Targeting insulin signaling and TRAF2/JNK pathway: a comprehensive *in silico* study of *Uncaria tomentosa* compounds

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SUPPLEMENTARY MATERIAL

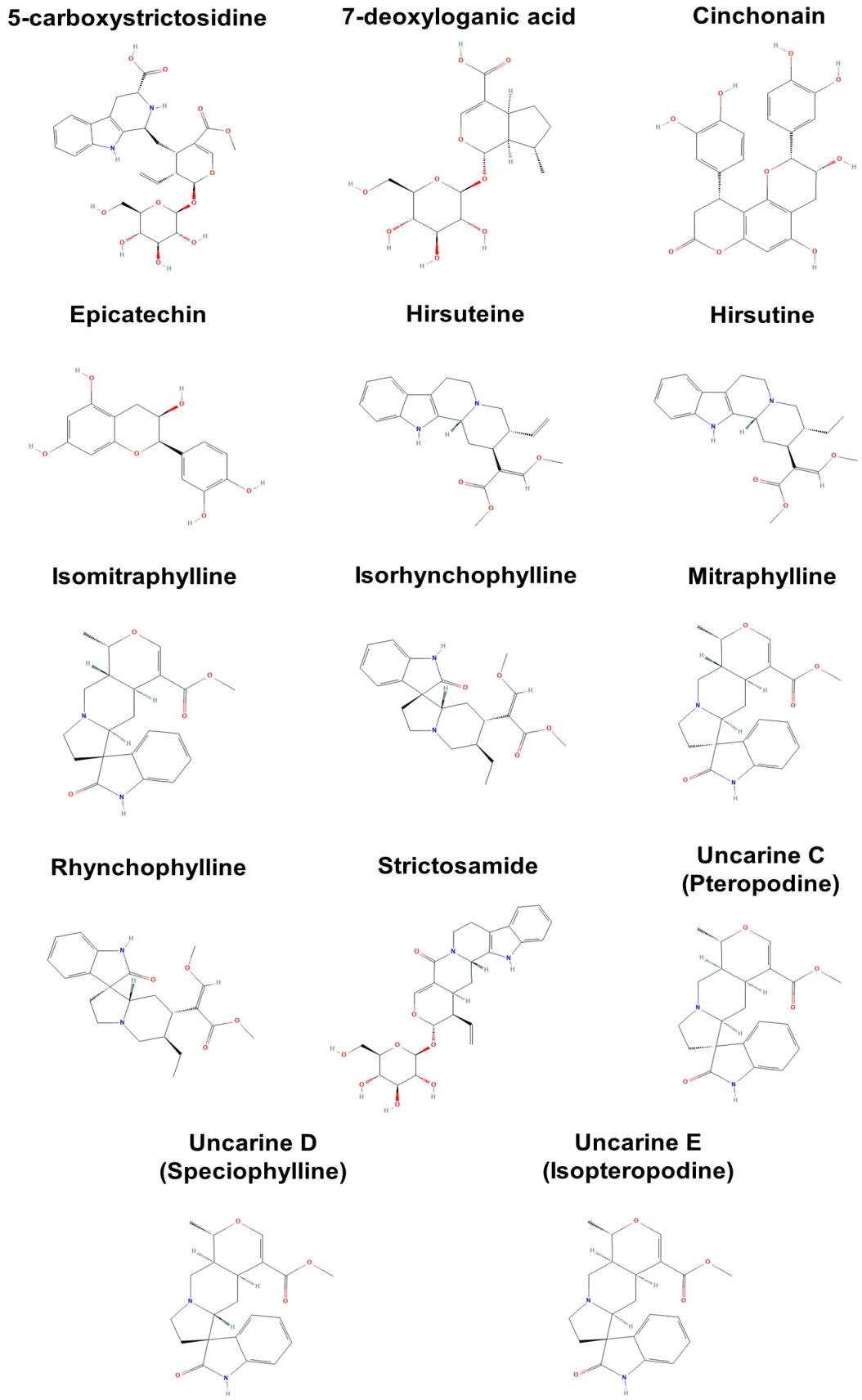

Figure S1. Chemical structures of the 14 compounds found in UT, obtained from the PubChem database

