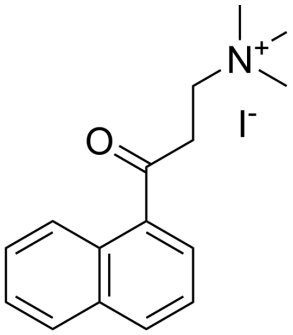
α-NETA

Cat. No.:	HY-138097
CAS No.:	115066-04-1
Molecular Formula:	$C_{16}H_{20}INO$
Molecular Weight:	369.24
Target:	Apoptosis; Cholinesterase (ChE); Aldehyde Dehydrogenase (ALDH); Chemerin Receptor
Pathway:	Apoptosis; Neuronal Signaling; Metabolic Enzyme/Protease; GPCR/G Protein
Storage:	4°C, protect from light, stored under nitrogen * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 83.33 mg/mL (225.68 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.7083 mL	13.5413 mL	27.0827 mL
	5 mM	0.5417 mL	2.7083 mL	5.4165 mL
	10 mM	0.2708 mL	1.3541 mL	2.7083 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (5.63 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.63 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.63 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

α-NETA is a potent and noncompetitive choline acetyltransferase (ChA) inhibitor with an IC_{50} of 9 μM. α-NETA is a potent ALDH1A1 (IC_{50}=0.04 μM) and chemokine-like receptor-1 (CMKLR1) antagonist. α-NETA weakly inhibits cholinesterase (ChE; IC_{50}=84 μM) and acetylcholinesterase (AChE; IC_{50}=300 μM). α-NETA has anti-cancer activity[1][2].

IC_{50} & Target	ALDH1	AChE

In Vitro

α-NETA (50-150 nM; 24 hours) decreases all cell lines viability in a dose-dependent manner[3].

α-NETA (2.5-10.0 μg/mL; 24 hours) leads to epithelial ovarian cancer (EOC) cell death associated with membrane blistering and cytoplasm leakage[3].
α-NETA treatment increases EOC cell expression of pyroptosis-associated proteins[3].
α-NETA is most potent in inhibiting aldehyde dehydrogenase 1 family, member A1 (ALDH1A1; IC_{50}=0.04 μM; purified enzymes assay), followed by CMKLR1 (IC_{50}=0.375 μM for β-ARR2 recruitment; Cell-based assay) and G9a histone lysine methyltransferase (IC_{50}=0.50 μM; purified enzymes assay). α-NETA selectively inhibits chemerin-stimulated CMKLR1 association with β-arrestin2[2].
α-NETA possesses fluorescent characteristics (excitation spectrum: maxima 255 and 297 nm; emission spectrum: maximum 437 nm) of naphthyl moiety[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[3]

Cell Line:	Ho8910, Ho8910PM, A2780, and Iose80 cells
Concentration:	50, 100, 150 nM
Incubation Time:	24 hours
Result:	Decreased all cell lines viability in a dose-dependent manner.

Apoptosis Analysis[3]

Cell Line:	Epithelial ovarian cancer (EOC) cell
Concentration:	2.5, 7.5, 10.0 μg/mL
Incubation Time:	24 hours
Result:	Led to EOC cell death associated with membrane blistering and cytoplasm leakage.

In Vivo

α-NETA (i.p.; 0.125 mg/kg; once every other day for 20 days) significantly decreases tumor volume and tumor weight[3].
α-NETA (s.c. injection; 3 mg/kg or 10 mg/kg; daily; for 30 days) significantly delays the onset of EAE with 3 mg/kg, and completely suppresses clinical signs for an average of nine days with 10 mg/kg beyond the first appearance of disease in control female C57BL/6 mice[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	BALB/c nude mice with skov3 cells[3]
Dosage:	0.125 mg/kg
Administration:	IP; once every other day for 20 days
Result:	Significantly decreased tumor volume and tumor weight.

CUSTOMER VALIDATION

- Hypertension. 2024 Feb 15.
- Eur J Pharmacol. 2022 Oct 25;175343.
- BMC Endocr Disord. 2023 Jan 10;23(1):9.
- Research Square Preprint. 2023 Sep 18.

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REFERENCES

[1]. Sastry BV, et al. Relationships between chemical structure and inhibition of choline acetyltransferase by 2-(alpha-naphthoyl)ethyltrimethylammonium and related compounds. Pharmacol Res Commun. 1988 Sep;20(9):751-71.

[2]. Graham KL, et al. A novel CMKLR1 small molecule antagonist suppresses CNS autoimmune inflammatory disease. PLoS One. 2014 Dec 1;9(12):e112925.

[3]. Qiao L, et al. α-NETA induces pyroptosis of epithelial ovarian cancer cells through the GSDMD/caspase-4 pathway. FASEB J. 2019 Nov;33(11):12760-12767.

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