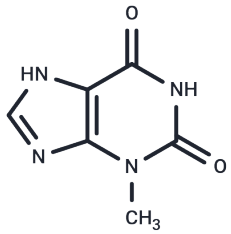
Data Sheet (Cat.No.PDK0014)

TargetMol

3-Methylxanthine

Chemical Properties



CAS No. : 1076-22-8

Formula: C6H6N4O2

Molecular Weight: 166.14

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	3-Methylxanthine, a xanthine derivative, is a cyclic guanosine monophosphate (GMP) inhibitor with an IC50 of 920 μM on guinea-pig isolated trachealis muscle. It inhibits xanthine crystallization and could protect patients with xanthinuria from developing renal xanthine calculi.
Targets(IC50)	Endogenous Metabolite
In vitro	To identify in vitro inhibitors of xanthine crystallization that have potential for inhibiting the formation of xanthine crystals in urine and preventing the development of the renal calculi in patients with xanthinuria. METHODS AND RESULTS: The formation of xanthine crystals in synthetic urine and the effects of 10 potential crystallization inhibitors were assessed using a kinetic turbidimetric system with a photometer. The maximum concentration tested for each compound was: 20 mg/L for 3-Methylxanthine (3-MX); 40 mg/L for 7-methylxanthine (7-MX), 1-methylxanthine (1-MX), theobromine (TB), theophylline, paraxanthine, and caffeine; 45 mg/L for 1-methyluric acid; 80 mg/L for 1,3-dimethyluric acid; and 200 mg/L for hypoxanthine. Scanning electron microscopy was used to examine the morphology of the crystals formed when inhibitory effects were observed. Only 7-MX, 3-MX, and 1-MX significantly inhibited xanthine crystallization at the tested concentrations. Mixtures of inhibitors had an additive effect rather than a synergistic effect on crystallization. CONCLUSIONS: Two of the inhibitors identified here-7-MX and 3-MX-are major metabolites of TB. In particular, after TB consumption, 20% is excreted in the urine as TB, 21.5% as 3-MX, and 36% as 7-MX. Thus, consumption of theobromine could protect patients with xanthinuria from the development of renal xanthine calculi. Clinical trials are necessary to demonstrate these effects in vivo.

Solubility Information

Solubility	1M NaOH: 50 mg/mL (300.95 mM),when pH is adjusted to 11 with 1 M NaOH. Sonication is recommended. DMSO: 2.61 mg/mL (15.71 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	6.019 mL	30.0951 mL	60.1902 mL
5 mM	1.2038 mL	6.019 mL	12.038 mL
10 mM	0.6019 mL	3.0095 mL	6.019 mL
50 mM	0.1204 mL	0.6019 mL	1.2038 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Xanthine urolithiasis: Inhibitors of xanthine crystallization. PLoS One. 2018 Aug 29;13(8):e0198881.