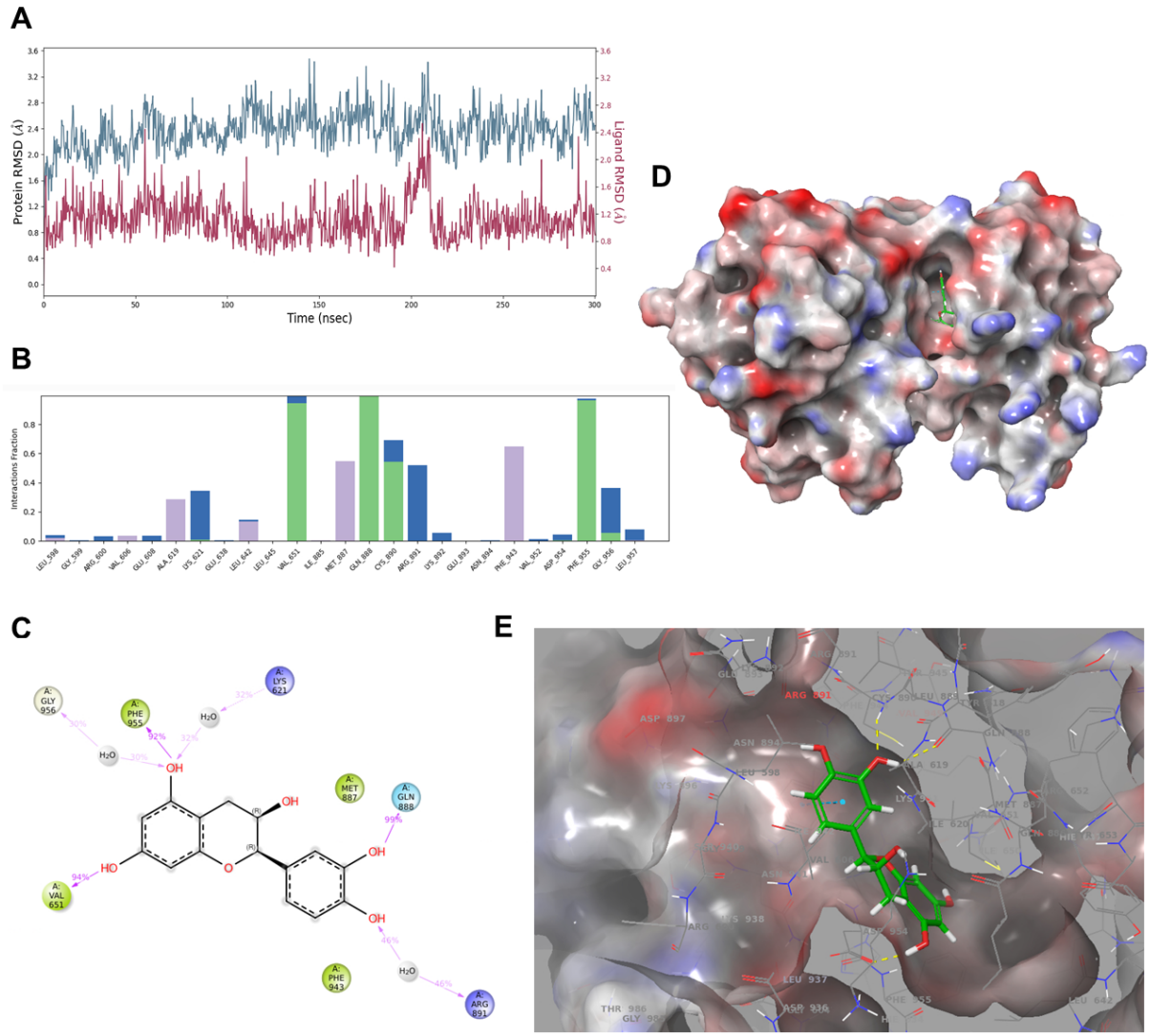

Figure S2. Molecular dynamics between PERK protein and the compound Epicatechin. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

