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Designing of Remdesivir Based New Molecules Binds to Protease Enzyme of Covid-19 Virus: An In-silico Study

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Abstract

In present day the pandemic character of Novel Corona Virus Covid-19 become the most life threatening problem for human health. Till date around 6.5 million of people were affected and 0.4 million were died of this. In spite of all types of precaution the rate of spreading increasing day after day and if it could not be ceased, whole human being in world will cease to exist. Remdesivir is an antiviral drug that was developed to block infection with related coronaviruses and even Ebola. It is one of the drugs the WHO is helping to investigate. It works against SARS-CoV-2 in cells in a dish in a lab as well as in mice infected with the virus. Remdesivir specifically targets key viral proteins involved in making new copies of the virus and prevents them from working. Due to the bulkier structure, Remdesivir violets Lipinski rule (MW>500 and No of H-bond accepters >10), shows very low GI track absorption and bioavailability (0.17). In this work, I tried to investigate the structural aspects of Remdesivir for the binding with viral protein and from the availed data tried to design (Insilico) a newer molecules which binds more effectively with the protein. My work will helpful to enrich the data base for the develop more efficient drug than Remdesivir.

Keywords—Corona Virus, Designing of New Molecules, Protease Inhibitor, Remdesivir based drug

Biography:

Dr. Md. Maidul Islam has completed his PhD at the age of 30 years from Indian Institute of Chemical Biology Kolkata (Jadavpur University) and postdoctoral studies from the same Institute. Presently he is working as Assistant Professor in Aliah University Kolkata. He has published a book and more than 35 papers in reputed journals. He has been serving as referee of several reputed journals. Till now he had been selected for two national and two international awards

Speaker Publications:

2nd Euroscicon Conference on Virology; Online Event- July 27, 2020.

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