Product Data Sheet

LabMol-319

Molecular Weight:

Cat. No.: HY-150234 CAS No.: 381188-63-2 Molecular Formula: $C_{22}H_{16}N_2O_5$

Target: Virus Protease; Flavivirus

388.37

Pathway: Anti-infection

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)

SOLVENT & SOLUBILITY

In Vitro

DMSO: 100 mg/mL (257.49 mM; Need ultrasonic)

| Preparing Stock Solutions | Solvent Mass Concentration | 1 mg | 5 mg | 10 mg |
|------------------------------|-------------------------------|-----------|------------|------------|
| | 1 mM | 2.5749 mL | 12.8743 mL | 25.7486 mL |
| | 5 mM | 0.5150 mL | 2.5749 mL | 5.1497 mL |
| | 10 mM | 0.2575 mL | 1.2874 mL | 2.5749 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 (6.44 mM); Clear solution

BIOLOGICAL ACTIVITY

| Description | LabMol-319 is a potent zika virus (ZIKV) NS5 RdRp inhibitor with an IC $_{50}$ of 1.6 μ M. LabMol-319 is an antiviral agent ^[1] . | |
|-------------|--|--|
| In Vitro | LabMol-319 shows 98% inhibition on NS5 RdRp activity at concentration of 20 μ M ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only. | |

REFERENCES

[1]. Melina Mottin, et al. Discovery of New Zika Protease and Polymerase Inhibitors through the Open Science Collaboration Project OpenZika. J Chem Inf Model. 2022 Dec 26;62(24):6825-6843.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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