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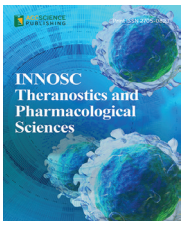

RESEARCH ARTICLE

Inhibitory Potential of Chitosan Derivatives against Severe Acute Respiratory Syndrome Coronavirus 2: An *In Silico* Prospective

Supplementary Files

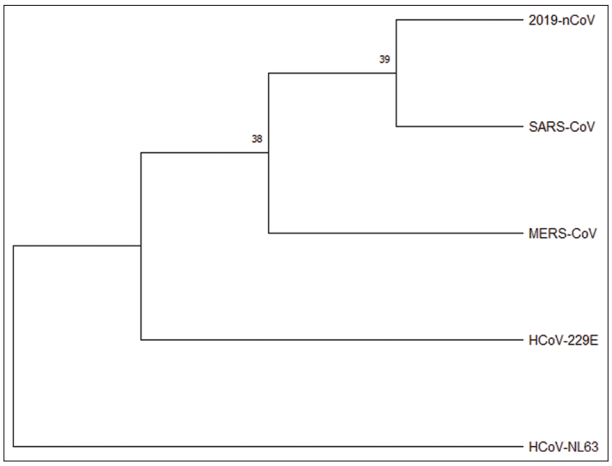

Figure S1. Phylogenetic analysis of severe acute respiratory syndrome coronavirus 2.

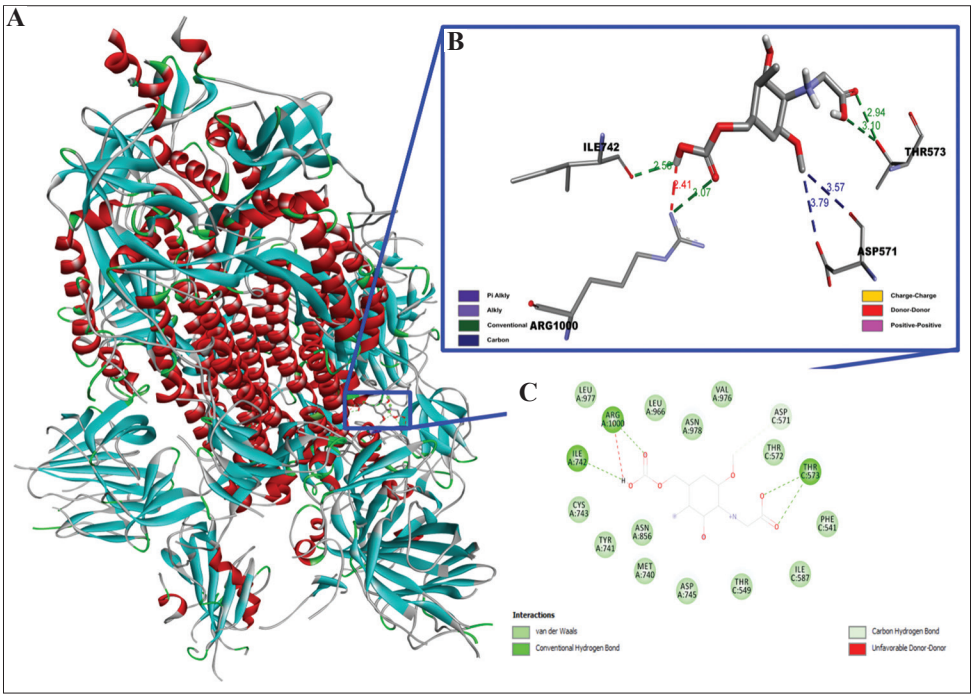

Figure S2. (A) Molecular docking of N,O-carboxy methyl chitosan with the S protein. (B) Brief 3D representation of N,O-carboxy methyl chitosan and S protein interaction, including bond types and length. (C) 2D representation of N,O-carboxy methyl chitosan and S protein with participating amino acids and types of bonds.

