Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary data for

Insights into the binding modes of CC chemokine receptor 4 (CCR4) inhibitors: A combined approach involving homology modelling, docking, and molecular dynamics simulation studies

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Fig. S1. Errat plot for the CCR4 model computed using SAVES server.

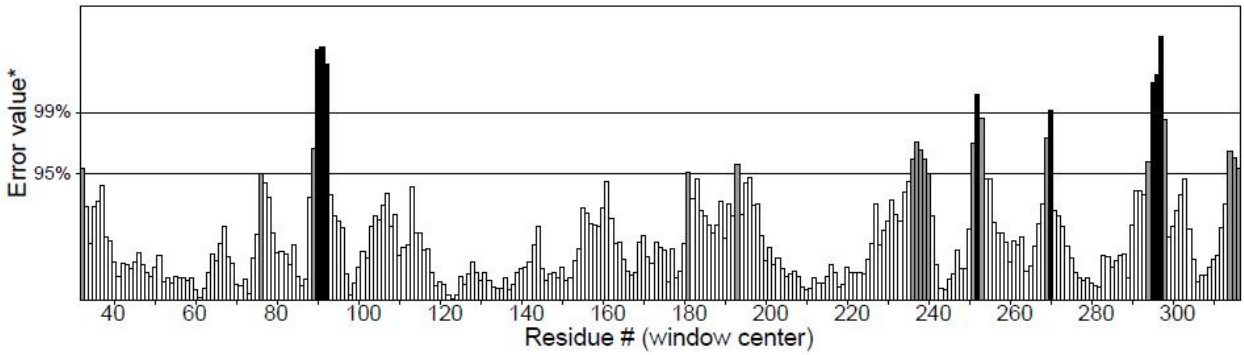

Fig. S2. Knowledge based energy profile of template (4MBS) and target (CCR4) calculated using ProSA server.

