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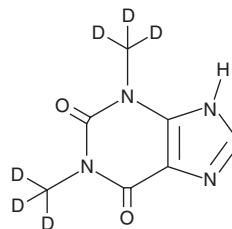
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PRODUCT INFORMATION



Theophylline-d₆ Item No. 9003566

CAS Registry No.: 117490-39-8
Formal Name: 3,9-dihydro-1,3-di(methyl-d₃)-1H-purine-2,6-dione
Synonym: 1,3-Dimethylxanthine-d₆
MF: C₇H₂D₆N₄O₂
FW: 186.2
Chemical Purity: ≥95% (Theophylline)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₆); ≤1% d₀
UV/Vis.: λ_{max}: 271 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



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

Laboratory Procedures

Theophylline-d₆ is intended for use as an internal standard for the quantification of theophylline (Item No. 23760) 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).

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

Description

Theophylline is an inhibitor of phosphodiesterase (PDE; K_i = 100 μM).¹ It is also an adenosine A₁ and A₂ receptor antagonist (K_i = 14 μM for both).² Theophylline induces relaxation of isolated cat bronchial smooth muscle segments precontracted with acetylcholine (EC₄₀ = 117 μM).³ It inhibits ovalbumin-induced increases in bronchoalveolar lavage fluid (BALF) eosinophil infiltration in an ovalbumin-sensitized mouse model of allergic asthma. Formulations containing theophylline have been used in the treatment of asthma and chronic obstructive pulmonary disease (COPD).

References

1. Butcher, R.W. and Sutherland, E.W. Adenosine 3',5'-phosphate in biological materials. I. Purification and properties of cyclic 3',5'-nucleotide phosphodiesterase and use of this enzyme to characterize adenosine 3',5'-phosphate in human urine. *J. Biol. Chem.* **237**(4), 1244-1250 (1962).
2. Daly, J.W., Padgett, W., Shamim, M.T., *et al.* 1,3-Dialkyl-8-(p-sulfophenyl)xanthines: Potent water-soluble antagonists for A₁- and A₂-adenosine receptors. *J. Med. Chem.* **28**(4), 487-492 (1985).
3. Leemans, J., Kirschvink, N., and Gustin, P. A comparison of *in vitro* relaxant responses to ipratropium bromide, β-adrenoceptor agonists and theophylline in feline bronchial smooth muscle. *Vet. J.* **193**(1), 228-233 (2012).

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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