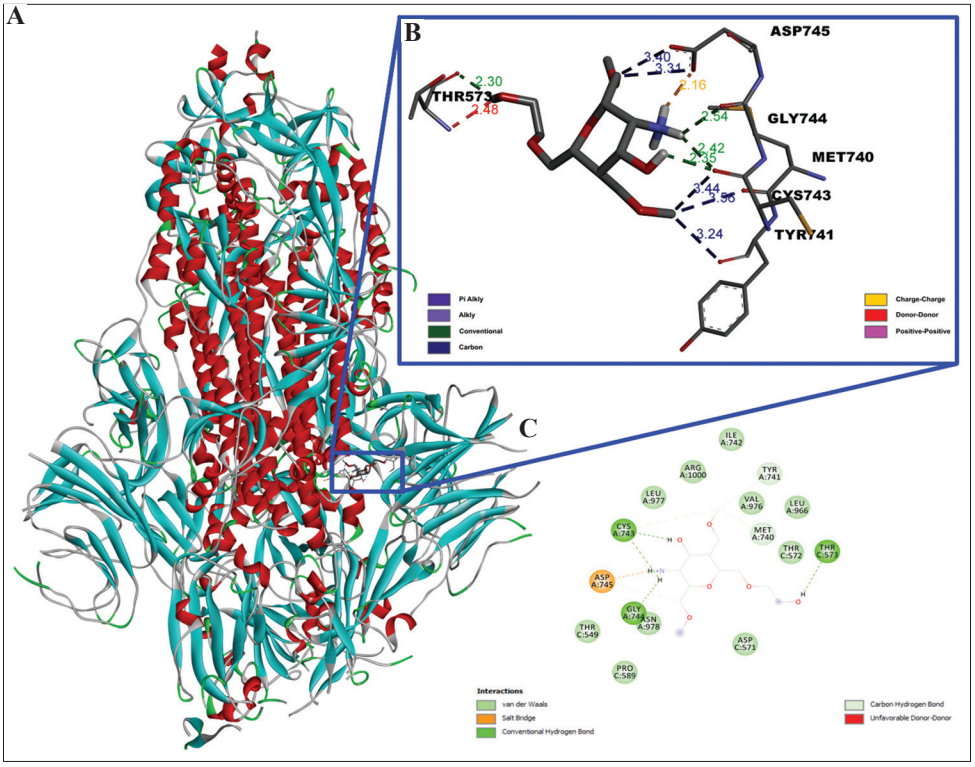

Figure S3. (A) Molecular docking of glycerol chitosan with the S protein. (B) Brief 3D representation of glycerol chitosan and S protein interaction, including bond types and length. (C) 2D representation of glycerol chitosan and S protein with participating amino acids and types of bonds.

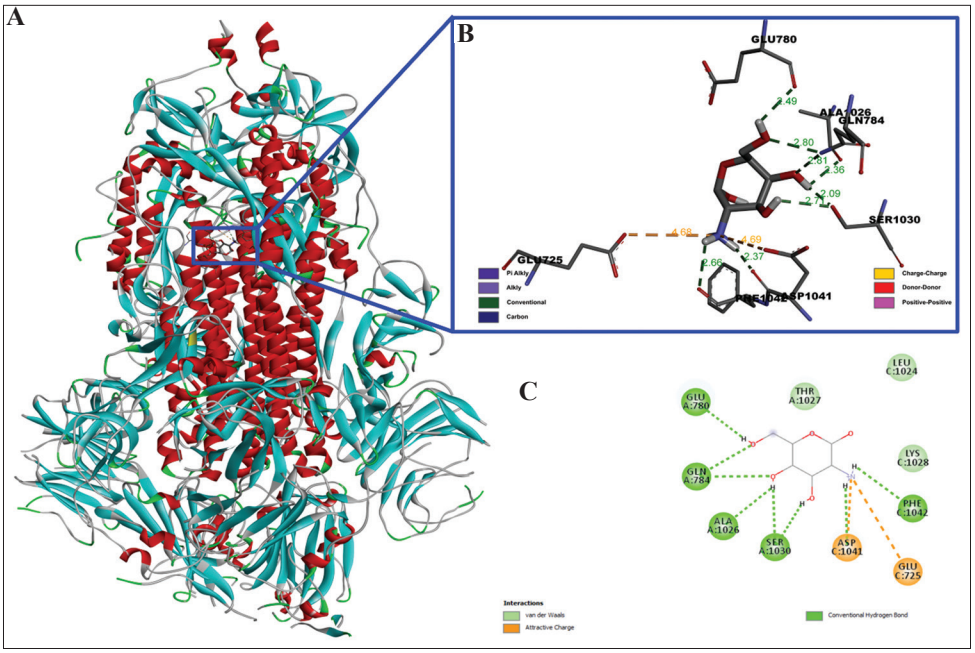

Figure S4. (A) Molecular docking of monomeric chitosan with the S protein. (B) Brief 3D representation of monomeric chitosan and S protein interaction, including bond types and length. (C) 2D representation of monomeric chitosan and S protein with participating amino acids and types of bonds.