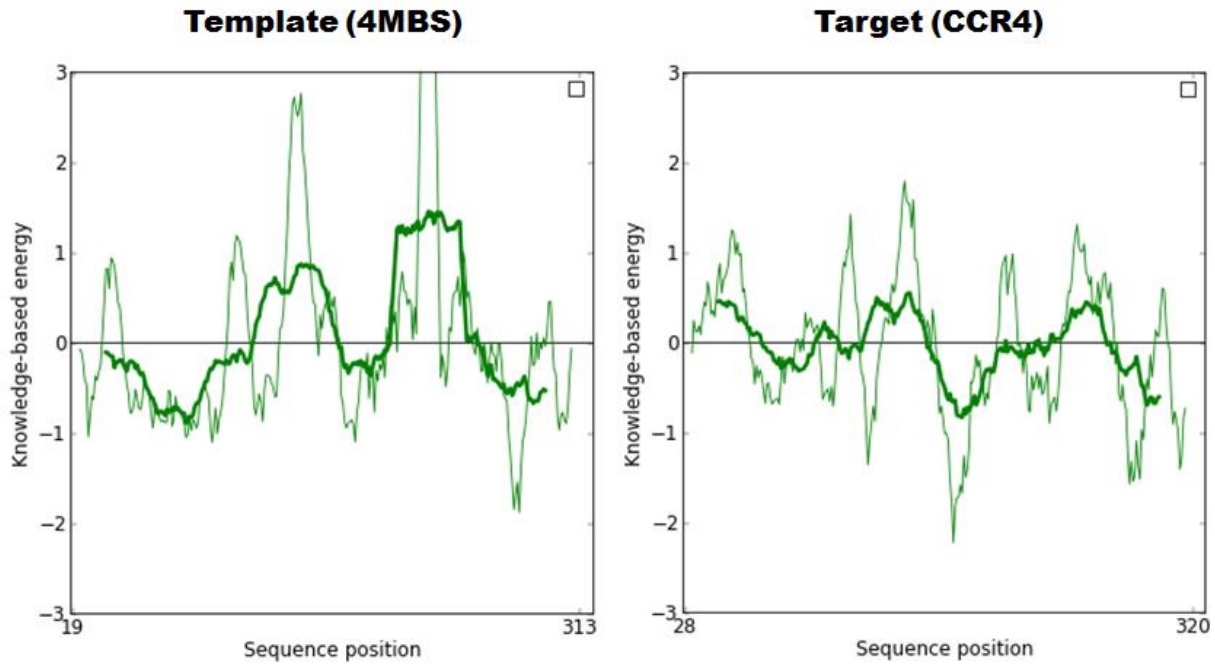

Fig. S3. Superposed docked orientations of compound **1** (yellow), compound **2** (magenta), compound **3** (gold) and compound **4** (cyan) over Maraviroc (green). Left side shows top view of the superposed orientations. TM helices were numbered at their top and CCR4 is shown in surface. Right side shows side view of the superposed docked modes. It shows all the docked inhibitors identify same binding site as Maraviroc does.

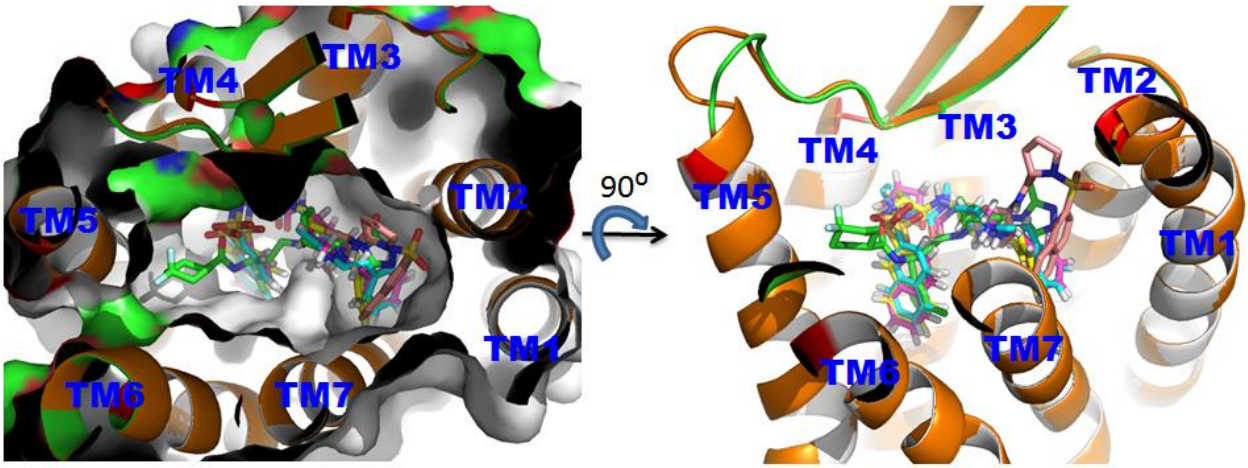

Fig. S4. 2D-schematic interaction plots for (A) **1**-CCR4 and (B) **2**-CCR4 after docking simulation. Red spokes on half moon represents hydrophobic interaction whereas green dash line represent H-bonds.

