molecules

MDPI

*Supplementary Materials*

# Inhibition of Aldose Reductase by Ginsenoside Derivatives via a Specific Structure Activity Relationship with Kinetics Mechanism and Molecular Docking Study

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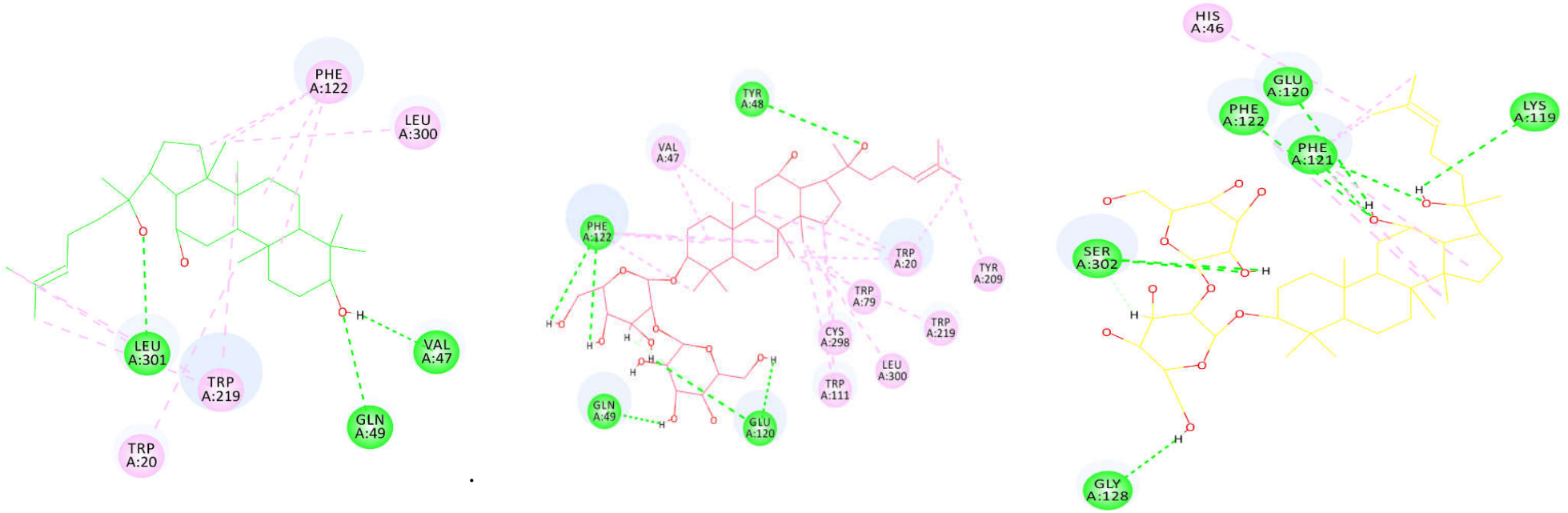
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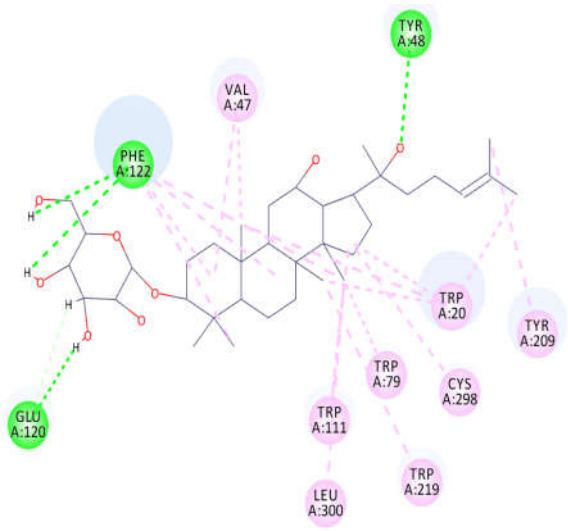
(**a**) (**b**) (**c**)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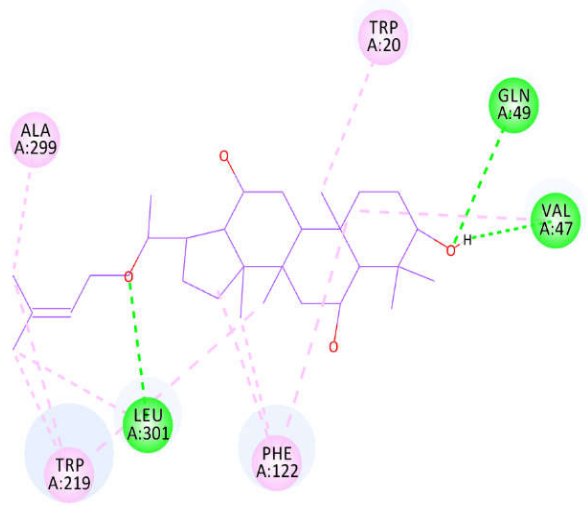
(**d**)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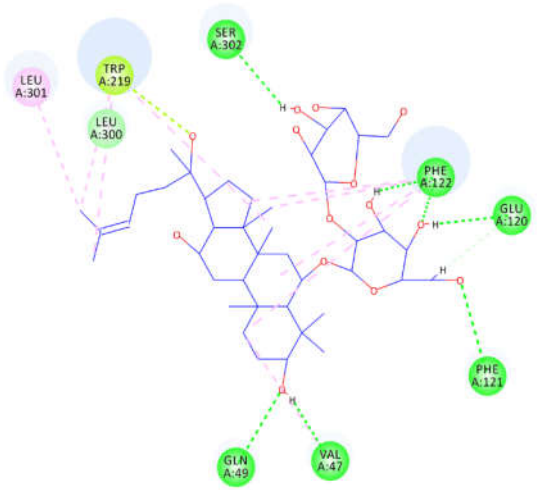
(**e**)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(**f**)

