Product Data Sheet

Product Name: BMS 599626 dihydrochloride
Cat. No.: GC14136

Chemical Properties

Cas. No.	1781932-33-9		
Chemical Name	(E)-(S)-morpholin-3-ylmethyl hydrogen ((Z)-4-((1-(3-fluorobenzyl)-1H-indazol-5-yl)imino)-5-methyl-1,4-dihydropyrrolo[2,1-f][1,2,4]triazin-6-yl)carbonimidate dihydrochloride		
SMILES	CC(C(/N=C(OC[C@]1([H])COCCN1)\O)=CN2NC=N/3)=C2C3=N\C4=CC=C5C(C=NN5CC6=CC(F)=CC=C6)=C4.Cl.Cl		
Formula	$C_{27}H_{27}FN_8O_3$.2HCl	M.Wt	603.48
Solubility	Soluble in DMSO > 10 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	BMS 599626 dihydrochloride		

Background

BMS 599626 dihydrochloride is a potent and selective inhibitor of EGFR and ErbB2 with IC50 values of 22 and 32 nM, respectively [1].

The epidermal growth factor receptor (EGFR) is the cell-surface receptor for epidermal growth factor and plays an important role in tumor invasion and cancer cell proliferation. Receptor tyrosine-protein kinase erbB-2 (ErbB2) is a human epidermal growth factor receptor and plays a critical role in breast cancer.

BMS 599626 dihydrochloride is a potent and selective EGFR and ErbB2 inhibitor. BMS-599626 inhibited HER4 with IC50 value of 190 nM. In Sal2, N87 and GEO tumor cells, BMS-599626 inhibited phosphorylation of HER1 and HER2 in a dose-dependent way and inhibited cell proliferation. In AU565 breast cancer cells, BMS-599626 (1μM) inhibited HER1/HER2 heterodimer formation [1]. In tumor cells that forming HER1/HER2 heterodimers, BMS-599626 inhibited heterodimerization [2].

In the L2987 human lung tumors xenograft models, BMS-599626 (60 mg/kg) inhibited and delayed tumor growth in a dose-dependent way [1].

References:
[1]. Gavai AV, Fink BE, Fairfax DJ, et al. Discovery and preclinical evaluation of [4-[[1-(3-fluorophenyl)methyl]-1H-indazol-5-ylamino]-5-methylpyrrolo[2,1-f][1,2,4]triazin-6-yl]carbamic acid, (3S)-3-morpholinylmethyl ester (BMS-599626), a selective and orally efficacious inhibitor of human epidermal growth factor receptor 1 and 2 kinases. J Med Chem, 2009, 52(21): 6527-6530.
[2]. Wong TW, Lee FY, Yu C, et al. Preclinical antitumor activity of BMS-599626, a pan-HER kinase inhibitor that inhibits HER1/HER2 homodimer and heterodimer signaling. Clin Cancer Res, 2006, 12(20 Pt 1): 6186-6193.

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