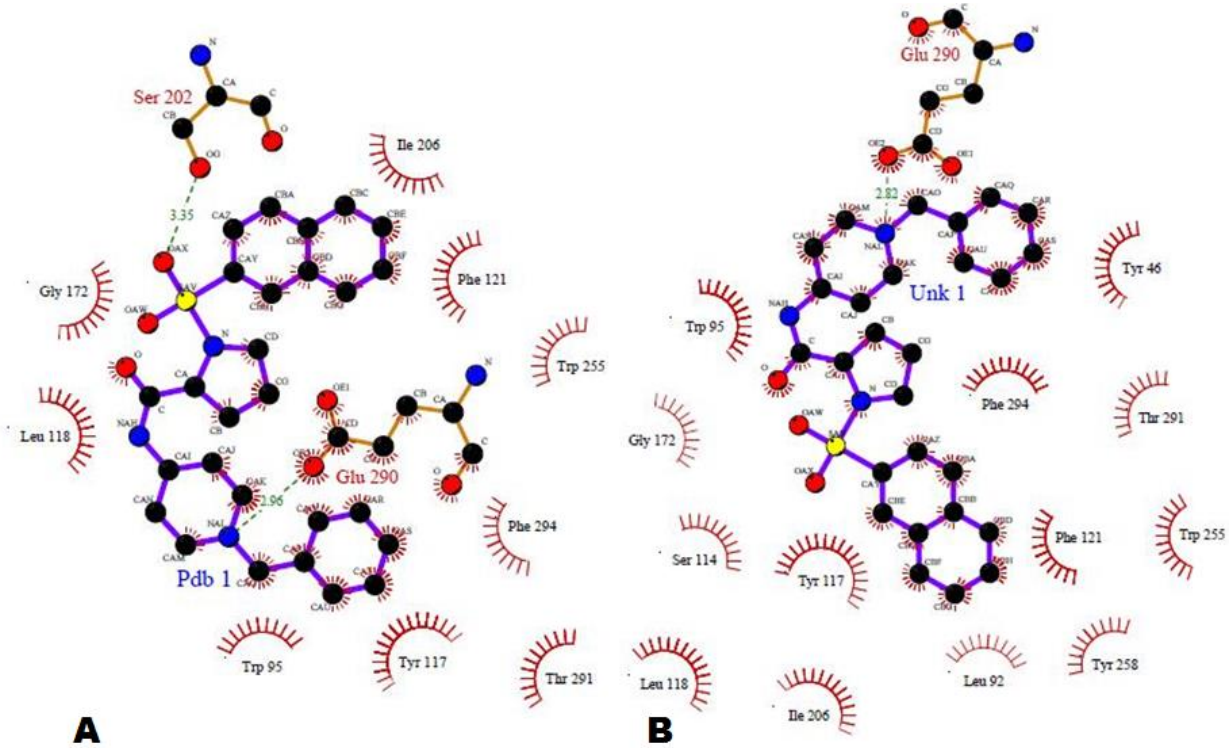

Fig. S5. 2D-schematic interaction plots for (A) **3**-CCR4 and (B) **4**-CCR4 after docking simulation. Red spokes on half moon represents hydrophobic interaction whereas green dash line represent H-bonds.

