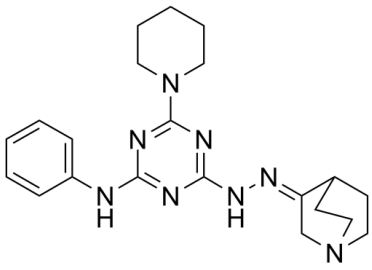
Data Sheet

Product Name:	ATB107
Cat. No.:	CS-M0770
CAS No.:	455325-51-6
Molecular Formula:	C21H28N8
Molecular Weight:	392.50
Target:	Others
Pathway:	Others
Solubility:	H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

ATB107 is a novel and potent inhibitor of indole-3-glycerol phosphate synthase (**IGPS**) with a K_D of 3 μM. IC50 & Target: KD: 3 μM (IGPS)[1] **In Vitro:** The minimum inhibitory concentration (MIC) of ATB107 is 0.1 μg/mL for M. tuberculosis H37Ra. ATB107 also has high activity against M. tuberculosis H37Rv, with an MIC of 0.1 μg/mL. All 50 fully susceptible clinical isolates tested are susceptible to ATB107 at 1 μg/mL; of these, 41 (82%) are susceptible to ATB107 at 0.1 μg/mL. The results also show that 67 (83.8%) multidrug-resistant TB (MDR-TB) isolates are susceptible to ATB107 at 1 μg/mL, and 25 (31.3%) isolates are susceptible to ATB107 at 0.1 μg/mL. Results show that the binding ability of ATB107 is well correlated with its concentrations. At the highest concentration of 200 μg/mL, ATB107 can inhibit cell proliferation, with cell survival of about 60%. With the lower concentration of 50 μg/mL, cell survival is more than 80% for ATB107[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]The concentration of mIGPS is determined. The substrate CdRP is chemically synthesized, with a yield of 30 mM. Ten microliters of 30 mM CdRP and 10 μL of 1.24 μM IGPS are added to 480 μL of 5 mM Tris/HCl (pH 7.0), and incubated at 37°C for 20 min. The enzyme activity is measured with a spectrophotometer by following the increase in absorbance of the solution at 280 nm. ATB107 is added to the assay mixture to obtain concentrations of 10^{-4} M, 7.5×10^{-5} M, 5×10^{-5} M, 2.5×10^{-5} M, and 10^{-5} M, respectively [1]. **Cell Assay:** [1]The tetrazolium dye reduction assay [3-[4,5-dim-ethylthiazol-2-yl]-2,5-diphenyl-tetrazolium bromide (MTT)] is used to determine the effect of ATB107 on cell survival and growth. At first, the THP-1 macrophage cells are inoculated at 8×10^4 cells/mL) into 96-well plates and incubated at 37°C in a 5% CO_2/95% air atmosphere for 24 h. ATB107 is added to give concentrations of 50,100, 150 and 200 μg/mL. After incubation of cells treated with ATB107 for 12 h, 20 μL (5 g/L) of MTT solution is added to each well; this is followed by incubation for another 4 h to allow the formation of formazan crystals. Finally, 10% SDS is added to dissolve the formazan crystals, and the plates are read on a microplate reader at 570 nm. Controls are included in which only culture media are added to wells containing cells[1].

References:

[1]. Shen H, et al. A novel inhibitor of indole-3-glycerol phosphate synthase with activity against multidrug-resistant Mycobacterium tuberculosis. FEBS J. 2009 Jan;276(1):144-54.

CAIndexNames:

1-Azabicyclo[2.2.2]octan-3-one, 2-[4-(phenylamino)-6-(1-piperidinyl)-1,3,5-triazin-2-yl]hydrazone

SMILES:

C1(N2CCCCC2)=NC(NC3=CC=CC=C3)=NC(N/N=C4CN5CCC\4CC5)=N1

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

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