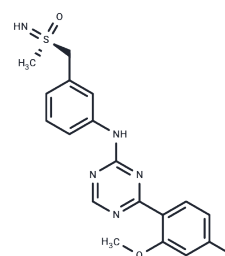


Atuveciclib S-Enantiomer

Chemical Properties

CAS No. :	2250279-81-1
Formula:	C ₁₈ H ₁₈ FN ₅ O ₂ S
Molecular Weight:	387.43
Appearance:	no data available
Storage:	Powder: -20°C for 3 years In solvent: -80°C for 1 year



Biological Description

Description	Atuveciclib S-Enantiomer (BAY-1143572 S-Enantiomer) is the (S)-enantiomer of BAY-1143572. Atuveciclib S-Enantiomer is a potent and selective CDK9 inhibitor, which inhibits CDK9 / CycT1 with an IC ₅₀ of 16 nM.
Targets(IC ₅₀)	CDK
In vitro	Atuveciclib (BAY-1143572) S-Enantiomer reveals very similar in vitro properties compared with Atuveciclib (BAY-1143572), well within the limits of measurement accuracy. However, with multiple batches of Atuveciclib (BAY-1143572) S-Enantiomer, there is a trend toward a slightly lower activity against CDK9 in the biochemical assay (IC ₅₀ CDK9/CycT1: 16 nM) and antiproliferative activity against HeLa cells (IC ₅₀ : 1100 nM) [1].
In vivo	Atuveciclib (BAY-1143572) S-Enantiomer exhibits blood/plasma ratios close to 1, suggesting a similarity in distribution. Compared to its parent compound, Atuveciclib (BAY-1143572), this enantiomer demonstrates comparable pharmacokinetic (PK) properties in rats, including a clearance rate (CL _b) of 1.2 L/kg per hour, a steady-state volume of distribution (V _{ss}) of 1.2 L/kg, a half-life (t _{1/2}) of 0.6 hours, and a bioavailability (F) of 53% [1].

Solubility Information

Solubility	DMSO: 113 mg/mL (291.67 mM), (< 1 mg/ml refers to the product slightly soluble or insoluble)
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A DRUG SCREENING EXPERT

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5811 mL	12.9056 mL	25.8111 mL
5 mM	0.5162 mL	2.5811 mL	5.1622 mL
10 mM	0.2581 mL	1.2906 mL	2.5811 mL
50 mM	0.0516 mL	0.2581 mL	0.5162 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Reference

Lücking U, et al. Identification of Atuveciclib (BAY 1143572), the First Highly Selective, Clinical PTEFb/CDK9 Inhibitor for the Treatment of Cancer. ChemMedChem. 2017 Nov 8;12(21):1776-1793.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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