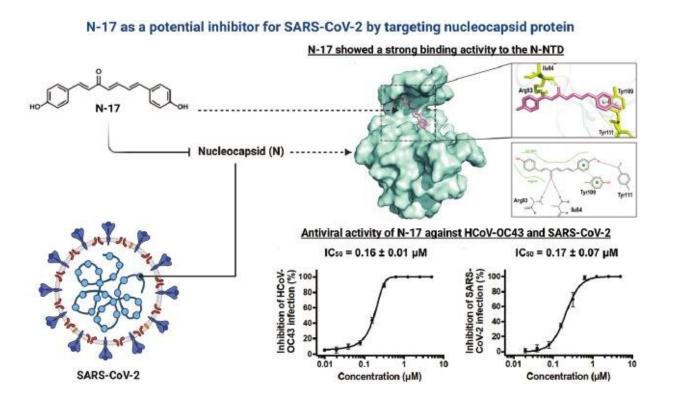


Newly-identified compound inhibits SARS-CoV-2 by targeting the nucleocapsid protein

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N-17 is a potential inhibitor of SARS-CoV-2 nucleocapsid protein, shows nanomolar activity against the HCoV-OC43 and SARS-CoV-2 viruses and may prevent SARS-CoV-2 replication and transcription by blocking the packaging process of viral RNA. Credit: *Acta Materia Medica* (2023). DOI: 10.15212/AMM-2023-0021

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has



spread globally since 2020. The nucleocapsid (N) protein plays a crucial role in the life cycle of SARS-CoV-2.

The authors of an article published in *Acta Materia Medica* have established a method to screen inhibitors of N protein by using microscale thermophoresis assays to obtain potential anti-SARS-CoV-2 agents. 1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one (N-17, a diphenylheptane) was identified as a compound with outstanding inhibitory activity.

The binding of N-17 to the N-terminal domain of N protein (N-NTD) was further validated by using drug affinity responsive target stability assays. The ability of N-17 to bind N protein was evaluated and the affinity of N-17 to the N-NTD with molecular docking and molecular dynamics simulation was predicted.

N-17 exhibited excellent anti-viral activity against HCoV-OC43 and SARS-CoV-2, with EC₅₀ values of $0.16 \pm 0.01 \mu$ M and $0.17 \pm 0.07 \mu$ M, respectively. Thus, a novel SARS-CoV-2 inhibitor targeting the N protein was discovered and its anti-viral activity in vitro was validated. The results may contribute to the development of promising therapeutic agents for COVID-19

More information: Yang Liu et al,

1,7-Bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one inhibits SARS-CoV-2 by targeting the nucleocapsid protein, *Acta Materia Medica* (2023). DOI: 10.15212/AMM-2023-0021

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