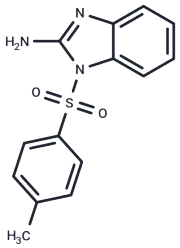
Data Sheet (Cat.No.T6591)

TargetMol

Nodinitib-1

Chemical Properties



CAS No. : 799264-47-4

Formula: C14H13N3O2S

Molecular Weight: 287.34

Appearance: no data available

Storage: keep away from direct sunlight,keep away from moisture
Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Biological Description

Description	Nodinitib-1 (CID-1088438) is a potent and selective NOD1 inhibitor with an IC50 of 0.56 μM.
Targets(IC50)	NOD-like Receptor (NLR),NOD,TNF
In vitro	Nodinitib-1 has shown selective inhibition of NOD1-induced NF-κB activation in HEK293 cells with no cytotoxicity and is selected as a probe candidate molecule. Nodinitib-1 is also confirmed in secondary assays by selectively inhibiting NOD1-dependent IL-8 secretion and also selectively inhibiting the NOD1-dependent pathway to NF-κB activation. [1] In another research, Nodinitib-1 is proved to cause conformational changes of NOD1 in vitro and alter NOD1 subcellular targeting in cells, providing chemical probes for interrogating mechanisms regulating NOD1 activity and tools for exploring the roles of NOD1 in various infectious and inflammatory diseases. [2]
Kinase Assay	NOD1 Dose Response assay: Day 1 Procedure 1) Harvest HEK-293-T NFKB-Luc at 100% confluency at 100% confluency. 2) Add NOD assay media with Multidrop. 3) Spin down plates at 1000 rpm for 1 min in centrifuge. 4) Serial compound dilutions. 5) Add gamma-tri-DAP to cell suspension at 0.75 ug/mL. 6) Seed 13000 cells/well in 4 uL/well to full plate HEK-293-T NFKB-Luc to TC-treated plate. 7) Spin down plates 500 RPM for 5 min on centrifuge. 8) Lid Plates. Sandwich 4 plates between 2 lidded 384 plates filled with Water. 9) Wrap plates securely in single layer of Plastic Wrap. 10) Incubate overnight (14 hours) in 37 ℃ and 5% CO2 incubator. Day 2 Procedure 1) Add 3 ul/well of SteadyGlo solution with Multidrop. 2) Shake plates on a plate shaker for 20 min. 3) Spin plates 1000 RPM for 1 min using centrifuge. 4) Read luminescence.IC50 values are calculated using GraphPad Prism 5.0.The average Z' for the screen is 0.6, the signal to background is 11.1, signal to noise is 78.6 and signal to window is 6.0.
Cell Research	Hepatic toxicity of compounds is determined with Fa2N-4 immortalized human hepatocytes using the ATP-lite 1-step assay. Fa2N-4 cells are seeded at 50,000 cells/well, and incubated with a range of concentrations of the test compound (0.01 μM-50 μM) in MFE support medium for 24 h at 37 ℃, 5% CO2. At the end of the experiment D-luciferin and luciferase are added. The emitted luminescent signal produced as a result of the reaction with cellular ATP is captured on the Infinite M200 plate reader. The concentration of each compound that killed 50% of the cells (LC50) is calculated by non-linear regression analysis using a log (inhibitior) vs response equation with a variable

	slope, using the statistic software package Prism4.(Only for Reference)

Solubility Information

Solubility	Ethanol: 2.9 mg/mL (10.09 mM),Sonication is recommended. DMSO: 28.7 mg/mL (99.88 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.4802 mL	17.401 mL	34.802 mL
5 mM	0.696 mL	3.4802 mL	6.9604 mL
10 mM	0.348 mL	1.7401 mL	3.4802 mL
50 mM	0.0696 mL	0.348 mL	0.696 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.

Reference

Khan PM et al. ACS Med Chem Lett, 2011, 2(10), 780-785.
Zhang Y, Li N, Yuan G, et al. Upregulation of NOD1 and NOD2 contribute to cancer progression through the positive regulation of tumorigenicity and metastasis in human squamous cervical cancer. BMC medicine. 2022, 20 (1): 1-15.
Correa RG et al. Chem Biol, 2011, 18(7), 825-832.
Ding L, Zheng G, Zhou A, et al.Development and Verification of Diagnosis Model for Papillary Thyroid Cancer Based on Pyroptosis-Related Genes: A Bioinformatic and in vitro Investigation.Journal of Inflammation Research. 2024: 7761-7776.