

Mechanisms of Ganweikang Tablets against Chronic Hepatitis B: A Comprehensive Study of Network Analysis, Molecular Docking and Chemical Profiling

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Supplementary figures:

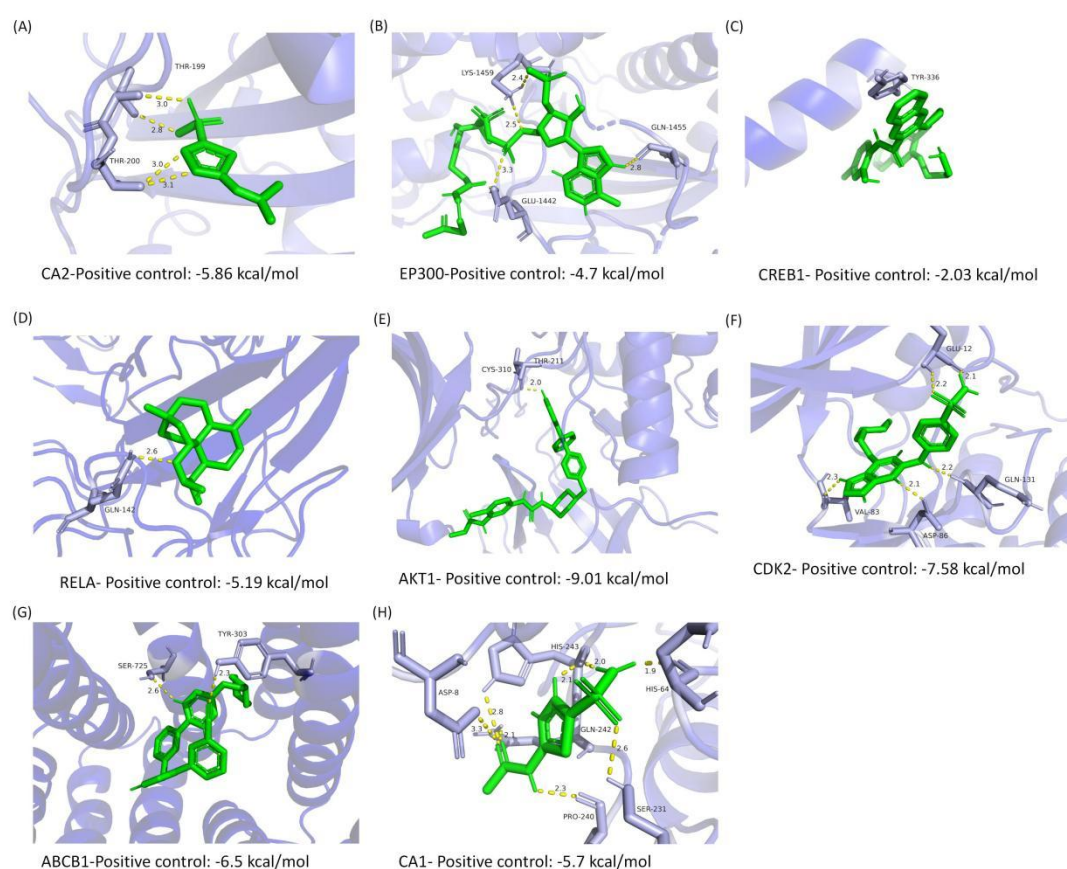
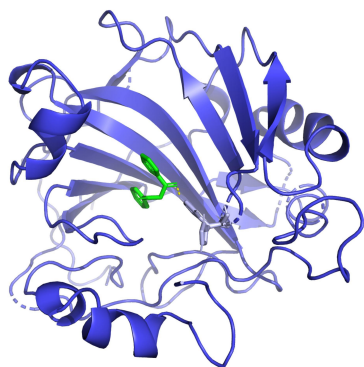


Figure S1 Schematic diagrams for the binding modes between targets and positive control small molecules

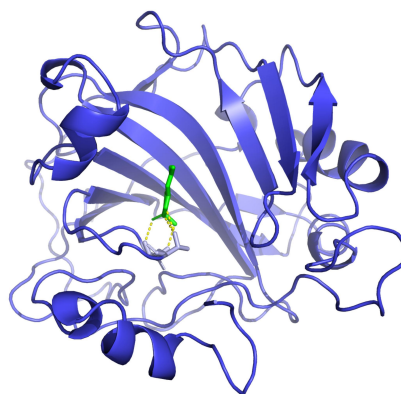
(A) CA2 with positive control; (B) EP300 with positive control; (C) CREB1 with positive control; (D) RELA with positive control; (E) AKT1 with positive control; (F) CDK2 with positive control; (G) ABCB1 with positive control; (H) CA1 with positive control

(A)



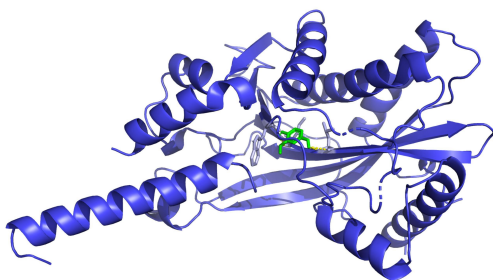
CA2- DBM : -6.33 kcal/mol

(B)



