PRODUCT INFORMATION



4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone

Item No. 16414

CAS Registry No.: Formal Name:	64091-91-4 4-(methylnitrosoamino)-1-(3-pyridinyl)-1-butanone	
Synonym:	NNK	
MF:	C ₁₀ H ₁₃ N ₃ O ₂	
FW:	207.2	
Purity:	≥98%	
UV/Vis.:	λ _{max} : 229 nm	N
Supplied as:	A solid	14
Storage:	-20°C	
Stability:	≥4 years	
Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.		

Laboratory Procedures

4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone is supplied as a solid. A stock solution may be made by dissolving the 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone in the solvent of choice, which should be purged with an inert gas. 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 4-(methylnitrosamino)-1-(3-pyridyl)-1butanone in ethanol and DMSO is approximately 25 mg/ml and approximately 30 mg/ml in DMF.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone can be prepared by directly dissolving the solid in aqueous buffers. The solubility of 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone in PBS, pH 7.2, is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) is a tobacco-specific nitrosamine carcinogen.¹ Reactive metabolites of NNK alkylate DNA, forming pyridyloxobutyl (POB) and pyridylhydroxybutyl (PHB) adducts, and induce DNA methylation. NNK (100 mg/kg, single dose) increases the protein levels of DNA methyltransferase 1 (DNMT1) in mouse bronchial epithelial cells within one day and increases hypermethylation of the tumor suppressor genes Chd13, Prdm2, and Runx3 in lung tissue within three days.² It induces tumor formation preferentially in the lung via various routes of administration in animal models.³ NNK induces adenomas and adenocarcinomas, which are present after 16 and 50 weeks, respectively, in mouse lung when administered at a single dose of 10 µmol/animal. Lifetime administration of NNK (63.5 mg/animal) to rats results in a 90% incidence of lung tumors.⁴

References

- 1. Carlson, E.S., Upadhyaya, P., Villalta, P.W., et al. Chem. Res. Toxicol. 31(5), 358-370 (2018).
- 2. Jin, H., Chen, J.X., Wang, H., et al. Nutr. Cancer 67(1), 167-176 (2016).
- 3. Hecht, S.S. Chem. Res. Toxicol. 11(6), 559-603 (1998).
- 4. Rivenson, A., Hoffmann, D., Prokopczyk, B., et al. Cancer Res. 48(23), 6912-6917 (1988).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFFTY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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1180 EAST ELLSWORTH RD ANN ARBOR, MI 48108 · USA PHONE: [800] 364-9897 [734] 971-3335 FAX: [734] 971-3640 CUSTSERV@CAYMANCHEM.COM WWW.CAYMANCHEM.COM