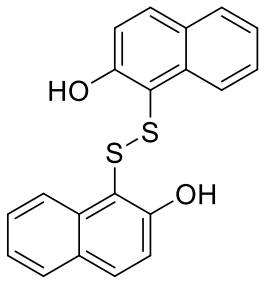
Product data sheet

MedKoo Cat#: 407179 Name: IPA-3 CAS: 42521-82-4 Chemical Formula: $C_{20}H_{14}O_2S_2$ Exact Mass: 350.0435 Molecular Weight: 350.45	
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:

IPA-3 is a potent and selective PAK1 inhibitor. IPA-3 inhibits the growth of liver cancer cells by suppressing PAK1 and NF-κB activation. IPA-3 treatment significantly inhibited the growth of HCC cells. The mechanisms through which IPA-3 treatment suppresses HCC cell growth are enhancement of apoptosis and blockage of activation of NF-κB. IPA-3 not only inhibits the HCC cell growth, but also suppresses the metastatic potential of HCC cells. Nude mouse xenograft assay demonstrated that IPA-3 treatment significantly reduced the tumor growth rate and decreased tumor volume, indicating that IPA-3 can suppress the in vivo tumor growth of HCC cells. Hepatocellular carcinoma (HCC) is one of the major malignancies worldwide and is associated with poor prognosis due to the high incidences of metastasis and tumor recurrence. Overexpression of p21-activated protein kinase 1 (PAK1) is frequently observed in HCC and is associated with a more aggressive tumor behavior, suggesting that PAK1 is a potential therapeutic target in HCC.

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	5.0	14.27
DMF:PBS (pH 7.2) (1:4)	0.2	0.57
DMSO	35.74	101.98
Ethanol	7.0	19.97

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.85 mL	14.27 mL	28.53 mL
5 mM	0.57 mL	2.85 mL	5.71 mL
10 mM	0.29 mL	1.43 mL	2.85 mL
50 mM	0.06 mL	0.29 mL	0.57 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. Wu Z, Wang L, Fan L, Tang H, Zuo X, Gu D, Lu X, Li Y, Wu J, Qin S, Xia Y, Zhu H, Wang L, Xu W, Li J, Jin H. Exploring the significance of PAK1 through chromosome conformation signatures in ibrutinib-resistant chronic lymphocytic leukaemia. Mol Oncol. 2022 Aug;16(16):2920-2935. doi: 10.1002/1878-0261.13281. Epub 2022 Jul 22. PMID: 35811334; PMCID: PMC9394240.
2. Li H, Li T, Zou W, Ni M, Hu Q, Qiu X, Yao Z, Fan J, Li L, Huang Q, Zhou R. IPA-3: An Inhibitor of Diadenylate Cyclase of Streptococcus suis with Potent Antimicrobial Activity. Antibiotics (Basel). 2022 Mar 21;11(3):418. doi: 10.3390/antibiotics11030418. PMID: 35326881; PMCID: PMC8944544.

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In vivo study

1. Verma A, Najahi-Missaoui W, Cummings BS, Somanath PR. Sterically stabilized liposomes targeting P21 (RAC1) activated kinase-1 and secreted phospholipase A2 suppress prostate cancer growth and metastasis. Oncol Lett. 2020 Nov;20(5):179. doi: 10.3892/ol.2020.12040. Epub 2020 Aug 31. PMID: 32934746; PMCID: PMC7471734.
2. Møller LLV, Jaurji M, Kjøbsted R, Joseph GA, Madsen AB, Knudsen JR, Lundsgaard AM, Andersen NR, Schjerling P, Jensen TE, Krauss RS, Richter EA, Sylow L. Insulin-stimulated glucose uptake partly relies on p21-activated kinase (PAK)2, but not PAK1, in mouse skeletal muscle. J Physiol. 2020 Dec;598(23):5351-5377. doi: 10.1113/JP280294. Epub 2020 Sep 17. PMID: 32844438; PMCID: PMC7771197.

7. Bioactivity

Biological target:

IPA-3 is a selective non-ATP competitive PAK1 inhibitor with IC_{50} of 2.5 μM, and shows no inhibition to group II PAKs (PAKs 4-6).

In vitro activity

IPA-3 suppressed the proliferation of MEC-1 in a dose-dependent manner (Fig. S3A). Of note, IPA-3 suppressed the viability of ibrutinib-resistant cells (MEC-1R) in the same manner (Fig. 6A). Annexin V and PI staining was then performed to investigate whether IPA-3 triggered cell apoptosis. Incubation of MEC-1R cells with higher doses of IPA-3 led to a higher percentage of apoptotic cells, suggesting that cells underwent apoptosis under IPA-3 treatment (Fig. 6B,C).

Reference: Mol Oncol. 2022 Aug;16(16):2920-2935. https://pubmed.ncbi.nlm.nih.gov/35811334/

In vivo activity

Twice-weekly administration of SSL-IPA3 (5 mg/kg) inhibited the growth of PC-3 tumor xenografts compared with that in the control group (Fig. 1A-C).

Reference: Oncol Lett. 2020 Nov;20(5):179. https://pubmed.ncbi.nlm.nih.gov/32934746/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.