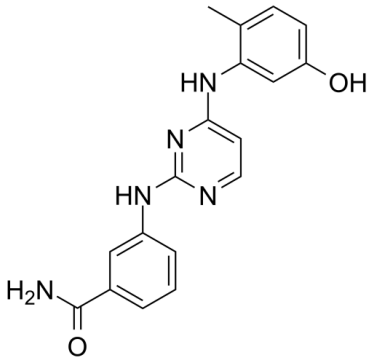
Data Sheet

Product Name:	Lck inhibitor 2
Cat. No.:	CS-1491
CAS No.:	944795-06-6
Molecular Formula:	C18H17N5O2
Molecular Weight:	335.36
Target:	Src
Pathway:	Protein Tyrosine Kinase/RTK
Solubility:	DMSO : 20 mg/mL (59.64 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Lck inhibitor 2 is a bis-anilinopyrimidine inhibitor of tyrosine kinases including LCK, BTK, LYN, SYK, and TXK. The IC50 values are 13nM, 9nM, 3nM, 26nM and 2nM for Lck, Btk, Lyn, Btk and Txk respectively IC50 Value: 13 nM(Lck) [1] Target: Src family kinase Lck inhibitor 2(Compound 9) inhibited 48 kinases with %control < 1 (33 of them tyrosine kinases, almost half of the 71 tyrosine kinases in the panel). A further 27 kinases were bound with %control < 10. Kd values for 16 kinases were determined and found to be below 100 nM. These included TXK (10 nM)[2].

References:

[1]. Bamborough, et al. Assessment of Chemical Coverage of Kinome Space and Its Implications for Kinase Drug Discovery. Journal of Medicinal Chemistry (2008), 51(24), 7898-7914.

[2]. Bamborough, Paul, et al. N-4-Pyrimidinyl-1H-indazol-4-amine inhibitors of Lck: Indazoles as phenol isosteres with improved pharmacokinetics. Bioorganic & Medicinal Chemistry Letters (2007), 17(15), 4363-4368.

[3]. Awale, Mahendra, et al. Molecular docking guided 3D-QSAR CoMFA analysis of N-4-Pyrimidinyl-1H-indazol-4-amine inhibitors of leukocyte-specific protein tyrosine kinase. Journal of Molecular Modeling (2008), 14(10), 937-947.

CAIndexNames:

Benzamide, 3-[[4-[(5-hydroxy-2-methylphenyl)amino]-2-pyrimidinyl]amino]-

SMILES:

OC1=CC=C(C)C(NC2=CC=NC(NC3=CC(C(N)=O)=CC=C3)=N2)=C1

Caution: Product has not been fully validated for medical applications. For research use only.

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