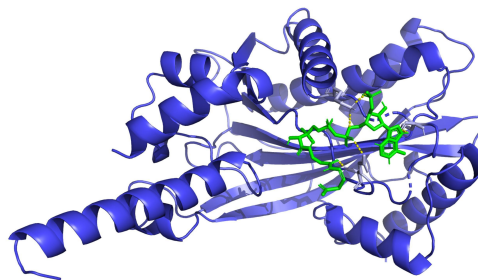
CA2- Positive control: -5.86 kcal/mol

(C)



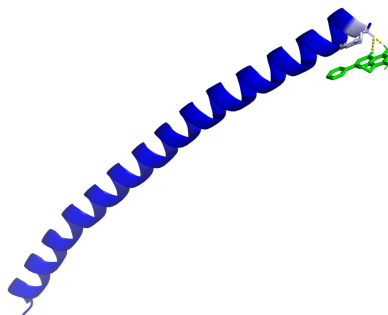
EP300-vanillin: -6.26 kcal/mol

(D)



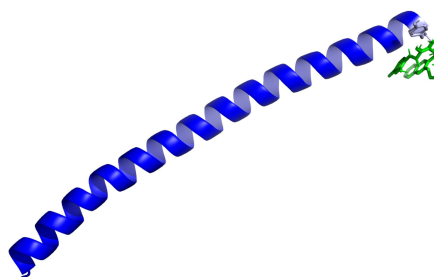
EP300-Positive control: -4.7 kcal/mol

(E)

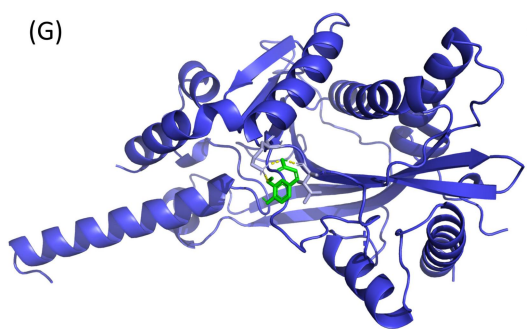


CREB1- wogonin: -3.67 kcal/mol

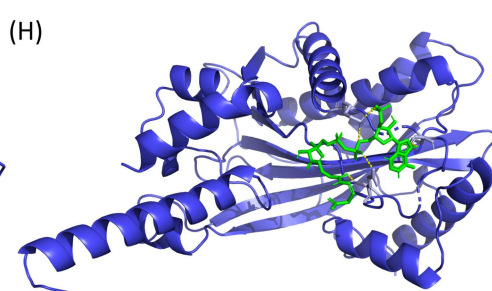
(F)



