Abstract



Insight into the screening of potential prodigiosin as a novel Anti-SARS-CoV-2 agent through pharmacoinformatics study

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Abstract:

The SARS-CoV-2 virus is a member of coronaviruses that causes a fatal respiratory pandemic named as COVID-19. At present, there are no approved treatments or vaccines to prevent or stop infection. Prodigiosin, a natural red pigment produced by Serratia marcescens and various bacterial species, has exhibited different promising therapeutic activities. It shows anticancer activity against 15 different types of cancers, It also has anti-diabetic effect, antioxidant effect, anti-inflammatory effect, antimalarial effect, antibacterial effect and dyeing effect .Prodigiosin was also identified as a possible therapy for diseases such as cystic fibrosis. The Pharmacophore modelling and docking analysis of Prodigiosin have illustrated the potential of the molecule to inhibit various viruses like HBV, HIV, and H1N1 through protein-ligand binding as described by (Suba et al., 2013). Therefore, the present investigation was carried out to identify the possible anti-SARSCoV-2 activity of prodigiosin by using pharmacoinformatics-based methods. The dynamic behavior of the prodigiosin molecule was explored through all-atoms molecular dynamics (MD) simulation study. Several parameters from the MD simulation have confirmed the stability of protein-ligand complexes. Thus, prodigiosin could be considered as a novel antiviral therapeutic agent against SARS-CoV-2 which could be beneficial against COVID-19.

Biography:

Shaimaa Ahmed Abdel-Mougood has completed her MSc degree from (IGSR) Alexandria University, Egypt and currently, beside her clinical pharmaceutical work she is a fr eelancer research associate aimed to get (PhD by publications). She has published her works in reputed international conferences and has been serving as an online tutor to help young medical staff. Her page has more than 45000 followers. She is interested in precision medicine, systems biology, drug design, bioinformatics, molecular biology & biotechnology.

Publication of speakers:

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