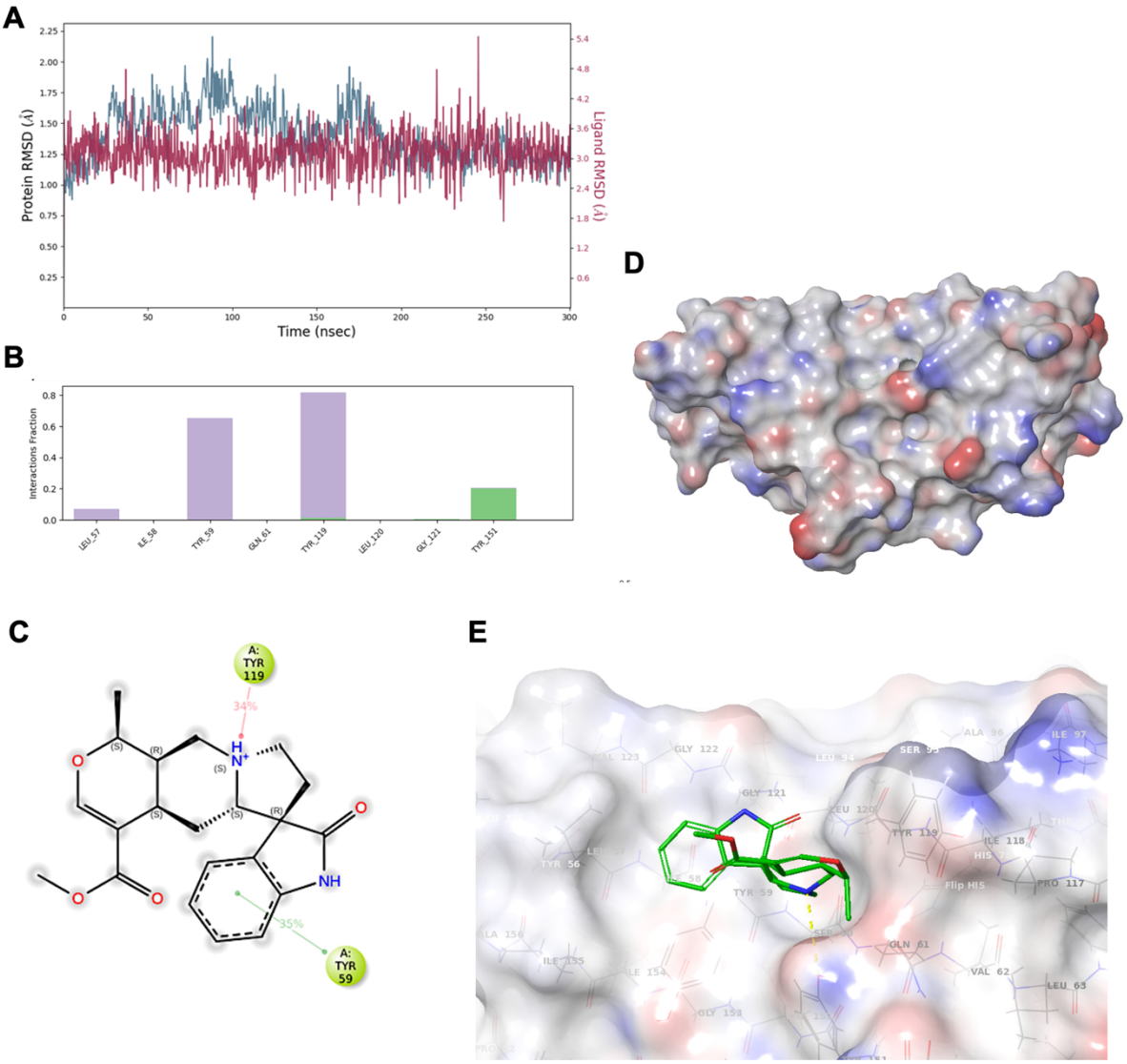

Figure S3. Molecular dynamics between TNF-α cytokine and the compound Mitraphylline. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

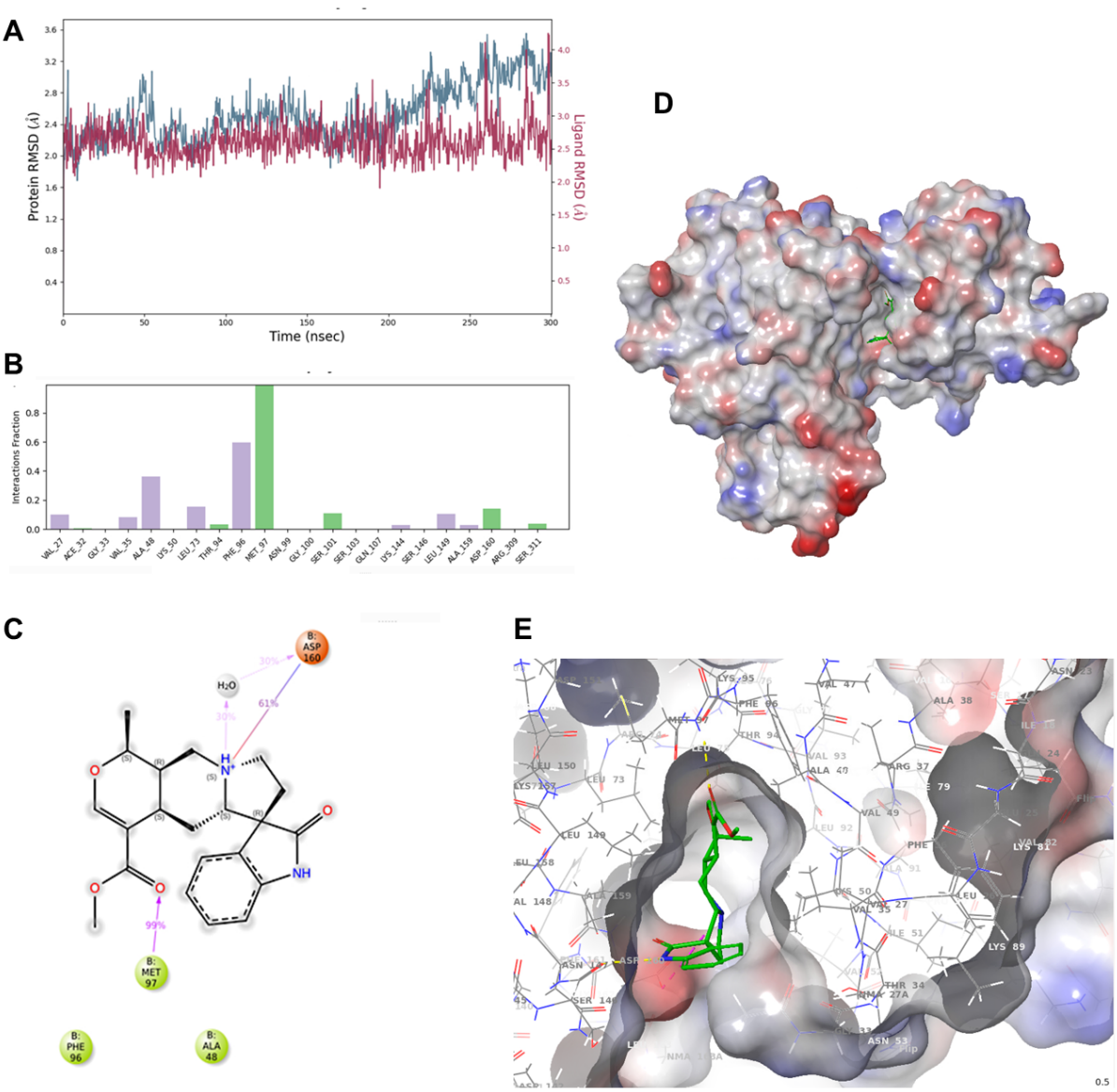

Figure S4. Molecular dynamics between TRAF2 protein and the compound Mitraphylline. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

