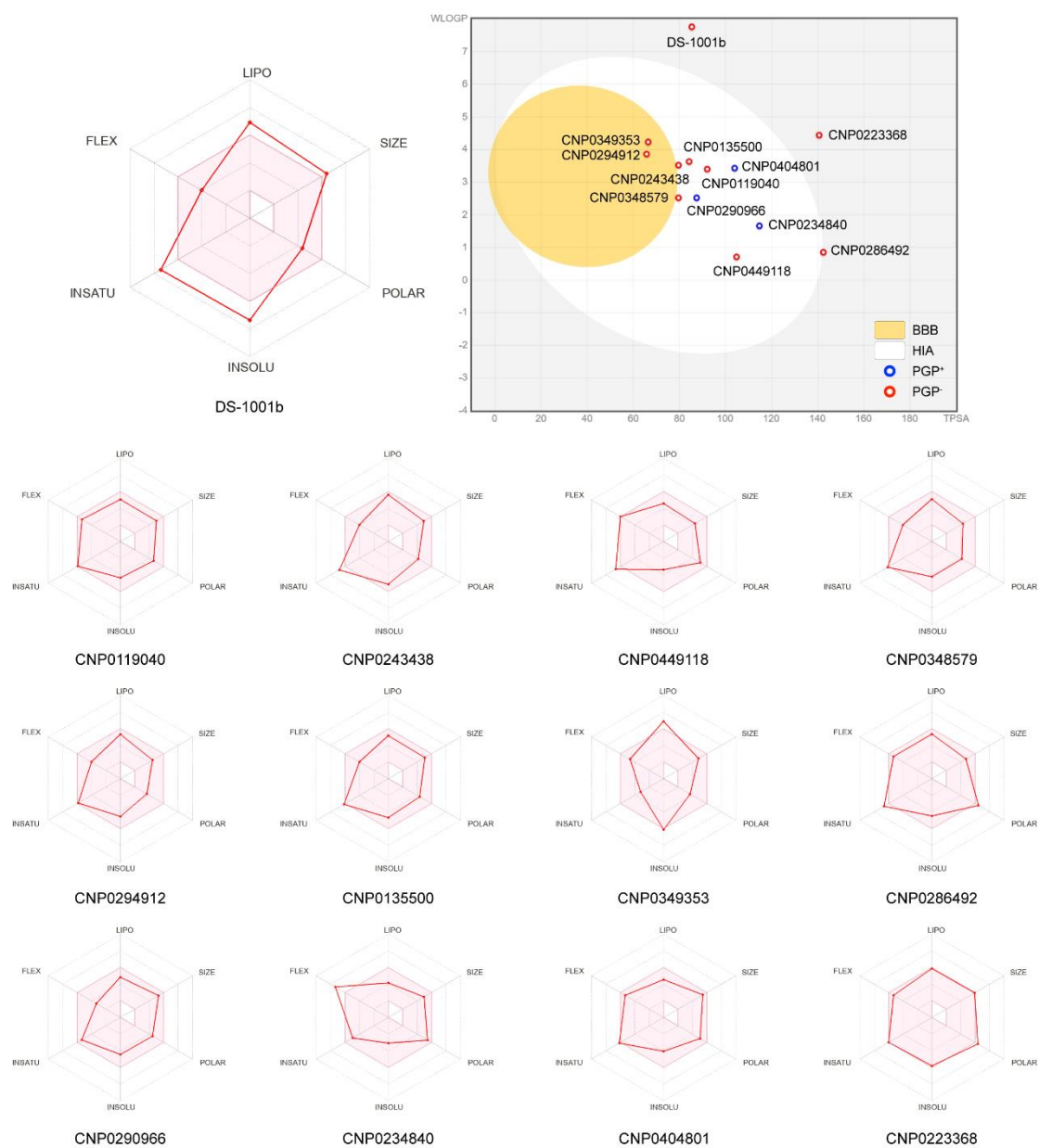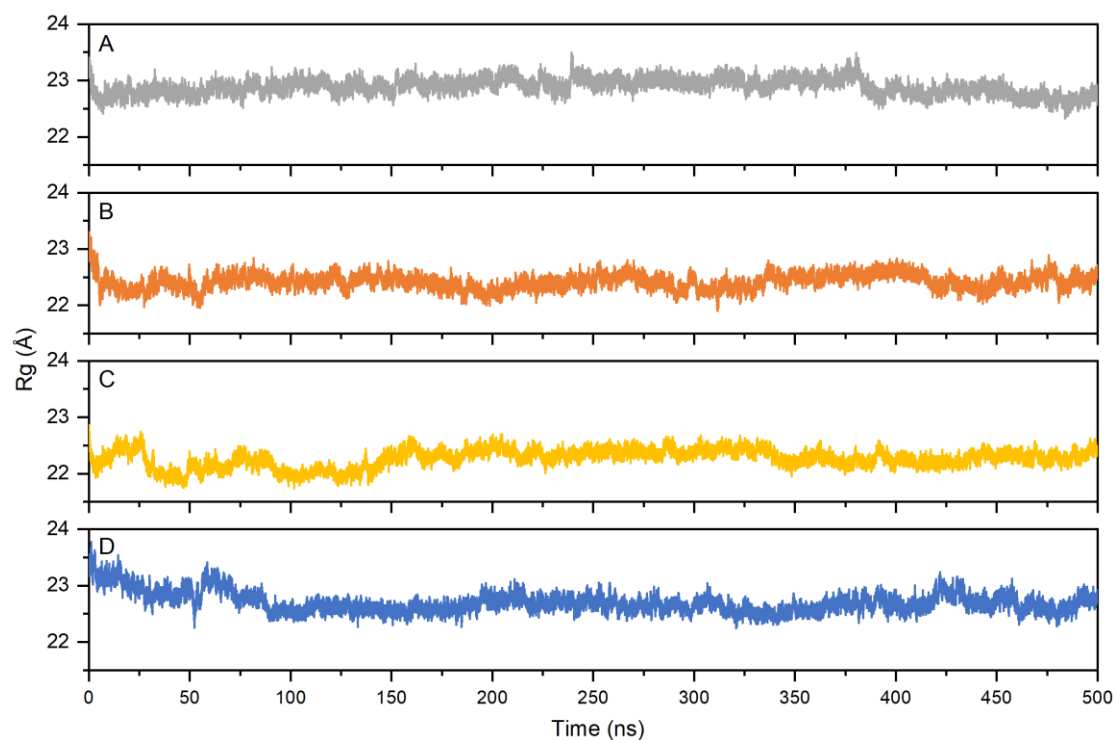**Figure S1.** The similarity matrix from fingerprint of 12 hits, coumarin and flavonoids

