

Product Data Sheet

Elemicin-d₃

Cat. No.: HY-N6807S Molecular Formula: $C_{12}H_{13}D_3O_3$ Molecular Weight: 211.27

Target: Bacterial; Influenza Virus; Stearoyl-CoA Desaturase (SCD); Isotope-Labeled

Compounds

Pathway: Anti-infection; Metabolic Enzyme/Protease; Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

BIOLOGICAL ACTIVITY

Description	Elemicin- d_3 is deuterated labeled Pemafibrate (HY-17618). Pemafibrate is a highly selective PPAR α agonist, with an EC $_{50}$ of 1 nM.
In Vitro	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 ^[1] . Elemicin (62.5, 125, 250, 500, 1000 μ M) has an IC ₅₀ value of 910 μ M in HepG2 cells ^[3] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Elemicin (500 mg/kg; orally gavage; every 24 h for 3 weeks) impairs liver function in mice. Elemicin inhibits liver SCD1, leading to a disequilibrium of lysophosphatidylcholines (LPCs) ^[4] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Yi-Kun Wang, et al. Role of Metabolic Activation in Elemicin-Induced Cellular Toxicity. J Agric Food Chem. 2019 Jul 24;67(29):8243-8252.

[2]. Yang XN, et al. Metabolic Activation of Elemicin Leads to the Inhibition of Stearoyl-CoA Desaturase 1. Chem Res Toxicol. 2019 Sep 10.

[3]. Xiao-Nan Yang, et al. Metabolic Activation of Elemicin Leads to the Inhibition of Stearoyl-CoA Desaturase 1. Chem Res Toxicol. 2019 Oct 21;32(10):1965-1976.

 $[4]. A yodeji\ Oluwabunmi\ Oriola, et\ al.\ Essential\ Oils\ and\ Their\ Compounds\ as\ Potential\ Anti-Influenza\ Agents.\ Molecules.\ 2022\ Nov\ 12;27(22):7797.$

 $[5]. \ Russak \ EM, et \ al. \ Impact \ of \ Deuterium \ Substitution \ on \ the \ Pharmacokinetics \ of \ Pharmaceuticals. \ Ann \ Pharmacother. \ 2019 \ Feb; \\ 53(2):211-216.$

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

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA