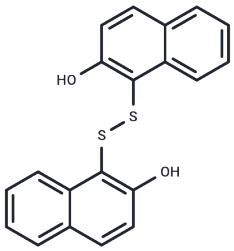
Data Sheet (Cat.No.T6546)

TargetMol

IPA-3

Chemical Properties



CAS No. : 42521-82-4

Formula: C20H14O2S2

Molecular Weight: 350.45

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	IPA-3 is a selective, non-ATP competitive Pak1 inhibitor with an IC50 of 2.5 μM, and it does not inhibit group II PAKs (PAKs 4-6).
Targets(IC50)	PAK
In vitro	IPA-3 is a non-ATP-competitive, allosteric inhibitor of p21-activated kinase 1 (Pak1), with PIR3.5 serving as its control compound. It effectively blocks Cdc42-stimulated and sphingosine-dependent autophosphorylation of Pak1 on Thr423, without targeting the protein's exposed cysteine residues. The efficacy of IPA-3 is dependent on its disulfide bond; reduction by dithiothreitol (DTT) nullifies its inhibitory action on Pak1. Notably, IPA-3 obstructs Pak1 activation by various activators but does not affect already preactivated Pak1; it also impedes PDGF-induced Pak activation in mouse embryonic fibroblasts. This inhibition is partially achieved through covalent binding to Pak1's regulatory domain, an interaction that is both time- and temperature-sensitive, and prevents Cdc42 engagement. Additionally, IPA-3 demonstrates a direct bond to the Pak1 autoregulatory domain and offers reversible inhibition of PMA-induced membrane ruffling in cells.
Kinase Assay	Pak1 (150 nM final) is pre-incubated with MBP (8.3 μM), indicated proteins, and IPA-3 or DMSO in Kinase buffer for 20 minutes at 4°C. Cdc42-GTPγS (3.2 μM) is then added and the reaction is pre-equilibrated 10 minutes at 30°C. Kinase reactions are started by the addition of ATP (to 30 μM) containing [32P]ATP and are incubated 10 min and analyzed by SDS-PAGE and autoradiography.
Cell Research	Human primary schwannoma cells are grown on 96 well plates for 2 days. Cells are left untreated or treated with 5 μM IPA-3, 20 μM IPA-3 or 20 μM PIR-3.5 for 24 hours. The MTS-solution is left on the cells for 3 hours, before the absorbance at 490 nm is measured. The experiments are conducted three times and mean and standard error of the mean is calculated with Excel.

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: 7 mg/mL (19.97 mM),Sonication is recommended. DMSO: 250 mg/mL (713.37 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

In vivo Formulation	10% DMSO+90% Corn oil: 10 mg/mL (28.53 mM),Solution. 10% DMSO+40% PEG300+5% Tween 80+45% Saline: < 10 mg/mL (28.53 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% Saline: < 10 mg/mL (28.53 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. 10% DMSO+90% (20% SBE-β-CD in Saline): < 10 mg/mL (28.53 mM),Lower concentrations may be soluble, but exact solubility limit is unknown. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.8535 mL	14.2674 mL	28.5347 mL
5 mM	0.5707 mL	2.8535 mL	5.7069 mL
10 mM	0.2853 mL	1.4267 mL	2.8535 mL
50 mM	0.0571 mL	0.2853 mL	0.5707 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

Deacon SW, et al. Chem Biol, 2008, 15(4), 322-331.
Viaud J, et al. Mol Cancer Ther, 2009, 8(9), 2559-2565.