عنوان مقاله:

Assessment and Molecular Docking of SARS-CoV-۲ NSP۳ and NSP۱۲ Mutants in Iranian Patients in Golestan Province

محل انتشار:

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خلاصه مقاله:

Background: Molecular analysis of SARS-CoV-۲ genome is important to predict viral pathogenicity. In addition to transmission, replication is a key factor in pathogenicity of the virus. Notably, mutations in non-structural proteins (NSP۳ and NSP۱۲) can affect host immune response and viral replication. Therefore, this study was conducted to investigate different mutations of SARS-CoV-۲ NSP۳, and NSP۱۲ during different waves of COVID-۱۹ infection.Methods: We recruited ۵۷ NGS sequences including ۸ NGS sequences from Golestan SARS-CoV-۲ RNA samples, obtained as part of clinical testing in different referral centers of Iran. After obtaining sequences from the global initiative on sharing all influenza data (GISAID), and evaluating and processing data, all sequences were aligned to the Wuhan variant genome (NC_۰۴۵۵۱۲.۲) using MEGA۶. The HDOCK server was used for molecular docking.Results: In NSP۳, mutations in positions (nts ۳۱۵, ۵۴۵, ۲۶۶۶, ۳۲۶۴) were more frequent and among them mutation in positions including nt ۵۴۵ (aa۱۸۲) and nt ۲۶۶۶ (aa۸۸۹) were associated with an increase in codon usage. In the term of NSP۱۲, mutations in positions such as nts ۴۰۶ (aa۱۳۷), ۹۶۵ (aa۳۲۳), ۱۲۳۳, ۱۶۵۳, ۱۸۳۶, ۲۷۳۳ were more frequent. The molecular docking results showed more affinity in some variants of NSP۳ and NSP۱۲ as well.Conclusion: This study has assessed mutation in SARS-CoV-۲ Nsp۳, and NSP۱۲ which are viral protease, and viral polymerase (RdRp). The mutations reported in this study may help this virus to replicate faster and evade the pharmaceutical agents which target viral polymerase activity and be very effective in viral pathogenesis. In addition, .this study highlights the importance of ongoing genomic variation studies to be performed on SARS-CoV-۲ variants

کلمات کلیدی:

NSP۳, NSP۱۲, Mutation, COVID-۱۹, Golestan