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产品名称: 1-[(4,6-二甲基-5-嘧啶基)羰基]-4-[(3S)-4-[(1R)-2-甲氧基-1-[4-(三氟甲基)苯基]乙基]-3-甲基-1-哌嗪基]-4-甲基哌啶马来酸盐  
产品别名: Vicriviroc maleate; SCH-417690 maleate; SCH-D maleate

生物活性:					
Description	Vicriviroc maleate (SCH-417690 maleate; SCH-D maleate) is a potent, selective, oral bioavailable and CNS penetrated antagonist of CCR5, with a $K_i$ of 2.5 nM, and also inhibits HIV-1 in PBMC cells, with $IC_{90}$ s of 3.3 nM (JrFL), 2.8 nM (ADA-M), 1.8 nM (301657), 4.9 nM (JV1083) and 10 nM (RU 570).				
	CCR5	HIV-1 (301657)	HIV-1 (ADA-M)		
IC <sub>50</sub> & Target	2.5 nM ( $K_i$ )	1.8 nM ( $IC_{90}$ , in PBMC cells)	2.8 nM ( $IC_{90}$ , in PBMC cells)		
	HIV-1 (JrFL)	HIV-1 (JV1083)	HIV-1 (RU 570)		
	3.3 nM ( $IC_{90}$ , in PBMC cells)	4.9 nM ( $IC_{90}$ , in PBMC cells)	10 nM ( $IC_{90}$ , in PBMC cells)		
In Vitro	Vicriviroc maleate (SCH-417690 maleate; SCH-D maleate) is a potent, selective and oral bioavailable inhibitor of CCR5, with a $K_i$ of 2.5 nM, and also inhibits HIV-1 in PBMC cells, with $IC_{90}$ s of 3.3 (JrFL), 2.8 (ADA-M), 1.8 (301657), 4.9 (JV1083) and 10 nM (RU 570). In addition, Vicriviroc maleate shows a mean $IC_{50}$ and $IC_{90}$ of 0.45 nM and 4 nM for a panel of HIV isolates, and has weak activity against hERG activity ( $IC_{50}$ , 5.8 $\mu$ M)[1]. Vicriviroc maleate inhibits chemotactic response to MIP-1 $\alpha$ with $IC_{50}$ values below 1 nM, and suppresses RANTES-induced signaling with a mean $IC_{50}$ of $4.2 \pm 1.3$ nM. Vicriviroc maleate potently suppresses all the viral isolates tested, with geometric mean $EC_{50}$ s of 0.04-2.3 nM and $IC_{90}$ s of 0.45-18 nM[2].				
In Vivo	Vicriviroc maleate (SCH-417690 maleate; SCH-D maleate; 10 mg/kg) has good oral availability in rats and monkeys, with no acute CNS or GI effects in rats[1].				
Solvent&Solubility	<b>In Vitro:</b> <b>DMSO : 50 mg/mL (76.96 mM; Need ultrasonic)</b> <b>H<sub>2</sub>O : 25 mg/mL (38.48 mM; Need ultrasonic and warming)</b>				
	Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
		1 mM	1.5392 mL	7.6959 mL	15.3917 mL
		5 mM	0.3078 mL	1.5392 mL	3.0783 mL
		10 mM	0.1539 mL	0.7696 mL	1.5392 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℃，6 months；-20℃，1 month。 -80℃ 储存时，请在 6 个月内使用，-20℃ 储存时，请在 1 个月内使用。  <b>In Vivo:</b>  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				



