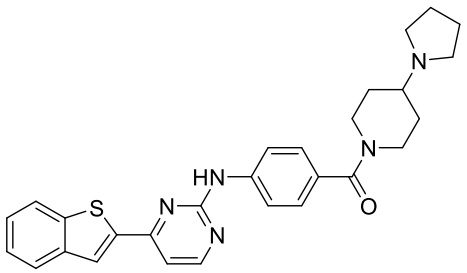
Product data sheet

MedKoo Cat#: 407163 Name: IKK-16 (free base) CAS#: 873225-46-8 (free base) Chemical Formula: $C_{28}H_{29}N_5OS$ Exact Mass: 483.20928 Molecular Weight: 483.63	
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:
IKK-16 is a potent and slective inhibitor of IκB kinase (IKK) (IC50 values are 40, 70 and 200 nM for IKKβ, IKK complex and IKKα respectively). KK-16 inhibits TNFα-stimulated expression of the adhesion molecules E-selectin, ICAM-1, and VCAM-1 in HUVEC cells.

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	27	55.83

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.07 mL	10.34 mL	20.68 mL
5 mM	0.41 mL	2.07 mL	4.14 mL
10 mM	0.21 mL	1.03 mL	2.07 mL
50 mM	0.04 mL	0.21 mL	0.41 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. Dietel E, Brobeil A, Tag C, Gattenloehner S, Wimmer M. PTPIP51 crosslinks the NFκB signaling and the MAPK pathway in SKBR3 cells. Future Sci OA. 2020 Mar 4;6(5):FSO463. doi: 10.2144/fsoa-2019-0136. PMID: 32518680; PMCID: PMC7273389.

2. Waelchli R, Bollbuck B, Bruns C, Buhl T, Eder J, Feifel R, Hersperger R, Janser P, Revesz L, Zerwes HG, Schlapbach A. Design and preparation of 2-benzamido-pyrimidines as inhibitors of IKK. Bioorg Med Chem Lett. 2006 Jan 1;16(1):108-12. doi: 10.1016/j.bmcl.2005.09.035. Epub 2005 Oct 19. PMID: 16236504.

In vivo study

1. Waelchli R, Bollbuck B, Bruns C, Buhl T, Eder J, Feifel R, Hersperger R, Janser P, Revesz L, Zerwes HG, Schlapbach A. Design and preparation of 2-benzamido-pyrimidines as inhibitors of IKK. Bioorg Med Chem Lett. 2006 Jan 1;16(1):108-12. doi: 10.1016/j.bmcl.2005.09.035. Epub 2005 Oct 19. PMID: 16236504.

7. Bioactivity
Biological target:
IKK 16 is a selective IκB kinase (IKK) inhibitor for the IKK2, IKK complex and IKK1 with IC50s of 40 nM, 70 nM and 200 nM, respectively. IKK16 also inhibits leucine-rich repeat kinase-2 (LRRK2) with an IC50 of 50 nM.

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In vitro activity

The treatment of SKBR3 cells with rising concentrations of IKK-16 resulted in a highly significant decrease in cell viability (5 μM $p < 0.0001$; 50 μM $p < 0.0001$). In contrast, applying IKK-16 to HaCat cells led to a slight but significant increase in cell viability for the application of 5 μM ($p < 0.05$). Increasing the concentration resulted in a highly significant decrease in cell viability ($p < 0.0001$; Figure 1). The application of 50 μM IKK-16 to the SKBR3 cell line severely diminished the seeded cell population leaving only cell debris. All applied concentrations of IKK-16 significantly reduced the RelA/PTPIP51 interaction (0.5 μM $p < 0.01$; 5 μM $p < 0.05$) in the breast cancer cell line SKBR3. On the contrary, the application of IKK-16 to HaCat cells enhanced the interaction of RelA and PTPIP51 for the highest tested concentration (50 μM $p < 0.05$).

Reference: Future Sci OA. 2020 Mar 4;6(5):FSO463. https://www.ncbi.nlm.nih.gov/pmc/articles/pmid/32518680/

In vivo activity

IKK-16 (compound 16) was also tested in two animal models. First, its efficacy to inhibit TNFα release into plasma upon LPS-challenge in the rat was determined. The compound was dosed sc (30 mg/kg) or orally (30 mg/kg) 1 h prior to the LPS-challenge. Four hours after the challenge, plasma was collected and the systemic TNFα levels were analyzed using a commercially available ELISA kit. Both routes of administration of inhibitor 16 at the indicated dose resulted in a significant inhibition of 86% (sc) and 75% (p.o.).12 In a second experiment, it was shown that compound 16 was also active in the thioglycollate-induced peritonitis model in the mouse. The maximal inhibition of neutrophil extravasation in this model was about 50% at a dose of 10 mg/kg sc.

Reference: Bioorg Med Chem Lett. 2006 Jan 1;16(1):108-12. https://linkinghub.elsevier.com/retrieve/pii/S0960-894X(05)01203-5