Potential repurposing of Valproic acid-CoA against SARS-CoV2

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We have performed an extensive computational analysis to find potential targets and drugs against SARS-CoV2. The work goes beyond docking, and includes binding energy calculation and 1000 ns MD simulation to assess the affinity of drugs for the target. Based on these and on our knowledge of drug potency, we have concluded that Valproic acid-CoA, an existing drug for epilepsy, should be able to inhibit the RNA-dependent RNA Polymerase (RdRp) of SARV-CoV2, an essential enzyme for virus survival [1,2]. Mainstream media have also covered the report [3-5], and another study, performed at the Scripps Institute (TSRI), La Jolla, USA also lists Valproic acid as one of the potential molecules for repurposing against the virus, thus being an independent validation of our work [6].

The molecule Valproic acid is an approved drug whose patent has expired recently. It is currently sold under brand names; Depakene, Depacon (Abbott) and Stavzor (Bionpharma). A few Indian companies have licenses to manufacture the drug.

The drug needs to be tested in cell culture and in animal models to determine the minimum inhibitory concentration (MIC) and to determine dosage. The drug can go immediately into clinical trials, as this is the repurposing of an existing approved drug. We sincerely request you to kindly facilitate the test and trial. Quick testing and determination of its potential efffectiveness will help India and the world in the fight against the SARV-CoV2 virus.

We are in the process of over-expressing and purifying CoV2-RdRp. We will then crystallize the protein and determine its three-dimensional structure. Later using Schrödinger and other packages we will perform structure-based inhibitor discovery and validation using SPR, ITC and NMR spectroscopy, which can then be taken up by our collaborators for *in vivo* screening.

References

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