

Figure 2. Docked complexes between ivermectin and RBD of spike protein and 3CL^{pro} of SARS-CoV-2. Interaction of ivermectin with RBD-spike protein (A). Interaction of ivermectin with subunit 1 of 3CL^{pro} (B), and subunit 2 of 3CL^{pro} (C).

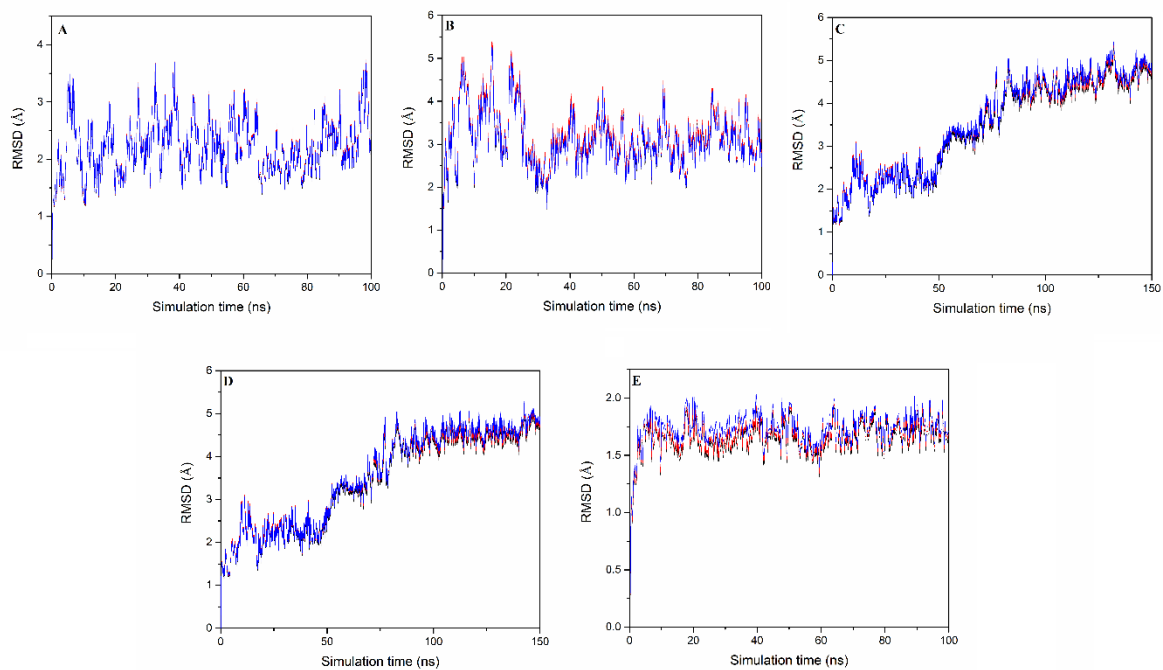


Figure 3. Root mean squared deviation (RMSD) values of Importin- α -IVM, Nsp9-IVM, RdRp-IVM, spike-protein-IVM, and 3CL^{pro}-IVM systems through MD simulations. A) Importin- α -IVM, B) Nsp9-IVM, C) RdRp-IVM, D) RBD-spike-IVM, and E) 3CL^{pro}-IVM complexes. Triplicate simulations are in black, blue, and red lines.

