BO-01 : Docking of nitrovinylfuran derivatives against SARS CoV-2 main protease for the treatment of covid-19

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Subject description: Covid-19 has become one of the most known pandemics in the world wide, it was appeared in late of December 2019 from Wuhan city of China. The research to fight covid19 is ongoing without finding any efficient treatment still now.

Objectives: This work aims to identify new anticovid19 agents by a virtual screening of the nitrovinylfuran derivatives as new inhibitors of the SARS CoV-2 main protease (Mpro), implicated in the replication of the virus.

Methods: A set of nitrovinylfuran derivatives were docked in the structure of Mpro (downloaded from PDB), and then filtered according to their good ADME-T profile using two web servers.

Results and discussion: Two nitrovinylfuran derivatives PubChem-57392921 and PubChem-88580143 showed good interaction energy scores with the binding site of SARS CoV-2 Mpro. In addition, they were found having good pharmacokenitic properties and a low toxicity.

Conclusion: Our research proposed two nitrovinylfuran derivatives as potential inhibitors of SARS CoV2 Mpro, other practical investigations on the nitrovinylfuran derivatives could enrich the treatment of covid19 by new antiviral agents.

Keywords: Covid-19, SARS CoV-2 main protease (Mpro), virtual screening, ADME-T profile.

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