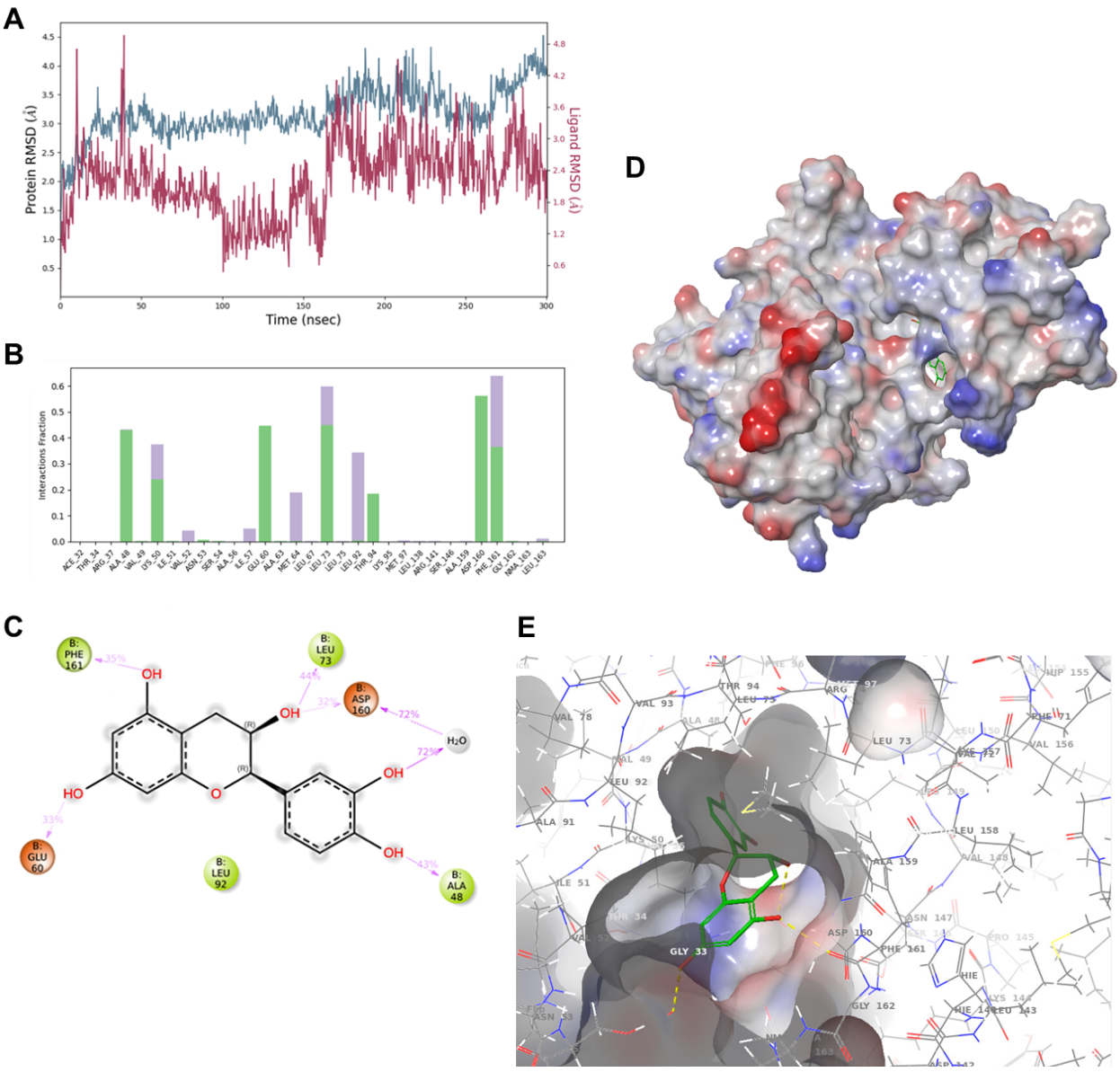

Figure S5. Molecular dynamics between TRAF2 protein and the compound Epicatechin. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

