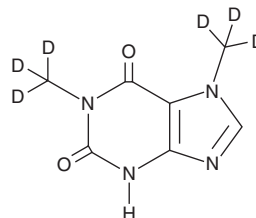


PRODUCT INFORMATION



Paraxanthine-d₆ Item No. 9003564

CAS Registry No.: 117490-41-2
Formal Name: 3,7-dihydro-1,7-di(methyl-d₃)-1H-purine-2,6-dione
Synonym: 1,7-Dimethylxanthine-d₆
MF: C₇H₂D₆N₄O₂
FW: 186.2
Chemical Purity: ≥95% (Paraxanthine)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₆); ≤1% d₀
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

Paraxanthine-d₆ is intended for use as an internal standard for the quantification of paraxanthine (Item No. 21068) 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).

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

Description

Paraxanthine is an active metabolite of caffeine (Item No. 14118).¹ It is formed via N3-demethylation of caffeine by the cytochrome P450 (CYP) isoform CYP1A2. Paraxanthine is an adenosine A₁ and A₂ receptor antagonist (K_s = 35 and 22 μM, respectively).² *In vivo*, paraxanthine (30 mg/kg) increases striatal cGMP and extracellular striatal dopamine levels and locomotor activity, as well as inhibits motor depression induced by the adenosine A₁ agonist CPA (N⁶-cyclopentyladenosine; Item No. 21448) or the adenosine A₂ receptor agonist CGS 21680 (Item No. 17126) in rats not habituated to caffeine.³ It also promotes wakefulness and increases locomotor activity and core temperature in narcoleptic transgenic mice without increasing behavioral anxiety.⁴

References

1. Tassaneeyakul, W., Birkett, D.J., McManus, M.E., *et al.* Caffeine metabolism by human hepatic cytochromes P450: contributions of 1A2, 2E1 and 3A isoforms. *Biochem. Pharmacol.* **47**(10), 1767-1776 (1994).
2. Chou, C.-C. and Vickroy, T.W. Antagonism of adenosine receptors by caffeine and caffeine metabolites in equine forebrain tissues. *Am. J. Vet. Res.* **64**(2), 216-224 (2003).
3. Orrú, M., Guitart, X., Karcz-Kubicha, M., *et al.* Psychostimulant pharmacological profile of paraxanthine, the main metabolite of caffeine in humans. *Neuropharmacology* **67**, 476-484 (2013).
4. Okuro, M., Fujiki, N., Kotorii, N., *et al.* Effects of paraxanthine and caffeine on sleep, locomotor activity, and body temperature in orexin/ataxin-3 transgenic narcoleptic mice. *Sleep* **33**(7), 930-942 (2010).

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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