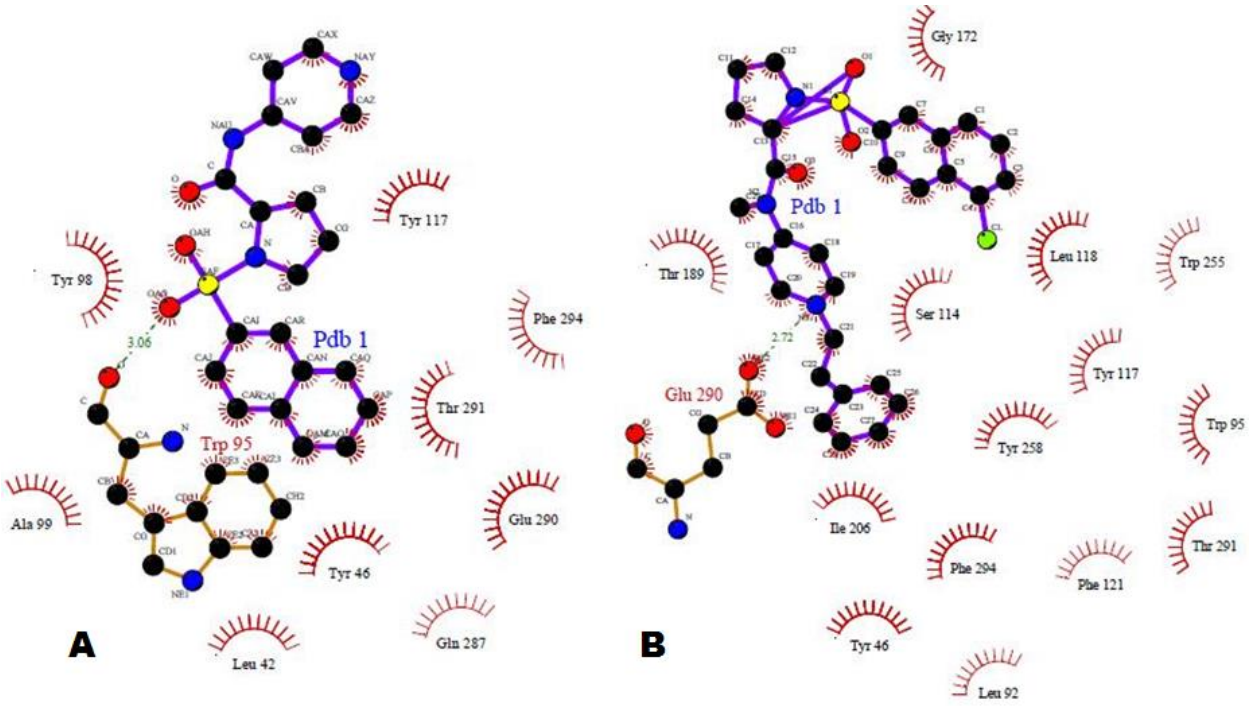

Fig. S6. Temperature and pressure of the simulated systems 1 (green), 2 (red), 3 (blue) and 4 (black) were plotted as time evolution. Average temperature was maintained at 323 K and pressure at 1 Bar for all the simulated system.

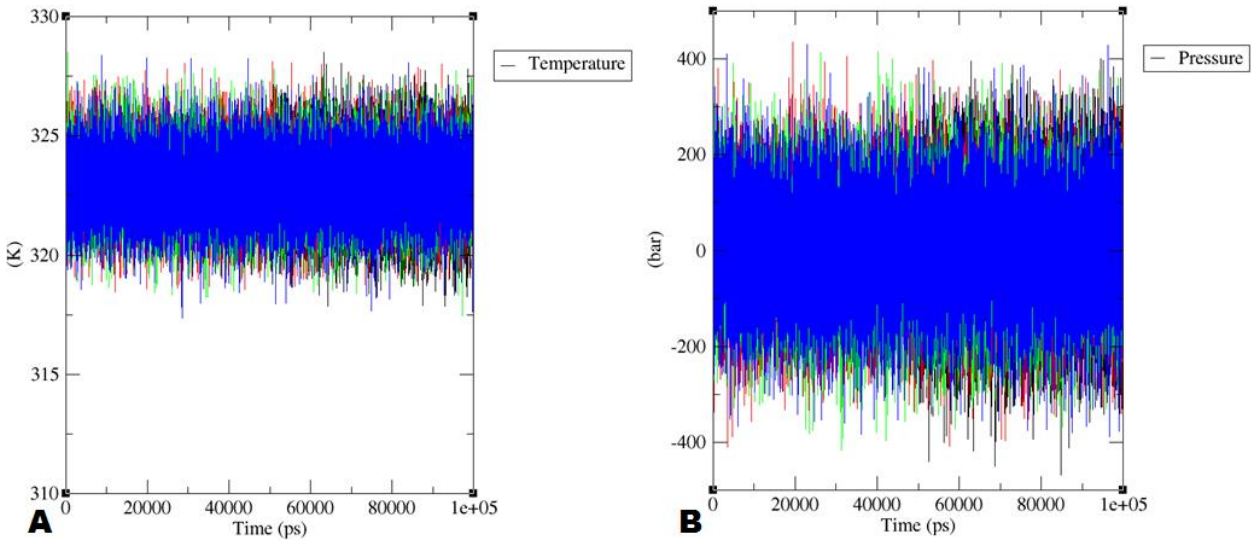

Fig. S7. PCA data were extracted for first three components for simulated systems. Backbone atoms information was used to generate matrix. Arrow shows direction of movement in the CCR4 structure during simulations.

