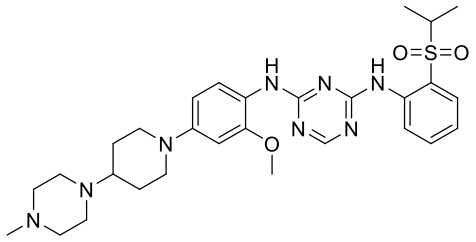
Product data sheet

MedKoo Cat#: 204450 Name: ASP-3026 CAS#: 1097917-15-1 Chemical Formula: $C_{29}H_{40}N_8O_3S$ Exact Mass: 580.29441 Molecular Weight: 580.74	
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:
ASP3026 is a novel and selective inhibitor for the ALK kinase. ASP3026 potently inhibited ALK kinase activity and was more selective than crizotinib in a Tyr-kinase panel. In an anchorage independent in vitro cell growth assay, ASP3026 inhibited the growth of NCI-H2228, a human NSCLC tumor cell line endogenously expressing EML4-ALK variant 3 and that of 3T3 cells expressing EML4-ALK variant 1, 2 and 3. The plasma and tumor concentrations of ASP3026 in mice xenografted with NCI-H2228 tumor were determined using high-performance liquid chromatography-tandem mass spectrometry. Significant tumor penetration was observed.

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
DMSO	20	34.44

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.72 mL	8.61 mL	17.22 mL
5 mM	0.34 mL	1.72 mL	3.44 mL
10 mM	0.17 mL	0.86 mL	1.72 mL
50 mM	0.03 mL	0.17 mL	0.34 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. Al Mamun Bhuyan A, Bissinger R, Cao H, Lang F. Inhibition of Erythrocyte Cell Membrane Scrambling by ASP3026. Cell Physiol Biochem. 2017;43(2):507-517. doi: 10.1159/000480477. Epub 2017 Sep 20. PMID: 28930717.

In vivo study

1. Iikubo K, Kondoh Y, Shimada I, Matsuya T, Mori K, Ueno Y, Okada M. Discovery of N-{2-Methoxy-4-[4-(4-methylpiperazin-1-yl)piperidin-1-yl]phenyl}-N'-[2-(propane-2-sulfonyl)phenyl]-1,3,5-triazine-2,4-diamine (ASP3026), a Potent and Selective Anaplastic Lymphoma Kinase (ALK) Inhibitor. Chem Pharm Bull (Tokyo). 2018;66(3):251-262. doi: 10.1248/cpb.c17-00784. PMID: 29491259.

7. Bioactivity
Biological target:

ASP3026 is a novel and selective inhibitor for ALK with IC50 of 3.5 nM.

In vitro activity

Product data sheet

Treatment with ASP3026 alone did not significantly modify annexin-V-binding or forward scatter. Energy depletion, oxidative stress and ionomycin, all markedly and significantly increased the percentage of annexin-V-binding erythrocytes, and decreased the forward scatter. ASP3026 significantly blunted the effect of energy depletion and oxidative stress, but not of ionomycin on annexin-V-binding. ASP3026 did not significantly influence the effect of any maneuver on forward scatter.

Reference: Cell Physiol Biochem. 2017;43(2):507-517. https://www.karger.com/?DOI=10.1159/000480477

In vivo activity

The antitumor activity of 14a was evaluated in mice xenografted with NCI-H2228, a human NSCLC tumor cell endogenously expressing EML4-ALK (Fig. 4). Compound 14a inhibited the growth of NCI-H2228 cells with an IC50 value of 65 nM.) Once-daily oral administration of 14a demonstrated tumor growth inhibition at doses of 0.3 mg/kg (4% inhibition) and 1 mg/kg (69% inhibition), and tumor regression at doses of 3 mg/kg (4% regression), 10 mg/kg (45% regression), and 30 mg/kg (78% regression) in a dose-dependent manner. Body weight was not affected by 14a at the doses used in this experiment.)

Reference: Chem Pharm Bull (Tokyo). 2018;66(3):251-262. https://doi.org/10.1248/cpb.c17-00784