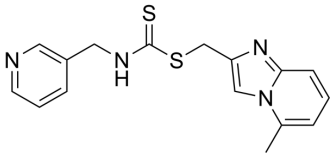
SARS-CoV-2 3CLpro-IN-13

Cat. No.:	HY-149264
CAS No.:	622794-09-6
Molecular Formula:	$C_{16}H_{16}N_4S_2$
Molecular Weight:	328.46
Target:	SARS-CoV
Pathway:	Anti-infection
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SARS-CoV-2 3CLpro-IN-13 is a potent SARS-CoV-2 3CL protease inhibitor with an IC_{50} value of 21 nM. SARS-CoV-2 3CLpro-IN-13 shows anti-coronavirus activity[1].
IC_{50} & Target	IC_{50}: 21 nM (SARS-CoV-2 3CL protease)[1]
In Vitro	SARS-CoV-2 3CLpro-IN-13 (compound 1) shows anti-coronavirus activity with IC_{50}s of 0.016, 0.021, 0.383, 2.00 μM for hCoV-229E (Alpha-CoV) 3CLpro, SARS-CoV-2 (Beta-CoV) 3CLpro, SARS-CoV (Beta-CoV) 3CLpro, MERS-CoV (Beta-CoV) 3CLpro, respectively[1]. SARS-CoV-2 3CLpro-IN-13 (0-300 μM) shows a selectivity profile against human cysteine proteases with IC_{50}s of 1.46, >300, 122 μM for 3CLpro SARS-CoV-2, human calpain 1, Cathepsin L respectively[1]. SARS-CoV-2 3CLpro-IN-13 (0.1-10 μM) shows antiviral activity with IC_{50} values of 1.06, 1.34 μM for SARS-CoV-2 and human coronavirus 229E, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Brier L, et al. Novel dithiocarbamates selectively inhibit 3CL protease of SARS-CoV-2 and other coronaviruses. Eur J Med Chem. 2023 Mar 15;250:115186.

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