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Neutron crystallography to inform drug design targeting SARS-CoV-2 main protease

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SARS-CoV-2 main protease (Mpro) is an important target for small-molecule COVID-19 antivirals. We use neutrons to determine protonation states of ionizable residues in Mpro informing computer-assisted and structure-based design. Several neutron crystal structures were determined, revealing protonation state modulation upon inhibitor binding. This information is used to design novel inhibitors and to perform structure-activity relationship studies guided by virtual reality structure analysis.

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