

Product data sheet



MedKoo Cat#: 558428 Name: NNK CAS: 64091-91-4 Chemical Formula: C ₁₀ H ₁₃ N ₃ O ₂ Exact Mass: 207.1008 Molecular Weight: 207.233		
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:

NNK is a procarcinogen, a major tobacco-specific toxicant that inhibits the expression of lysyl oxidase, a tumor suppressor.

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	30.0	144.76
DMSO	43.75	211.12
Ethanol	25.0	120.64
PBS (pH 7.2)	10.0	48.26

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	4.83 mL	24.13 mL	48.26 mL
5 mM	0.97 mL	4.83 mL	9.65 mL
10 mM	0.48 mL	2.41 mL	4.83 mL
50 mM	0.10 mL	0.48 mL	0.97 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. Sun Y, Wang H, Chen H, Zhang S, Li J, Zhang J, Tian J, Zhang Y, Hou H, Hu Q. Nicotine Inhibits the Cytotoxicity and Genotoxicity of NNK Mediated by CYP2A13 in BEAS-2B Cells. *Molecules*. 2022 Jul 29;27(15):4851. doi: 10.3390/molecules27154851. PMID: 35956805; PMCID: PMC9369970.
2. Jin Z, Gao F, Flagg T, Deng X. Tobacco-specific nitrosamine 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone promotes functional cooperation of Bcl2 and c-Myc through phosphorylation in regulating cell survival and proliferation. *J Biol Chem*. 2004 Sep 17;279(38):40209-19. doi: 10.1074/jbc.M404056200. Epub 2004 Jun 21. PMID: 15210690.

In vivo study

1. Arimoto-Kobayashi S, Sasaki K, Hida R, Miyake N, Fujii N, Saiki Y, Daimaru K, Nakashima H, Kubo T, Kiura K. Chemopreventive effects and anti-tumorigenic mechanisms of 2,6-dimethoxy-1,4-benzoquinone, a constituent of *Vitis coignetiae* Pulliat (crimson glory vine, known as yamabudo in Japan), toward 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)-induced lung tumorigenesis in A/J mice. *Food Chem Toxicol*. 2021 Aug;154:112319. doi: 10.1016/j.fct.2021.112319. Epub 2021 Jun 1. PMID: 34087405.
2. Carlson ES, Upadhyaya P, Villalta PW, Ma B, Hecht SS. Analysis and Identification of 2'-Deoxyadenosine-Derived Adducts in Lung and Liver DNA of F-344 Rats Treated with the Tobacco-Specific Carcinogen 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone

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and Enantiomers of its Metabolite 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanol. Chem Res Toxicol. 2018 May 21;31(5):358-370. doi: 10.1021/acs.chemrestox.8b00056. Epub 2018 Apr 19. PMID: 29651838; PMCID: PMC5995121.

7. Bioactivity

Biological target:

NNK simultaneously stimulates Bcl2 phosphorylation exclusively at Ser⁷⁰ and c-Myc at Thr⁵⁸ and Ser⁶² through activation of both ERK1/2 and PKC α .

In vitro activity

NNK simultaneously stimulates Bcl2 phosphorylation exclusively at Ser(70) and c-Myc at Thr(58) and Ser(62) through activation of both ERK1/2 and PKC α , which is required for NNK-induced survival and proliferation of human lung cancer cells. Treatment of cells with staurosporine or PD98059 blocks both Bcl2 and c-Myc phosphorylation and results in suppression of NNK-induced proliferation.

Reference: J Biol Chem. 2004 Sep 17;279(38):40209-19. <https://pubmed.ncbi.nlm.nih.gov/15210690/>

In vivo activity

This study found that oral intake of yamabudo-fr or DBQ affords significant protection against a tobacco-specific nitrosamine, 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)-induced mouse model of lung tumorigenesis. Yamabudo juice and DBQ inhibited the mutagenicity of NNK in the Ames test using Salmonella typhimurium TA1535 but not S. typhimurium YG7108, an alkylguanine DNA alkyltransferase-deficient strain (same as TA1535 but Δ ada_{st}::Km^r, Δ ogt_{st}::Cm^r). Yamabudo juice and DBQ might accelerate the repair of DNA damage caused by NNK and reduce DNA damage to cells.

Reference: Chem Res Toxicol. 2018 May 21;31(5):358-370. <https://pubmed.ncbi.nlm.nih.gov/34087405/>

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.