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# SARS-CoV-2: Prediction of Critical Charged Amino Acid Mutations

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**Abstract :** Viruses change with time through mutations and result in new variants that may persist or disappear. A Mutation refers to an actual change in the virus genetic sequence, and a variant is a viral genome that may contain one or more mutations. Critical mutations may cause the virus to be more transmissible, with high disease severity, and more vulnerable to diagnostics, therapeutics, and vaccines. Thus, variants carrying such mutations may increase the risk to human health and are considered variants of concern (VOC). Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) - the contagious in humans, positive-sense single-stranded RNA virus that caused coronavirus disease 2019 (COVID-19) - has been studied thoroughly, and several variants were revealed across the world with their corresponding mutations. SARS-CoV-2 has four structural proteins, known as the S (spike), E (envelope), M (membrane), and N (nucleocapsid) proteins, but prior study and vaccines development focused on genetic mutations in the S protein due to its vital role in allowing the virus to attach and fuse with the membrane of a host cell. Specifically, subunit S1 catalyzes attachment, whereas subunit S2 mediates fusion. In this perspective, we studied all charged amino acid mutations of the SARS-CoV-2 viral spike protein S1 when bound to Antibody CC12.1 in a crystal structure and assessed the effect of different mutations. We generated all missense mutants of SARS-CoV-2 protein amino acids (AAs) within the SARS-CoV-2:CC12.1 complex model. To generate the family of mutants in each complex, we mutated every charged amino acid with all other charged amino acids (Lysine (K), Arginine (R), Glutamic Acid (E), and Aspartic Acid (D)) and studied the new binding of the complex after each mutation. We applied Poisson-Boltzmann electrostatic calculations feeding into free energy calculations to determine the effect of each mutation on binding. After analyzing our data, we identified charged amino acids keys for binding. Furthermore, we validated those findings against published experimental genetic data. Our results are the first to propose in silico potential life-threatening mutations of SARS-CoV-2 beyond the present mutations found in the five common variants found worldwide.

**Keywords :** SARS-CoV-2, variant, ionic amino acid, protein-protein interactions, missense mutation, AESOP
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