# PRODUCT INFORMATION

## 1,3,7-Trimethyluric Acid-$d_9$

*Item No. 9003567*

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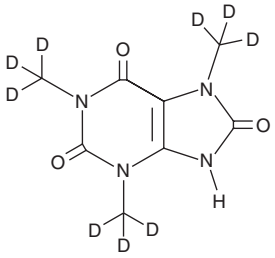
| **CAS Registry No.:** | 117490-42-3 |
| **Formal Name:** | 7,9-dihydro-1,3,7-tri(methyl-$d_3$)-1H-purine-2,6,8(3H)-trione |
| **Synonyms:** | 8-oxo Caffeine-$d_9$, TMU-$d_9$ |
| **MF:** | $C_8HD_9N_4O_3$ |
| **FW:** | 219.2 |
| **Chemical Purity:** | ≥95% (1,3,7-Trimethyluric Acid) |
| **Deuterium Incorporation:** | ≥99% deuterated forms ($d_1$-$d_9$); ≤1% $d_0$ |
| **UV/Vis.:** | $\lambda_{max}$: 236, 290 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

1,3,7-Trimethyluric acid-$d_9$ is intended for use as an internal standard for the quantification of 1,3,7-trimethyluric acid (Item No. 16949) 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).

1,3,7-Trimethyluric acid-$d_9$ is supplied as a crystalline solid. A stock solution may be made by dissolving the 1,3,7-trimethyluric acid-$d_9$ in the solvent of choice, which should be purged with an inert gas. 1,3,7-Trimethyluric acid-$d_9$ is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 1,3,7-trimethyluric acid-$d_9$ in ethanol is approximately 1 mg/ml and approximately 30 mg/ml in DMSO and DMF.

### Description

1,3,7-Trimethyluric acid is a derivative of uric acid (Item No. 16219) and a metabolite of caffeine (Item No. 14118).[1] It is formed from caffeine by the cytochrome P450 (CYP) isoform CYP3A4. 1,3,7-Trimethyluric acid (500 µM) scavenges hydroxyl radicals in a cell-free assay and inhibits *t*-butyl hydroperoxide-induced lipid peroxidation by 56.5% in isolated human erythrocyte membranes.[2]

### 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. Bhat, V.B., Sridhar, G.R., and Madyastha, K.M. Efficient scavenging of hydroxyl radicals and inhibition of lipid peroxidation by novel analogues of 1,3,7-trimethyluric acid. *Life Sci.* **70(4)**, 381-393 (2001).





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