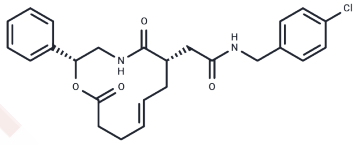
Data Sheet (Cat.No.T26110)

TargetMol

Robotnikinin

Chemical Properties



CAS No. : 1132653-79-2

Formula: C25H27ClN2O4

Molecular Weight: 454.95

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	Robotnikinin is an Shh signaling inhibitor in a concentration-dependent manner. It acts by exhibiting significant repression of Shh-induced Gli1/Gli2.
Targets(IC50)	Others,Hedgehog/Smoothened

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.198 mL	10.9902 mL	21.9804 mL
5 mM	0.4396 mL	2.198 mL	4.3961 mL
10 mM	0.2198 mL	1.099 mL	2.198 mL
50 mM	0.044 mL	0.2198 mL	0.4396 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Hitzenberger M, Schuster D, Hofer TS. The Binding Mode of the Sonic Hedgehog Inhibitor Robotnikinin, a Combined Docking and QM/MM MD Study. Front Chem. 2017 Oct 23;5:76. doi: 10.3389/fchem.2017.00076. eCollection 2017. PubMed PMID: 29109946; PubMed Central PMCID: PMC5660280.

Dockendorff C, Nagiec MM, Weïwer M, Buhrlage S, Ting A, Nag PP, Germain A, Kim HJ, Youngsaye W, Scherer C, Bennion M, Xue L, Stanton BZ, Lewis TA, Macpherson L, Palmer M, Foley MA, Perez JR, Schreiber SL. Macrocyclic Hedgehog Pathway Inhibitors: Optimization of Cellular Activity and Mode of Action Studies. ACS Med Chem Lett. 2012 Oct 11;3(10):808-813. Epub 2012 Aug 30. PubMed PMID: 23074541; PubMed Central PMCID: PMC3469069.

Hassounah NB, Bunch TA, McDermott KM. Molecular pathways: the role of primary cilia in cancer progression and therapeutics with a focus on Hedgehog signaling. Clin Cancer Res. 2012 May 1;18(9):2429-35. doi: 10.1158/1078-0432.CCR-11-0755. Epub 2012 Mar 13. PubMed PMID: 22415315; PubMed Central PMCID: PMC3738179.

Hwang S, Thangapandian S, Lee Y, Sakkiah S, John S, Lee KW. Discovery and evaluation of potential sonic hedgehog signaling pathway inhibitors using pharmacophore modeling and molecular dynamics simulations. J Bioinform Comput Biol. 2011 Dec;9 Suppl 1:15-35. PubMed PMID: 22144251.

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