

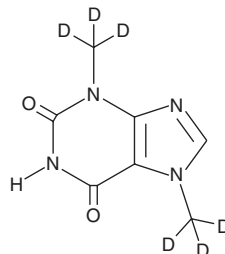
PRODUCT INFORMATION



Theobromine-d₆

Item No. 9003565

CAS Registry No.: 117490-40-1
Formal Name: 3,7-dihydro-3,7-di(methyl-d₃)-1H-purine-2,6-dione
MF: C₇H₂D₆N₄O₂
FW: 186.2
Chemical Purity: ≥95% (Theobromine)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₆); ≤1% d₀
UV/Vis.: λ_{max}: 273 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years
Item Origin: Synthetic



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Theobromine-d₆ is intended for use as an internal standard for the quantification of theobromine (Item No. 21745) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

Theobromine-d₆ is supplied as a crystalline solid. A stock solution may be made by dissolving the theobromine-d₆ in the solvent of choice, which should be purged with an inert gas. Theobromine-d₆ is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of theobromine-d₆ in ethanol is approximately 1 mg/ml and approximately 10 mg/ml in DMSO and DMF.

Description

Theobromine is a methylxanthine alkaloid and derivative of caffeine (Item No. 14118) that has been found in cocoa beans and has diverse biological activities.¹⁻³ It is an adenosine A₁ receptor antagonist (IC₅₀s = 200-280 μM in radioligand binding assays using rat brain membranes).² Theobromine (150 μg/ml) increases AMPK phosphorylation and inhibits adipocyte differentiation, ERK and JNK phosphorylation, and IL-6 and TNF-α production in 3T3-L1 preadipocytes cultured in differentiation medium.¹ It inhibits decreases in renal cortex SIRT1 activity and increases in NADPH oxidase-dependent reactive oxygen species (ROS) production, as well as reduces kidney hypertrophy and albuminuria in a spontaneously hypertensive rat model of streptozotocin-induced diabetes when administered at a dose of 5 mg/kg per day.³ Theobromine is toxic to dogs with an LD₅₀ value of 250 to 500 mg/kg.⁴

References

1. Jang, Y.J., Koo, H.J., Sohn, E.-H., *et al.* Theobromine inhibits differentiation of 3T3-L1 cells during the early stage of adipogenesis via AMPK and MAPK signaling pathways. *Food Funct.* **6**(7), 2365-2374 (2015).
2. Daly, J.W., Butts-Lamb, P., and Padgett, W. Subclasses of adenosine receptors in the central nervous system: Interaction with caffeine and related methylxanthines. *Cell. Mol. Neurobiol.* **3**(1), 69-80 (1983).
3. Papadimitriou, A., Silva, K.C., Peixoto, E.B.M.I., *et al.* Theobromine increases NAD⁺/Sirt-1 activity and protects the kidney under diabetic conditions. *Am. J. Physiol. Renal Physiol.* **308**(3), D209-F225 (2015).
4. Lawrence, L.P. Chocolate toxicosis. *The 5-minute veterinary consult: Canine and feline.* Smith, F.W.K. Jr., editor, 3rd edition, Lippincott Williams & Wilkins (2004).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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