Product Data Sheet

Product Name: CHMFL-ABL-053
Cat. No.: GC17294

Chemical Properties

Cas. No.	1808287-83-3		
Chemical Name	2-((3-amino-4-methylphenyl)amino)-N-(2-methyl-5-(3-(trifluoromethyl)benzamido)phenyl)-4-(methylamino)pyrimidine-5-carboxamide		
SMILES	CC1=CC=C(NC2=NC(NC)=C(C(NC3=CC(NC(C4=CC=CC(C(F)(F)F)=C4)=O)=CC=C3C)=O)C=N2)C=C1N		
Formula	$C_{28}H_{26}F_3N_7O_2$	M.Wt	549.55
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	CHMFL-ABL-053		

Background

CHMFL-ABL-053 (compound 18a) is a BCR-ABL inhibitor with ABL1: IC50 of 70 nM. CHMFL-ABL-053 is derived from a dihydropyrimidopyrimidine core scaffold based compound 27 (GNF 7). [1]

CHMFL-ABL-053 inhibited the proliferation of CML cell lines K562 (GI50 = 14 nM), KU812 (GI50 = 25 nM) and MEG 01 (GI50 = 16 nM), through significant suppression of the BCR-ABL auto phosphorylation (EC50 = 100 nM) and downstream mediators such as STAT5, Crkl and ERK's phosphorylation. In the TEL fused isogenic BaF3 cells, CHMFL-ABL-053 exhibited strong binding ability against BLK, DDR1, DDR2, EPHA8, EphB6, HCK, LCK, p38α and SRC kinases. CHMFL-ABL-053 exhibited an IC50 of 70 nM against ABL1 kinase, inhibited p38α (IC50: 62 nM) and SRC kinase (IC50: 90 nM) by Invitrogen Select Screen biochemical assay. CHMFL-ABL-053 showed less potent to DDR1 (IC50: 292 nM) and

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DDR2 (IC50: 457 nM). CHMFL-ABL-053 did not exhibit apparent potency against c-KIT kinase (IC50: over 10000 nM). [1]

Pharmacokinetic study showed that CHMFL-ABL-053 had over 4 hours half-life and 24% bioavailability in rats. 50mg/kg/day dosage treatment could almost completely suppress the tumor progression in the K562 cells inoculated xenograft mouse model. As a potential useful drug candidate for CML, 18a is under extensive preclinical safety evaluation now. [1]

Reference:

1.Discovery of 2-((3-Amino-4-methylphenyl)amino)-N-(2-methyl-5-(3-(trifluoromethyl) benzamido)phenyl)-4-(methylamino)pyrimidine-5-carboxamide (CHMFL-ABL-053) as a Potent, Selective, and Orally Available BCR-ABL/SRC/p38 Kinase Inhibitor for Chronic Myeloid Leukemia.J Med Chem. 2016 Feb 5. [Epub ahead of print]

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