Supporting Information

Molecular dockings and molecular dynamics simulations reveal the potency of different inhibitors against xanthine oxidase

Yue Pan[1], Zhongkui Lu[1], Congcong Li[1], Renrui Qi[1], Hao Chang[2], Lu Han[1,*] and Weiwei Han[1,*]

[1] Key Laboratory for Molecular Enzymology and Engineering of Ministry of Education, School of Life Science, Jilin University, 2699 Qianjin Street, Changchun 130012, China;
[2] Jilin Province TeyiFood Biotechnology Company Limited, Erdao District, Changchun 130012, China

Figure S1. Figure: a. The location of guanine after autodock vina (The Carbon atoms are white) docking and the location of guanine in original structure (The Carbon atoms are pink) b. The interaction between guanine and protein in the structure of the original structure c. The interaction between guanine and protein in the structure of Autodock Vina（RMSD=0.4867） docking.

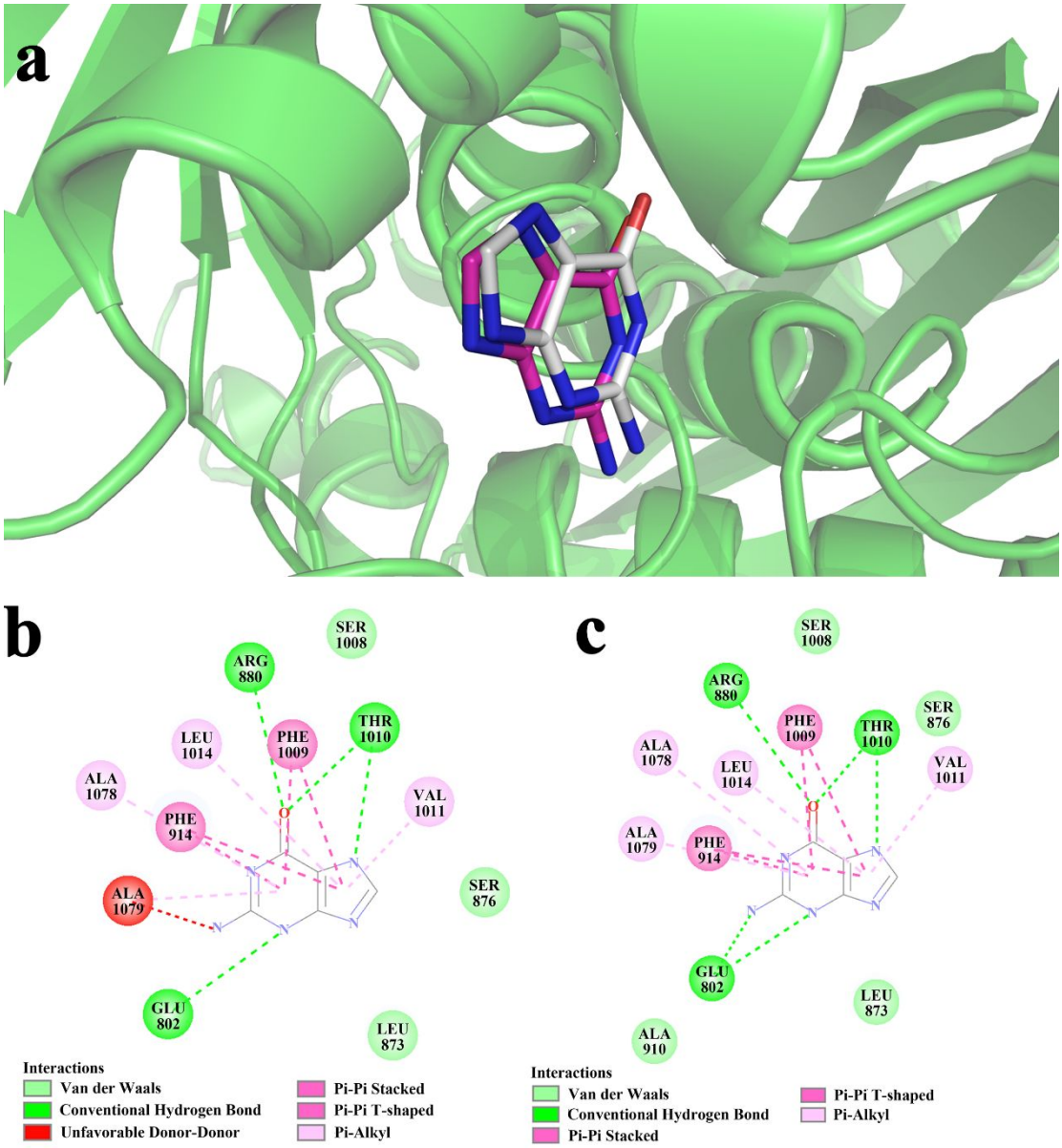

Figure S2. Dynamic changes of the secondary structure profile for **a.** free protein, **b.** XO-allopurinol, **c.** XO-daidzin and **d.** XO−puerarin. The colored bar represented different secondary structures as follows: coil (C), 3-helix (I), 5-helix (G), α-helix (H), β-sheet (B), β-Bridge (E), turn (T).

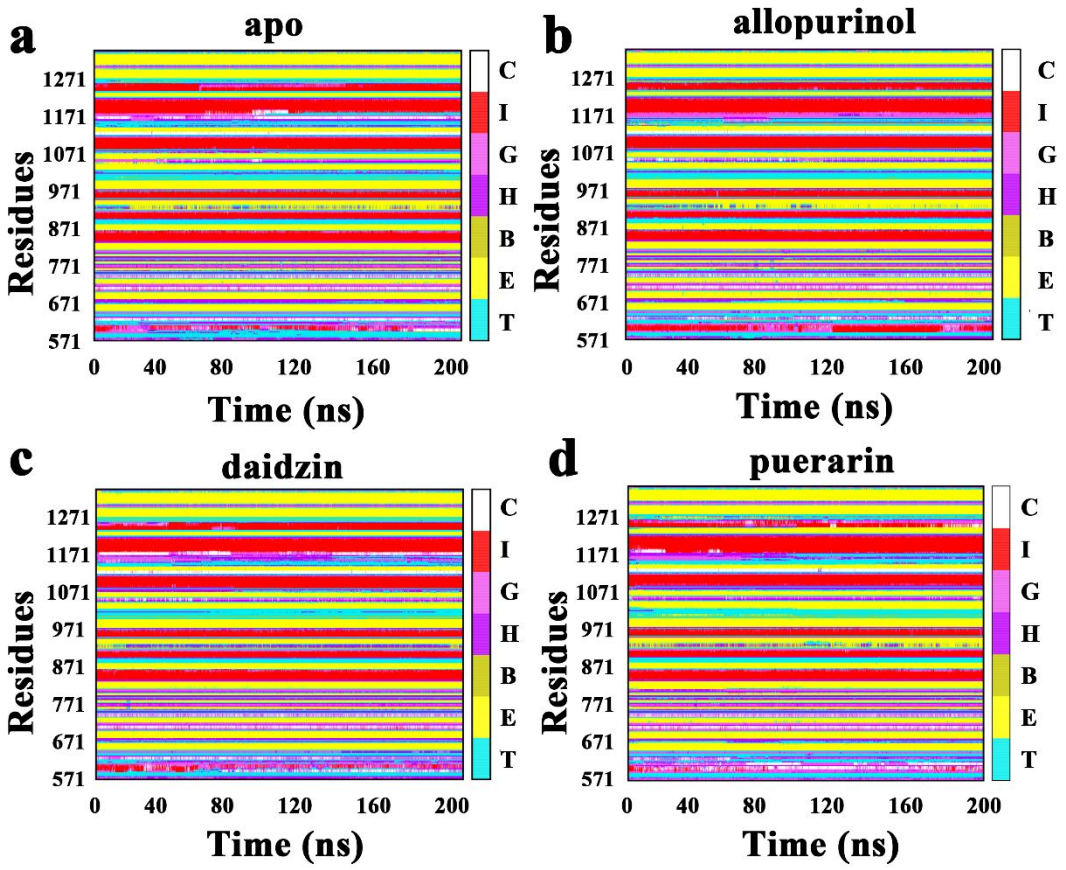

Figure S3. The percentage of the total variance of the atom positional fluctuations corresponding to the eigenvalue.

