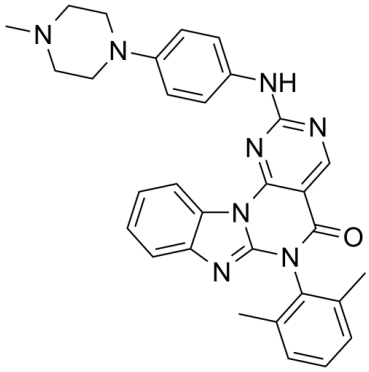
Data Sheet

Product Name:	Lck Inhibitor
Cat. No.:	CS-1448
CAS No.:	847950-09-8
Molecular Formula:	C31H30N8O
Molecular Weight:	530.62
Target:	Src
Pathway:	Protein Tyrosine Kinase/RTK
Solubility:	DMSO : 100 mg/mL (188.46 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Lck Inhibitor is a new class of compounds that are potent inhibitors of Lck with an IC50 value of 7 nM. IC50 Value: 7 nM [1] Target: Lck in vitro: Lck Inhibitor (compound 25) exhibited good potency in the T-cell receptor-induced IL-2 secretion assay (IL- 2) and also inhibited subsequent T-cell proliferation (T-cell prolif.) in the same human T -cells. in vivo: A once daily dose of 25was administered orally at 10, 30, and 60 mg/kg from day 9 today 17. Paw volume was measured daily from day 9 through day 18. The compound showed a dose-dependent inhibition of arthritis, with an ED50 estimated at 24 mg/kg (Figure 6). Based on the measured plasma levels from the three dose groups, the exposure of 25 at the ED50 was estimated to be 2.7 μM·h (Cmax≈ 0.7 μM) [1]. Clinical trial: N/A

References:

[1]. Martin, Matthew W.; Newcomb, John; Nunes, Joseph J.; et al. Structure-Based Design of Novel 2-Amino-6-phenyl-pyrimido[5',4':5,6]pyrimido[1,2-a]benzimidazol-5(6H)-ones as Potent and Orally Active Inhibitors of Lymphocyte Specific Kinase (Lck): Synthesis, SAR, and In Vivo Anti-Inflammatory Activity. Journal of Medicinal Chemistry (2008), 51(6), 1637-1648.

[2]. Liew, Chin Y.; Ma, Xiao H.; Liu, Xianghui; Yap, Chun W. SVM Model for Virtual Screening of Lck Inhibitors. Journal of Chemical Information and Modeling (2009), 49(4), 877-885.

CAIndexNames:

Pyrimido[5',4':5,6]pyrimido[1,2-a]benzimidazol-5(6H)-one, 6-(2,6-dimethylphenyl)-2-[[4-(4-methyl-1-piperazinyl)phenyl]amino]-

SMILES:

O=C1N(C2=C(C)C=CC=C2C)C3=NC4=CC=CC=C4N3C5=NC(NC6=CC=C(N7CCN(C)CC7)C=C6)=NC=C15

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

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