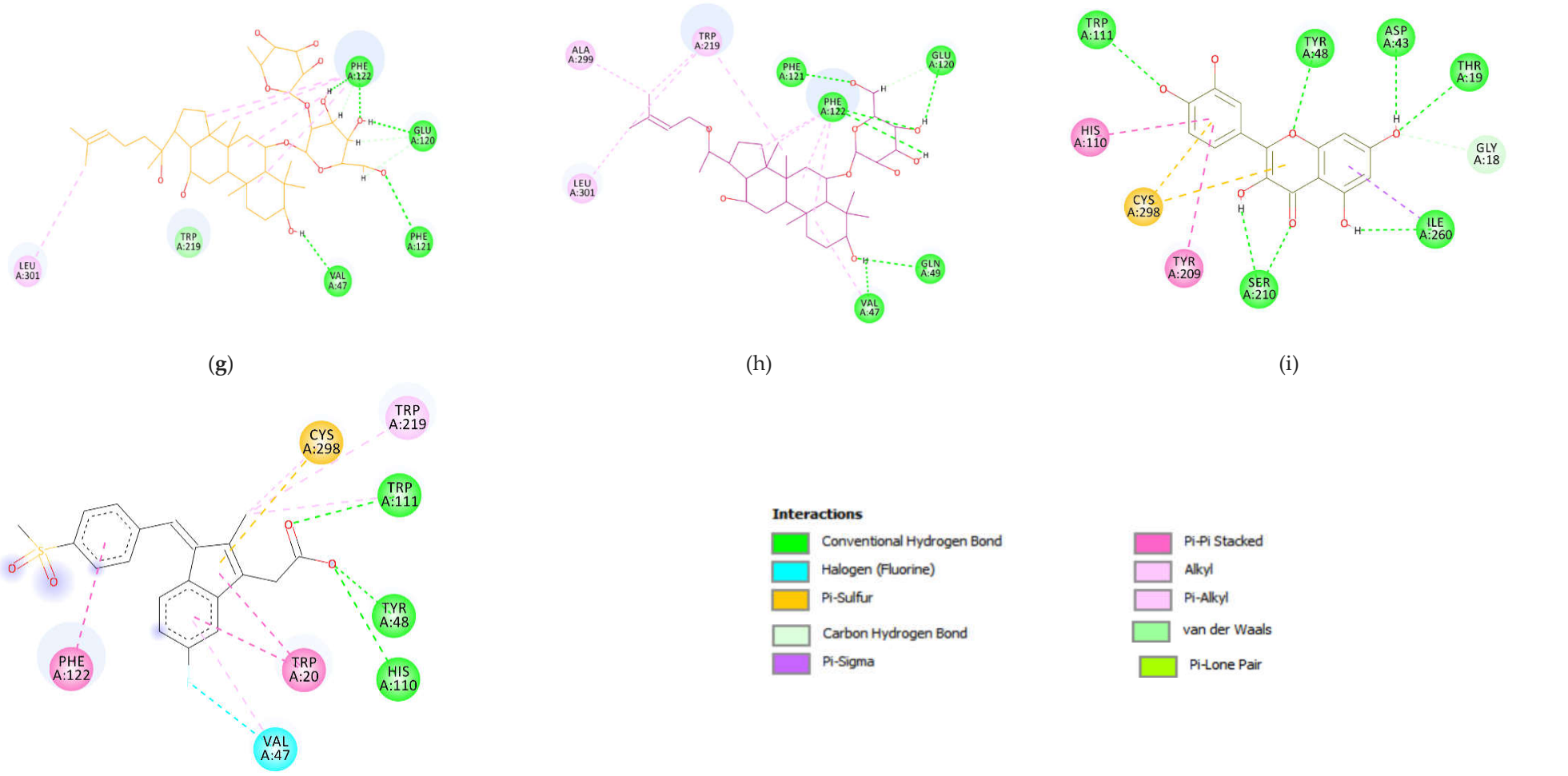