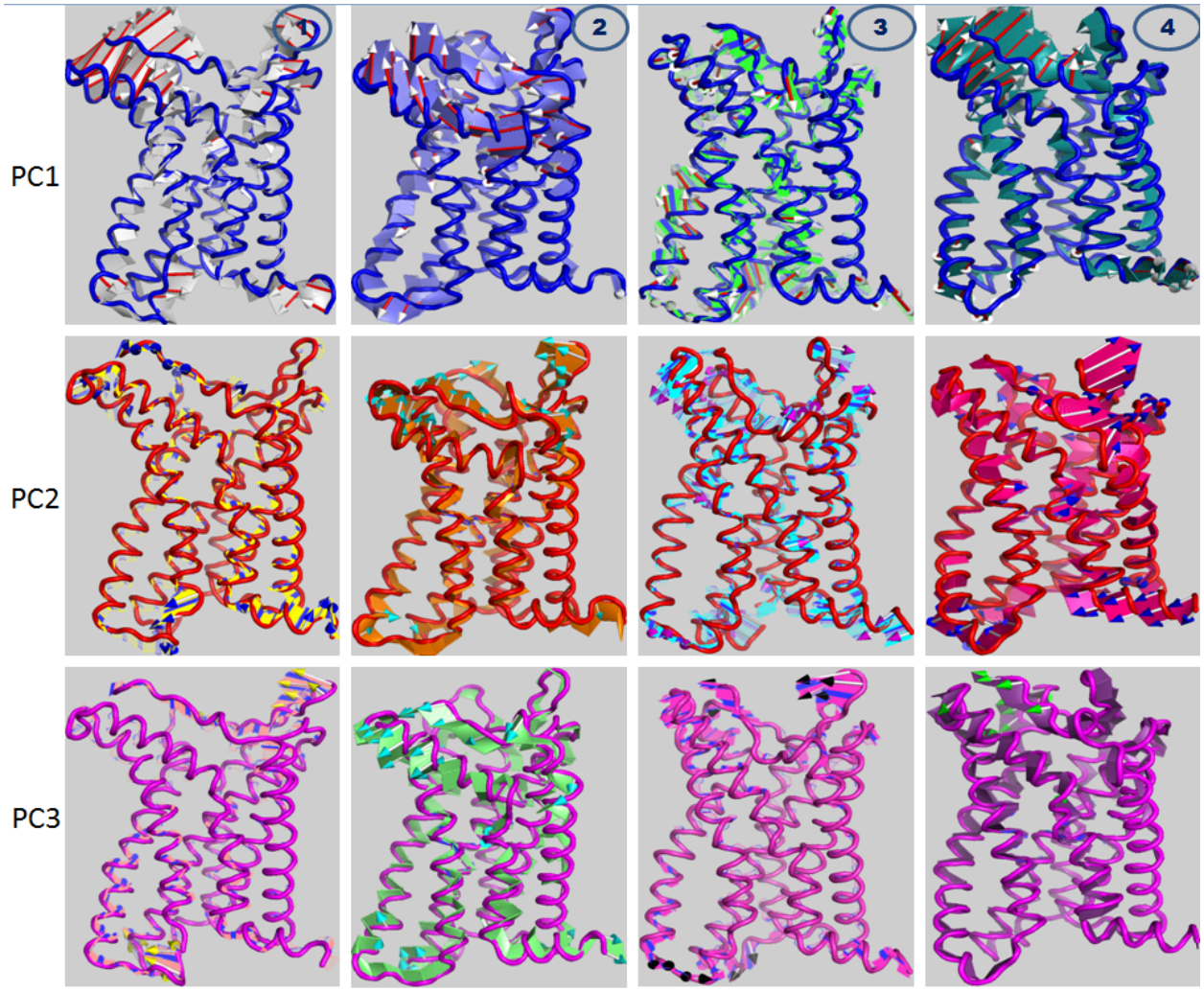

Fig. S8. H-bonds occurred between (A) **1**-CCR4, (B) **2**-CCR4, (C) **3**-CCR4 and (D) **4**-CCR4 during MD simulation.

