**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:** C₇H₈N₄O₂  
**FW:** 180.2  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 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 inhibitor of phosphodiesterase 9 (PDE9) and an antagonist of adenosine receptors A₁ and A₂ (Kᵢₛ = 35 and 22 μM, respectively in equine forebrain tissues).<sup>1,2</sup> It is the main metabolite of caffeine (Item No. 14118) in humans, making up 80% of the three dimethylxanthine metabolites produced by caffeine demethylation.<sup>1,3</sup> Paraxanthine increases locomotor activity and counteracts adenosine receptor agonist-induced motor depression in rats not habituated to caffeine.<sup>1</sup> At a dose of 30 mg/kg, paraxanthine induces a significant increase in striatal cGMP and extracellular striatal dopamine concentrations in vivo. It also promotes wakefulness and increases locomotor activity and core temperature in narcoleptic transgenic mice without increasing behavioral anxiety.<sup>3</sup>

**References**