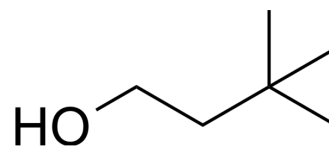


3,3-Dimethyl-1-butanol

Cat. No.:	HY-W012977		
CAS No.:	624-95-3		
Molecular Formula:	C ₆ H ₁₄ O		
Molecular Weight:	102		
Target:	TGF-beta/Smad; NF-κB; Endogenous Metabolite		
Pathway:	Stem Cell/Wnt; TGF-beta/Smad; NF-κB; Metabolic Enzyme/Protease		
Storage:	Pure form	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (980.39 mM; Need ultrasonic)
 H₂O : 9.09 mg/mL (89.12 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	9.8039 mL	49.0196 mL	98.0392 mL
	5 mM	1.9608 mL	9.8039 mL	19.6078 mL
	10 mM	0.9804 mL	4.9020 mL	9.8039 mL

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

In Vivo

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
 Solubility: ≥ 2.5 mg/mL (24.51 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
 Solubility: ≥ 2.5 mg/mL (24.51 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil
 Solubility: ≥ 2.5 mg/mL (24.51 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

3,3-Dimethyl-1-butanol (DMB) is an orally active inhibitor of trimethylamine (TMA) and trimethylamine N-oxide (TMAO). 3,3-Dimethyl-1-butanol inhibits the signaling pathway of p65 NF-κB and TGF-β1/Smad3. 3,3-Dimethyl-1-butanol has potential applications in cardiovascular disease (CVD)^{[1][2][3]}.

In Vitro

3,3-Dimethyl-1-butanol is a cosurfactant of lauryl sulfobetaine/water system^[4].
 MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

3,3-Dimethyl-1-butanol (1% DMB soluble in water; p.o.; 6 weeks) significantly reduces the cardiac hypertrophy and fibrosis in heart failure (HF) mice^[1].

3,3-Dimethyl-1-butanol (0.2% and 1.0% DMB soluble in water; p.o.; 21 d) increases the serum TMAO level with dose-dependent manner in ICR mice. 3,3-Dimethyl-1-butanol has been proved that the interaction between the gut and the brain has a regulatory effect on social behavior^[2].

3,3-Dimethyl-1-butanol (1.0% DMB soluble in water; p.o.; gestation period and suckling period) prevents the 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) induced hypertension in offspring of pregnant Sprague-Dawley rats^[3].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	C57BL6/J male mice (8-10 weeks old) with heart failure ^[1] .
Dosage:	1% DMB soluble in water.
Administration:	Oral gavage; 6 weeks.
Result:	Reduced the plasma trimethylamine N-oxide (TMAO) levels, the cross-sectional area of LV cardiomyocytes, and the area of LV interstitial fibrosis. Decreased the expression of ANP, BNP, β -MHC, collagen I α , collagen III and CTGF. Inhibited TNF- α , IL-6, IL-1 β , p65, TGF- β and Smad3 expression.

Animal Model:	Male and female ICR mice (8-weeks old) ^[2] .
Dosage:	0.2% and 1.0% DMB soluble in water.
Administration:	Oral gavage; 21 d.
Result:	Showed insignificantly effect on body weight, water intake, food intake, sexual preference, anxiety, depression and memory formation. Weakened the social dominance of mice.

Animal Model:	Pregnant Sprague-Dawley rats ^[3] .
Dosage:	1.0% DMB soluble in water.
Administration:	Oral gavage; gestation period and suckling period.
Result:	Increased kidney weight, plasma trimethylamine (TMA) level and acetic acid, reduced diastolic. Had significantly effect on gut microbiota composition.

REFERENCES

- [1]. Wang G, et al. 3,3-Dimethyl-1-butanol attenuates cardiac remodeling in pressure-overload-induced heart failure mice. *J Nutr Biochem*. 2020 Apr;78:108341.
- [2]. Mao J, et al. Repeated 3,3-Dimethyl-1-butanol exposure alters social dominance in adult mice. *Neurosci Lett*. 2021 Jul 27;758:136006.
- [3]. Hsu CN, et al. Maternal 3,3-Dimethyl-1-Butanol Therapy Protects Adult Male Rat Offspring against Hypertension Programmed by Perinatal TCDD Exposure. *Nutrients*. 2021 Aug 30;13(9):3041.
- [4]. Valiente M, et al. 1-Butanol and 3, 3-dimethyl-1-butanol as cosurfactants of the laurylsulfobetaine/water system[J]. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2001, 183: 235-246.

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

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