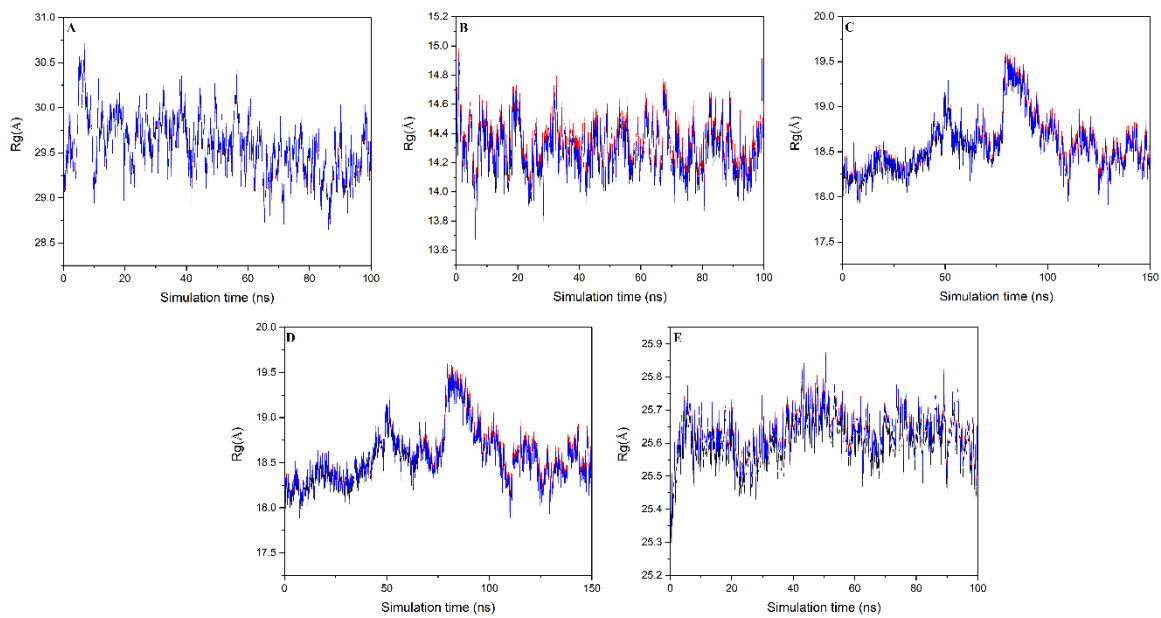


Figure 4. The radius of gyration (Rg) values of Importin- α -IVM, Nsp9-IVM, RdRp-IVM, spike-protein-IVM, and 3CL^{pro}-IVM systems through MD simulations. A) Importin- α -IVM, B) Nsp9-IVM, C) RdRp-IVM, D) RBD-spike-IVM, and E) 3CL^{pro}-IVM complexes. Triplicate simulations are in black, blue, and red lines.

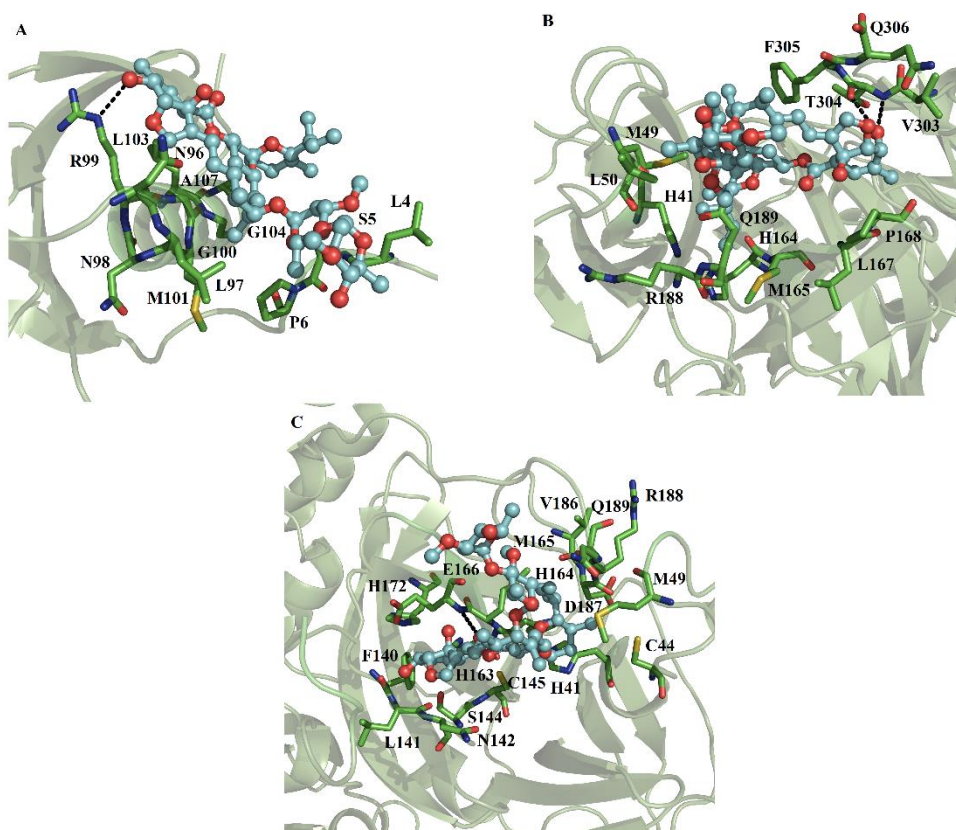


Figure 5. Complexes between ivermectin with Nsp9 replicase and 3CL^{pro} of SARS-CoV-2 through MD simulations. Interaction of ivermectin with Nsp9 replicase (A). Interaction of ivermectin with subunit 1 of 3CL^{pro} (B) and subunit 2 of 3CL^{pro} (C).