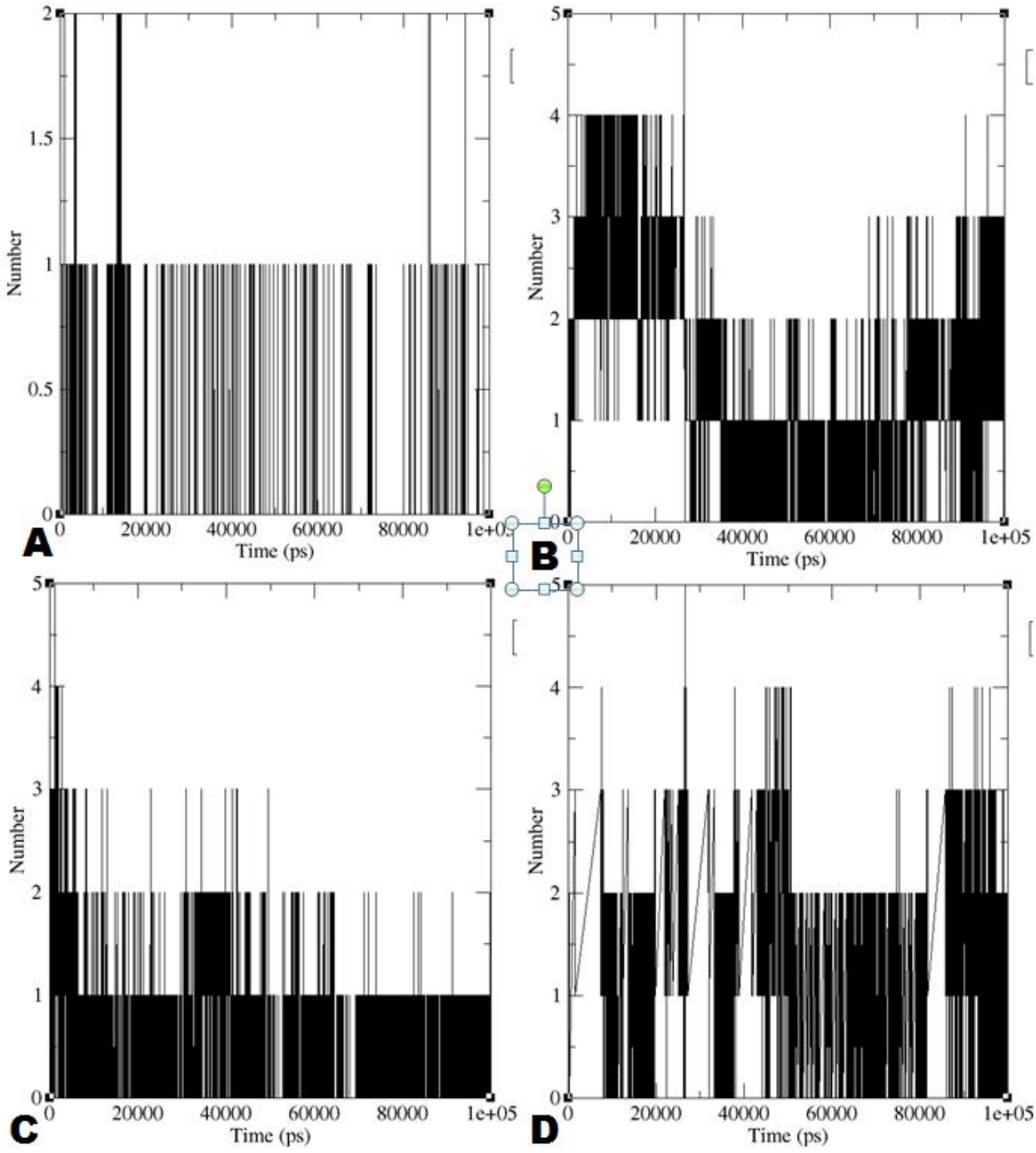

Fig. S9. 2D-schematic interaction plots for (A) **1**-CCR4 and (B) **2**-CCR4 after MD simulation. Red spokes on half moon represents hydrophobic interactions with the ligands.