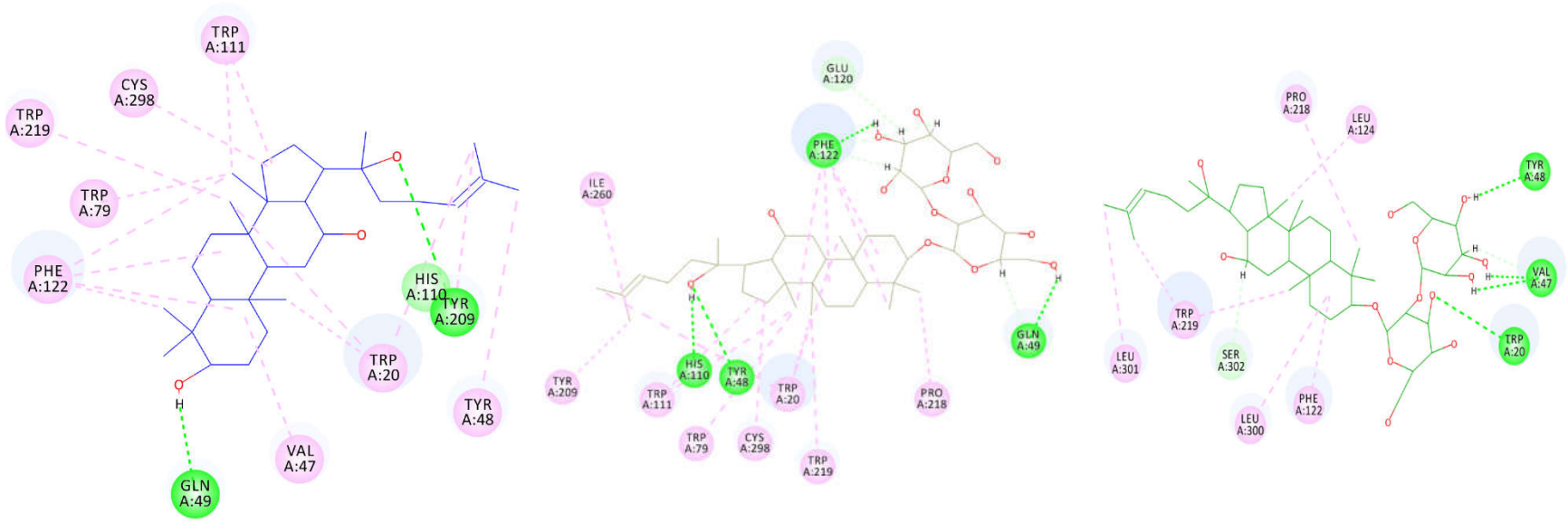



**Figure S1.** 2D interactions of ginsenosides inside the active pocket of rat lens aldose reductase (RLAR). The interactions are represented by green (conventional hydrogen bonding), yellow (π-sulfur interactions), tea pink (π-π T-shaped and π-π stacked interactions), cyan (fluorine) and yellow (π-sulfur). Protopanaxadiol (**a**), (20*S*) ginsenoside Rg3 (**b**), (20*R*) ginsenoside Rg3 (**c**), ginsenoside Rh2 (**d**), protopanaxatriol (**e**), ginsenoside Rf (**f**), (20*S*) ginsenoside Rg2 (**g**), and ginsenoside Rh1(**h**), quercetin (**i**), and sulindac (**j**).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LEU A:124
TYR A:48
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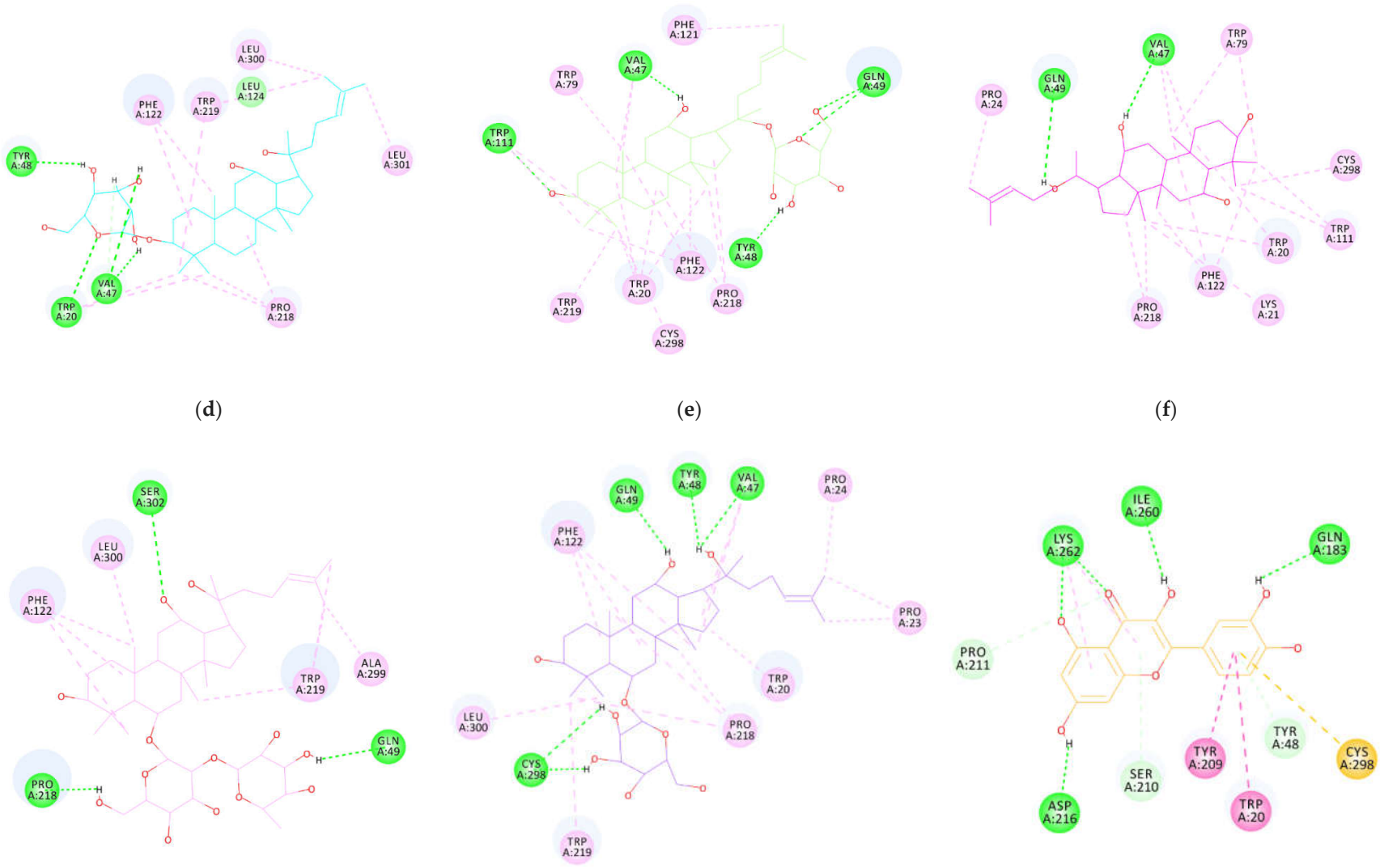
LEU A:300

