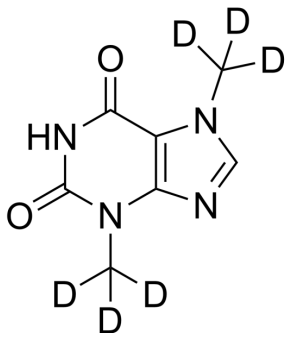
Theobromine-d_6

Cat. No.:	HY-N0138S
CAS No.:	117490-40-1
Molecular Formula:	$C_7H_2D_6N_4O_2$
Molecular Weight:	186.2
Target:	Adenosine Receptor; Endogenous Metabolite; Isotope-Labeled Compounds
Pathway:	GPCR/G Protein; Metabolic Enzyme/Protease; Others
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 : 2.86 mg/mL (15.36 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	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

Theobromine-d_6 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).

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