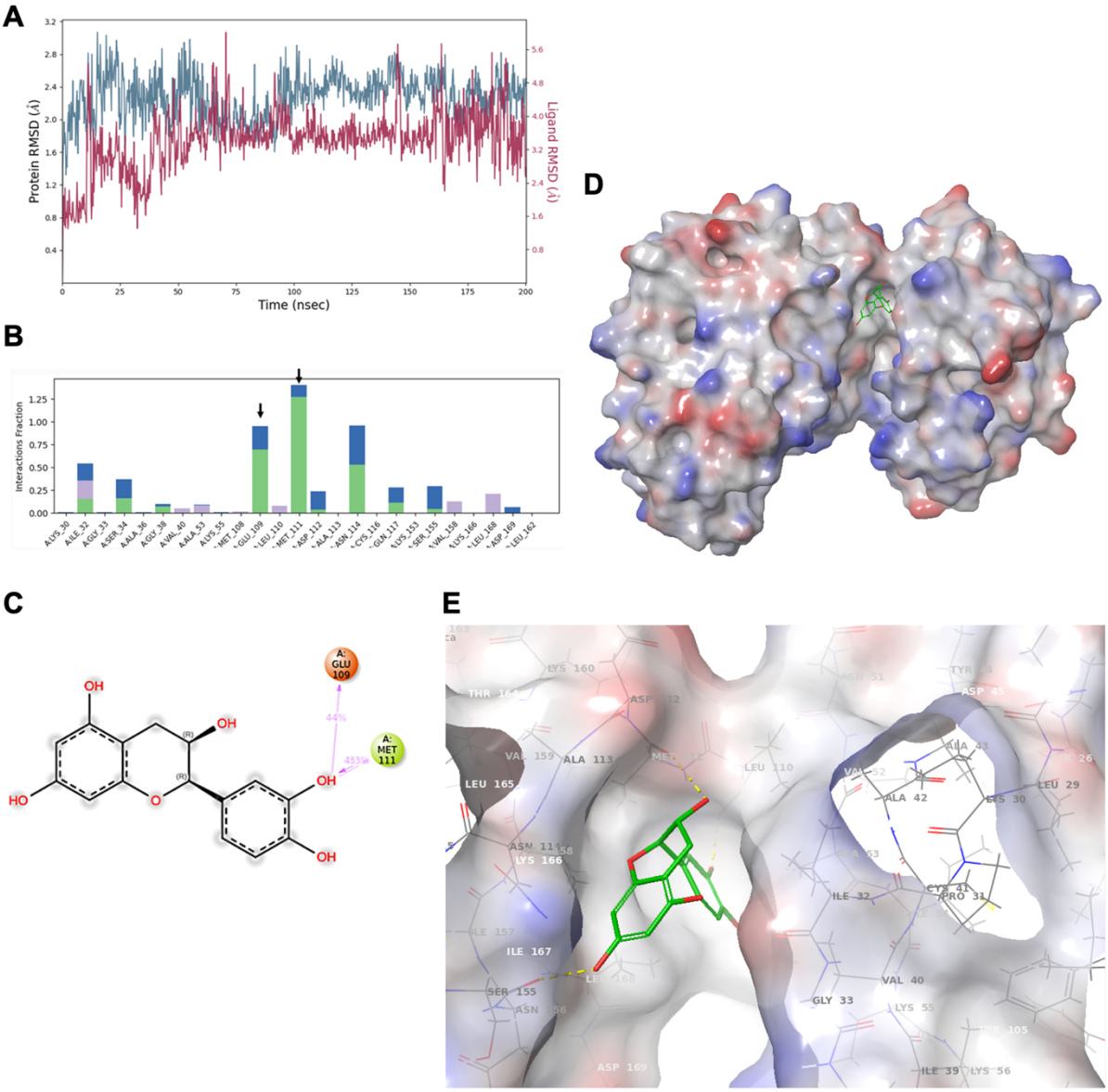

Figure S6. Molecular dynamics between JNK protein and the compound Epicatechin. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

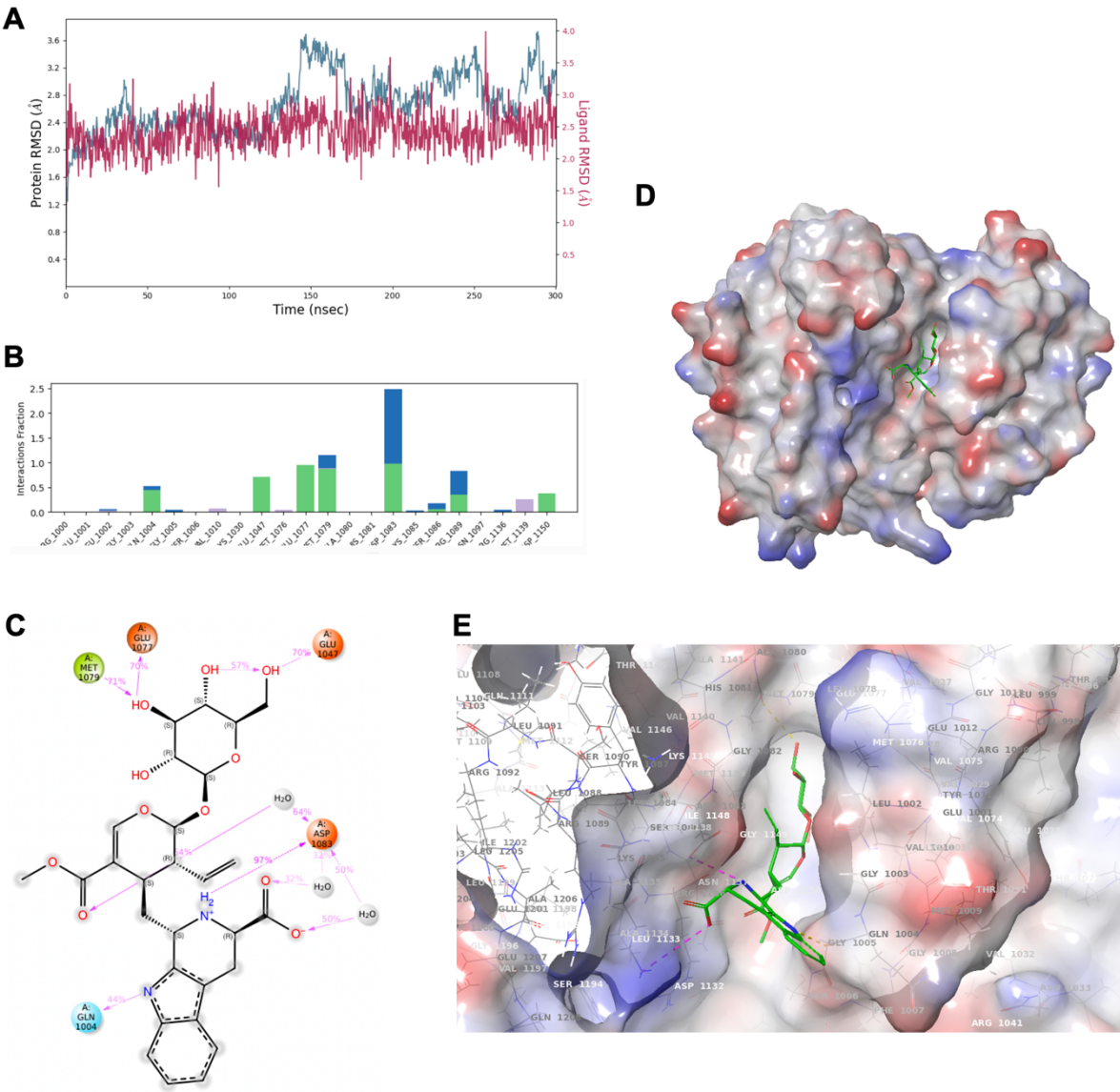

Figure S7. Molecular dynamics between IRS-1 protein and the compound 5-Carboxystrictosidine. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