(**a**) (**b**) (**c**)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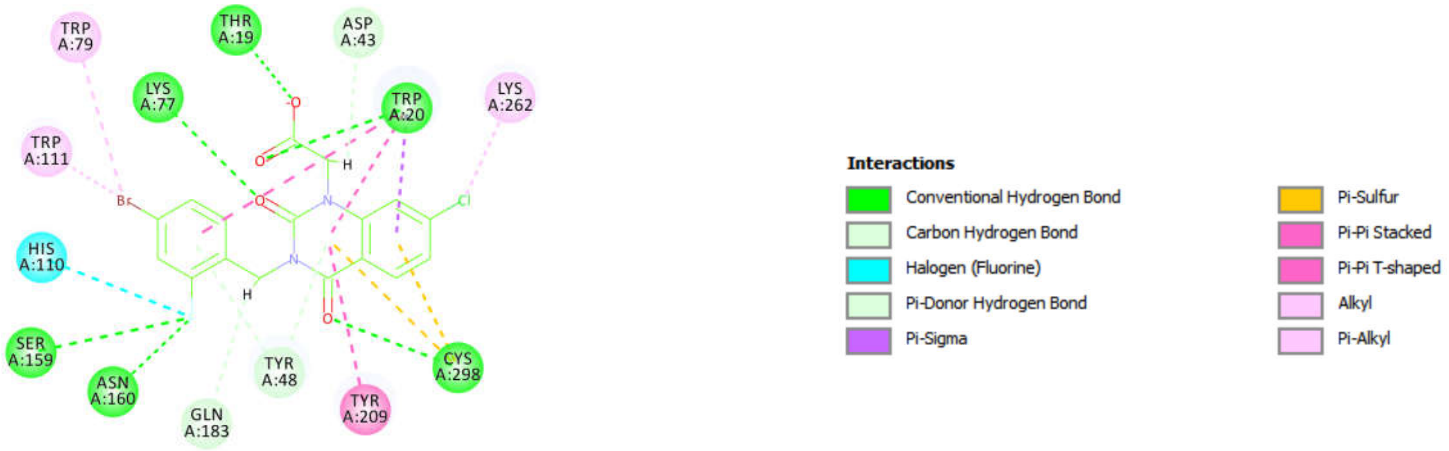
(**d**) (**e**) (**f**)

(**g**) (**h**) (**i**)




(j)

**Figure S2.** 2D interactions of ginsenosides inside the active pocket of human aldose reductase (HRAR). The interactions are represented by green (conventional hydrogen bonding), yellow (π-sulfur interactions), tea pink (π-π T shaped and π-π stacked interactions), cyan (fluorine) and yellow (π-sulfur). Protopanaxadiol (a), (20*S*) ginsenoside Rg3 (b), (20*R*) ginsenoside Rg3 (c), ginsenoside Rh2 (d), compound K (e), protopanaxatriol (f), (20*R*) ginsenoside Rg2 (g), ginsenoside Rh1(h), quercetin (i), and zenaresta (j)