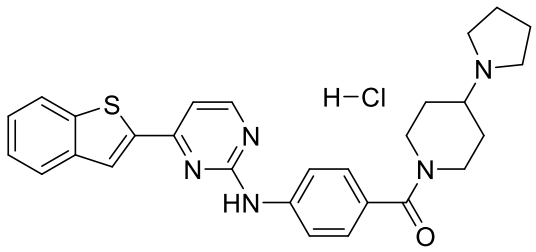
Product data sheet

MedKoo Cat#: 407298 Name: IKK-16 HCl CAS: 1186195-62-9 (HCl) Chemical Formula: $C_{28}H_{30}ClN_5OS$ Exact Mass: 519.186 Molecular Weight: 520.092	
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
DMF	5.0	9.61
DMSO	45.33	87.16
DMSO:PBS (pH 7.2) (1:2)	0.3	0.58

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.92 mL	9.61 mL	19.23 mL
5 mM	0.38 mL	1.92 mL	3.85 mL
10 mM	0.19 mL	0.96 mL	1.92 mL
50 mM	0.04 mL	0.19 mL	0.38 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. Thein S, Pham A, Bayer KU, Tao-Cheng JH, Dosemeci A. IKK regulates the deubiquitinase CYLD at the postsynaptic density. Biochem Biophys Res Commun. 2014 Jul 18;450(1):550-4. doi: 10.1016/j.bbrc.2014.06.019. Epub 2014 Jun 10. PMID: 24928390; PMCID: PMC4126652.
2. Tandon M, Johnson J, Li Z, Xu S, Wipf P, Wang QJ. New pyrazolopyrimidine inhibitors of protein kinase d as potent anticancer agents for prostate cancer cells. PLoS One. 2013 Sep 23;8(9):e75601. doi: 10.1371/journal.pone.0075601. PMID: 24086585; PMCID: PMC3781056.

In vivo study

1. Sordi R, Chiazza F, Johnson FL, Patel NS, Brohi K, Collino M, Thiemermann C. Inhibition of IκB Kinase Attenuates the Organ Injury and Dysfunction Associated with Hemorrhagic Shock. Mol Med. 2015 Jun 18;21(1):563-75. doi: 10.2119/molmed.2015.00049. PMID: 26101953; PMCID: PMC4607620.
2. Coldewey SM, Rogazzo M, Collino M, Patel NS, Thiemermann C. Inhibition of IκB kinase reduces the multiple organ dysfunction caused by sepsis in the mouse. Coldewey SM, Rogazzo M, Collino M, Patel NS, Thiemermann C. Inhibition of IκB kinase reduces the

multiple organ dysfunction caused by sepsis in the mouse. Dis Model Mech. 2013 Jul;6(4):1031-42. doi: 10.1242/dmm.012435. Epub 2013 May 2. PMID: 23649820; PMCID: PMC3701222.doi: 10.1242/dmm.012435. Epub 2013 May 2. PMID: 23649820; PMCID: PMC3701222.

7. Bioactivity

Biological target:

IKK 16 hydrochloride is a selective IκB kinase (IKK) inhibitor for IKK2, IKK complex and IKK1 with IC_{50}s of 40 nM, 70 nM and 200 nM, respectively. IKK16 also inhibits leucine-rich repeat kinase-2 (LRRK2) with an IC_{50} of 50 nM.

In vitro activity

Phosphorylation of CYLD under basal conditions was inhibited by IKK16. NMDA treatment further promoted phosphorylation of CYLD at the PSD, but IKK16 failed to block the NMDA-induced effect. In vitro experiments using purified proteins demonstrated direct phosphorylation and activation of CYLD by the beta catalytic subunit of IKK. Activation of IKK in isolated PSDs also promoted phosphorylation of CYLD and an increase in endogenous deubiquitinase activity for K63-linked polyubiquitins. Altogether, the results suggest that in the absence of excitatory conditions, constitutive IKK activity at the PSD regulates CYLD and maintains basal levels of K63-linkage specific deubiquitination at the synapse.

Reference: Biochem Biophys Res Commun. 2014 Jul 18;450(1):550-4. https://pubmed.ncbi.nlm.nih.gov/24928390/

In vivo activity

Treatment of septic mice with IKK 16 at 1 hour after surgery significantly attenuated (P<0.05) the rises in serum creatinine (Fig. 2D) and lung MPO activity (Fig. 2F), and ameliorated the rise in ALT (Fig. 2E, P>0.05). Thus, treatment of septic mice with IKK 16 attenuated the sepsis-induced MOD (multiple organ dysfunction).

Reference: Dis Model Mech. 2013 Jul;6(4):1031-42. https://pubmed.ncbi.nlm.nih.gov/23649820/

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.