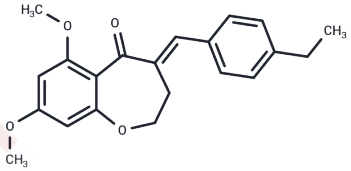
Data Sheet (Cat.No.T39984)

TargetMol

PKM2-IN-3

Chemical Properties



CAS No. : 2408841-19-8

Formula: C21H22O4

Molecular Weight: 338.403

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	PKM2-IN-3 is a potent PKM2 kinase inhibitor, displaying an IC 50 value of 4.1 μM. The compound effectively suppresses PKM2-mediated glycolysis and NLRP3 activation, thereby exerting an anti-neuroinflammatory effect.
Targets(IC50)	Others,PKM
In vitro	PKM2-IN-3 (compound 10i) effectively suppresses TNF-α secretion in LPS-induced RAW264.7 macrophages with an IC50 of 5.2 μM and demonstrates minimal toxicity with a CC50 of 43.6 μM[1]. At concentrations of 0.1-100 μM over 20 minutes, it selectively inhibits PKM2 kinase activity with an IC50 of 4.1 μM[1].
In vivo	PKM2-IN-3, at a dosage of 1 and 10 mg/kg administered intraperitoneally (i.p.) daily for three days, significantly reversed behavior changes in LPS-induced mice during open field tests. Similarly, when administered intravenously (i.v.) at 4 hours and 24 hours post-ischemia, it notably reduced infarct volume and ameliorated neurological deficits in tMCAO rat models. In the first scenario, the treatment involved male mice aged 6-8 weeks and weighing 20.0-22.0 g, while in the second, male Sprague-Dawley rats aged 8-10 weeks and weighing 250.0-280.0 g were used.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.9551 mL	14.7754 mL	29.5508 mL
5 mM	0.591 mL	2.9551 mL	5.9102 mL
10 mM	0.2955 mL	1.4775 mL	2.9551 mL
50 mM	0.0591 mL	0.2955 mL	0.591 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

Gao CL, et al. Synthesis and Target Identification of Benzoxepane Derivatives as Potential Anti-Neuroinflammatory Agents for Ischemic Stroke. Angew Chem Int Ed Engl. 2020;59(6):2429-2439.

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