

Investigation of the Effects of N-Linked Glycans on the Stability of the Spike Protein in SARS-CoV-2 by Molecular Dynamics Simulations

E.Deniz TEKİN¹

¹Turk Hava Kurumu Universitesi

April 16, 2024

Abstract

We perform all-atom molecular dynamics simulations to study the effects of the N-linked glycans on the stability of the spike glycoprotein in SARS-CoV-2. After a 100 ns of simulation on the spike proteins without and with the N-linked glycans, we found that the presence of glycans increases the local stability in their vicinity; even though their effect on the full structure is negligible.

Hosted file

Manuscript_EDTekin.docx available at <https://authorea.com/users/738513/articles/712748-investigation-of-the-effects-of-n-linked-glycans-on-the-stability-of-the-spike-protein-in-sars-cov-2-by-molecular-dynamics-simulations>