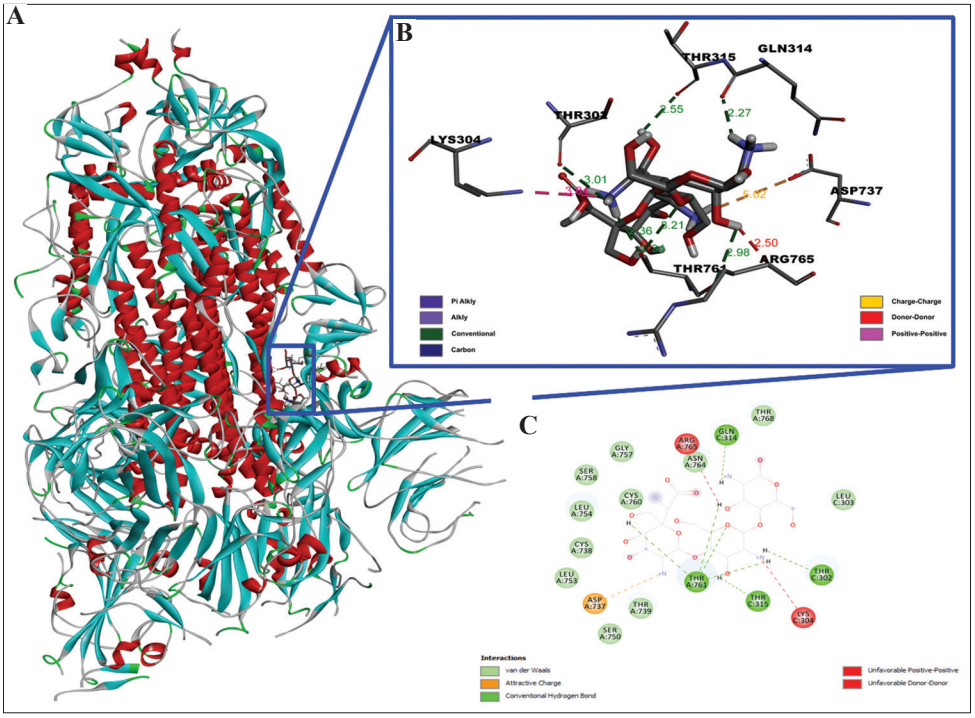

Figure S5. (A) Molecular docking of carboxy ethyl chitosan with the S protein. (B) Brief 3D representation of carboxy ethyl chitosan and S protein interaction, including bond types and length. (C) 2D representation of carboxy ethyl chitosan and S protein with participating amino acids and types of bonds.

