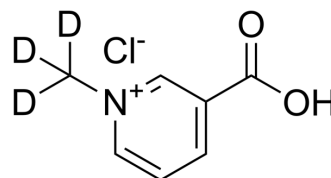


Trigonelline-d₃ chloride

Cat. No.:	HY-N0415S
Molecular Formula:	C ₇ H ₅ D ₃ ClNO ₂
Molecular Weight:	176.62
Target:	Fungal; HSV; Bacterial; Isotope-Labeled Compounds
Pathway:	Anti-infection; Others
Storage:	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 5 mg/mL (28.31 mM; ultrasonic and warming and heat to 60°C)

Concentration	Mass			
	1 mg	5 mg	10 mg	
1 mM	5.6619 mL	28.3094 mL	56.6187 mL	
5 mM	1.1324 mL	5.6619 mL	11.3237 mL	
10 mM	0.5662 mL	2.8309 mL	5.6619 mL	

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

Trigonelline-d₃ (chloride) is the deuterium labeled Trigonelline chloride. Trigonelline chloride, an alkaloid with potential antidiabetic activity, is present in considerable amounts in coffee. Trigonelline chloride has anti-HSV-1, antibacterial, and antifungal activities.

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]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. *Ann Pharmacother*. 2019;53(2):211-216.
- [2]. Ilavenil S, et al. Trigonelline protects the cardiocyte from hydrogen peroxide induced apoptosis in H9c2 cells. *Asian Pac J Trop Med*. 2015 Apr;8(4):263-8.
- [3]. Joanna Folwarczna, et al. Effects of Trigonelline, an Alkaloid Present in Coffee, on Diabetes-Induced Disorders in the Rat Skeletal System. *Nutrients*. 2016 Mar; 8(3): 133.

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

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