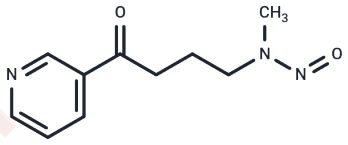
Data Sheet (Cat.No.T20533)

TargetMol

NNK

Chemical Properties



CAS No. : 64091-91-4

Formula: C10H13N3O2

Molecular Weight: 207.23

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	NNK is a nitrosated derivative of nicotine that activates the ERK1/2 and PKCα signaling pathways, induces Bcl2 phosphorylation at Ser70, and activates c-Myc at Thr58 and Ser62, thereby promoting the proliferation and survival of human lung cancer cells, and is commonly used to establish lung cancer mouse models.
Targets(IC50)	Lipoxygenase
In vitro	**METHODS**: CL1.0 cells were seeded in 96-well plates and treated with 0, 3 or 10 nM NNK for 24 h, followed by MTT to measure cell viability. Cells treated with 0 or 10 nM NNK for 24 h were collected and analyzed by RT-PCR. The expression of α3, α4, α5 and α7 was detected. GAPDH was used as internal control. Cells were also preincubated with -bungarotoxin (Bun, 10 nM) for 2 h and then stimulated with NNK (+, 10 nM) without (–) for 24 h. Study contactin-1 protein levels and mRNA expression. **RESULTS** NNK increased contactin-1 protein levels and up-regulated contactin-1 mRNA in a dose-dependent manner, indicating that NNK may directly stimulate gene transcription and cause CL1.0 cells to exhibit weaker toxic effects. [3]
In vivo	**METHODS**: Female A/J mice (7 weeks old) were treated with eight consecutive doses of NNK (3 μmol per week) by intragastric gavage (i.g.) or intraperitoneal injection, and the carcinogenesis of the mice was observed. **RESULTS** After 26 weeks, all mice developed lung adenomas. [1] **METHODS**: F344 rats were administered subcutaneously three times a week for 20 weeks with a total dose of 702 mg. The carcinogenesis of the mice was observed after 12 months. **RESULTS** 67% of the rats developed lung cancer. [2]

Solubility Information

Solubility	DMSO: 247.5 mg/mL (1194.33 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 20 mg/mL (96.51 mM),Solution. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.8256 mL	24.1278 mL	48.2556 mL
5 mM	0.9651 mL	4.8256 mL	9.6511 mL
10 mM	0.4826 mL	2.4128 mL	4.8256 mL
50 mM	0.0965 mL	0.4826 mL	0.9651 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Hecht SS, et al. Lung tumor induction in A/J mice by the tobacco smoke carcinogens 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone and benzo[a]pyrene: a potentially useful model for evaluation of chemopreventive agents. Carcinogenesis. 1994 Dec;15(12):2721-5.

Han G, Sinjab A, Rahal Z, et al.An atlas of epithelial cell states and plasticity in lung adenocarcinoma.Nature.2024, 627(8004): 656-663.

Hecht SS,et al. Comparative carcinogenicity in F344 rats of the tobacco-specific nitrosamines, N'-nitrosonornicotine and 4-(N-methyl-N-nitrosamino)-1-(3-pyridyl)-1-butanone. Cancer Res. 1980 Feb;40(2):298-302.

Hung YH,et al. 4-(Methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) enhances invasiveness of lung cancer cells by up-regulating contactin-1 via the alpha7 nicotinic acetylcholine receptor/ERK signaling pathway. Chem Biol Interact. 2009 May 15;179(2-3):154-9.

Tong M, Yu R, Silbermann E, Zabala V, Deochand C, de la Monte SM. Differential Contributions of Alcohol and Nicotine-Derived Nitrosamine Ketone (NNK) to White Matter Pathology in the Adolescent Rat Brain. Alcohol Alcohol. 2015 Nov;50(6):680-9. doi: 10.1093/alcalc/agv102. Epub 2015 Sep 15. PubMed PMID: 26373813; PubMed Central PMCID: PMC4608624.