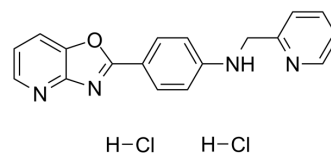


## DC07090 dihydrochloride

<b>Cat. No.:</b>	HY-123517
<b>CAS No.:</b>	1158264-37-9
<b>Molecular Formula:</b>	C <sub>18</sub> H <sub>16</sub> Cl <sub>2</sub> N <sub>4</sub> O
<b>Molecular Weight:</b>	375.25
<b>Target:</b>	Enterovirus
<b>Pathway:</b>	Anti-infection
<b>Storage:</b>	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



### SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 100 mg/mL (266.49 mM; Need ultrasonic)					
		Solvent Concentration	Mass	1 mg	5 mg	10 mg
	<b>Preparing Stock Solutions</b>	1 mM		2.6649 mL	13.3244 mL	26.6489 mL
		5 mM		0.5330 mL	2.6649 mL	5.3298 mL
		10 mM		0.2665 mL	1.3324 mL	2.6649 mL
Please refer to the solubility information to select the appropriate solvent.						
<b>In Vivo</b>	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: 2.5 mg/mL (6.66 mM); Clear solution; Need ultrasonic					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: 2.5 mg/mL (6.66 mM); Clear solution; Need ultrasonic					
	3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: 2.5 mg/mL (6.66 mM); Clear solution; Need ultrasonic					

### BIOLOGICAL ACTIVITY

<b>Description</b>	DC07090 dihydrochloride is a low toxicity, potent, reversible and competitive non-peptidyl human enterovirus 71 3C protease inhibitor with an IC <sub>50</sub> and a K <sub>i</sub> value for 21.72 μM and 23.29 μM. DC07090 dihydrochloride could also inhibit coxsackievirus A16 (CVA16) replication with an EC <sub>50</sub> value of 27.76 μM <sup>[1]</sup> .
<b>IC<sub>50</sub> &amp; Target</b>	IC <sub>50</sub> : 21.72 μM (EV71 3C protease) <sup>[1]</sup> . K <sub>i</sub> : 23.29 μM (EV71 3C protease) <sup>[1]</sup> . EC <sub>50</sub> : 27.76 μM (coxsackievirus A16) <sup>[1]</sup>
<b>In Vitro</b>	DC07090 dihydrochloride forms stable hydrogen-bonding interactions with the main chains of S128, G145, G164 and

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hydrophobic interactions with F25, L125, L127 and F170. DC07090 dihydrochloride (0.01~10  $\mu\text{M}$ ) shows micromolar potency against EV71 3Cpro. DC07090 dihydrochloride exhibits a highly inhibitory potency on EV71 replication with an EC50 value of 22.09  $\mu\text{M}$ . DC07090 dihydrochloride inhibits CVA16 with an EC50 value of 27.76  $\mu\text{M}$ <sup>[1]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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## REFERENCES

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[1]. Ma GH, et al. Identification and biochemical characterization of DC07090 as a novel potent small molecule inhibitor against human enterovirus 71 3C protease by structure-based virtual screening. *Eur J Med Chem.* 2016 Nov 29;124:981-991.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

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