Product Data Sheet

Chemical Properties

Product Name: CHIR-090

Cas No.: 728865-23-4

M.Wt: 437.49

Formula: C24H27N3O5

Synonyms: CHIR 090; CHIR090

Chemical Name: N-[(2S,3R)-3-hydroxy-1-(hydroxyamino)-1-oxobutan-2-yl]-4-[2-[4-(morpholin-4-ylmethyl)phenyl]ethynyl]benzamide

Canonical SMILES: CC(C(C(=O)NO)NC(=O)C1=CC=C(C=C1)C#CC2=CC=C(C=C2)CN3CCOCC3)O

Solubility: $\geq 21.85$ mg/mL in DMSO

Storage: Store at $-20^\circ C$

General tips: For obtaining a higher solubility, please warm the tube at $37^\circ C$ and shake it in the ultrasonic bath for a while. Stock solution can be stored below $-20^\circ C$ 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: Others

Pathways: LpxC

Description:

CHIR-090 is a very potent, low, tight-binding inhibitor of LpxC with Ki value of 4.0 nM [1]. LpxC is a zinc-dependent amidase and present in almost all Gram-negative bacteria. LpxC is a promising target for the development of novel antibiotic substances against multigrug-resistant Gram-negative bacteria [2].

CHIR-090 is a potent LpxC inhibitor and has a different selectivity with the reported LpxC inhibitor
L-161. When tested with Escherichia coli LpxC, administration of CHIR-090 showed tight inhibition with Ki value of 4.0 nM, Ki*=0.5 nM, K5=1.9/min and K6=0.18/min [1]. In bacterial P.aeruginosa efflux pump mutants, CHIR-090 treatment showed inhibition function on MexAB-Oprm, MexCD-OprJ and MexEF-OprN [2]. CHIR-090 showed remarkable antibiotic activity against both E.coli and P.aeruginosa by inhibiting LpxC orthologs at low nM concentrations [3]. In E.coli W3110RL with R.leguminosarum lpxC replacement of E.coli lpxC, CHIR-090 (1 to 10 μg/ml) treatment had no effect on strain growth on LB agar plates while wild-type cells stopped growing after about 2 h in the presence of 1 μg/ml CHIR-090 [1].

Reference:

Protocol

Cell experiment:

Cell lines wild-type E. coli W3110 and E. coli W3110RL

Preparation method The solubility of this compound in DMSO is >21.9mg/mL. General tips for obtaining a higher concentration: Please warm the tube at 37°C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Reacting conditions

Applications In the presence of 1 μg/mL CHIR-090, wild-type E. coli W3110 stopped growing after about 2 h. The E. coli W3110RL, in which R. leguminosarum lpxC replaces the chromosomal copy of E. coli lpxC, was resistant to CHIR-090. The MIC of CHIR-090 against W3110RL in liquid medium was 100 μg/mL, compared to 0.25 μg/ mL for W3110.

Reference:

Caution
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.