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	<p>Solubility: <math>\geq 2.5</math> mg/mL (3.85 mM); Clear solution</p> <p>此方案可获得 <math>\geq 2.5</math> mg/mL (3.85 mM, 饱和度未知) 的澄清溶液。</p> <p>以 1 mL 工作液为例, 取 100 <math>\mu</math>L 25.0 mg/mL 的澄清 DMSO 储备液加到 400 <math>\mu</math>L PEG300 中, 混合均匀向上述体系中加入 50 <math>\mu</math>L Tween-80, 混合均匀; 然后继续加入 450 <math>\mu</math>L 生理盐水定容至 1 mL。</p> <p>2. 请依序添加每种溶剂: 10% DMSO <math>\rightarrow</math> 90% (20% SBE-<math>\beta</math>-CD in saline)</p> <p>Solubility: <math>\geq 2.5</math> mg/mL (3.85 mM); Clear solution</p> <p>此方案可获得 <math>\geq 2.5</math> mg/mL (3.85 mM, 饱和度未知) 的澄清溶液。</p> <p>以 1 mL 工作液为例, 取 100 <math>\mu</math>L 25.0 mg/mL 的澄清 DMSO 储备液加到 900 <math>\mu</math>L 20% 的 SBE-<math>\beta</math>-CD 生理盐水水溶液中, 混合均匀。</p> <p>3. 请依序添加每种溶剂: 10% DMSO <math>\rightarrow</math> 90% corn oil</p> <p>Solubility: <math>\geq 2.5</math> mg/mL (3.85 mM); Clear solution</p> <p>此方案可获得 <math>\geq 2.5</math> mg/mL (3.85 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。</p> <p>以 1 mL 工作液为例, 取 100 <math>\mu</math>L 25.0 mg/mL 的澄清 DMSO 储备液加到 900 <math>\mu</math>L 玉米油中, 混合均匀。</p>
References	<p>[1]. Tagat JR, et al. Piperazine-based CCR5 antagonists as HIV-1 inhibitors. IV. Discovery of 1-[(4,6-dimethyl-5-pyrimidinyl)carbonyl]-4-[4-[2-methoxy-1(R)-4-(trifluoromethyl)phenyl]ethyl-3(S)-methyl-1-piperazinyl]-4-methylpiperidine (Sch-417690/Sch-D), a potent, highly selective, and orally bioavailable CCR5 antagonist. J Med Chem. 2004 May 6;47(10):2405-8.</p> <p>[2]. Strizki JM, et al. Discovery and characterization of vicriviroc (SCH 417690), a CCR5 antagonist with potent activity against human immunodeficiency virus type 1. Antimicrob Agents Chemother. 2005 Dec;49(12):4911-9.</p>
实验参考:	
Cell Assay	<p>Ficoll-purified peripheral blood mononuclear cells (PBMCs) are stimulated in vitro with phytohemagglutinin (PHA) (5 <math>\mu</math>g/mL) and interleukin-2 (IL-2) (50 U/mL) for 3 to 7 days. The cells are resuspended at <math>4 \times 10^5</math>/mL in complete medium (RPMI, 10% fetal bovine serum [FBS], 50 U/mL IL-2), seeded into 96-well plates (<math>2 \times 10^5</math>/well), incubated with an equal volume of culture medium containing compound (Vicriviroc) for 1 h at 37°C, and infected in triplicate with 25 to 100 50% tissue culture infectious doses (TCID<sub>50</sub>) per well of viral inoculum for 3 to 4 h. Cells are washed twice in phosphate-buffered saline (PBS) to remove residual virus and are cultured with compound for 4 to 6 days. HIV-1 replication is quantified by measurement of extracellular p24 antigen in the supernatants by enzyme-linked immunosorbent assay. The 50% effective concentrations (EC<sub>50</sub>s) and EC<sub>90</sub>s for each virus are determined using Graphpad PRISM software[2].</p>
References	<p>[1]. Tagat JR, et al. Piperazine-based CCR5 antagonists as HIV-1 inhibitors. IV. Discovery of 1-[(4,6-dimethyl-5-pyrimidinyl)carbonyl]-4-[4-[2-methoxy-1(R)-4-(trifluoromethyl)phenyl]ethyl-3(S)-methyl-1-piperazinyl]-4-methylpiperidine (Sch-417690/Sch-D), a potent, highly selective, and orally bioavailable CCR5 antagonist. J Med Chem. 2004 May 6;47(10):2405-8.</p>



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	[2]. Strizki JM, et al. Discovery and characterization of vicriviroc (SCH 417690), a CCR5 antagonist with potent activity against human immunodeficiency virus type 1. Antimicrob Agents Chemother. 2005 Dec;49(12):4911-9.
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