Product Data Sheet

Product Name: B-Raf inhibitor 1 dihydrochloride
Cat. No.: GC14907

Chemical Properties

Cas. No.	1191385-19-9		
Chemical Name	1-N-(4-chlorophenyl)-6-methyl-5-N-[3-(7H-purin-6-yl)pyridin-2-yl]isoquinoline-1,5-diamine;dihydrochloride		
SMILES	CC1=C(C2=C(C=C1)C(=NC=C2)NC3=CC=C(C=C3)Cl)NC4=C(C=CC=N4)C5=C6C(=NC=N5)N=CN6.Cl.Cl		
Formula	$C_{26}H_{21}Cl_3N_8$	M.Wt	551.86
Solubility	DMF: 1mg/mL,DMSO: 10mg/mL,DMSO:PBS (pH 7.2) (1:2): 0.3mg/mL	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	B-Raf inhibitor 1 dihydrochloride		

Background

B-Raf inhibitor 1 is an inhibitor of B-Raf kinase with IC50 values of 0.31μM and 0.72μM for cell proliferation, respectively in A375 and HCT116 [1].

B-Raf is important in signal transduction and some mutant B-Raf occurs in cancer cells. The most common mutation of these is V600E, which makes B-Raf kinase constitutively active. B-Raf inhibitor 1 belongs to the type IIA inhibitors and binds to the DFG-out ATP-binding site of B-Raf. The selectivity of B-Raf inhibitor 1 is less than of other type inhibitors. Besides mutant B-Raf, it can also inhibit wild type B-Raf and other tyrosine kinase. In cells with wild type B-Raf, B-Raf inhibitor 1 can activate the RAF-MEK-ERK signaling pathway via Raf dimerization. The preclinical toxicity test shows B-Raf inhibitor 1 can induce hyperplasia in a mouse model [1, 2].

References:
[1] Wang X, Kim J. Conformation-specific effects of Raf kinase inhibitors. J Med Chem. 2012 Sep 13;55(17):7332-41.
[2] Smith AL, DeMorin FF, Paras NA, Huang Q, Petkus JK, Doherty EM, Nixey T, Kim JL, Whittington DA, Epstein LF, Lee MR, Rose MJ, Babij C, Fernando M, Hess K, Le Q, Beltran P, Carnahan J. Selective inhibitors of the mutant B-Raf pathway: discovery of a potent and orally bioavailable aminoisoquinoline. J Med Chem. 2009 Oct 22;52(20):6189-92.

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