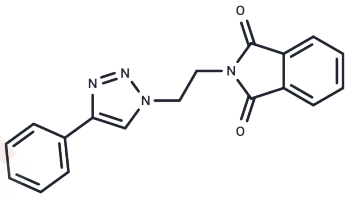
Data Sheet (Cat.No.T60836)

TargetMol

PT4

Chemical Properties



CAS No. : 1280738-47-7

Formula: C18H14N4O2

Molecular Weight: 318.33

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	PT4 is a treatment agent for Cutaneous leishmaniasis (CL). PT4 decreases of mitochondrial membrane potential and increases reactive oxygen species production, therefore leads to parasite death. PT4 is effective against both species of Leishmania. The IC50 values of PT4 against L. amazonensis and L. braziliensis are 125.18 and 233.18 μM , respectively. PT4 also shows potent anti-inflammatory activity in vivo [1].
Targets(IC50)	Others,Reactive Oxygen Species,Parasite
In vitro	PT4 (0-1256.5 μM, 48 hours) effectively inhibits the viability of mammalian cells and demonstrates significant antiparasitic activity against L. amazonensis and L. braziliensis promastigotes and amastigotes, with dosages ranging from 314.1-19.6 μM over 48 hours. It induces mitochondrial membrane depolarization in these parasites, leading to an increase in reactive oxygen species (ROS) within the mitochondria. In cytotoxicity assays, PT4 showed varying inhibitory effects on Balb/c mice peritoneal exudate cells (mPEC), J774A.1 macrophages, and fibroblasts, with half-maximal cytotoxic concentration (CC50) values of 981.37 μM, 521.47 μM, and 895.17 μM, respectively. Additionally, cell proliferation assays revealed that PT4 inhibited the proliferation of L. amazonensis and L. braziliensis promastigotes with half-maximal inhibitory concentration (IC50) values of 70.46 μM and 181.73 μM, respectively, and their amastigote forms with IC50 values of 125.18 μM and 233.18 μM, respectively.
In vivo	The pharmacokinetic and toxicological analysis of PT4 demonstrates its chemical characteristics and effects within specified parameters. It adheres to the Hydrogen Bond Acceptor (HBA) criterion of 4 (≤10), lacks Hydrogen Bond Donors (HBD) with a count of 0 (≤5), and possesses a LogP value of 2.23 (≤5), indicating moderate lipophilicity. The molecular weight (MW) is well within the acceptable range at 318.33 g/mol (≤500). PT4 exhibits an optimal number of rotatable bonds (n-ROTB) at 4 (≤10) and a Topological Polar Surface Area (TPSA) of 68.09 Å², aligning with effective permeability characteristics. It is acknowledged for its ability to cross the blood-brain barrier (BBB Yes), demonstrates a high gastrointestinal absorption (GIA High), and is not a P-Glycoprotein (P-GP) substrate. Skin permeability is indicated by a log value of -6.85 cm/s. Its interaction with Cytochrome P450 enzymes shows it as an inhibitor of 2C9, 2C19, and 1A2, while not inhibiting 2D6 and 3A4, highlighting selective metabolic interactions. The total clearance rate is noted at a log value of 0.117 ml/min/kg, with no significant reaction as a renal Organic Cation Transporter 2 (OCT2) substrate. The lethal dose 50 (LD50) is recorded at 4700 mg/kg, suggesting a relatively safe profile within

In vivo	certain exposure limits.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.1414 mL	15.707 mL	31.4139 mL
5 mM	0.6283 mL	3.1414 mL	6.2828 mL
10 mM	0.3141 mL	1.5707 mL	3.1414 mL
50 mM	0.0628 mL	0.3141 mL	0.6283 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.