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Produktinformation

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- Trockeneiszuschlag
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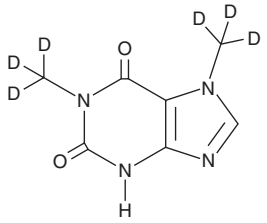
PRODUCT INFORMATION

Paraxanthine-d_6

Item No. 9003564

CAS Registry No.:	117490-41-2
Formal Name:	3,7-dihydro-1,7-di(methyl-d_3)-1H-purine-2,6-dione
Synonym:	1,7-Dimethylxanthine-d_6
MF:	$C_7H_2D_6N_4O_2$
FW:	186.2
Chemical Purity:	≥95% (Paraxanthine)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_6); ≤1% d_0
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

Paraxanthine-d_6 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-d_6 is supplied as a crystalline solid. A stock solution may be made by dissolving the paraxanthine-d_6 in the solvent of choice, which should be purged with an inert gas. Paraxanthine-d_6 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of paraxanthine-d_6 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 A_1 and A_2 receptor antagonist (K_is = 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 A_1 agonist CPA (N^6-cyclopentyladenosine; Item No. 21448) or the adenosine A_2 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).

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