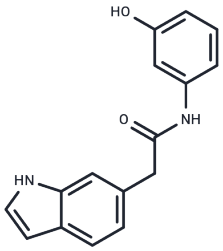
Data Sheet (Cat.No.T60442)

TargetMol

NLRP3/AIM2-IN-3

Chemical Properties



CAS No. : 1787787-60-3

Formula: C16H14N2O2

Molecular Weight: 266.29

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	NLRP3/AIM2-IN-3 is a unique molecule that inhibits NLRP3 and AIM2 inflammasome activation in a species-specific manner. It has an IC50 value for cell lysis of 0.077 ± 0.008 μ M. NLRP3/AIM2-IN-3 is a potent inhibitor of NLRP3 and AIM2 inflammasome-dependent cell lysis with an IC50 value for cell lysis of 0.077 ± 0.008 μ M. NLRP3/AIM2-IN-3 inhibits LPS/nigericin NLRP3/AIM2-IN-3 inhibits LPS/nigericin-stimulated cell lysis in THP-1 macrophages with an IC50 value of 0.077 ± 0.008 μM. NLRP3/AIM2-IN-3 interferes with the interaction of NLRP3 or AIM2 with the bridging protein ASC, inhibiting oligomerization of ASC.
Targets(IC50)	NOD-like Receptor (NLR),NOD,Pyroptosis,AIM2
In vitro	NLRP3/AIM2-IN-3 (0-100 μM) exhibits significant inhibitory activity against NLRP3 and AIM2 in human THP-1 macrophages, without affecting NLRC4-dependent activation of caspase-1 or IL-1b release. It inhibits IL-1b secretion from THP-1 macrophages with an IC50 of 0.098 μM, which is nearly 150-fold and 500-fold more potent compared to its effects on J774A.1 (14.62 μM) and Bone Marrow-Derived Macrophages (BMDM) (48.98 μM), respectively. [1]

Solubility Information

Solubility	DMSO: 225 mg/mL (844.94 mM),Sonication is recommended. Methanol: 45 mg/mL (168.99 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween-80+45% Saline: 3.3 mg/mL (12.39 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.7553 mL	18.7765 mL	37.553 mL
5 mM	0.7511 mL	3.7553 mL	7.5106 mL
10 mM	0.3755 mL	1.8777 mL	3.7553 mL
50 mM	0.0751 mL	0.3755 mL	0.7511 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

Jiao Y, et al. Discovery of a novel and potent inhibitor with differential species-specific effects against NLRP3 and AIM2 inflammasome-dependent pyroptosis. Eur J Med Chem. 2022;232:114194.
Wang D, et al. Systemic pharmacology reveal the mechanism by which the Qiangjin Zhuanggu Qufeng mixture inhibits LPS-induced pyroptosis of rat nucleus pulposus cells [published online ahead of print, 2023 Jul 27]. Phytomedicine. 2023;119:154998.