سمینار هفتگی ماده چگال نرم

Transition from the down state to the up state of RBD protein in SARS-CoV-2

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Abstract

Since the first observed case in December 2019, millions of people have been infected by Coronavirus disease 2019 (COVID-19), which is caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Located on the viral membrane, trimeric spike glycoprotein is one of the most crucial parts of the virus' structure as it is responsible for the attachment and entry of the virus to host cells. The spike glycoprotein undergoes hinge-like conformational movements and its receptor-binding domains (RBD) can be in either an accessible (up) state or an inaccessible (down) state to the host cell receptors, such as ACE2. Having performed Molecular Dynamics Simulations and Targeted Molecular Dynamics (TMD), here in this work, we have investigated important properties of the down and up states and the transition between them, respectively. Moreover, we oxidized 2 amino acids located in the vicinity of RBD and assessed the effects of such oxidation on the mobility of RBD and its transition from the down to the up state. What we have found is that the RBD has less mobility in its down state, whether it is oxidized or native. This might happen due to some hydrogen and ionic bonds existing between the RBD and other parts of the spike protein, especially one of the three monomers, since during the transition some of those bonds break. In addition, we have found out that glycans such as N165B, N343B, and N343A play an important role in the establishment of hydrogen bonds. We have also shown that the oxidation not only makes the transition smoother and slower, but under oxidation more work is needed. This could result in the harder transition and as the transition gets harder, the probability by which the virus attaches to host cells would decline consequently.

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