

[Inicio](#) > Small molecule interactions with the SARS-CoV-2 main protease: In silico all-atom microsecond MD simulations, PELE Monte Carlo simulations, and determination of in vitro activity inhibition

Small molecule interactions with the SARS-CoV-2 main protease: In silico all-atom microsecond MD simulations, PELE Monte Carlo simulations, and determination of in vitro activity inhibition

URL: <https://linkinghub.elsevier.com/retrieve/pii/S1093326321002217>

Authors: [Liang, Julia](#) / [Pitsillou, Eleni](#) / [Ververis, Katherine](#) / [Guallar, Victor](#) / [Hung, Andrew](#) / [Karagiannis, Tom](#)

Publication: Journal of Molecular Graphics and Modelling

Volume / Pagination: /

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 27 Mar 2023 - 03:29): <https://www.bsc.es/es/research-and-development/publications/small-molecule-interactions-the-sars-cov-2-main-protease>