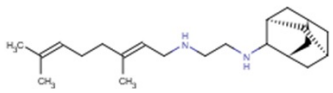
# Data Sheet (Cat.No.T16925)

TargetMol
A DRUG SCREENING EXPERT

SQ109

## Chemical Properties



| | |
|---|---|
| CAS No.: | 502487-67-4 |
| Formula: | C22H38N2 |
| Molecular Weight: | 330.55 |
| Appearance: | N/A |
| Storage: | 0-4℃ for short term (days to weeks), or -20℃ for long term (months). |

## Biological Description

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|---|---|
| Description | SQ109 is an effective inhibitor of the trypomastigote form of the parasite (IC50 for cell killing: 50±8 nM). SQ109 is an antitubercular agent. |
| Targets($IC_{50}$) | trypomastigote cell: 50±8 nM |
| In vitro | SQ109 also inhibits extracellular epimastigotes (IC50: 4.6±1 μM) and the clinically relevant intracellular amastigotes (IC50: ~0.5 to 1 μM). It has a selectivity index of ~10 to 20. SQ109 has little effect (EC50: ~80 μM) in a red blood cell hemolysis assay [1]. |
| In vivo | SQ109 (0.1-25 mg/kg per day, p.o., mice for 28 days) causes dose-dependent reductions of mycobacterial load in both spleen and lung comparable to that of EMB administered at 100 mg/kg per day but is less potent than isoniazid at 25 mg/kg per day. 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. The elimination t1/2 of SQ109 is 3.5 (i.v.) and 5.2 h (p.o.). The oral bioavailability is 4%. The terminal half-life (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 determined to be 12% and 5%, respectively [2][3]. |

## Solubility Information

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|---|---|
| Solubility | DMSO: 25 mg/mL (75.63 mM)<br>(< 1 mg/ml refers to the product slightly soluble or insoluble) |

Preparing Stock Solutions

| | 1mg | 5mg | 10mg |
|---|---|---|---|
| 1 mM | 3.025 mL | 15.126 mL | 30.253 mL |
| 5 mM | 0.605 mL | 3.025 mL | 6.051 mL |
| 10 mM | 0.303 mL | 1.513 mL | 3.025 mL |
| 50 mM | 0.061 mL | 0.303 mL | 0.605 mL |

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Veiga-Santos P, et al. SQ109, a new drug lead for Chagas disease. Antimicrob Agents Chemother. 2015 Apr;59(4):1950-61.
2. Jia L, et al. Pharmacodynamics and pharmacokinetics of SQ109, a new diamine-based antitubercular drug. Br J Pharmacol. 2005 Jan;144(1):80-7
3. Jia L, et al. Interspecies pharmacokinetics and in vitro metabolism of SQ109. Br J Pharmacol. 2006 Mar;147(5):476-85.



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