3,3-Dimethyl-1-butanol

Cat. No.:	HY-W01297	7	
CAS No.:	624-95-3		
Molecular Formula:	$C_{6}H_{14}O$		
Molecular Weight:	102		
Target:	TGF-beta/S	mad; NF-ı	kB; Endogenous Metabolite
Pathway:	Stem Cell/V	Vnt; TGF-b	peta/Smad; NF-кВ; 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) H ₂ O : 9.09 mg/mL (89.12 mM; Need ultrasonic)				
Preparing Stock Solutions		Solvent Mass Concentration	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	1. 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				
	2. 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				
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (24.51 mM); Clear solution				

Description3,3-Dimethyl-1-butanol (DMB) is an orally active inhibitor of trimethylamine (TMA) and trimethylamine N-oxide (TMAO).Dimethyl-1-butanol inhibits the signaling pathway of p65 NF-κB and TGF-β1/Smad3. 3,3-Dimethyl-1-butanol has potent applications in cardiovascular disease (CVD) ^{[1][2][3]} .	3,3- tial
In Vitro3,3-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.	







Product Data Sheet

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 dosedependent 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 2,3,7,8tetrachlorodibenzo-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 Iα, collagen III and CTGF. Inhibited TNF-α, IL-6, IL-1β, 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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