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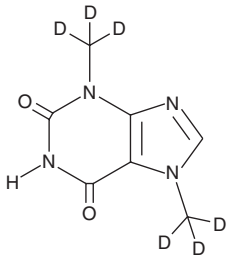
PRODUCT INFORMATION

Theobromine-d_6

Item No. 9003565

CAS Registry No.:	117490-40-1
Formal Name:	3,7-dihydro-3,7-di(methyl-d_3)-1H-purine-2,6-dione
MF:	$C_7H_2D_6N_4O_2$
FW:	186.2
Chemical Purity:	≥95% (Theobromine)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_6); ≤1% d_0
UV/Vis.:	λ_{max}: 273 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥2 years
Item Origin:	Synthetic



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

Laboratory Procedures

Theobromine-d_6 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-d_6 is supplied as a crystalline solid. A stock solution may be made by dissolving the theobromine-d_6 in the solvent of choice, which should be purged with an inert gas. Theobromine-d_6 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of theobromine-d_6 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 A_1 receptor antagonist (IC_{50}s = 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 LD_{50} 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).

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