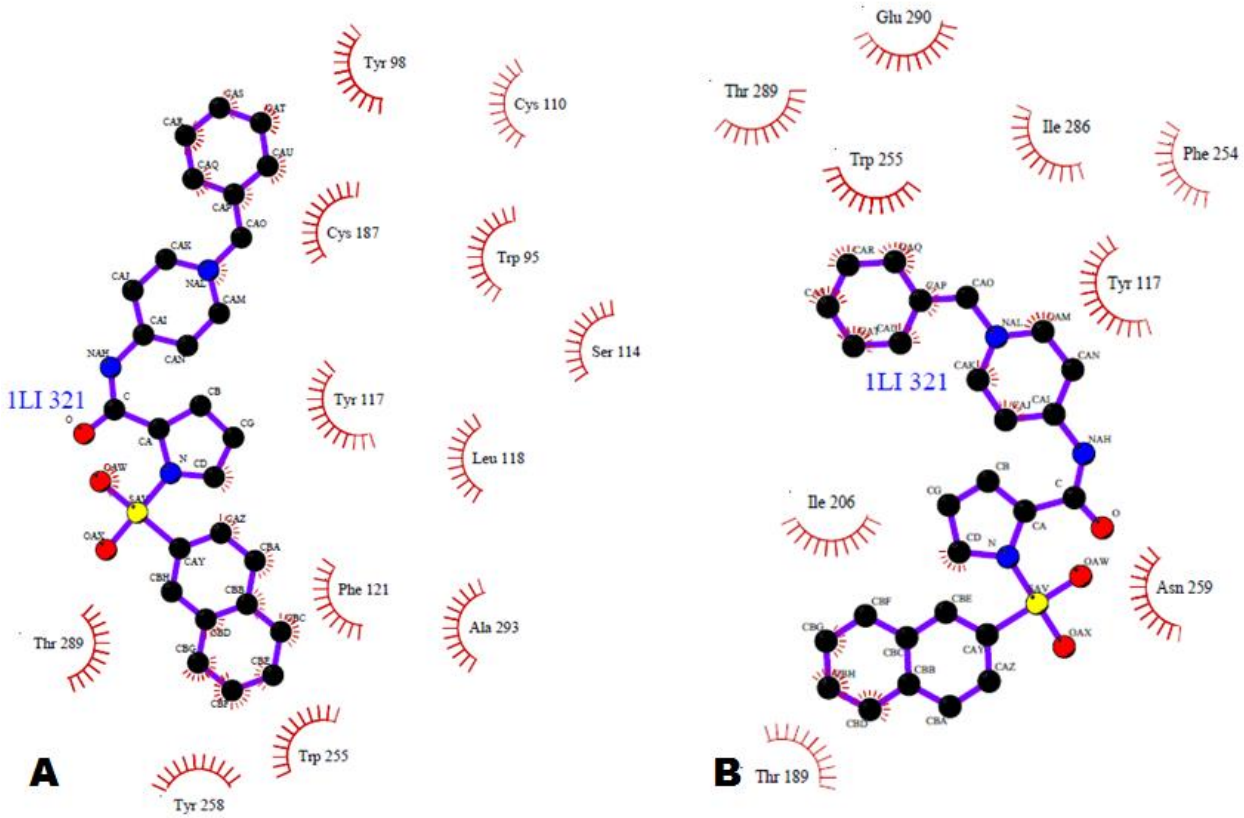

Fig. S10. 2D-schematic interaction plots for (A) **3**-CCR4 and (B) **4**-CCR4 after MD simulation. Red spokes on half moon represents hydrophobic interaction whereas green dash line represent H-bond.