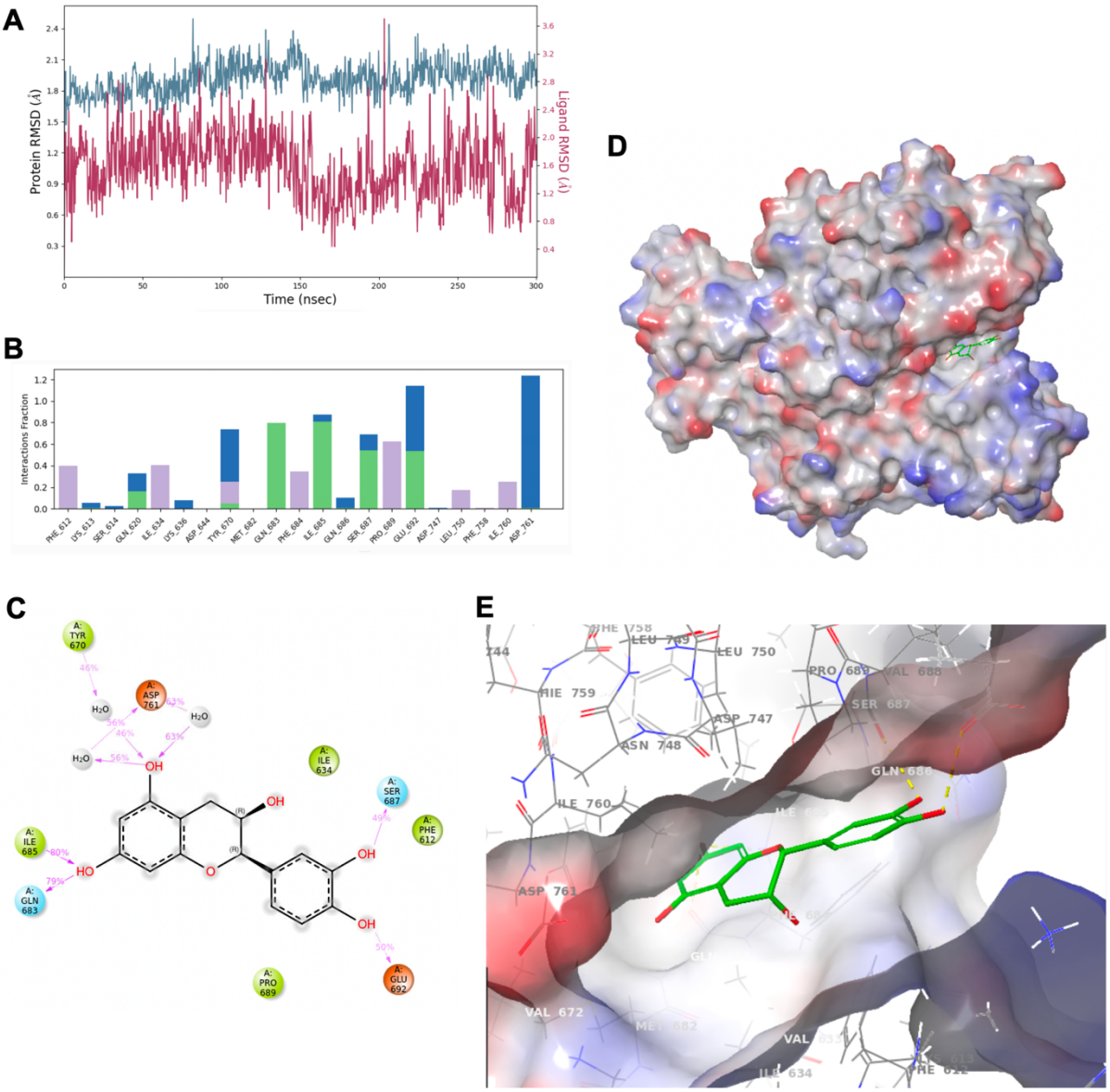

Figure S8. Molecular dynamics between PI3K protein and the compound Epicatechin. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

