IQ-1S free acid

Cat. No.: HY-100233

CAS No.: 23146-22-7

Molecular Formula: $C_{15}H_9N_3O$

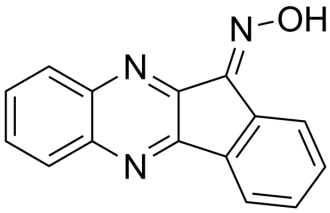
Molecular Weight: 247.25

Target: JNK

Pathway: MAPK/ERK Pathway

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 16.67 mg/mL (67.42 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	4.0445 mL	20.2224 mL	40.4449 mL
	5 mM	0.8089 mL	4.0445 mL	8.0890 mL
	10 mM	0.4044 mL	2.0222 mL	4.0445 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.67 mg/mL (6.75 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1.67 mg/mL (6.75 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.67 mg/mL (6.75 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

IQ-1S free acid is a prospective inhibitor of NF-κB/activating protein 1 (AP-1) activity with an IC_{50} of 2.3±0.41 μM. IQ-1S free acid has binding affinity (K_d values) in the nanomolar range for all three JNKs with K_ds of 100 nM, 240 nM, and 360 nM for JNK3, JNK1, and JNK2, respectively.

IC_{50} & Target

JNK3 100 nM (Kd)	JNK1 240 nM (Kd)	JNK2 360 nM (Kd)	CK1δ 0.38 μM (Kd)
PI3Kγ	MKNK2		

	0.47 μM (Kd)	0.92 μM (Kd)
In Vitro	Compound IQ-1S is a potent, noncytotoxic inhibitor of pro-inflammatory cytokine [interleukin (IL)-1α, IL-1β, IL-6, IL-10, tumor necrosis factor (TNF)-α, interferon-γ, and granulocyte-macrophage colony-stimulating factor] and nitric oxide production by human and murine monocyte/macrophages. The effect of IQ-1S is evaluated on LPS-induced cytokine production in human PBMCs. Among the 12 cytokines analyzed, LPS (200 ng/mL) consistently induces five (IL-1α, IL-1β, IL-6, IL-10, and TNF-α) in PBMCs compared with DMSO-treated control cells. Production of all of these cytokines is significantly inhibited by 20 μM IQ-1S. Among them, TNF-α production is inhibited completely by IQ-1 (>99%), the levels of IL-1α, IL-1β, and IL-10 are decreased by 85%, and IL-6 production is decreased by 33%[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.	
In Vivo	When mice are dosed with 12.5 and 30 mg/kg IQ-1S (The sodium salt of IQ-1S) i.p., the serum exposure of the compound is also good, with AUC_{0-12h} values of 2.9 and 7.4 μM/h, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

PROTOCOL

Cell Assay [1]	Human PBMCs are plated in 96-well plates at a density of 2×10^5 cells/well in culture medium supplemented with 3% (v/v) endotoxin-free FBS. PBMCs are pretreated with 20 μM IQ-1S or DMSO for 30 min, followed by addition of 200 ng/ml LPS for 24 h. A human cytokine MultiAnalyte ELISArray Kit is used to evaluate various cytokines (IL-1α, IL-1β, IL-2, IL-4, IL-6, IL-8, IL-10, IL-12, IL-17A, interferon (IFN)-γ, TNF-α, and granulocyte-macrophage colony-stimulating factor in supernatants of PBMCs[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Mice[1] For in vivo analysis, 12.5 or 30 mg/kg i.p. doses of IQ-1S (The sodium salt of IQ-1) are administered to BALB/c mice (15-20 animals/group), and the mice are sacrificed at various time points after compound administration. For quantification, a calibration curve is established using mouse serum samples spiked with known concentrations of IQ-1S (0.1-20 μM), and a linear dependence of the peak area with IQ-1S concentration is obtained (correlation coefficient r=0.997). The area under the serum concentration-time curve (AUC_{0-12h}) is calculated using the linear trapezoidal method up to the last measured concentration[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Patent. US20180263995A1.

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REFERENCES

[1]. Schepetkin IA, et al. Identification and characterization of a novel class of c-Jun N-terminal kinase inhibitors. Mol Pharmacol. 2012 Jun;81(6):832-45.

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