

Product Data Sheet

Product Name: Theobromine-d6

Cat. No.: GC48162

Chemical Properties

Cas. No. 117490-40-1

SMILES O=C(C(N(C([2H])([2H])[2H])C=N1)=C1N2C([2H])([2H])[2H])NC2=O

Formula C7H2D6N4O2

M.Wt 186.2

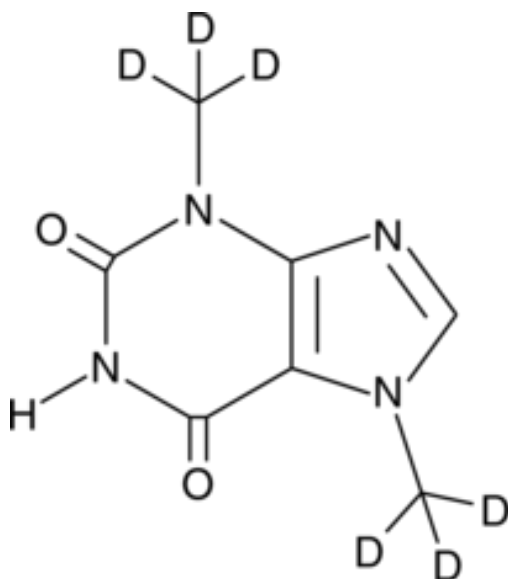
Solubility DMF: 10 mg/ml, DMSO: 10 mg/ml, Ethanol: 1 mg/ml, PBS (pH 7.2): 1 mg/ml

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

Theobromine-d₆ is intended for use as an internal standard for the quantification of theobromine by GC- or LC-MS. Theobromine is a methylxanthine alkaloid and derivative of caffeine that has been found in cocoa beans and has diverse biological activities.^{1,2,3} It is an adenosine A₁ receptor

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

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antagonist (IC_{50} s = 200-280 μ M in radioligand binding assays using rat brain membranes).²

Theobromine (150 μ g/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

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 pathwaysFood 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 methylxanthinesCell. 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 conditionsAm. J. Physiol. Renal Physiol.308(3)F209-F225(2015) 4.Lawrence, L.P.Chocolate toxicosisThe 5-minute veterinary consult: Canine and feline(2004)

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