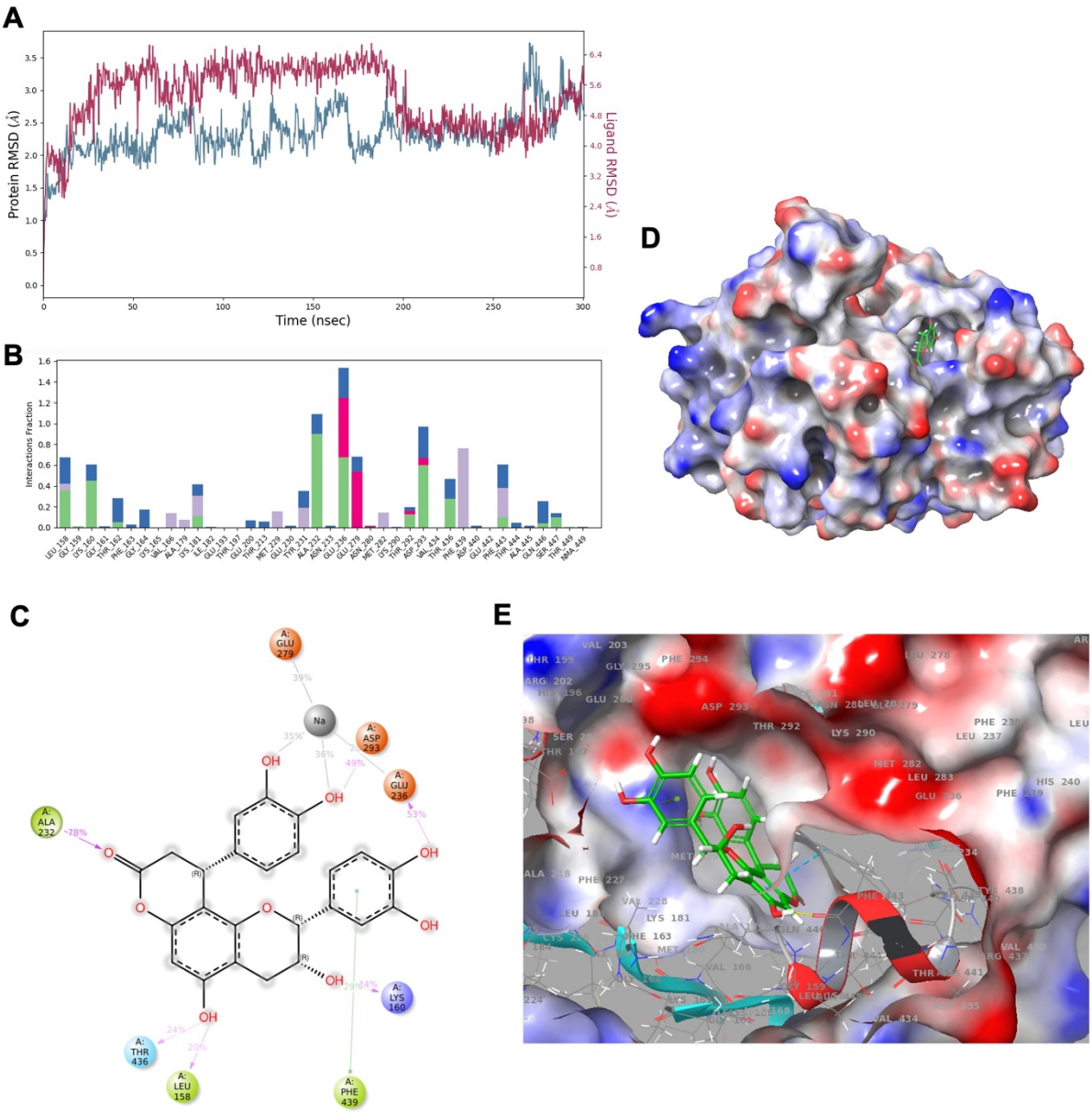

Figure S9. Molecular dynamics between AKT protein and the compound Cinchonain. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

