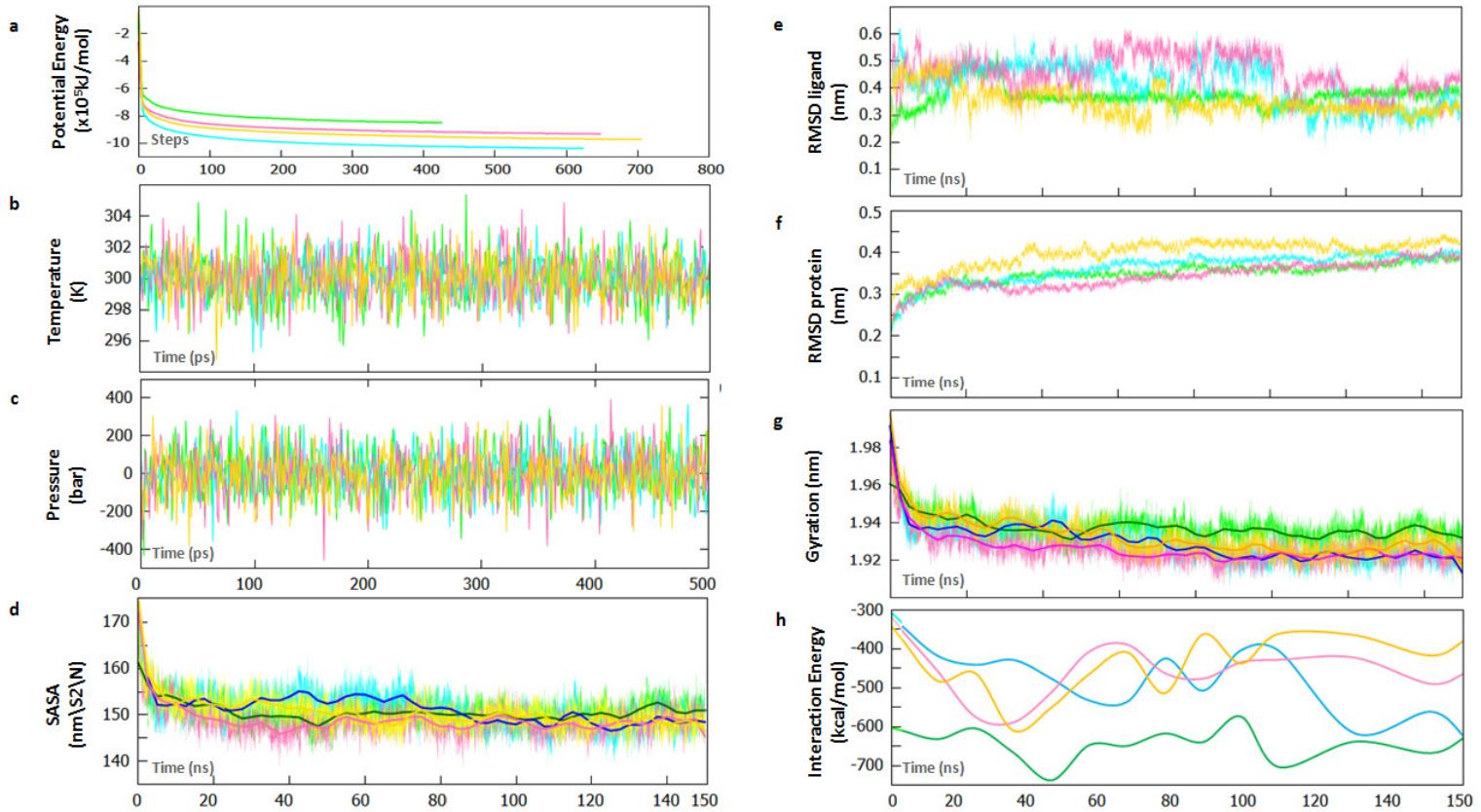


**Supplementary Figure 1**

**Ramachandran plot for the pPAF-AH models.**

**A.** wild pPAF-AH; **B.** pPAF-AH-V279F; **C.** pPAF-AH-Q281R, and **D.** pPAF-AH-DM.



## Supplementary Figure 2

### Molecular dynamics trajectory for the complexes of pPAF-AH with substrate PAF.

Period of equilibration: (a) potential energy; (b) temperature; (c) pressure; and Molecular dynamics production run: (d) solvent accessible surface area, (e) RMSD for ligand; (f) RMSD for protein; (g) radius of gyration; (h) Interaction energy. The plots for complexes of wild pPAF-AH: PAF, pPAF-AH-V279F: PAF, pPAF-AH-Q281R: PAF and pPAF-AH-DM: PAF, are shown in green, cyan, pink and yellow respectively.