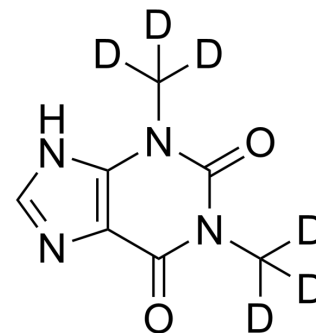


Theophylline-d₆

Cat. No.:	HY-B0809S	
CAS No.:	117490-39-8	
Molecular Formula:	C ₇ H ₂ D ₆ N ₄ O ₂	
Molecular Weight:	186.2	
Target:	Phosphodiesterase (PDE); Adenosine Receptor; Autophagy; Endogenous Metabolite	
Pathway:	Metabolic Enzyme/Protease; GPCR/G Protein; Autophagy	
Storage:	Powder	-20°C 3 years 4°C 2 years
	In solvent	-80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 10 mg/mL (53.71 mM)
 DMF : ≥ 10 mg/mL (53.71 mM)
 PBS (pH 7.2) : ≥ 1 mg/mL (5.37 mM)
 Ethanol : ≥ 1 mg/mL (5.37 mM)
 * "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent		1 mg	5 mg	10 mg
	Concentration	Mass			
	1 mM		5.3706 mL	26.8528 mL	53.7057 mL
	5 mM		1.0741 mL	5.3706 mL	10.7411 mL
	10 mM		0.5371 mL	2.6853 mL	5.3706 mL

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

BIOLOGICAL ACTIVITY

Description

Theophylline-d₆ is the deuterium labeled Theophylline. Theophylline is a nonselective phosphodiesterase (PDE) inhibitor, adenosine receptor blocker, and histone deacetylase (HDAC) activator.

In Vitro

Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs^[1].

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

REFERENCES

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- [1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019;53(2):211-216.
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- [3]. Marques LJ, et al. Pentoxifylline inhibits TNF-alpha production from human alveolar macrophages. *Am J Respir Crit Care Med.* 1999 Feb;159(2):508-11.
- [4]. Daly JW, et al. Adenosine receptors: development of selective agonists and antagonists. *Prog Clin Biol Res.* 1987;230:41-63.
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Caution: Product has not been fully validated for medical applications. For research use only.

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