Product Data Sheet

Product Name: Atuveciclib S-Enantiomer (BAY-1143572 S-Enantiomer)
Cat. No.: GC34421

Chemical Properties

Cas. No.			
SMILES	N=[S@@](CC1=CC(NC2=NC(C3=CC=C(F)C=C3OC)=NC=N2)=CC=C1)(C)=O		
Formula	$C_{18}H_{18}FN_5O_2S$	M.Wt	387.43
Solubility	DMSO : ≥ 113 mg/mL (291.67 mM)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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			

Background

Atuveciclib S-Enantiomer (BAY-1143572 S-Enantiomer) is a potent and selective CDK9 inhibitor, which inhibits CDK9/CycT1 with an IC50 of 16 nM.

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 (IC50 CDK9/CycT1: 16 nM) and antiproliferative activity against HeLa cells (IC50: 1100 nM) [1].

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 (CLb: 1.2 L/kg per hour, Vss: 1.2 L/kg, t1/2: 0.6 h, F: 53 %)[1].

[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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