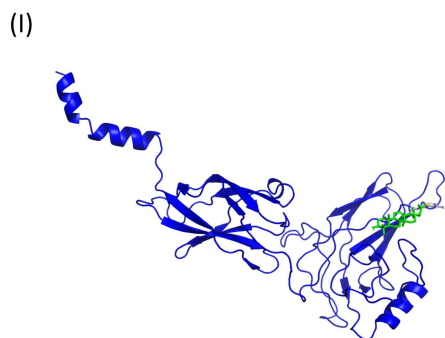
CREB1-Positive control: -2.03 kcal/mol



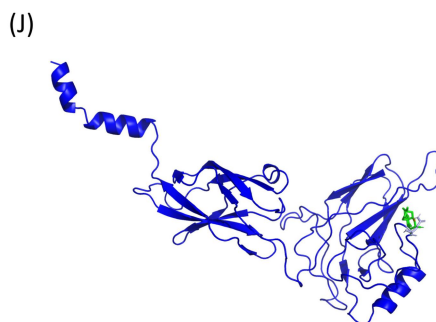
EP300-cis-ferulic acid: - 5.47kcal/mol



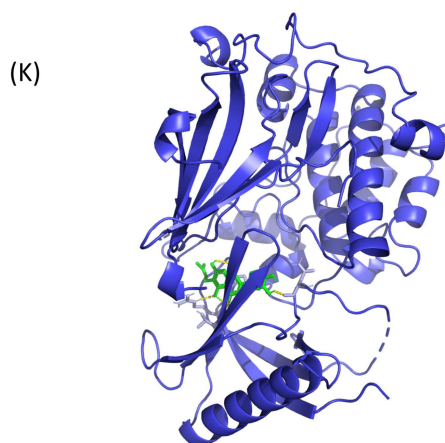
EP300-Positive control: - 4.7kcal/mol



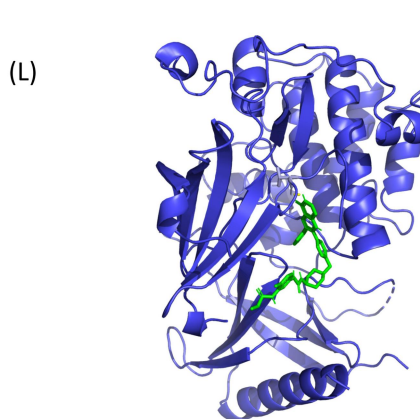
RELA- oleanolic acid: -6.87 kcal/mol



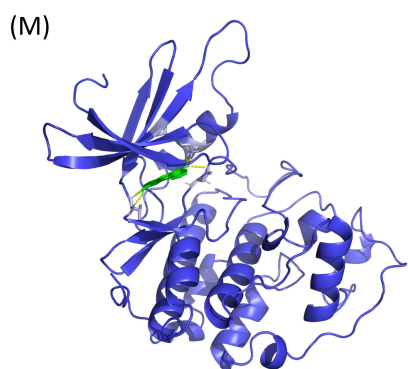
RELA-Positive control: -5.19 kcal/mol



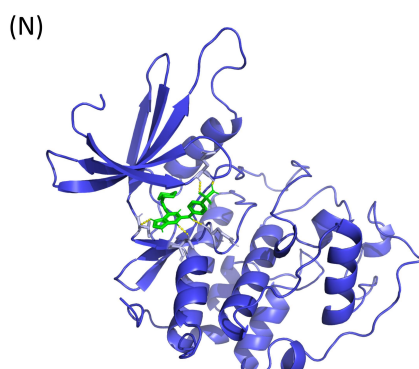
AKT1- chromone O: -8.8 kcal/mol



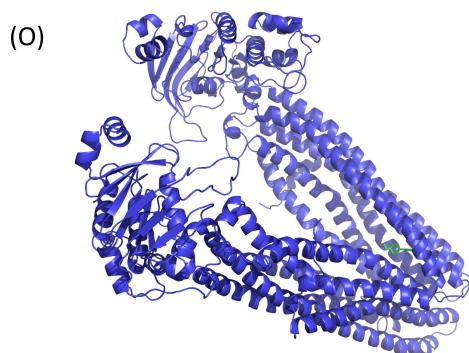
AKT-1-Positive control: -9.01 kcal/mol



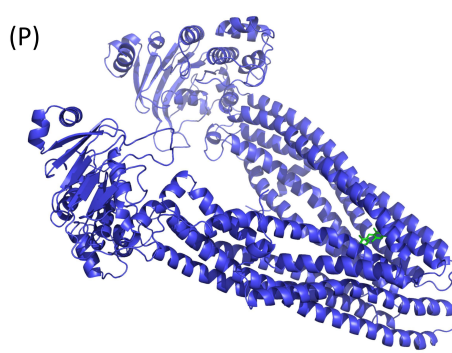
CDK2- 3,4-methylenedioxy:
-7.99 kcal/mol



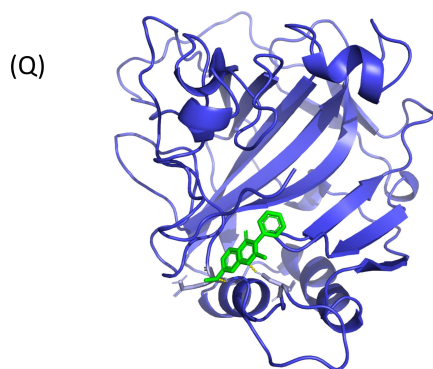
CDK2-Positive control: -7.58 kcal/mol



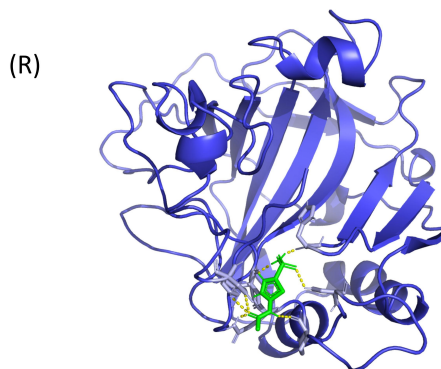
ABCB1-formononetin: -7.19
kcal/mol



ABCB1-Positive control: -6.27
kcal/mol



CA1- 7-methoxy-2 methylisoflavone: -
7.18 kcal/mol



CA1-Positive control: -5.7
kcal/mol

FigureS2 The binding patterns between active ingredients, positive control and targets

(A) CA2 with Karenzu DK2; (B) CA2 with positive control; (C) EP300 with vanillin; (D) EP300 with positive control; (E) CREB1 with wogonin; (F) CREB1 with positive control; (G) EP300 with cis-ferulic acid; (H) EP300 with positive control; (I) RELA with oleanolic acid; (J) RELA with positive control; (K) AKT1 with chromone O; (L) AKT1 with positive control; (M) CDK2 with 3,4-methylenedioxy; (N) CDK2 with positive control; (O) ABCB1 with formononetin; (P) ABCB1 with positive control; (Q) CA1 with 7-methoxy-2-methylisoflavone; (R) CA1 with positive control