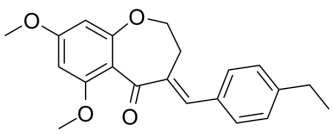
PKM2-IN-3

Cat. No.:	HY-139667
CAS No.:	2408841-19-8
Molecular Formula:	$C_{21}H_{22}O_4$
Molecular Weight:	338.4
Target:	Pyruvate Kinase
Pathway:	Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	PKM2-IN-3 is an inhibitor of PKM2 kinase with an IC_{50} value of 4.1 μM. PKM2-IN-3 exhibits an anti-neuroinflammatory effect by inhibiting PKM2-mediated glycolysis and NLRP3 activation[1].
IC_{50} & Target	PKM2 4.1 μM (IC_{50})
In Vitro	PKM2-IN-3 (compound 10i) inhibits the TNF-α release of LPS-stimulated RAW264.7 macrophages, with an IC_{50} value of 5.2 μM. PKM2-IN-3 exhibits the lowest toxicity with a CC_{50} value of 43.6 μM[1]. PKM2-IN-3 (0.1-100 μM; 20 min) inhibits PKM2 kinase activity in a cell-free molecular level with an IC_{50} value of 4.1 μM[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	PKM2-IN-3 (1, 10 mg/kg; i.p.; daily for 3 days) significantly reverses the LPS-induced mice behavior changes in open field test[1]. PKM2-IN-3 (1, 10 mg/kg; i.v.; injected at 4 hours and 24 hours after ischemia onset) reduces the infarct volume and improves neurological deficits of tMCAO rats[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	LPS-induced mice (male 6-8 weeks old; 20.0-22.0 g)[1]
Dosage:	1, 10 mg/kg
Administration:	i.p.; daily for 3 days
Result:	Reversed the LPS-induced mice behavior changes in open field test.

Animal Model:	tMCAO Sprague-Dawley rats (Male 8-10 weeks old; 250.0-280.0 g)[1]
Dosage:	1, 10 mg/kg
Administration:	i.v.; injected at 4 hours and 24 hours after ischemia onset
Result:	Reduced the infarct volume and improved neurological deficits of tMCAO rats.

REFERENCES

[1]. 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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