Product Data Sheet

Chemical Properties

Product Name: SQ109
Cas No.: 502487-67-4
M.Wt: 330.55
Formula: C22H38N2
Synonyms: NSC 722041; SQ-109; SQ 109

Chemical Name: N’-(2-adamantyl)-N-[(2E)-3,7-dimethylocta-2,6-dienyl]ethane-1,2-diamine
Canonical SMILES: CC(=CCCC(=CCNCCNC1C2CC3CC(C2)CC1C3)C)C
Solubility: Soluble in DMSO
Storage: Store at -20°C
General tips: For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.
Shopping Condition: Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

Biological Activity

Targets: Microbiology & Virology
Pathways: Antibiotic

Description:

SQ109 is a novel antitubercular drug with IC50 value of 0.2 μg/ml on XDR [1]. Tuberculosis is a serious infection disease caused by Mycobacterium tuberculosis (Mtbb). It is the
leading single-agent killer with highest fatality rate. About more than three million lives were killed by tuberculosis every year. Even so, the existed drugs for TB treatment are facing many challenges including the side effects and the development of multidrug-resistant tuberculosis (MDR-TB). As a novel antitubercular drug, SQ109 has a distinguished mechanism of action and improved potency. The target of it is the mycolic acid transporter MmpL3 required for the synthesis of mycolic acid in cell wall of Mtb [1 and 2].

SQ109 was screened out from a big chemical library designed around the active pharmacophore of ethambutol (EMB). Even so, SQ109 had different chemical structure, potency and mechanism with EMB. Among the top 27 candidates, SQ109 showed the highest selectivity index value and lowest IC50 value in vitro of 16.7 and 0.78 μg/ml, respectively. SQ109 displayed potent activity against all the substrains of Mtb including XDR- and MDR-TB clinical strains with IC50 values of 0.2 μg/ml. Besides that, SQ109 also showed significant effects on other pathogenic Mycobacteria with MIC values in the range of 4 to 16 μg/ml [1].

SQ109 showed low oral bioavailability in PK studies. The carbamate prodrug of it with improved oral bioavailability (from 21.4% to 91.4 %) exerted a high tissue distribution in rats. In the infected mice, treatment of SQ109 at dose of 10 mg/kg significantly attenuated the symptom of weight loss. In the chronic TB model in mice, 10 mg/kg of SQ109 showed better potency than EMB at dose of 100 mg/kg. Besides that, it was reported that the combination treatment of SQ109 and bedaquiline demonstrated a durable cure in infected mice model [1 and 3].

Reference:

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.