



上海源叶生物科技有限公司
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产品名称: **THZ531**
CAS 号: **1702809-17-3**
产品货号: **S88471**

生物活性:

Description	THZ531 是选择性的 CDK12 和 CDK13 的共价抑制剂, IC ₅₀ 值分别为 158 nM 和 69 nM。			
IC ₅₀ & Target[1]	CDK12 158 nM (IC ₅₀)	CDK13 69 nM (IC ₅₀)	CDK7 8.5 μM (IC ₅₀)	CDK9 10.5 μM (IC ₅₀)
Cellular Effect	Cell Line	Type	Value	Description
	BT-474	GI ₅₀	0.044 μM	Antiproliferative activity against trastuzumab-sensitive HER2-positive human BT-474 cells by Cell Titer Glo assay
	Bel-7402	IC ₅₀	650 nM	Antiproliferative activity against human Bel-7402 cells assessed as inhibition of cell growth measured after 96 hrs by SRB assay
	HCT-116	IC ₅₀	89 nM	Antiproliferative activity against human HCT-116 cells assessed as inhibition of cell growth measured after 96 hrs by SRB assay
	HeLa	IC ₅₀	106 nM	Antiproliferative activity against human HeLa cells assessed as inhibition of cell growth measured after 96 hrs by SRB assay
	JIMT-1	GI ₅₀	1.84 μM	Antiproliferative activity against trastuzumab-resistant HER2-positive human JIMT-1 cells by Cell Titer Glo assay
	Kelly	IC ₅₀	253.8 nM	Antiproliferative activity against human Kelly cells harboring CDK12 C1039F mutant assessed as reduction in cell viability incubated for 72 hrs by CellTiter-Glo assay
	Kelly	IC ₅₀	93 nM	Antiproliferative activity against human Kelly cells harboring wild type CDK12 assessed as reduction in cell viability incubated for 72 hrs by CellTiter-Glo assay
	L02	IC ₅₀	119 nM	Cytotoxicity against human L02 cells assessed as inhibition of cell growth measured after 96 hrs by SRB assay
	MDA-MB-231	IC ₅₀	133 nM	Antiproliferative activity against human MDA-MB-231 cells assessed as inhibition of cell growth measured after 96 hrs by SRB assay
	MDA-MB-231	IC ₅₀	17.9 μM	Antiproliferative activity against human MDA-MB-231 cells assessed as inhibition of cell growth incubated for 48 hrs by MTT assay
	MDA-MB-231	IC ₅₀	3.5 μM	Antiproliferative activity against human MDA-MB-231 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay
	MDA-MB-231	IC ₅₀	44.2 μM	Antiproliferative activity against human MDA-MB-231 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay
	MDA-MB-231	IC ₅₀	7.1 μM	Antiproliferative activity against human MDA-MB-231 cells assessed as inhibition of cell growth incubated for 72 hrs by MTT assay