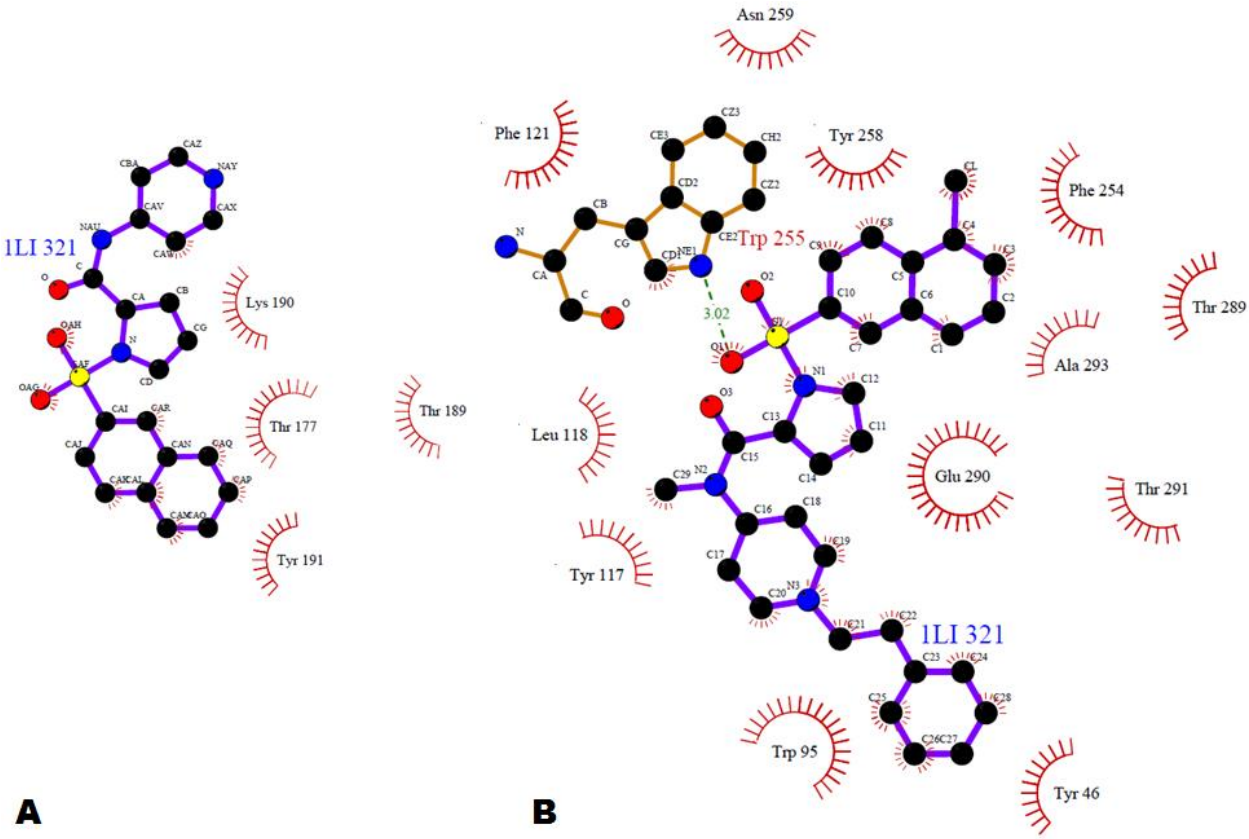

Fig. S11. Graph plot of pIC50 of simulated ligands versus predicted binding energy between ligands-CCR4.