Product Data Sheet

Product Name: ZINC12613047
Cat. No.: GC10231

Chemical Properties

Cas. No.	1069521-64-7		
Chemical Name	N-[[1-(2,3-dihydro-1H-inden-2-yl)-3-piperidinyl]methyl]-N-(2-methoxyethyl)-2-naphthalenecarboxamide		
SMILES	COCCN(C(C1=CC(C=CC=C2)=C2C=C1)=O)CC3CCCN(C4CC(C=CC=C5)=C5C4)C3		
Formula	$C_{29}H_{34}N_2O_2$	M.Wt	442.6
Solubility	≤5mg/ml in ethanol;10mg/ml in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	ZINC12613047		

Background

IC50: 21 nM for human BChE

ZINC12613047 is a BChE inhibitor.

Butyrylcholinesterase (BChE) is considered as a promising drug target as its levels and activity increase significantly in the late stages of Alzheimer’s disease.

In vitro: In previous study, the complex structure between ZINC12613047 and BChE revealed the molecular basis of the high affinity binding. In contrast, the pocket was comparatively smaller in AChE likely explaining why ZINC12613047 displayed low affinity. In addition, ZINC12613047 was tested at 10 μM, where it showed significant Aβ1-42-antiaggregation effects with 61.7% inhibition. The cytotoxicity profile was assessed using the human neuroblastoma SH-SY5Y cell line and the MTS assay. ZINC12613047 at 10 μM was completely noncytotoxic. Moreover, to compare neuronal death induced by Aβ1-42 with or without various concentrations of ZINC12613047, the MTS assay was performed. Results showed that incubation of SH-SY5Y cells with 5 μM Aβ1-42 led to significant toxicity; the cell-death was about 35% higher than in the control. A clear dose-response neuroprotective

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effect was observed when the cells were incubated with Aβ1-42 in the presence of ZINC12613047. ZINC12613047 at 10 μM could completely protect the human neuronal SH-SY5Y cells from Aβ1-42 peptide toxicity [1].

In vivo: There is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:

[1] B. Brus, U. Kosak, S. Turk, et al. Discovery, biological evaluation, and crystal structure of a novel nanomolar selective butyrylcholinesterase inhibitor. Journal of Medicinal Chemistry 57(19), 8167-8179 (2014).