عنوان مقاله:

Molecular Analysis of ۵-COR Derivatives of Uracil and Evaluating their Affinity Against the MPro Target of COVID-۱۹

محل انتشار:

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خلاصه مقاله:

Molecular analysis of ۵-COR (R: H, CH۳, NH۲, OH, F, Cl, Br, I) functionalized derivatives of uracil (U) were explored in this work using computational procedures. Next, binding affinity of each U compound was examined against the main protease (MPro) target of COVID-۱۹ pandemic to maybe inhibit it from further growth. The results indicated that the models of U detected effects of structural modifications by showing variations in their molecular features. Molecular orbital properties indicated that the electronic features of models were changed through functionalization processes. Further analysis of performing molecular docking (MD) simulations also indicated that the models could contribute to different types of interactions with the MPro target, in which the model with ۵-COI additional group was highlighted for strong contribution to make the strongest complex of ligand-target system. As a consequence, such structural modification of U helped the models for proper interaction with MPro to maybe inhibit the growth of COVID-۱۹ pandemic.

کلمات کلیدی:

Uracil, Coronavirus, COVID-۱۹, Main protease, Computational, Docking