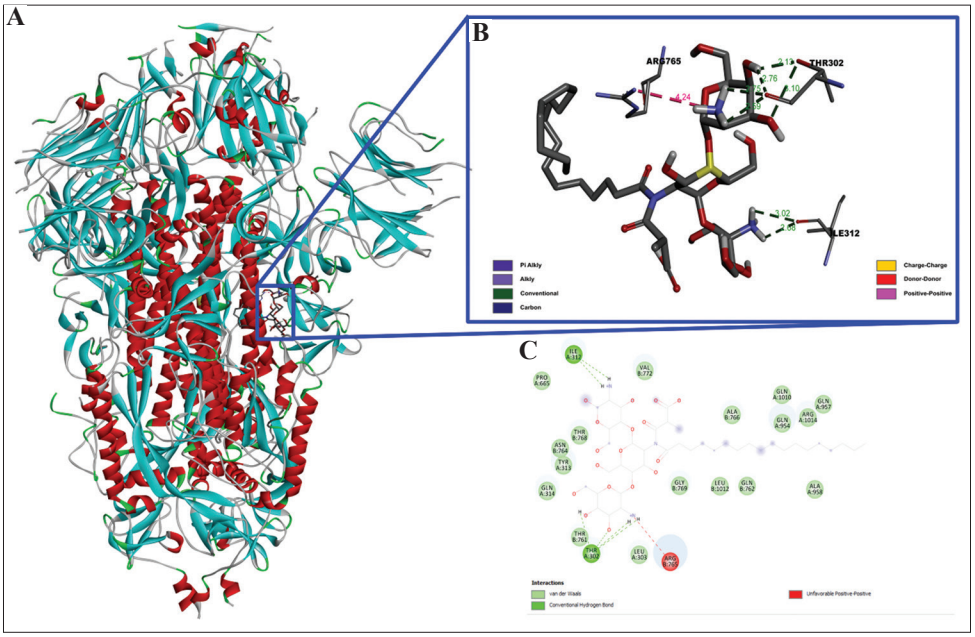

Figure S6. (A) Molecular docking of N-octadecanoyl-N-3-carboxy propionyl chitosan with the S protein. (B) Brief 3D representation of N-octadecanoyl-N-3-carboxy propionyl chitosan and S protein interaction, including bond types and length. (C) 2D representation of N-octadecanoyl- N-3-carboxy propionyl chitosan and S protein with participating amino acids and types of bonds.

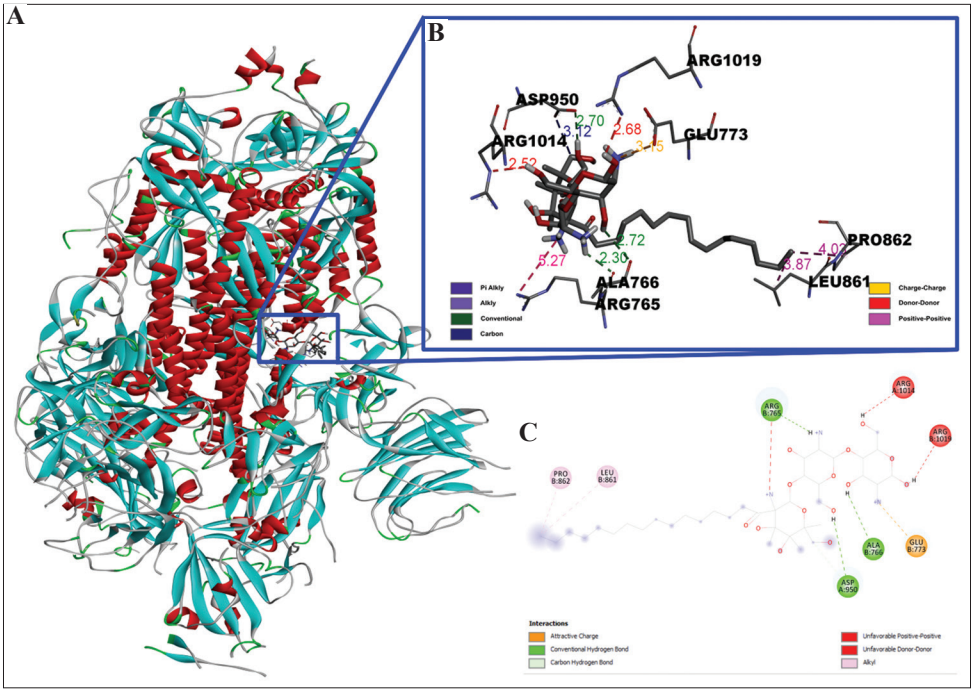

Figure S7. (A) Molecular docking of palmitoyl-trimethyl-chitosan chitosan with the S protein. (B) Brief 3D representation of palmitoyl-trimethyl-chitosan and S protein interaction, including bond types and length. (C) 2D representation of palmitoyl-trimethyl-chitosan and S protein with participating amino acids and types of bond.

Figure S8. Protein–protein interaction depicting five lowest binding energy for S Protein–ACE2 complex in the presence mHTCC. Green- lowest binding energy 1, Yellow- lowest binding energy 2, Blue- lowest binding energy 3, Cyans- lowest binding energy 4, Magentas- lowest binding energy 5, and Red- S Protein.