

Product Data Sheet

Product Name: Lck inhibitor 2

Cat. No.: GC36430

Chemical Properties

Cas. No. 944795-06-6

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

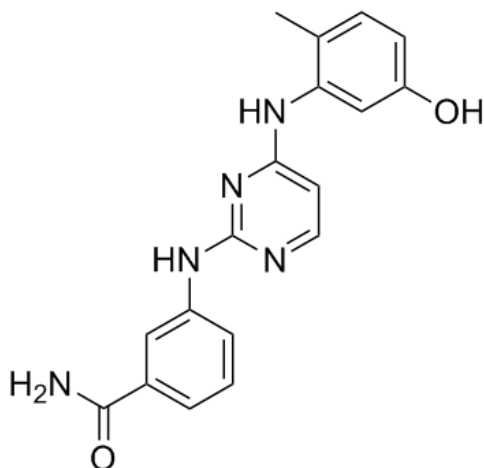
Formula $C_{18}H_{17}N_5O_2$ M.Wt 335.36

Solubility DMSO: 20 mg/mL (59.64 mM) Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C 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



Background

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

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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 kinaseLck 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].

[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.

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