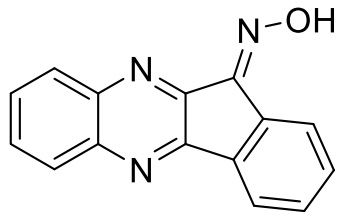
Product data sheet

MedKoo Cat#: 526823 Name: IQ-1S CAS: 23146-22-7 Chemical Formula: $C_{15}H_9N_3O$ Exact Mass: 247.0746 Molecular Weight: 247.257	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
IQ-1S is a potent and selective c-Jun N-Terminal Kinase Inhibitor. IQ-1S inhibits murine delayed-type hypersensitivity. IQ-1S is highly specific for JNK and that its neutral form is the most abundant species at physiologic pH. IQ-1S can reduce inflammation and cartilage loss associated with CIA and can serve as a small-molecule modulator for mechanistic studies of JNK function in rheumatoid arthritis.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	15.0	60.67
DMF:PBS (pH 7.2) (1:2)	0.3	1.21
DMSO	30.33	122.68
Ethanol	1.0	4.04

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	4.04 mL	20.22 mL	40.44 mL
5 mM	0.81 mL	4.04 mL	8.09 mL
10 mM	0.40 mL	2.02 mL	4.04 mL
50 mM	0.08 mL	0.40 mL	0.81 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Jin W, Stokes JM, Eastman RT, Itkin Z, Zakharov AV, Collins JJ, Jaakkola TS, Barzilay R. Deep learning identifies synergistic drug combinations for treating COVID-19. Proc Natl Acad Sci U S A. 2021 Sep 28;118(39):e2105070118. doi: 10.1073/pnas.2105070118. PMID: 34526388; PMCID: PMC8488647.
2. Schepetkin IA, Kirpotina LN, Hammaker D, Kochetkova I, Khlebnikov AI, Lyakhov SA, Firestein GS, Quinn MT. Anti-Inflammatory Effects and Joint Protection in Collagen-Induced Arthritis after Treatment with IQ-1S, a Selective c-Jun N-Terminal Kinase Inhibitor. J Pharmacol Exp Ther. 2015 Jun;353(3):505-16. doi: 10.1124/jpet.114.220251. Epub 2015 Mar 17. PMID: 25784649; PMCID: PMC4429673.

In vivo study

1. Plotnikov MB, Chernysheva GA, Smolyakova VI, Aliev OI, Trofimova ES, Sherstoboev EY, Osipenko AN, Khlebnikov AI, Anfinogenova YJ, Schepetkin IA, Atochin DN. Neuroprotective Effects of a Novel Inhibitor of c-Jun N-Terminal Kinase in the Rat

Model of Transient Focal Cerebral Ischemia. Cells. 2020 Aug 8;9(8):1860. doi: 10.3390/cells9081860. PMID: 32784475; PMCID: PMC7464312.
2. Atochin DN, Schepetkin IA, Khlebnikov AI, Seledtsov VI, Swanson H, Quinn MT, Huang PL. A novel dual NO-donating oxime and c-Jun N-terminal kinase inhibitor protects against cerebral ischemia-reperfusion injury in mice. Neurosci Lett. 2016 Apr 8;618:45-49. doi: 10.1016/j.neulet.2016.02.033. Epub 2016 Feb 26. PMID: 26923672; PMCID: PMC5491393.

7. Bioactivity

Biological target:

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.

In vitro activity

IQ-1S is a JNK inhibitor with K_d = 87, 360, and 390 nM for JNK3, JNK2, and JNK1, respectively. It demonstrated an IC50 = 6.3 μM against SARS-CoV-2 in a Vero E6 cell CPE assay.

Reference: Proc Natl Acad Sci U S A. 2021 Sep 28;118(39):e2105070118. https://pubmed.ncbi.nlm.nih.gov/34526388/

In vivo activity

Administration of IQ-1S at a dose of 25 mg/kg reduced JNK-dependent phosphorylation of c-Jun by 20%. These findings suggest that IQ-1S inhibits JNK enzymatic activity in the hippocampus and protects against stroke injury when administered in the therapeutic and prophylactic regimen in the rat model of FCI.

Reference: Cells. 2020 Aug 8;9(8):1860. https://pubmed.ncbi.nlm.nih.gov/32784475/