Product Data Sheet

Inhibitors

Screening Libraries

Trans-Anethole-d₃

 $\begin{array}{lll} \textbf{Cat. No.:} & \textbf{HY-N0367S} \\ \textbf{CAS No.:} & 444904-67-0 \\ \textbf{Molecular Formula:} & \textbf{C}_{10}\textbf{H}_{9}\textbf{D}_{3}\textbf{O} \\ \end{array}$

Molecular Weight: 151.22

Target: Endogenous Metabolite; Isotope-Labeled Compounds

Pathway: Metabolic Enzyme/Protease; Others

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

Analysis.

BIOLOGICAL ACTIVITY

| Description | Trans-Anethole- d_3 is deuterated labeled α -Terpineol (HY-N5142). α -Terpineol is isolated from Eucalyptus globulus Labill, exhibits strong antimicrobial activity against periodontopathic and cariogenic bacteria ^[1] . α -Terpineol possesses antifungal activity against T. mentagrophytes, and the activity might lead to irreversible cellular disruption ^[2] . |
|-------------|--|
| 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] . MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

REFERENCES

[1]. Tabanca N, et al. Estrogenic activity of isolated compounds and essential oils of Pimpinella species from Turkey, evaluated using a recombinant yeast screen. Planta Med. 2004 Aug;70(8):728-35.

[2]. Nakagawa Y, et al. Cytotoxic and xenoestrogenic effects via biotransformation of trans-anethole on isolated rat hepatocytes and cultured MCF-7 human breast cancer cells. Biochem Pharmacol. 2003 Jul 1;66(1):63-73.

 $\hbox{\hbox{$[3]$. Fahlbusch, et al. "Flavors and Fragrances", Ullmann's Encyclopedia of Industrial Chemistry, Weinheim: Wiley-VCH.}\\$

[4]. 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.

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