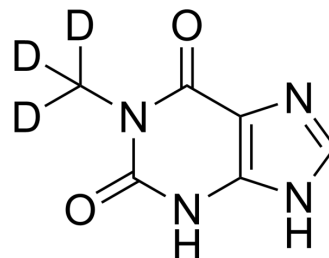


1-Methylxanthine-d₃

Cat. No.:	HY-W008449S2
CAS No.:	1216430-61-3
Molecular Formula:	C ₆ H ₃ D ₃ N ₄ O ₂
Molecular Weight:	169.16
Target:	Drug Metabolite; Endogenous Metabolite; Isotope-Labeled Compounds
Pathway:	Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	1-Methylxanthine-d ₃ is deuterated labeled 1-Methylxanthine (HY-W008449). 1-Methylxanthine, a caffeine derivative, is an essential human urinary metabolite of caffeine and theophylline (1,3-dimethylxanthine, TP) ^[1] . 1-Methylxanthine enhances the radiosensitivity of tumor cells ^[2] .
In Vitro	<p>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].</p> <p>1-Methylxanthine (1-MTX; 3 mM; for 30 min) increases the radiation-induced clonogenic and apoptotic cell (RKO human colorectal cancer cells carrying wild type protein 53 kDa (p53)) death^[3].</p> <p>1-Methylxanthine (1MX) exhibits similar activities to other naturally occurring methylxanthines. Unlike caffeine, TP, and theobromine, 3-Methylxanthine (3MX) and 1-methylxanthine do not occur naturally at high levels in plants^[2].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>

REFERENCES

- [1]. Algharrawi KH, et al. Direct conversion of theophylline to 3-methylxanthine by metabolically engineered E. coli. *Microb Cell Fact.* 2015 Dec 21;14:203.
- [2]. Youn H, et al. 1-Methylxanthine enhances the radiosensitivity of tumor cells. *Int J Radiat Biol.* 2009 Feb;85(2):167-74.
- [3]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother.* 2019 Feb;53(2):211-216.

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

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