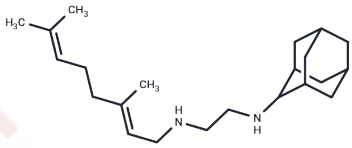
Data Sheet (Cat.No.T16925)

TargetMol

SQ109

Chemical Properties



CAS No. : 502487-67-4

Formula: C22H38N2

Molecular Weight: 330.55

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

Biological Description

Description	SQ109 (NSC-722041) is an effective inhibitor of the trypomastigote form of the parasite (IC50 = 50 nM). SQ109 is an antitubercular agent and targets MmpL3.
Targets(IC50)	Antibacterial,Antibiotic,Parasite
In vitro	SQ109 causes major ultrastructural changes in all three life cycle forms. SQ109 inhibits extracellular epimastigotes (IC50 = 4.6μM) and the clinically relevant intracellular amastigotes (IC50 = 0.5 - 1 μM), with a selectivity index of 10 to 20. SQ109 has little effect (EC50 = 80 μM) in a red blood cell hemolysis assay[1].
In vivo	The t1/2 of SQ109 in dogs (12-29 h, mean 29.3 h) is longer than in rats (7-8 h, mean 7.4 h), as reflected by the significantly larger volume of distribution of SQ109 in dogs. The oral bioavailability of SQ109 in rats and dogs is 12% and 5%, respectively[2]. SQ109 (0.1-25 mg/kg) to the mice for 28 days results in dose-dependent reductions of mycobacterial load in both spleen and lung comparable to that of EMB(100 mg/kg), but is less potent than isoniazid(25 mg/kg). Pharmacokinetic profiles of SQ109 in mice following a single administration showed its Cmax as 1038 (i.v.) and 135 ng/mL (p.o.), with an oral Tmax of 0.31 h and an oral bioavailability of 4%. The elimination t1/2 of SQ109 is 3.5 (i.v.) and 5.2 h (p.o.)[3].

Solubility Information

Solubility	DMSO: 21 mg/mL (63.53 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (6.05 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.0253 mL	15.1263 mL	30.2526 mL
5 mM	0.6051 mL	3.0253 mL	6.0505 mL
10 mM	0.3025 mL	1.5126 mL	3.0253 mL
50 mM	0.0605 mL	0.3025 mL	0.6051 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.

Reference

Veiga-Santos P, et al. SQ109, a new drug lead for Chagas disease. Antimicrob Agents Chemother. 2015 Apr;59(4):1950-61.

Jia L, et al. Pharmacodynamics and pharmacokinetics of SQ109, a new diamine-based antitubercular drug. Br J Pharmacol. 2005 Jan;144(1):80-7

Jia L, et al. Interspecies pharmacokinetics and in vitro metabolism of SQ109. Br J Pharmacol. 2006 Mar;147(5):476-85.