Table S1. The Druglikeness and PAINS of the top 12 compounds.
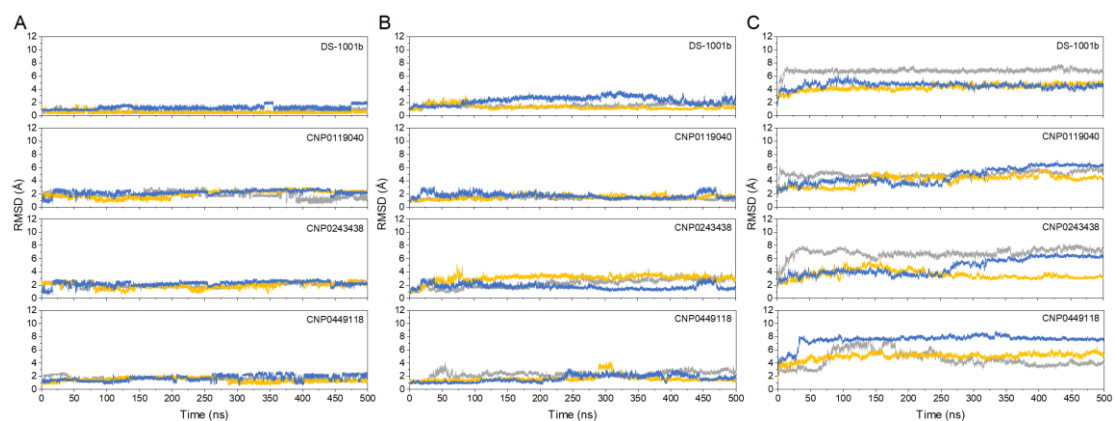
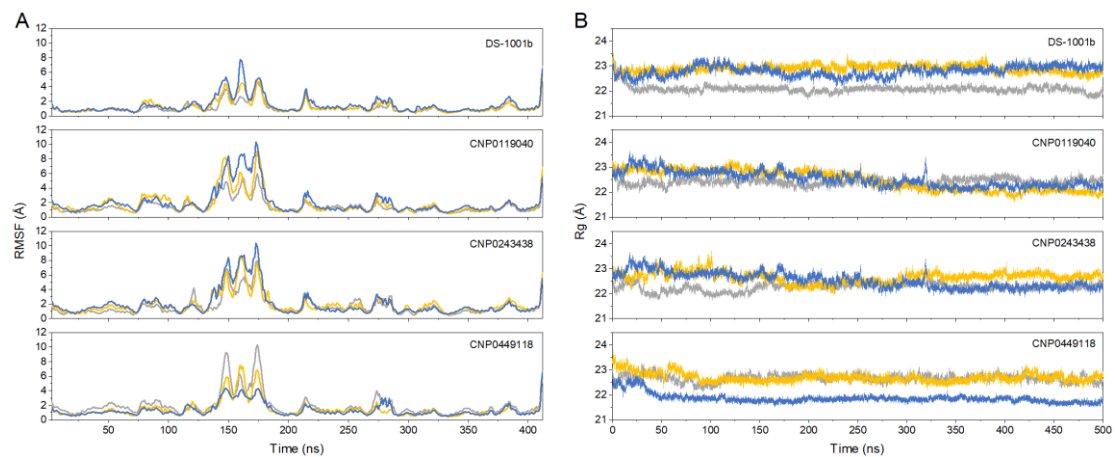| ID	Druglikeness						PAINS
	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score	
DS-1001b	No	No	Yes	No	No	0.56	0 alert
CNP0119040	Yes	Yes	Yes	Yes	Yes	0.55	0 alert
CNP0243438	Yes	Yes	Yes	Yes	Yes	0.56	0 alert
CNP0449118	Yes	Yes	Yes	Yes	Yes	0.56	0 alert
CNP0348579	Yes	Yes	Yes	Yes	Yes	0.56	0 alert
CNP0294912	Yes	Yes	Yes	Yes	Yes	0.55	0 alert
CNP0135500	Yes	Yes	Yes	Yes	Yes	0.55	0 alert
CNP0349353	Yes	Yes	Yes	Yes	No	0.85	0 alert
CNP0286492	Yes	Yes	No	No	Yes	0.56	0 alert
CNP0290966	Yes	Yes	Yes	Yes	Yes	0.55	0 alert
CNP0234840	Yes	Yes	No	Yes	Yes	0.55	0 alert
CNP0404801	Yes	Yes	Yes	Yes	Yes	0.55	0 alert
CNP0223368	Yes	No	No	No	Yes	0.55	0 alert

Figure S2. The bioactivity radar and BOILED-Egg plot of the 12 compounds

Figure S3. The Rg values of the DS-1001b, CNP0119040, CNP0243438, and CNP0449118 (frame interval=1).

Figure S4. The superposition of RMDS for triplicate sample, ligand(A), pocket(B) and backbone(C).

Figure S5. The superposition of RMSF(A) and Rg(B) for triplicate sample.