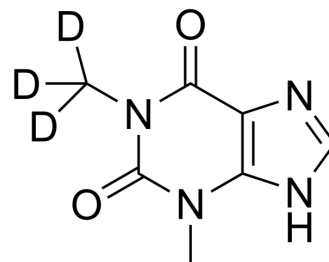


## Theophylline-d<sub>3</sub>

|                           |   |
|---------------------------|---|
| <b>Cat. No.:</b>          | HY-B0809S1  |
| <b>CAS No.:</b>           | 65566-68-9  |
| <b>Molecular Formula:</b> | C <sub>7</sub> H <sub>5</sub> D <sub>3</sub> N <sub>4</sub> O <sub>2</sub>  |
| <b>Molecular Weight:</b>  | 183.18  |
| <b>Target:</b>            | Endogenous Metabolite; Adenosine Receptor; HDAC; TNF Receptor; Interleukin Related; Phosphodiesterase (PDE); Apoptosis; Isotope-Labeled Compounds |
| <b>Pathway:</b>           | Metabolic Enzyme/Protease; GPCR/G Protein; Cell Cycle/DNA Damage; Epigenetics; Apoptosis; Immunology/Inflammation; Others                         |
| <b>Storage:</b>           | Please store the product under the recommended conditions in the Certificate of Analysis.   |



### BIOLOGICAL ACTIVITY

|                    |   |
|--------------------|---|
| <b>Description</b> | <p>Theophylline-d<sub>3</sub> is deuterated labeled Theophylline (HY-B0809). Theophylline (1,3-Dimethylxanthine) is a potent phosphodiesterase (PDE) inhibitor, adenosine receptor antagonist, and histone deacetylase (HDAC) activator. Theophylline (1,3-Dimethylxanthine) inhibits PDE3 activity to relax airway smooth muscle. Theophylline (1,3-Dimethylxanthine) has anti-inflammatory activity by increase IL-10 and inhibit NF-κB into the nucleus. Theophylline (1,3-Dimethylxanthine) induces apoptosis. Theophylline (1,3-Dimethylxanthine) can be used for asthma and chronic obstructive pulmonary disease (COPD) research<sup>[1][2][3][4][5]</sup>.</p>  |
| <b>In Vitro</b>    | <p>Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs<sup>[1]</sup>.</p> <p>Theophylline (1,3-Dimethylxanthine) (1-1000 μM) inhibits cAMP hydrolysis by PDE in homogenates of bronchial tissue to relax human bronchus and pulmonary arteries<sup>[2]</sup>.</p> <p>Theophylline (1,3-Dimethylxanthine) (10 μg/mL; 24 h; eosinophils) induces apoptosis through a reduction in the antiapoptotic protein Bcl-2<sup>[3]</sup>.</p> <p>Theophylline (1,3-Dimethylxanthine) (0-500 μM; 2 h; A549 cells) inhibits NF-κB activation, I kappa B alpha (I-κBα) degradation and decreases the level of IL-6 in a concentration-dependent manner<sup>[4]</sup>.</p> <p>Theophylline (1,3-Dimethylxanthine) (0-1000 μM; 30 min; A549 cells) induces histone deacetylase activity to decrease inflammatory gene expression<sup>[5]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> |
| <b>In Vivo</b>     | <p>Theophylline (1,3-Dimethylxanthine) (100 mg/kg; i.p.; daily, for 9 d; male Swiss mice) has anti-inflammatory activity in mice and increases IL-6 and IL-10 levels and inhibits TNF-α and NO<sup>[2]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>  |

### REFERENCES

- [1]. Rabe KF, et, al. Theophylline and selective PDE inhibitors as bronchodilators and smooth muscle relaxants. *Eur Respir J.* 1995 Apr;8(4):637-42.
- [2]. Németh ZH, et, al. Amrinone and theophylline differentially regulate cytokine and nitric oxide production in endotoxemic mice. *Shock.* 1997 May;7(5):371-5.
- [3]. Ichiyama T, et, al. Theophylline inhibits NF-kappa B activation and I kappa B alpha degradation in human pulmonary epithelial cells. *Naunyn Schmiedebergs Arch*

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Pharmacol. 2001 Dec;364(6):558-61.

[4]. Ito K, et, al, Adcock IM, Barnes PJ. A molecular mechanism of action of theophylline: Induction of histone deacetylase activity to decrease inflammatory gene expression. Proc Natl Acad Sci U S A. 2002 Jun 25;99(13):8921-6.

[5]. Barnes PJ. Theophylline. Am J Respir Crit Care Med. 2013 Oct 15;188(8):901-6.

[6]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

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