# LY1

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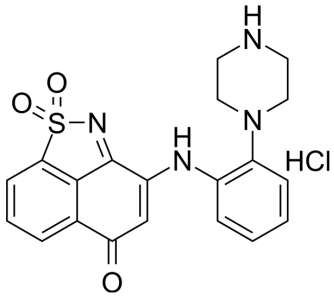
| **Cat. No.:** | HY-152101 |
| **CAS No.:** | 2883813-32-7 |
| **Molecular Formula:** | $C_{20}H_{19}ClN_4O_3S$ |
| **Molecular Weight:** | 430.91 |
| **Target:** | SARS-CoV |
| **Pathway:** | Anti-infection |
| **Storage:** | 4°C, protect from light, stored under nitrogen<br>* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light, stored under nitrogen) |




## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : 50 mg/mL (116.03 mM; Need ultrasonic)

| Preparing Stock Solutions | Mass / Solvent / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|---|
| | 1 mM | 2.3207 mL | 11.6034 mL | 23.2067 mL |
| | 5 mM | 0.4641 mL | 2.3207 mL | 4.6413 mL |
| | 10 mM | 0.2321 mL | 1.1603 mL | 2.3207 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: ≥ 2.5 mg/mL (5.80 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.80 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

LY1 is a potent, selective and covalent inhibitor against both SARS-CoV-2 $PL^{pro}$ and $M^{pro}$ with $K_d$ values of 1.5 μM and 2.3 μM for $M^{pro}$ C145A protein and $PL^{pro}$ C111A protein, respectively. LY1 potent against the viral proteases, with $IC_{50}$s of 0.12 μM and 0.99 μM against $M^{pro}$ and $PL^{pro}$. LY1 shows high selectivity over other kinases, human proteases and metalloenzyme[1].

**$IC_{50}$ & Target**

Kd: 1.5 μM ($M^{pro}$ C145A protein) and 2.3 μM ($PL^{pro}$ C111A protein)[1].
IC50: 0.12 μM ($M^{pro}$ protease) and 0.99 μM ($PL^{pro}$ protease)[1].

**In Vitro**

In SARS-CoV-2-infected Vero E6 cells, LY1 causes a dramatic reduction in the viral nucleoprotein (NP) levels with 5 μM. A 99.99% reduction in the viral RdRP RNA levels is observed with 15 μM LY1[1].
LY1 against cathepsin B and cathepsin L with the $IC_{50}$ values of 8.8 μM and 2.2 μM, respectively[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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| **In Vivo** | In the 8 week toxicity study, rats are orally administered with LY1 up to 300 mg/kg for 4 weeks and then recovered for another 4 weeks; no significant change in body weight and food consumption is observed in any group[1].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## REFERENCES

[1]. Wenying Yu, et al. Structure-Based Design of a Dual-Targeted Covalent Inhibitor Against Papain-like and Main Proteases of SARS-CoV-2. J Med Chem. 2022 Dec 22;65(24):16252-16267.



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