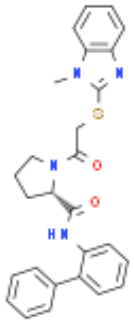
Product Data Sheet

Cas No.:	916141-36-1	Cat. No:	PC10674
Product Name:	TCS 1102		
Product synonym:	(2S)-N-[1,1'-联苯]-2-基-1-[2-[(1-甲基-1H-苯并咪唑-2-基)硫基]乙酰基]-2-吡咯烷甲酰胺;TCS1102 抑制剂		
Chemical name:	TCS 1102		
MF:	C27H26N4O2S	FW:	470.58594
Purity:	≥98%	Batch No.:	-
Storage:			
Structural formula:			
λmax:	-	Formulation:	-
Solubility :			
SMILES :	O=C([C@H]1N(C(CSC2=NC3=CC=CC=C3N2C)=O)CCC1)NC4=CC=CC=C4C5=CC=CC=C5		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

OX2和OX1受体的拮抗剂,TCS 1102是食欲肽OX受体拮抗剂，对OX2和OX1受体的Ki分别为0.2和3 nM。

生物活性	TCS 1102 is a potent, dual orexin receptor antagonist, with Ki values of 0.2 nM and 3 nM for **OX2** and **OX1** receptors, respectively. TCS 1102 demonstrates excellent brain peneration and moderate bioavailability in rats.
IC50 & Target[1][2]	OX_1 Receptor: 3 nM (Ki); OX_2 Receptor: 0.2 nM (Ki)
体外研究(In Vitro)	TCS 1102 (10 μM) inhibits Ca responses to Orexin A (human, rat, mouse) (HY-106224) and Yan 7874 (an Orexin receptor agonist) in CHO-hOX2 cells. **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>
TCS 1102 (compound 18) (15, 50, 100 mg/kg; i.p; single dose) induces locomotion inhibition in rat in a dose dependent manner. TCS-1102 (10 and 20 mg/kg; i.p.; single dose) decreases fear and anxiety in rats after exposure to footshock. Furthermore, TCS-1102 (10 mg/kg; i.p.; single dose) also shows anxiolytic effects for high responders (HR) rat when tested in the elevated T-maze.
PK of TCS 1102 in Rat (100 mg/kg; i.p.; measured at 30 min)
<table>
<tr><th>CL (mL/min/kg)</th><th>$T_{1/2}$ (h)</th><th>F (%)</th><th>Brain/plasma/CSF (nM)</th></tr>
<tr><td>3.7</td><td>0.3</td><td>11</td><td>2370/3500/43</td></tr>
</table>
Medlife has not independently confirmed the accuracy of these methods. They are for reference only.
<table>
<tr><td>Animal Model:</td><td>Male Sprague–Dawley rats (130-160 g)</td></tr>
<tr><td>Dosage:</td><td>10 and 20 mg/kg</td></tr>
<tr><td>Administration:</td><td>Intraperitoneal injection; 30 min before received the footshocks</td></tr>
<tr><td>Result:</td><td>Decreased fear and anxiety in rats 14 days after exposure to footshock.</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>
</table>

溶解度数据

体外研究:

DMSO : ≥ 100 mg/mL (212.50 mM)

* "≥" means soluble, but saturation unknown.

配制储备溶液	溶剂体积 质量 浓度	1 mg	5 mg	10 mg
	1 mM	2.1250 mL	10.6250 mL	21.2499 mL
	5 mM	0.4250 mL	2.1250 mL	4.2500 mL
	10 mM	0.2125 mL	1.0625 mL	2.1250 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 40% PEG300 5% Tween-80 45% saline

   Solubility: ≥ 2.5 mg/mL (5.31 mM); Clear solution

   此方案可获得 ≥ 2.5 mg/mL (5.31 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生理盐水定容至 1 mL。

   将 0.9 g 氯化钠，完全溶解于 100 mL ddH?O 中，得到澄清透明的生理盐水溶液

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

   Solubility: ≥ 2.5 mg/mL (5.31 mM); Clear solution

   此方案可获得 ≥ 2.5 mg/mL (5.31 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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