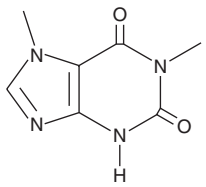
PRODUCT INFORMATION

Paraxanthine

Item No. 21068

CAS Registry No.:	611-59-6
Formal Name:	3,7-dihydro-1,7-dimethyl-1H-purine-2,6-dione
Synonyms:	1,7-Dimethylxanthine, NSC 400018
MF:	$C_7H_8N_4O_2$
FW:	180.2
Purity:	≥98%
UV/Vis.:	λ_{max}: 269 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

Paraxanthine is supplied as a crystalline solid. A stock solution may be made by dissolving the paraxanthine in the solvent of choice. Paraxanthine is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of paraxanthine in these solvents is approximately 0.5, 30, and 20 mg/ml, respectively.

Paraxanthine is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, paraxanthine should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Paraxanthine has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

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).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM