Trimethylamine N-oxide dihydrate

Cat. No.: HY-108915 CAS No.: 62637-93-8 Molecular Formula: $C_3H_{13}NO_3$

Molecular Weight: 111.14

Target: Endogenous Metabolite; NOD-like Receptor (NLR); Reactive Oxygen Species; TGF-

beta/Smad

Metabolic Enzyme/Protease; Immunology/Inflammation; NF-κB; Stem Cell/Wnt; TGF-Pathway:

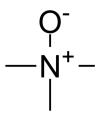
beta/Smad

Storage: Powder -20°C 3 years

> 4°C 2 years

In solvent -80°C 6 months

> -20°C 1 month



Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

H₂O: 100 mg/mL (899.77 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	8.9977 mL	44.9883 mL	89.9766 mL
	5 mM	1.7995 mL	8.9977 mL	17.9953 mL
	10 mM	0.8998 mL	4.4988 mL	8.9977 mL

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

In Vivo

- 1. Add each solvent one by one: PBS
 - Solubility: 120 mg/mL (1079.72 mM); Clear solution; Need ultrasonic
- 2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (22.49 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (22.49 mM); Clear solution
- 4. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (22.49 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Trimethylamine N-oxide dihydrate is a gut microbe-dependent metabolite of dietary choline and other trimethylaminecontaining nutrients. Trimethylamine N-oxide dihydrate induces inflammation by activating the ROS/NLRP3 inflammasome. Trimethylamine N-oxide dihydrate also accelerates fibroblast-myofibroblast differentiation and induces cardiac fibrosis by

	activating the TGF- β /smad2 signaling pathway [1][2][3].				
IC ₅₀ & Target	Human Endogenous Metabolite	NLRP3	Microbial Metabolite		
In Vitro	The size and migration of fibroblasts are increased after Trimethylamine N-oxide (TMAO) dihydrate treatment compared with non-treated fibroblasts in vitro. Trimethylamine N-oxide dihydrate increases TGF- β receptor I expression, which promotes the phosphorylation of Smad2 and up-regulates the expression of α -SMA and collagen I. The ubiquitination of TGF- β RI is decreased in neonatal mouse fibroblasts after Trimethylamine N-oxide dihydrate treatment. Trimethylamine N-oxide dihydrate also inhibits the expression of smurf2 ^[2] . ?Trimethylamine N-oxide is frequently found in the tissues of a variety of marine organisms that protects against the adverse effects of temperature, salinity, high urea and hydrostatic pressure ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.				
In Vivo	Trimethylamine N-oxide (TMAO) dihydrate contributes to cardiovascular diseases by promoting inflammatory responses. C57BL/6 mice are fed a normal diet, high-choline diet and/or 3-dimethyl-1-butanol (DMB) diet. The levels of Trimethylamine N-oxide dihydrate and choline are increased in choline-fed mice. Left ventricular hypertrophy, pulmonary congestion, and diastolic dysfunction are markedly exacerbated in heart failure with preserved ejection fraction (HFpEF) mice fed high-choline diets compared with mice fed the control diet. Myocardial fibrosis and inflammation were markedly increased in HFpEF mice fed high-choline diets compared with animals fed the control diet ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.				

CUSTOMER VALIDATION

- Phytomedicine. 2022 Mar 21;100:154067.
- Clin Chim Acta. 2023 Dec 16:117726.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Wei Shuai, et al. High-choline Diet Exacerbates Cardiac Dysfunction, Fibrosis, and Inflammation in a Mouse Model of Heart Failure With Preserved Ejection Fraction. J Card Fail. 2020 May 14;S1071-9164(19)31802-0.

[2]. Wenlong Yang, et al. Gut Microbe-Derived Metabolite Trimethylamine N-oxide Accelerates Fibroblast-Myofibroblast Differentiation and Induces Cardiac Fibrosis. J Mol Cell Cardiol. 2019 Sep;134:119-130.

[3]. Manuel T Velasquez, et al. Trimethylamine N-Oxide: The Good, the Bad and the Unknown. Toxins (Basel). 2016 Nov 8;8(11):326.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA