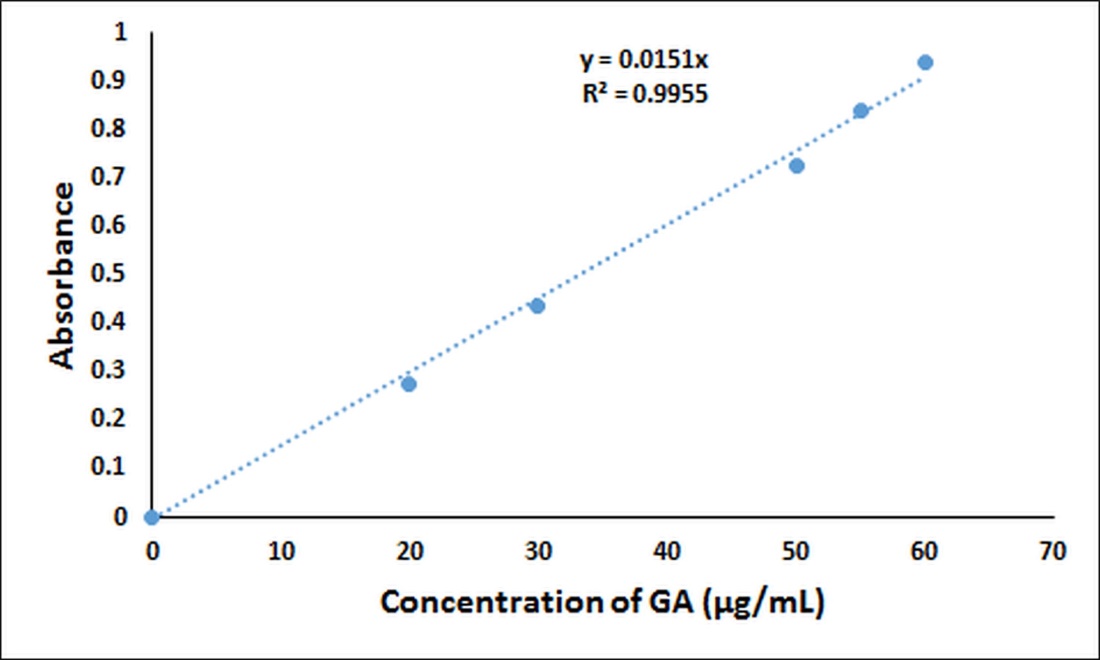
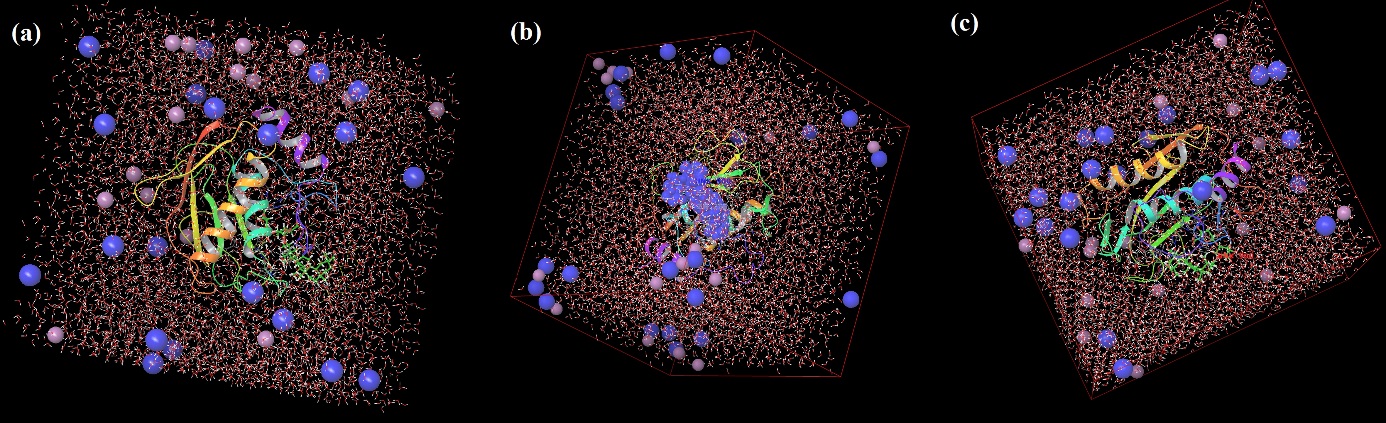
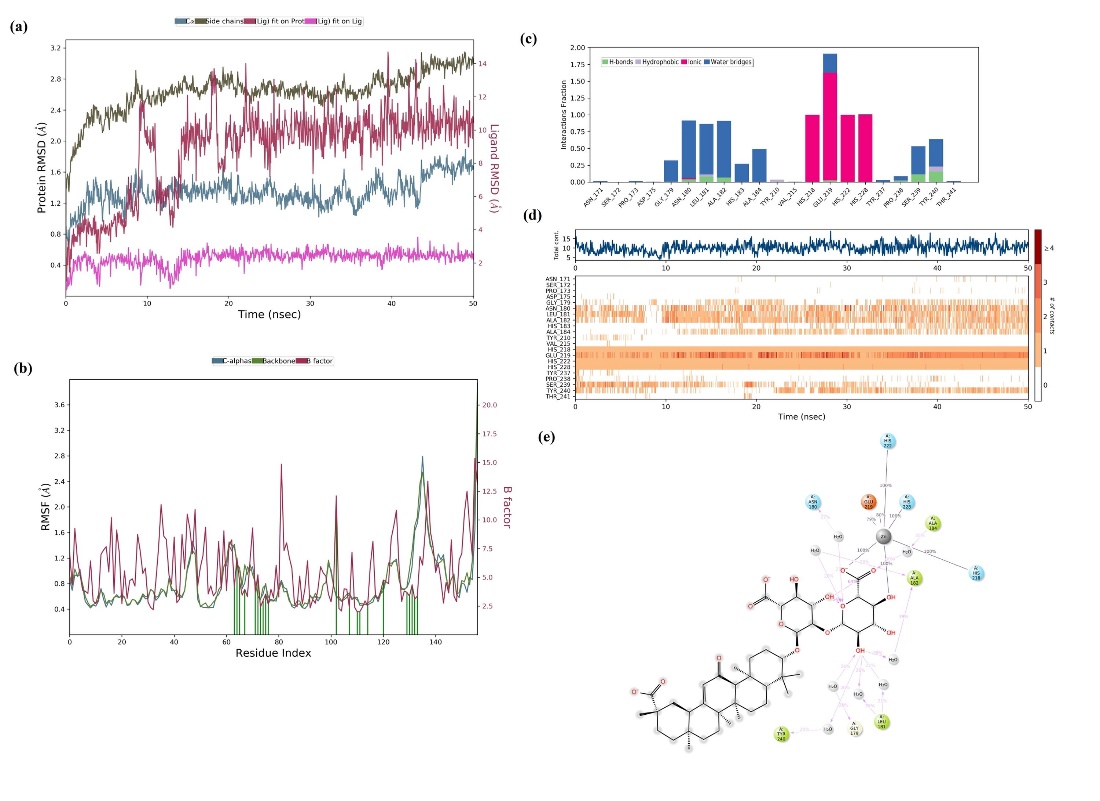
**SUPPLEMENTARY**



