

Supplemental Material

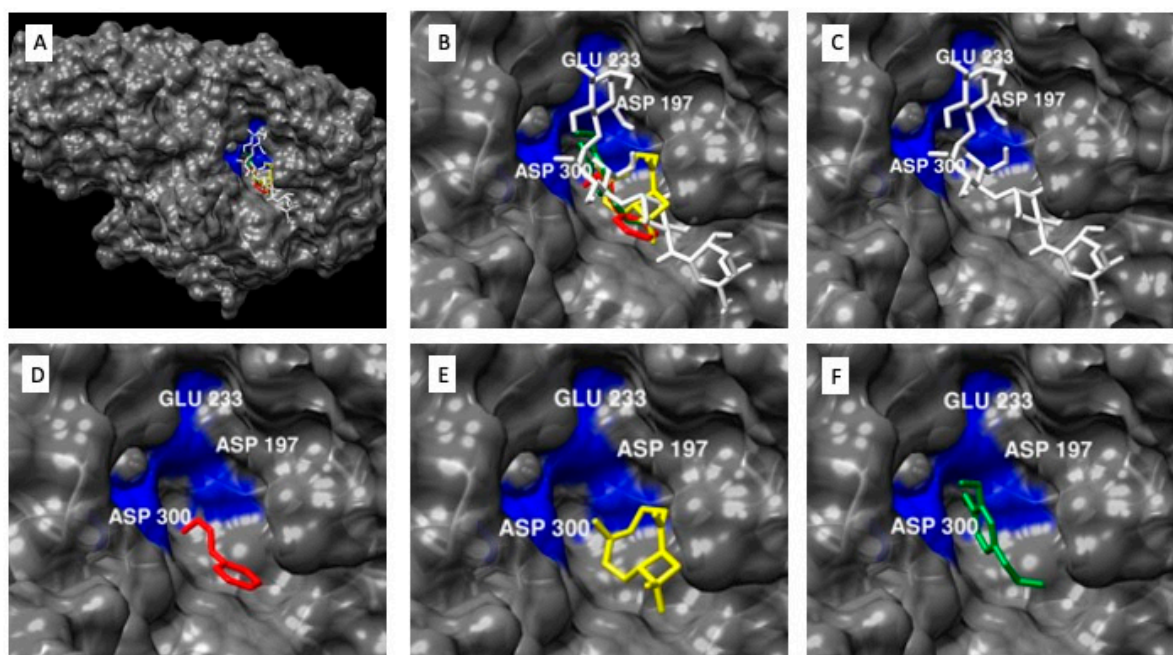


Figure S1. Molecular modeling of cinnamon essential oil constituents docked with alpha-amylase. (A) Alpha-amylase antagonist acarbose and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of alpha-amylase; (B) Close view of alpha-amylase antagonist acarbose and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of alpha-amylase, specifically near residues ASP197, GLU233, and ASP300; (C): Acarbose docked in the active pocket of alpha-amylase, with a binding affinity of -7.3 kcal/mol; (D) Cinnamaldehyde docked in the active pocket of alpha-amylase, with a binding affinity of -5.4 kcal/mol; (E) Beta-caryophyllene docked in the active pocket of alpha-amylase, with a binding affinity of -6.9 kcal/mol; (F) Eugenol docked in the active pocket of alpha-amylase, with a binding affinity of -5.6 kcal/mol.

