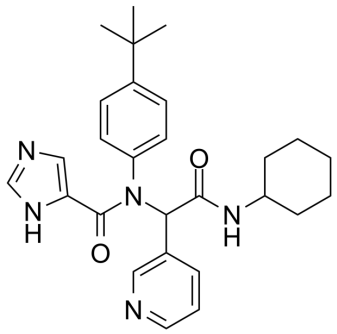
(Rac)-X77

Cat. No.:	HY-136298
CAS No.:	2144491-78-9
Molecular Formula:	$C_{27}H_{33}N_5O_2$
Molecular Weight:	459.58
Target:	SARS-CoV
Pathway:	Anti-infection

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (543.97 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.1759 mL	10.8795 mL	21.7590 mL
	5 mM	0.4352 mL	2.1759 mL	4.3518 mL
	10 mM	0.2176 mL	1.0879 mL	2.1759 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (4.53 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (4.53 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (4.53 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

(Rac)-X77 is a racemate of X77. X77 is a potent non-covalent inhibitor of the main protease of SARS-CoV-2 (SARS-CoV-2 M^{pro}) [1]. X77 binds to SARS-CoV-2 M^{pro} with a K_d value of 0.057 μM[2].

IC_{50} & Target

Kd: 0.057 μM (SARS-CoV-2 M^{pro})[2]

In Vitro

X77 can bind to SARS-CoV-2 M^{pro} (PDB code: 6W63). SARS-CoV-2 M^{pro} (PDB code: 6W63) is the main protease of SARS-CoV-2 and is one of the most important drug targets among coronaviruses[1].

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

REFERENCES

[1]. Sohini Chakraborti, et al. Drug Repurposing Approach Targeted Against Main Protease of SARS-CoV-2 Exploiting 'Neighbourhood Behaviour' in 3D Protein Structural Space and 2D Chemical Space of Small Molecules.

[2]. Alexander M Andrianov, et al. Computational discovery of small drug-like compounds as potential inhibitors of SARS-CoV-2 main protease. J Biomol Struct Dyn

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