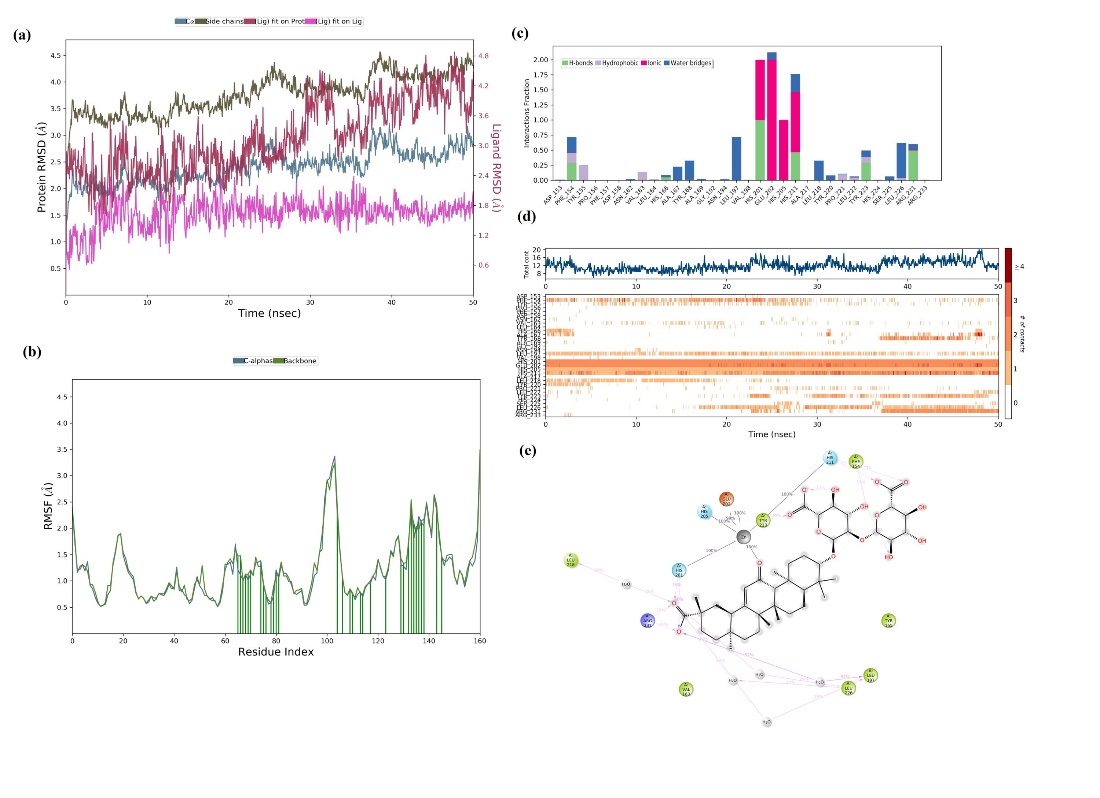
**Figure S1.** The calibration curve of GA



