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Data Sheet

Product Name:AminothiazoleCat. No.:CS-3404CAS No.:96-50-4Molecular Formula: $C_3H_4N_2S$ Molecular Weight:100.14Target:Bacterial; FungPathway:Anti-infectionSolubility:DMSO : \geq 50 m

CS-3404 96-50-4 $C_3H_4N_2S$ 100.14 Bacterial; Fungal; Virus Protease Anti-infection DMSO : \geq 50 mg/mL;H₂O : \geq 100 mg/mL

BIOLOGICAL ACTIVITY:

Aminothiazole (2-Aminothiazole), a typical heterocyclic amine, is a precursor for the synthesis of biologically active molecules including sulfur agents, biocides, fungicides, antibiotics, dyes and chemical reaction accelerators^{[1][2]}. *In Vitro:* Aminothiazole can be used as a thyroid inhibitor in the research of hyperthyroidism and it has antibacterial activity^[1]. Aminothiazole can be used for the synthesis of antitubercular and antibacterial agents^[3].

PROTOCOL (Extracted from published papers and Only for reference)

Animal administration [1] Aminothiazole analog (e.g., 4.5 g of 27) was added to 15 mL of pure PEG400, vortexed and sonicated to ensure dissolution, then stored at -4 °C until needed. This highly concentrated PEG400 solution was subsequently diluted to final dosing concentrations, where the volume added was composed of homogenized solid rodent feed, cocoa (taste masking agent), and water. Wild-type FVB mice weigh ~25 gm and typically drink 20 mL of liquid diet per day, allowing an estimate of daily drug consumption. A single dosing cohort consisted of three mice in a shared cage and liquid diet was provided at the start of the study in sufficient volume to last for the entire three-day trial (~200 mL). At the end of the three-day dosing period, animals were euthanized by CO2, followed by collection of plasma (cardiac puncture) and removal of whole brain. Heparinized blood was centrifuged to separate plasma and both plasma and brain samples were stored at -80 °C prior to analysis. Plasma samples were prepared for analysis by precipitating proteins and reconstituting the remaining fraction with HPLC mobile phase. Brain samples were typically prepared by four-fold dilution with water after weighing, then homogenized using bead-beater or PolytronTM resulting in a highly concentrated solution that was further diluted with mobile phase as appropriate in preparation for bioanalytical analysis using LC-MS. Analysis was by LC-MS (Shimadzu dual-HPLC pumps, C18 analytical column, with detection using an Applied Biosystems API-4000 triple quadrupole mass spectrometer). Specific LC-MS methods were developed for each compound analyzed and the stability of the compounds in brain and plasma were demonstrated for the time period of sample handling, workup, and LC-MS analysis.

References:

[1]. Gallardo-Godoy A, et al. 2-Aminothiazoles as therapeutic leads for prion diseases. J Med Chem. 2011 Feb 24;54(4):1010-21.

[2]. Khalifa ME, et, al. Recent Developments and Biological Activities of 2-Aminothiazole Derivatives. Acta Chim Slov. 2018 Mar;65(1):1-22.

[3]. Ran K, et, al. Identification of novel 2-aminothiazole conjugated nitrofuran as antitubercular and antibacterial agents. Bioorg Med Chem Lett. 2016 Aug 1;26(15):3669-74.

CAIndexNames:

2-Thiazolamine

SMILES:

NC1=NC=CS1

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

Tel: 610-426-3128

Fax: 888-484-5008

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

E-mail: sales@ChemScene.com