SARS-CoV-2-IN-36

Cat. No.: HY-151988

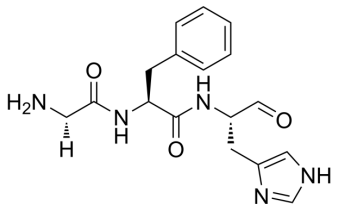
Molecular Formula: $C_{17}H_{21}N_5O_3$

Molecular Weight: 343.38

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-IN-36 is a potent SARS-CoV-2 Mpro (SARS-CoV) inhibitor with an IC_{50} of 2.37 μM and a K_d of 1.19 μM in enzymatic assays. SARS-CoV-2-IN-36 shows antiviral activity against UC-1074, RG2674, and NVDBB-2220 SARS-CoV-2 variants in Vero cells[1].

In Vitro

SARS-CoV-2-IN-36 (compound 58) inhibit the replication of the Wuhan (UC-1074),South African (RG2674), and UK (NVDBB-2220) SARS-CoV-2 variants, with IC50 values of 5.0 μM, 39.9 μM, and 5.2 μM, respectively. SARS-CoV-2-IN-36 alters cell morphology only at concentrations above ≥100 μM and does not inhibit Vero cell growth up to a concentration >100 μM[1]. SARS-CoV-2-IN-36 (compound 58) lacks antiviral activity against two herpesviruses (varicella-zoster virus and human cytomegalovirus) in human embryonic lung fibroblasts. SARS-CoV-2-IN-36 shows a very low cytotoxicity also against embryonic lung fibroblasts[1].

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

In Vivo

PK analysis of plasma concentrations, with ± SD, after intranasal (IN) and oral (PO) administration in male C57BL6 mice[1].

Route	Dose (mg/kg)	Concentration (mg/mL)	Number of animals	C_{max} (ng/mL)	T_{max} (h)	$AUC_{t/dose}$ (h*kg*ng/mL/mg)
IN	0.5	1.0	3	177.97±26.15	0.25±0.00	188.05±32.52
IN	1.25	2.5	3	325.95±42.45	0.25±0.00	150.62±23.80
PO	10	10	3	22.72±4.42	0.75±0.43	3.07±0.92
PO	25	2.5	3	33.67±3.42	0.5±0.43	2.00±0.51

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

REFERENCES

[1]. Simone Di Micco, et al. Rational design of the zonulin inhibitor AT1001 derivatives as potential anti SARS-CoV-2. Eur J Med Chem. 2022 Dec 15;244:114857.

Caution: Product has not been fully validated for medical applications. For research use only.

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