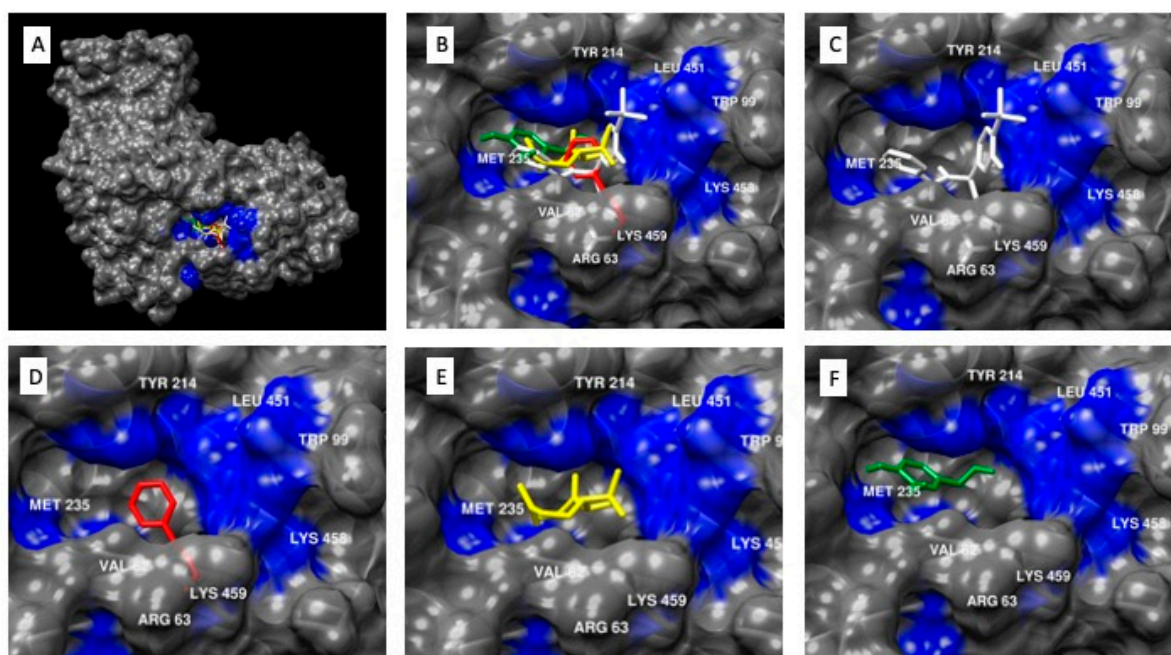


Figure S2. Molecular modeling of cinnamon essential oil constituents docked with glucokinase. (A) Glucokinase agonist piragliatin and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of glucokinase; (B) Close view of glucokinase agonist piragliatin and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of alpha-glucosidase, specifically near residues VAL 62, ARG 63, TRP 99, TYR 214, MET 235, LYS 458, LYS 459, and LEU 451; (C) Piragliatin docked in the active pocket of glucokinase, with a binding affinity of -9.5 kcal/mol; (D) Cinnamaldehyde docked in the active pocket of glucokinase, with a binding affinity of -5.8 kcal/mol; (E) Beta-caryophyllene docked in the active pocket of glucokinase, with a binding affinity of -6.3 kcal/mol; (F) Eugenol docked in the active pocket of glucokinase, with a binding affinity of -6.0 kcal/mol.

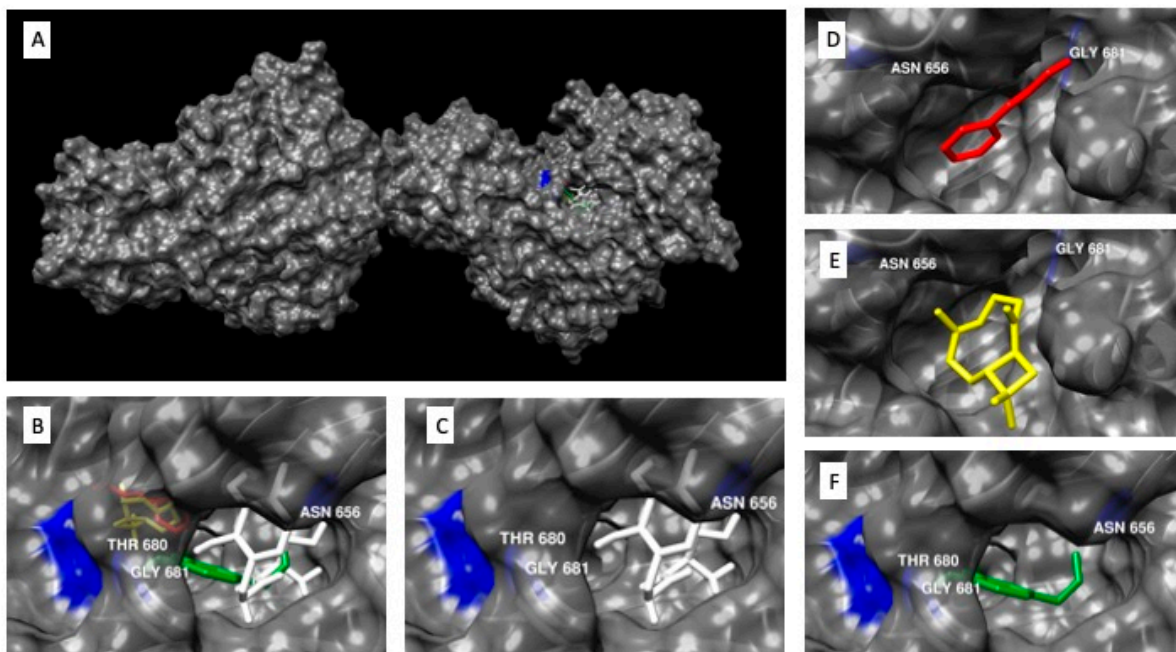


Figure S3. Molecular modeling of cinnamon essential oil constituents docked with hexokinase-II (HK-II). **(A)** HK-II antagonist benserazide and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of HK-II; **(B)** Close view of HK-II antagonist benserazide and essential oil compounds cinnamaldehyde, beta-caryophyllene, and eugenol docked in the active site of HK-II, specifically near residues ASN656, THR680, and GLY681; **(C)** Benserazide docked in the active pocket of HK-II, with a binding affinity of -7.4 kcal/mol; **(D)** Cinnamaldehyde docked in the active pocket of HK-II, with a binding affinity of -5.5 kcal/mol; **(E)** Beta-caryophyllene docked in the active pocket of HK-II, with a binding affinity of -6.6 kcal/mol; **(F)** Eugenol docked in the active pocket of HK-II, with a binding affinity of -5.6 kcal/mol.