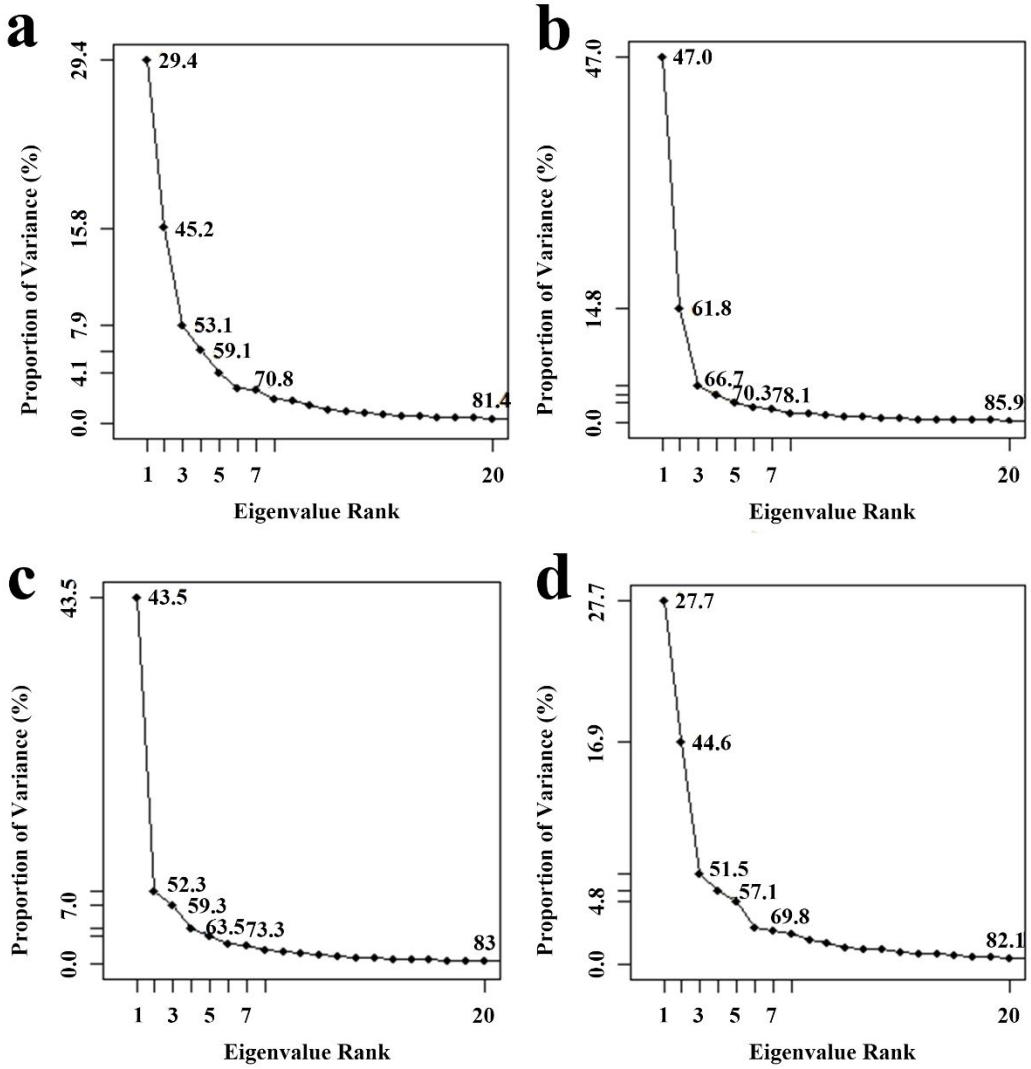

Figure S4. The cluster analysis for **a.** free protein, **b.** XO-allopurinol, **c.** XO-daidzin and **d.** XO–puerarin.