Methyl 2-Octynoate-d₅

BIOLOGICAL ACTIVITY

Cat. No.:	HY-W013576S	
Molecular Formula:	C ₉ H ₉ D ₅ O ₂	
Molecular Weight:	159.24	0
Target:	Isotope-Labeled Compounds	
Pathway:	Others	
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.	D

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Description	Methyl 2-Octynoate-d ₅ is deuterated labeled Estragole (HY-N5060). Estragole (4-Allylanisole), a relatively nontoxic volatile terpenoid ether, is a major component of the essential oil of many plants. Estragole dose-dependently blocks nerve excitability ^[1] . Estragole displays anti-toxoplasma activity ^[2] .	
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, large tracers for quantitation during the drug development process. Deuteration has gained attention because of its pot 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]. Ryan J Schutte, et al. Molecular docking predictions of fragrance binding to human leukocyte antigen molecules. Contact Dermatitis. 2019 Sep;81(3):174-183.

[2]. 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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