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Aspirin, the Feasibility as a Binding Inhibitor

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Introduction

Aspirin is a popular flu medicine and trying to use in curing Covid-19 patients; however, the effectiveness was mixed results, and the variant types were not provided in the reports [1-3]. *In silico* analysis demonstrated that it did not inhibit the binding of Delta S-RBD with ACE-2. Rather, it bridges the binding of Delta S-RBD K478 with ACE-2 R317 (Figure 1A) [4]. The binding affinity of current spreading BQ.1 and XBB.1.5 (MIFS: 309.9 and 373.9 kcal mol^{-1}, respectively) is weaker than that of the Delta variant (594.2 kcal mol^{-1}), and they do not contain extra basic amino acids at the binding site [5]. Therefore, the feasibility of aspirin binding inhibition was studied.

Results and discussion

The initial location of three aspirin locations is shown as the molecular color in Figure 1B, as demonstrated for other compounds [4,5]. After optimization of these complexes using an MM2 program, the aspirin-bound BQ.1 and XBB.1.5 S-RBD complexes were repulsed from ACE-2. The aspirin binding site is completely repulsed in Figures 1C and 1D due to the ion-ion repulsion. The *in silico* analysis of molecular interactions indicated that aspirin should also inhibit the binding like other carboxylic compounds among 170 compounds analyzed [4,5].

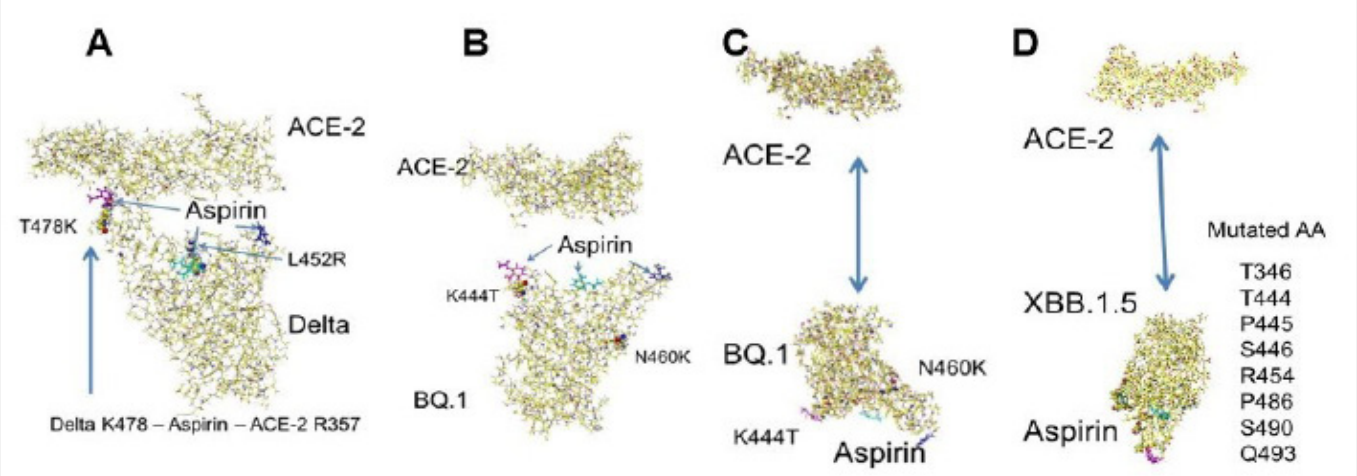

Figure 1: A: Binding of Delta with ACE-2; B: Initial lobation of ACE-2 and aspirin bound BQ.-1 S-RBD; C and D: Optimized complexes exhibit aspirin bound BQ.1 and XBB.1.5 S-RBD are repulsed from ACE-2.

Conclusion

Such *in silico* analysis of molecular interactions should help to understand the feasibility of binding inhibitors. The actual experiment using viruses is required before studying animal tests. Overdose of medicines should be avoided, as overtaking vitamins and amino acids has caused health problems.

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