Product Data Sheet

Product Name: MPC-3100
Cat. No.: GC14322

Chemical Properties

Cas. No.	958025-66-6		
Chemical Name	(2S)-1-[4-[2-[6-amino-8-[(6-bromo-1,3-benzodioxol-5-yl)sulfanyl]purin-9-yl]ethyl]piperidin-1-yl]-2-hydroxypropan-1-one		
SMILES	CC(C(=O)N1CCC(CC1)CCN2C3=C(C(=NC=N3)N)N=C2SC4=C(C=C5C(=C4)OCO5)Br)O		
Formula	$C_{22}H_{25}BrN_6O_4S$	M.Wt	549.4
Solubility	Soluble in DMSO	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	MPC-3100		

Background

MPC-3100 is a purine-based inhibitor of Hsp90 with IC50 value of 60nM [1].

MPC-3100 targets the N-terminal ATP-binding site of Hsp90 and blocks the activity of ATPase. In the Her2-luciferase degradation assay, MPC-3100 reduces this client protein of Hsp90 with IC50 value of 60nM. In HCT-116 cell lines, MPC-3100 inhibits cell proliferation with IC50 value of 540nM. Besides that, MPC-3100 shows a broad spectrum anti-proliferative activity against various cancer cell lines, such as NCI-N87 and DU-145. MPC-3100 also inhibits tumor growth in the NCI-N87 gastric cancer xenograft mode. Moreover, PK studies show that MPC-3100 displays a superior oral PK profile, good overall exposure and a reasonable hepatic clearance rate. Phase I clinical studies demonstrate MPC-3100 is safe and tolerated when administered at doses below 600 mg per day [1].

References:
[1] Kim SH, Bajji A, Tangallapally R, Markovitz B, Trovato R, Shenderovich M, Baichwal V, Bartel P, Cimbora D, McKinnon R, Robinson R, Papac D, Wettstein D, Carlson R, Yager KM. Discovery of (2S)-1-[4-(2-{6-amino-8-[(6-bromo-1,3-benzodioxol-5-yl)sulfanyl]-9H-purin-9-yl}ethyl)piperidin-1-yl]-2-hydroxypropan-1-one (MPC-3100), a purine-based Hsp90 inhibitor. J Med Chem. 2012 Sep 13;55(17):7480-501.

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