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产品名称: 6-(2,6-二甲基苯基)-2-[[4-(4-甲基-1-哌嗪基)苯基]氨基]-嘧啶并
[5',4':5,6]嘧啶并[1,2-A]苯并咪唑-5(6H)-酮
产品别名: Lck Inhibitor

生物活性:				
Description	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 $\mu\text{M} \cdot \text{h}$ ($\text{Cmax} \approx 0.7 \mu\text{M}$) [1]. Clinical trial: N/A			
	In Vitro: DMSO : 100 mg/mL (188.46 mM; Need ultrasonic)			
Solvent&Solubility	Preparing	Solvent / Mass / Concentration	1 mg	5 mg
	Stock Solutions	1 mM	1.8846 mL	9.4229 mL
		5 mM	0.3769 mL	1.8846 mL
		10 mM	0.1885 mL	0.9423 mL
			1.8846 mL	
*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液。一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。 储备液的保存方式和期限 -80°C, 6 months; -20°C, 1 month。 -80°C 储存时，请在 6 个月内使用，-20°C 储存时，请在 1 个月内使用。 In Vivo: 请根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都请先按照 In Vitro 方式配制澄清的储备液，再依次添加助溶剂： ——为保证实验结果的可靠性，澄清的储备液可以根据储存条件，适当保存；体内实验的工作液，建议您现用现配，当天使用； 以下溶剂前显示的百分比是指该溶剂在您配制终溶液中的体积占比；如在配制过程中出现沉淀、析出现象，可以通过加热和/或超声的方式助溶 1.请依序添加每种溶剂： 10% DMSO→40% PEG300 →5% Tween-80 → 45% saline Solubility: $\geq 2.5 \text{ mg/mL}$ (4.71 mM); Clear solution 此方案可获得 $\geq 2.5 \text{ mg/mL}$ (4.71 mM, 饱和度未知) 的澄清溶液。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀向上述体系中加入 50 μL Tween-80，混合均匀；然后继续加入 450 μL 生理盐水分定容至 1 mL。 2.请依序添加每种溶剂： 10% DMSO →90% corn oil Solubility: $\geq 2.5 \text{ mg/mL}$ (4.71 mM); Clear solution 此方案可获得 $\geq 2.5 \text{ mg/mL}$ (4.71 mM, 饱和度未知) 的澄清溶液，此方案不适用于实验周期在半个月以上的实验。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。				



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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.



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