

1 **Supplementary Materials**

2 **Blocking the Key Mutated hotspot residues in the RBD of Omicron variant**  
3 **(B.1.1.529) with medicinal compounds to disrupt the RBD-hACE2 complex**  
4 **using Molecular screening and Simulation approach**

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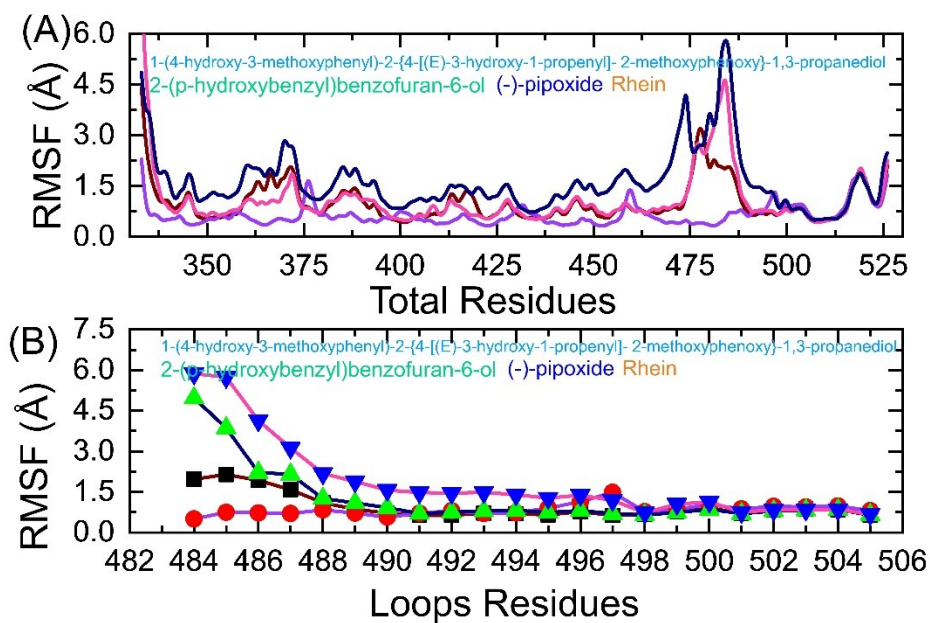
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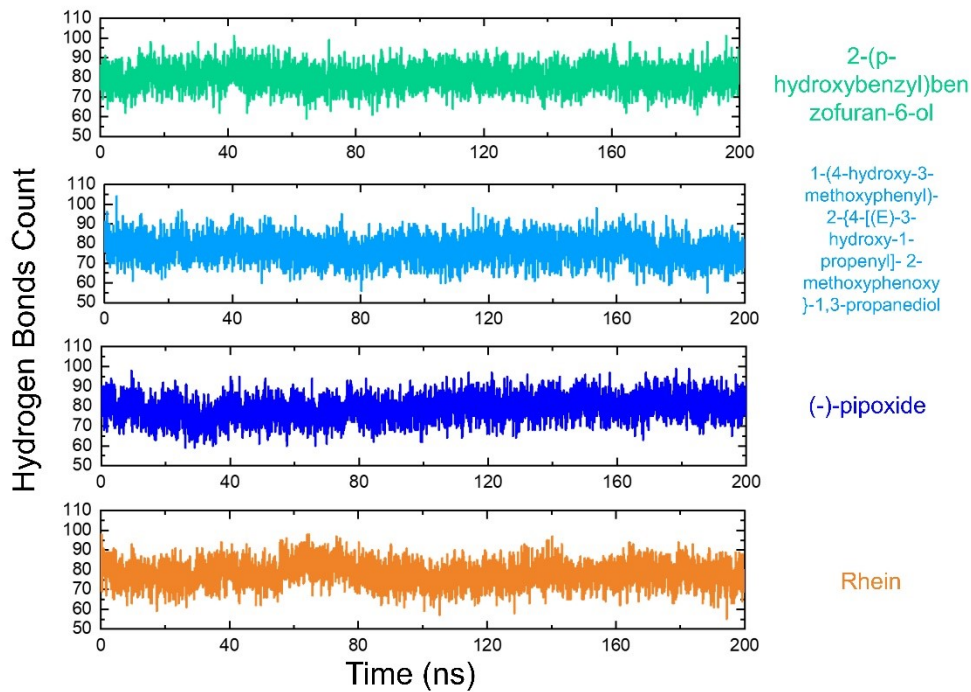
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 30 **Figure S1:** RMSF analysis of the top complexes replica 2. (A) Whole structure RMSF, (B) loop  
 31 residues RMSF.



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 33 **Figure S2:** Hydrogen bonding analysis of the top complexes replica 2.  
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