gabapentin that provides sustained dose-proportional exposure to gabapentin and predictable bioavailability. in vitro: The prodrug (XP-13512) demonstrated active apical to basolateral transport across Caco-2 cell monolayers and pH-dependent passive permeability across artificial membranes. XP13512 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. XP13512 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]. Toxicity: Gabapentin's most common side effects in adult patients include dizziness, fatigue, weight gain, drowsiness, and peripheral edema (swelling of extremities).

References:

[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 Pharmacol Exp Ther. 2004 Oct;311(1):315-23.

[2]. Cundy KC, et al. Clinical pharmacokinetics of XP13512, a novel transported prodrug of gabapentin. J Clin Pharmacol. 2008 Dec;48(12):1378-88.

CAIndexNames:

Cyclohexaneacetic acid, 1-[[[[1-(2-methyl-1-oxopropoxy)ethoxy]carbonyl]amino]methyl]-

SMILES:

O=C(O)CC1(CNC(OC(OC(C(C)C)=O)C)=O)CCCCC1

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

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

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