	MDA-MB-436	IC ₅₀	14.3 μM	Antiproliferative activity against human MDA-MB-436 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay	
	MDA-MB-436	IC ₅₀	18.1 μM	Antiproliferative activity against human MDA-MB-436 cells assessed as inhibition of cell growth incubated for 48 hrs by MTT assay	
	MDA-MB-436	IC ₅₀	4.6 μM	Antiproliferative activity against human MDA-MB-436 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay	
	MDA-MB-436	IC ₅₀	6.4 μM	Antiproliferative activity against human MDA-MB-436 cells assessed as inhibition of cell growth incubated for 72 hrs by MTT assay	
	MDA-MB-468	IC ₅₀	14.4 μM	Antiproliferative activity against human MDA-MB-468 cells assessed as inhibition of cell growth incubated for 48 hrs by MTT assay	
	MDA-MB-468	IC ₅₀	3.4 μM	Antiproliferative activity against human MDA-MB-468 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay	
	MDA-MB-468	IC ₅₀	47.7 μM	Antiproliferative activity against human MDA-MB-468 cells assessed as inhibition of cell growth incubated for 24 hrs by MTT assay	
	MDA-MB-468	IC ₅₀	5.8 μM	Antiproliferative activity against human MDA-MB-468 cells assessed as inhibition of cell growth incubated for 72 hrs by MTT assay	
In Vitro	THZ531 激酶检测显示其强效抑制 CDK12 和 CDK13, 其 IC50 分别为 158 nM 和 69 nM, 而对 CDK7 和 CDK9 的抑制效果较弱, IC50 分别为 8.5 和 10.5 μM. THZ531 处理显著且不可逆地减少 Jurkat 细胞增殖, IC50 为 50 nM; FACS 细胞周期分析显示随着剂量和时间的增加, 具有亚 G1 内容的细胞比例增加[1]。				
Solvent&Solubility	细胞实验: DMSO 中的溶解度 : 250 mg/mL (447.97 mM; 超声助溶; 吸湿的 DMSO 对产品的溶解度有显著影响, 请使用新开封的 DMSO)				
	Preparing Stock Solutions	Solvent / Mass Concentration	1 mg	5 mg	10 mg
		1 mM	1.7919 mL	8.9594 mL	17.9189 mL
		5 mM	0.3584 mL	1.7919 mL	3.5838 mL
		10 mM	0.1792 mL	0.8959 mL	1.7919 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。 动物实验: 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 方案 一 请依序添加每种溶剂： 10% DMSO → 40% PEG300 → 5% Tween-80 → 45% Saline Solubility: ≥ 1.43 mg/mL (2.56 mM); 澄清溶液 此方案可获得 ≥ 1.43 mg/mL（饱和度未知）的澄清溶液。 以 1 mL 工作液为例，取 100 μL 14.3 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；再向上述体系中加入 50 μL Tween-80，混合均匀；然后再继续加入 450 μL 生理盐水 定容至 1 mL。 生理盐水的配制：将 0.9 g 氯化钠，溶解于 ddH₂O 并定容至 100 mL，可以得到澄清透明的生理盐水溶液。 方案 二 请依序添加每种溶剂： 10% DMSO → 90% (20% SBE-β-CD in Saline) Solubility: 1.43 mg/mL (2.56 mM); 悬浊液; 超声助溶 此方案可获得 1.43 mg/mL 的均匀悬浊液，悬浊液可用于口服和腹腔注射。 以 1 mL 工作液为例，取 100 μL 14.3 mg/mL 的澄清 DMSO 储备液加到 900 μL 20% 的 SBE-β-CD 生理盐水水溶液 中，混合均匀。 2 g SBE-β-CD（磺丁基醚 β-环糊精）粉末定容于 10 mL 的生理盐水中，完全溶解至澄清透明。 方案 三 请依序添加每种溶剂： 10% DMSO → 90% Corn Oil Solubility: ≥ 1.43 mg/mL (2.56 mM); 澄清溶液 此方案可获得 ≥ 1.43 mg/mL（饱和度未知）的澄清溶液，此方案实验周期在半个月以上的动物实验酌情使用。 以 1 mL 工作液为例，取 100 μL 14.3 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。
参考文献	[1]. Zhang T, et al. Covalent targeting of remote cysteine residues to develop CDK12 and CDK13 inhibitors. Nat Chem Biol. 2016 Oct;12(10):876-84.

完整储备液配制表：

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。

可选溶剂	质量 溶剂体积 浓度	1 mg	5 mg	10 mg	25 mg
DMSO	1 mM	1.7919 mL	8.9594 mL	17.9189 mL	44.7972 mL
	5 mM	0.3584 mL	1.7919 mL	3.5838 mL	8.9594 mL
	10 mM	0.1792 mL	0.8959 mL	1.7919 mL	4.4797 mL
	15 mM	0.1195 mL	0.5973 mL	1.1946 mL	2.9865 mL



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	20 mM	0.0896 mL	0.4480 mL	0.8959 mL	2.2399 mL
	25 mM	0.0717 mL	0.3584 mL	0.7168 mL	1.7919 mL
	30 mM	0.0597 mL	0.2986 mL	0.5973 mL	1.4932 mL
	40 mM	0.0448 mL	0.2240 mL	0.4480 mL	1.1199 mL
	50 mM	0.0358 mL	0.1792 mL	0.3584 mL	0.8959 mL
	60 mM	0.0299 mL	0.1493 mL	0.2986 mL	0.7466 mL
	80 mM	0.0224 mL	0.1120 mL	0.2240 mL	0.5600 mL
	100 mM	0.0179 mL	0.0896 mL	0.1792 mL	0.4480 mL



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