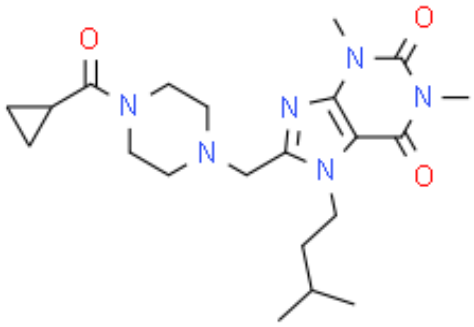
Product Data Sheet

Cas No.:	1802088-50-1	Cat. No:	PC12612
Product Name:	NCT-501		
Product synonym:	NCT-501		
Chemical name:	NCT-501		
MF:	C21H32N6O3	FW:	416.5172
Purity:	≥98%	Batch No.:	-
Storage:			
Structural formula:			
λmax：	-	Formulation：	-
Solubility :			
SMILES :	O=C(C1([H])C([H])([H])C1([H])[H])N1C([H])([H])C([H])([H])N(C([H])([H])C2=NC3=C(C(N(C([H])([H])[H])C(N3C([H])([H])[H])=O)=O)N2C([H])([H])C([H])([H])C([H])(C([H])([H])[H])C([H])([H])[H])C([H])([H])C1([H])[H]		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

ALDH1A1的强效选择性抑制剂，NCT-501是一种茶碱类的有效醛脱氢酶1A1 (ALDH1A1) 选择性抑制剂, 抑制hALDH1A1时IC50值为40 nM, 选择性超过其它ALDH同工酶和其它脱氢酶 (作用于hALDH1B1, hALDH3A1, 和hALDH2时, IC50值 >57 UM)。

生物活性	NCT-501 is a potent and selective theophylline-based inhibitor of **aldehyde dehydrogenase 1A1 (ALDH1A1)**, inhibits hALDH1A1 with **IC_{50}** of 40 nM, typically shows better selectivity over other ALDH isozymes and other dehydrogenases (hALDH1B1, hALDH3A1, and hALDH2, **IC_{50}** >57 μM).
IC50 & Target[1][2]	IC50: 40 nM (hALDH1A1)
体外研究(In Vitro)	NCT-501 shows a 16% decrease in the Cal-27 CisR cell line at 20 nM concentration, though the difference was not statistically significant. **Medlife has not independently confirmed the accuracy of these methods. They are for reference only.**

<table>
<tr><td>体内研究(In Vivo)</td><td>NCT-501 (100 µg/animal; i.t.; every alternate day for 20 days) shows a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts.

Medlife has not independently confirmed the accuracy of these methods. They are for reference only.
<table><tr><td>Animal Model:</td><td>5-6 weeks old male Hsd: Athymic Nude-Foxn1nu (immuno-deficient-mice bearing Cal-27 CisR cells)</td></tr><tr><td>Dosage:</td><td>100µg/animal</td></tr><tr><td>Administration:</td><td>Intra-tumorally (i.t); every alternate day for 20 days</td></tr><tr><td>Result:</td><td>Showed a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts.</td></tr></table></td></tr>
<tr><td>包装储存</td><td><table><tr><td>Powder</td><td>-20°C</td><td>3 years</td></tr><tr><td></td><td>4°C</td><td>2 years</td></tr><tr><td>In solvent</td><td>-80°C</td><td>6 months</td></tr><tr><td></td><td>-20°C</td><td>1 month</td></tr></table></td></tr>
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溶解度数据

体外研究:

DMSO : 12.5 mg/mL (**30.01 mM;** ultrasonic and warming and heat to 60°C)

配制储备溶液	溶剂体积 / 质量 / 浓度	1 mg	5 mg	10 mg
	1 mM	2.4008 mL	12.0042 mL	24.0085 mL
	5 mM	0.4802 mL	2.4008 mL	4.8017 mL
	10 mM	0.2401 mL	1.2004 mL	2.4008 mL

* 产品不同，其溶解度不同。建议根据产品选择合适的溶剂配制储备溶液；配成溶液后，**建议分装保存，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，建议在 6 个月内使用，-20°C 储存时，建议在 1 个月内使用。

体内研究:

建议根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都建议先按照 **体外研究** 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. 建议依照次序添加每种溶剂： 10% DMSO 90% (20% SBE-β-CD in saline)

   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution

   此方案可获得 ≥ 1.25 mg/mL (3.00 mM，饱和度未知) 的澄清溶液。

   以 1 mL 工作液为例，取 100 μL 12.5 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。

   将 2 g 磺丁基醚 β-环糊精加入 5 mL 生理盐水中，再用生理盐水定容至 10 mL，完全溶解，澄清透明

2. 建议依照次序添加每种溶剂： 10% DMSO 90% corn oil

   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution

   此方案可获得 ≥ 1.25 mg/mL (3.00 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 12.5 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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