

Data Sheet

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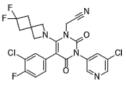
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Product Name : Secutrelvir
Cat. No. : PC-24181
CAS No. : 2996148-73-1
Molecular Formula : C₂₃H₁₆Cl₂F₃N₅O₂

Molecular Weight: 522.31

Target : SARS-CoV-2 Inhibitors

Solubility : 10 mM in DMSO



CAS: 2996148-73-1

Biological Activity

Secutrelvir (S-892216) is a potent, selective, reversible and covalent, oral **SARS-CoV-2** 3C-like protease (**3CLpro**) inhibitor with IC50 of 0.665 nM, and antiviral EC50 of 2.48 nM in CPE inhibition assays.

S-892216 has no inhibitory activity against caspase-2, chymotrypsin, cathepsin B/D/G/L, thrombin, or HIV-1 protease at 10 µM

S-892216 exhibits potent antiviral activities against various SARS-CoV-2 variants, including the Omicron JN.1 strain, with EC50 values of 2.27 to 12.5 nM in VeroE6/TMPRSS2 cells without cytotoxicity.

S-892216 displays anti-SARS-CoV-2 activity in VeroE6/TMPRSS2 cells with P-gp inhibitor and A549-Dual hACE2-TMPRSS2 cells, a human cell line derived from lung cancer overexpressing ACE2 and TMPRSS2, with EC50 values of 3.36 and 2.21 nM, respectively.

S-892216 demonstrates antiviral activity against the Omicron variants, with EC90 values of 2.31 to 2.41 nM in human airway epithelial cells (hAECs).

S-892216 exhibits promising antiviral activity against other beta-coronaviruses, including severe acute respiratory syndrome coronavirus (SARS-CoV), Middle East respiratory syndrome coronavirus (MERS-CoV), and human coronavirus OC43 (HCoV-OC43), with EC50 values of 6.61, 57.3, and 92.0 nM, respectively.

S-892216 (0.1, 0.3, 1, 3, and 10 mg/kg bid, oral) exhibits in vivo antiviral efficacy in mice infected with SARS-CoV-2.

References

Patent WO2025005305 A1.

2. Unoh Y, et al. J Med Chem. 2025 Jul 5. doi: 10.1021/acs.jmedchem.5c00754.

Caution: Product has not been fully validated for medical applications. Lab Use Only!

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