Docking and molecular interaction studies of covid-19 viral targets with sulphated polysaccharides

P.S. Gowtham and B. Vanavil*

Department of Biotechnology, Kalasalingam Academy of Research and Education, Krishnankoil-626126, Tamilnadu.

*Corresponding author

ABSTRACT

Sulphated polysaccharides exhibit innumerable pharmacological activities and have been reported to possess anti-viral activities against dengue, malaria, human immuno deficiency virus, hepatitis-B virus. COVID-19 is the recent pandemic caused by Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2) that threatens the whole world by infecting over 1 million and leading to death of more than 500,000people. SARS-CoV-2 virus mainly consists of four structural proteins including spike glycoprotein, small envelope glycoprotein, membrane glycoprotein, and nucleocapsid protein that are responsible for the pathogenesis. Many scientists are researching all over the world to find an inhibitor for treatment of COVID-19. It is the need of the hour to find a potential inhibitor that prevents this viral infection and hence can save millions of lives in the world. In this perspective, the present study was focused on exploring the potential of sulphated polysaccharides such as fucoidan, carrageenan, ulvan and curdlan sulfate as anti-viral agents against SARS-CoV-2 by *in silico* analysis through molecular docking of sulphated polysaccharides with target structural proteins. Structures of spike protein and nucleocapsid protein were retrieved from Protein Data Bank while the structures of small membrane protein and envelope protein were modeled using SWISS Model. Structures of sulphated polysaccharides were retrieved from PubChem. Among all sulphated polysaccharides, ulvan has a maximum binding affinity with the nucleocapsid protein which is followed by kappa carrageenan. Further, interacting amino acids differ with the different sulphated polysaccharides. Hence this study will be an asset in assessing the potential of sulphated polysaccharides for the development of anti-viral agents for COVID-19.

Keywords: Sulphated polysaccharides, SARS-CoV-2, COVID-19, Anti-viral agent

ISBN: 978-81-947843-4-0; DOI: 10.21467/abstracts.109