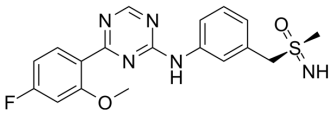
Atuveciclib S-Enantiomer

Cat. No.:	HY-12871C
CAS No.:	2250279-81-1
Molecular Formula:	$C_{18}H_{18}FN_5O_2S$
Molecular Weight:	387.43
Target:	CDK
Pathway:	Cell Cycle/DNA Damage
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 113 mg/mL (291.67 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	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

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

Atuveciclib S-Enantiomer (BAY-1143572 S-Enantiomer) is a potent and selective CDK9 inhibitor, which inhibits CDK9/CycT1 with an IC_{50} of 16 nM.

IC_{50} & Target

IC50: 16 nM (CDK9/CycT1)[1]

In Vitro

In comparison with Atuveciclib (BAY-1143572), Atuveciclib (BAY-1143572) S-Enantiomer reveals very similar in vitro properties, 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].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Atuveciclib (BAY-1143572) S-Enantiomer exhibits blood/plasma ratios of about 1. Relative to Atuveciclib (BAY-1143572), Atuveciclib (BAY-1143572) S-Enantiomer reveals very similar rat PK properties in vivo (CL_b: 1.2 L/kg per hour, V_{ss}: 1.2 L/kg, $t_{1/2}$: 0.6 h, F: 53 %)[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. 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.

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