

Table S1. Average RMSD, RMSF, RoG and SASA values of DPP-IV in complex with chlorogenic acid and Diprotin A.

Complexes	Average RMSD (Å)	Average RMSF (Å)	Average ROG (Å)	Average SASA (Å)
DPP-IV + Chlorogenic acid	1.76 ± 0.14	1.08 ± 0.50	26.95 ± 0.08	24324.70 ± 328.06
DPP-IV + Diprotin A	1.96 ± 0.20	1.18 ± 0.56	26.96 ± 0.10	24636.10 ± 371.14
DPP-IV	1.69 ± 0.16	1.13 ± 0.78	27.18 ± 0.10	24982.98 ± 367.09