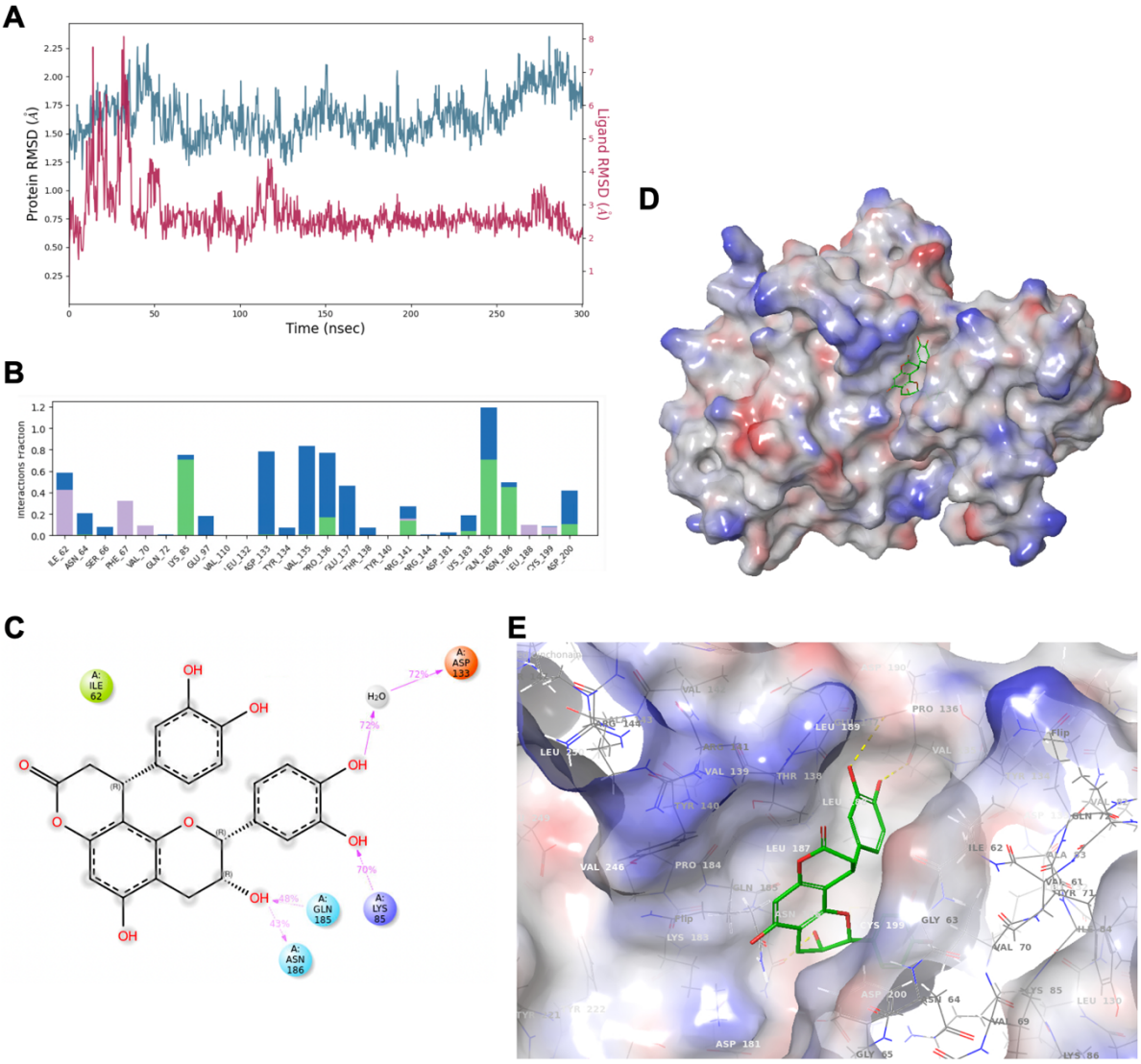

Figure S10. Molecular dynamics between GSK3β protein and the compound Cinchonain. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site

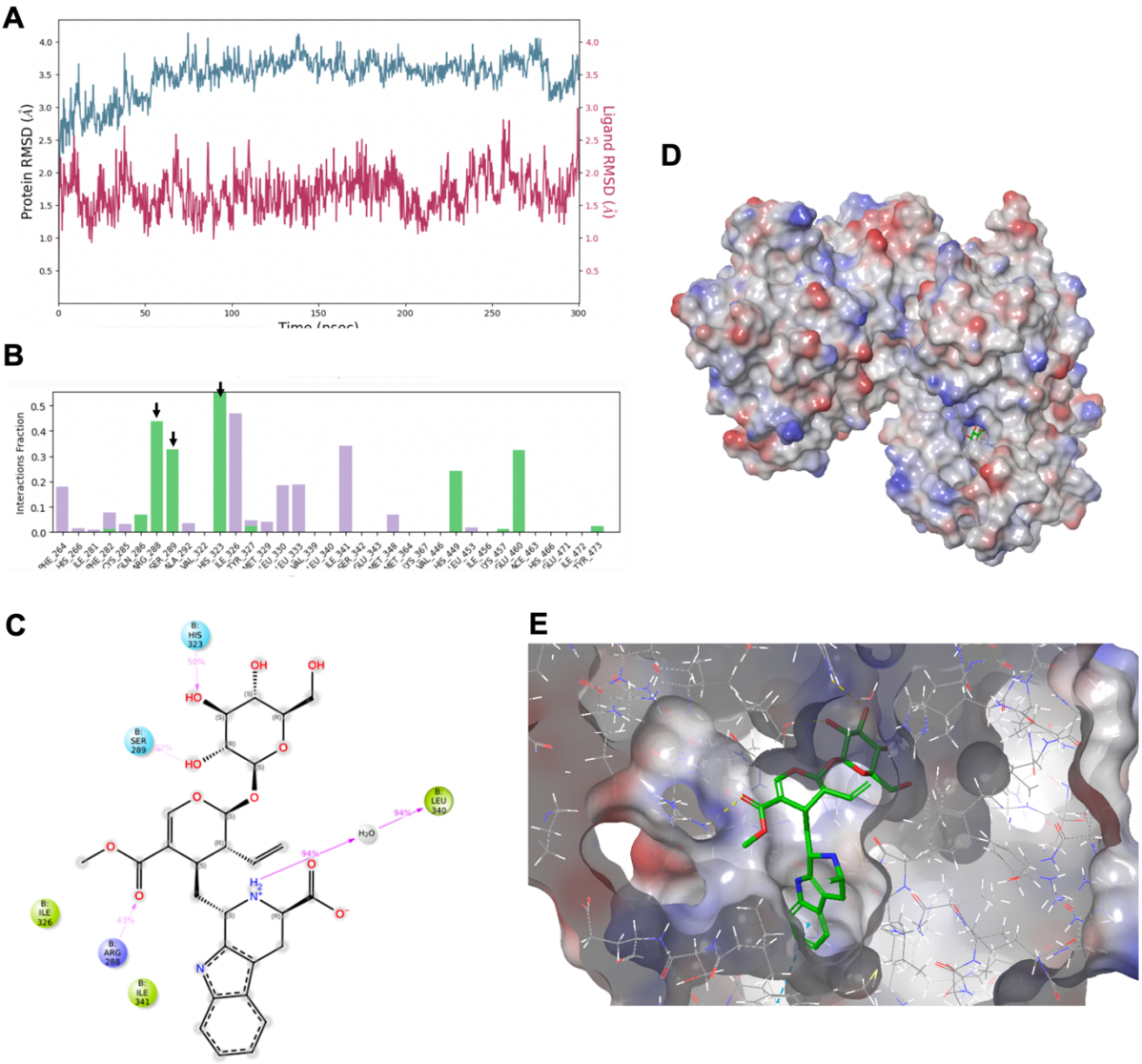

Figure S11. Molecular dynamics between PPARγ protein and the compound 5-Carboxystrictosidine. A) RMSD values for the protein-ligand complex (compound); **B and C)** Occurrence of hydrophilic or hydrophobic interactions, with certain residues, during the dynamics simulation; **D and E)** Three-dimensional demonstration of the interactions between the compound and the protein binding site