Supplementary materials for

Computational modeling of human coreceptor CCR5 antagonist as a HIV-1 entry inhibitor: using an integrated homology modeling, docking, and membrane molecular dynamics simulation analysis approach

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Supplementary Figure S1. ERRAT plot for the generated CCR5 model.

Chain#: 1
Overall quality factor**: 95.324

Supplementary Figure S2. ProSA energy plot for the generated CCR5 model (the overall Z score was -3.03).

Supplementary Figure S3. (A) Temperature and (B) pressure stabilized plot during NVT (100 ps) and NPT simulation (1000 ps).

Supplementary Figure S4. Maintenance of systems (A: 14-CCR5, B: 25-CCR5, C: 37-CCR5) pressure (1 bar) during MD simulations.

Supplementary Figure S5. Ramachandran plot for the CCR5 after MDS of **25**-CCR5 system.

Supplementary Figure S6. Ramachandran plot for the CCR5 after MDS of **37**-CCR5 system.

Supplementary Figure S7. (A) ERRAT plot for **25-CCR5** and (B) **37-CCR5** after 20000 ps of MD simulations.

Supplementary Figure S8. ProSA energy plot for the energy minimized CCR5 structures after MD simulations in (A) 25-CCR5 and (B) 37-CCR5 systems.

Supplementary Figure S9. Radius of gyration for CCR5 during MD simulations.

Supplementary Figure S10. RMS fluctuations (RMSF) for backbone (C, N, C α) atoms of CCR5 during MD simulations in different systems (**14-CCR5**, **25-CCR5** and **37-CCR5**).

Supplementary Figure S11. An average CCR5 structure (14-CCR5) was calculated from MD trajectories and represented by b-factors. Red indicates hot region, green intermediate regions, and blue indicates cool regions.

Supplementary Figure S12. An average CCR5 structure (**25**-CCR5) was calculated from MD trajectories and represented by b-factors. Red indicates hot region, green intermediate regions, and blue indicates cool regions.

Supplementary Figure S13. An average CCR5 structure (**37**-CCR5) was calculated from MD trajectories and represented by b-factors. Red indicates hot region, green intermediate regions, and blue indicates cool regions

Supplementary Figure S14. Backbone RMSDs for (A) ICL1, (B) ICL2 and (C) ICL3 as a function of time.