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## [Investigation of small molecule inhibitors of the SARS-CoV-2 papain-like protease by all-atom microsecond modelling, PELE Monte Carlo simulations, and in vitro activity inhibition](#)

**URL:** <https://linkinghub.elsevier.com/retrieve/pii/S0009261421009775>

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**Publication:** Chemical Physics Letters

**Volume / Pagination:** /

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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**Source URL (retrieved on 20 Mar 2023 - 23:18):** <https://www.bsc.es/es/research-and-development/publications/investigation-small-molecule-inhibitors-the-sars-cov-2-papain>