Screening Libraries

Inhibitors

Product Data Sheet

Actinine chloride

Cat. No.: HY-113270A CAS No.: 6249-56-5 Molecular Formula: $C_7H_{16}CINO_2$ Molecular Weight: 181.66

Target: **Endogenous Metabolite** Pathway: Metabolic Enzyme/Protease

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

H₂O: 100 mg/mL (550.48 mM; Need ultrasonic) DMSO: 30 mg/mL (165.14 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	5.5048 mL	27.5239 mL	55.0479 mL
	5 mM	1.1010 mL	5.5048 mL	11.0096 mL
	10 mM	0.5505 mL	2.7524 mL	5.5048 mL

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

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (13.76 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- β -CD in saline) Solubility: ≥ 2.5 mg/mL (13.76 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (13.76 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Actinine (γ-Butyrobetaine) chloride is angiopathic substance produced as an intermediary metabolite by gut microbiota that feed on carnitine in dietary red meat.
In Vivo	(3-Carboxypropyl)trimethylammonium chloride is produced as an intermediary metabolite by gut microbes of L-Carnitine to TMAO ^[1] . (3-Carboxypropyl)trimethylammonium chloride is implicated in arteriosclerosis and long-term cardiovascular death ^[2] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES [1]. Koeth RA, et al. γ-Butyrobetaine is a proatherogenic intermediate in gut microbial metabolism of L-carnitine to TMAO. Cell Metab. 2014 Nov 4;20(5):799-812.

[2]. Susumu Ogawa, et al. The Dynamics of Carnitine, γ -butyrobetaine and Trimethylamine N-oxide in Diabetics and the Effects of Changes in Renal Function. Ogawa et al., J Nephrol Ren Dis 2017, 1:2

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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

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