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Computational Insights on the Potential of Some NSAIDs for Treating COVID-19: Priority Set and Lead Optimization

The discovery of drugs capable of inhibiting SARS-CoV-2 is a priority for human beings due to the severity of the global health pandemic caused by COVID-19. To this end, repurposing of FDA-approved drugs such as NSAIDs against COVID-19 can provide therapeutic alternatives that could be utilized as an effective safe treatment for COVID-19. The anti-inflammatory activity of NSAIDs is also advantageous in the treatment of COVID-19, as it was found that SARS-CoV-2 is responsible for provoking inflammatory cytokine storms resulting in lung damage. In this study, 40 FDA-approved NSAIDs were evaluated through molecular docking against the main protease of SARS-CoV-2. Among the tested compounds, sulfinpyrazone 2, indomethacin 3, and auranofin 4 were proposed as potential antagonists of COVID-19 main protease. Molecular dynamics simulations were also carried out for the most promising members of the screened NSAID candidates (2, 3, and 4) to unravel the dynamic properties of NSAIDs at the target receptor. The conducted quantum mechanical study revealed that the hybrid functional B3PW91 provides a good description of the spatial parameters of auranofin 4. Interestingly, a promising structure–activity relationship (SAR) was concluded from our study that could help in the future design of potential SARS-CoV-2 main protease inhibitors with expected anti-inflammatory effects as well. NSAIDs may be used by medicinal chemists as lead compounds for the development of potent SARS-CoV-2 (M^{pro}) inhibitors. In addition, some NSAIDs can be selectively designated for treatment of inflammation resulting from COVID-19.