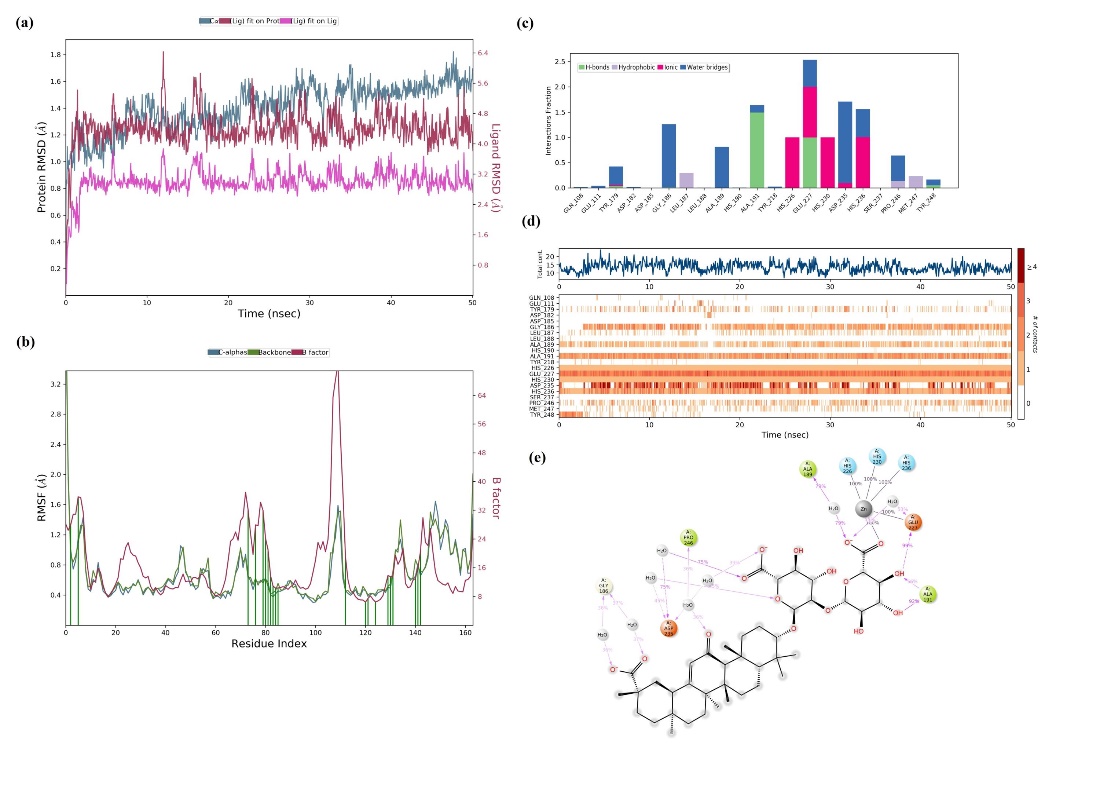
**Figure S2.** MD system of GA in complex with MMP-1(PDB ID: 966C) **(a)**, MMP-3(PDB ID: 2JT6) **(b)**, MMP-9(PDB ID: 5CUH) **(c)**



**Figure S3.**  MD simulation analysis of GA in complex with MMP-1(PDB ID: 966C). RMSD of GA-966C complex (Protein Cα-atoms RMSD is shown in green while RMSD of GA with respect to protein are shown in purple **(a)**, Protein amino acids RMSF **(b)**, Protein–ligand contact diagram **(c)**, timeline representation of the interactions and contacts **(d)**, ligand 2D interaction histogram obtained from MD trajectory **(e)**.



**Figure S4.** MD simulation analysis of GA in complex with MMP-3(PDB ID: 2JT6).  RMSD of GA-2JT6 complex (Protein Cα-atoms RMSD is shown in green while RMSD of GA with respect to protein are shown in purple **(a)**, Protein amino acids RMSF **(b)**, Protein–ligand contact diagram **(c)**, timeline representation of the interactions and contacts **(d)**, ligand 2D interaction histogram obtained from MD trajectory **(e)**.



**Figure S5.** MD simulation analysis of GA in complex with MMP-9(PDB ID: 5CUH). RMSD of GA-5CUH complex (Protein Cα-atoms RMSD is shown in green while RMSD of GA with respect to protein are shown in purple **(a)**, Protein amino acids RMSF **(b)**, Protein–ligand contact diagram **(c)**, timeline representation of the interactions and contacts **(d)**, ligand 2D interaction histogram obtained from MD trajectory **(e)**.