Supplemental Information

Binding of Raloxifene to Human Complement fragment 5a (hC5a): A Perspective on Cytokine Storm and COVID19.

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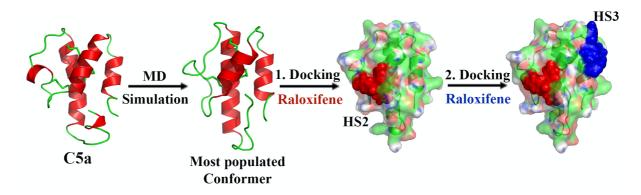


Figure S1. Schematic illustration of sequential docking of raloxifene to the ^hC5a or its representative conformers populated during MD simulation.

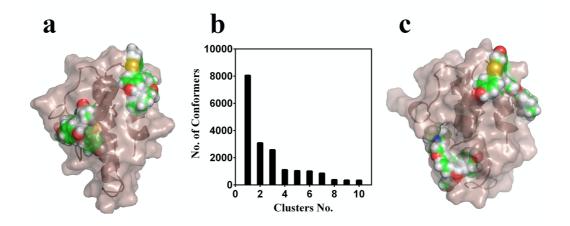


Figure S2. (a) The ^hC5a, respectively bound to two molecules of raloxifene at "HS2" and "HS3" subjected to 1 μs MD at 300K. (b) Cluster analysis of the raloxifene bound ^hC5a MD trajectory, displaying the number of conformers in the first ten major clusters. (c) The representative central conformer extracted from the first major cluster populated over 1 μs MD, indicating the physical viability and stability of the overall complex.