

5.1 Selection Criteria for Chemicals

One of the important points to be considered in the treatment or the drug development for COVID 19 is time constraint. Currently Drug repurposing [1] is the best option that can be considered for the development of drugs in the treatment of the COVID victims.

In view of the above comparative analysis between MERS CoV and Novel Corona Virus 2019 which revealed a close genetic relation, all the medications that were successful in treating MERS can be used in the therapy of COVID with the molecular mechanism studied. All the drugs and their structures are obtained from two important public databases which are PUBCHEM [2] and CHEBI [3].

A Selection of Chemicals

1. Remdesivir:

This is an active inhibitor for the RNA dependent RNA polymerase enzyme which was already tested and proved to be effective against MERS [4] (<https://www.jbc.org/content/early/2020/02/24/jbc.AC120.013056>).

One of the study by Elfiky et al. [5] on MERS therapy stated that Guanosine derivatives are good inhibitors for virus polymerases (<https://www.tandfonline.com/doi/full/10.1080/07391102.2020.1758789>) and can be used in treating MERS which was validated by in silico docking studies. Thus these derivatives along with the proposed other drugs can be tested for COVID therapy. The compounds tested in the study were as follows:

2. Guanosine triphosphate (GTP)
3. Uridine triphosphate (UTP),
4. IDX-184 (GTP derivative),
5. Sofosbuvir (UTP derivative)
6. Ribavirin (wide acting antiviral drug)

B. Collection of chemicals and their properties from Databases:

The data has been retrieved from two data bases CHEBI and PUBCHEM

1. Remdesivir [6] (CHEBI: 145994)

Formula: C₂₇H₃₅N₆O₈P

Molecular Mass: 602.6

Log P: 1.9

H bond donor: 4

H bond acceptor: 13

2. Guanosine triphosphate [7] (GTP) (CHEBI:16690)

Formula: C₁₀H₁₈N₅O₂₀P₅

Molecular Mass: 683.14

Log P: -5.7

H bond donor: 8

H bond acceptors: 16