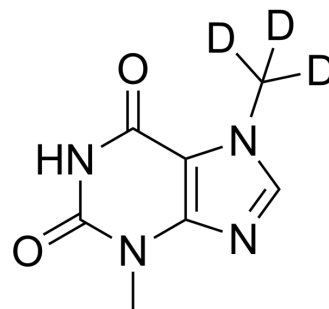


Theobromine-d₃

Cat. No.:	HY-N0138S1		
CAS No.:	65566-69-0		
Molecular Formula:	C ₇ H ₅ D ₃ N ₄ O ₂		
Molecular Weight:	183.18		
Target:	Adenosine Receptor; Endogenous Metabolite		
Pathway:	GPCR/G Protein; Metabolic Enzyme/Protease		
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 : 1.1 mg/mL (6.01 mM; Need ultrasonic)
 H₂O : 1.1 mg/mL (6.01 mM; Need ultrasonic)
 H₂O : 1.1 mg/mL (6.01 mM; Need ultrasonic)
 DMSO : 1.1 mg/mL (6.01 mM; Need ultrasonic)

	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	5.4591 mL	27.2956 mL	54.5911 mL
	5 mM	1.0918 mL	5.4591 mL	10.9182 mL
	10 mM	---	---	---

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

BIOLOGICAL ACTIVITY

Description

Theobromine-d₃ is the deuterium labeled Theobromine. Theobromine is a methylxanthine found in cacao beans which can inhibit adenosine receptor A1 (AR1) signaling.

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

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019;53(2):211-216.

[2]. Mitani T, et al. Theobromine suppresses adipogenesis through enhancement of CCAAT-enhancer-binding protein β degradation by adenosine receptor A1.

[3]. Martín-Peláez S, et al. Effect of cocoa's theobromine on intestinal microbiota of rats. Mol Nutr Food Res. 2017 Oct;61(10).

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

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