
Product Data Sheet

Product Name: ATB107
Cat. No.: GC32200

Chemical Properties

Cas. No. 455325-51-6

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

Formula $C_{21}H_{28}N_8$ M.Wt 392.5

Solubility Water : < 0.1 mg/mL (insoluble) 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.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure

Protocol**Kinase experiment:**

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 μ L of 1.24 μ M IGPS are added to 480 μ L 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 \times 10⁻⁵ M, 5 \times 10⁻⁵ M, 2.5 \times 10⁻⁵ M, and 10⁻⁵ M, respectively[1].

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

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Cell experiment:

The tetrazolium dye reduction assay [3-[4,5-dimethylthiazol-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% CO₂/95% 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.

Background

ATB107 is a novel and potent inhibitor of indole-3-glycerol phosphate synthase (IGPS)

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with a KD of 3 μ M.

The minimum inhibitory concentration (MIC) of ATB107 is 0.1 μ g/mL for *M. tuberculosis* H37Ra. ATB107 also has high activity against *M. tuberculosis* H37Rv, with an MIC of 0.1 μ g/mL. All 50 fully susceptible clinical isolates tested are susceptible to ATB107 at 1 μ g/mL; of these, 41 (82%) are susceptible to ATB107 at 0.1 μ g/mL. The results also show that 67 (83.8%) multidrug-resistant TB (MDR-TB) isolates are susceptible to ATB107 at 1 μ g/mL, and 25 (31.3%) isolates are susceptible to ATB107 at 0.1 μ g/mL. Results show that the binding ability of ATB107 is well correlated with its concentrations. At the highest concentration of 200 μ g/mL, ATB107 can inhibit cell proliferation, with cell survival of about 60%. With the lower concentration of 50 μ g/mL, cell survival is more than 80% for ATB107[1].

[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.

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