Pharmacoinformatics and UPLC-QTOF/ESI-MS-Based Phytochemical Screening of *Combretum indicum* against Oxidative Stress and Alloxan-Induced Diabetes in Long–Evans Rats

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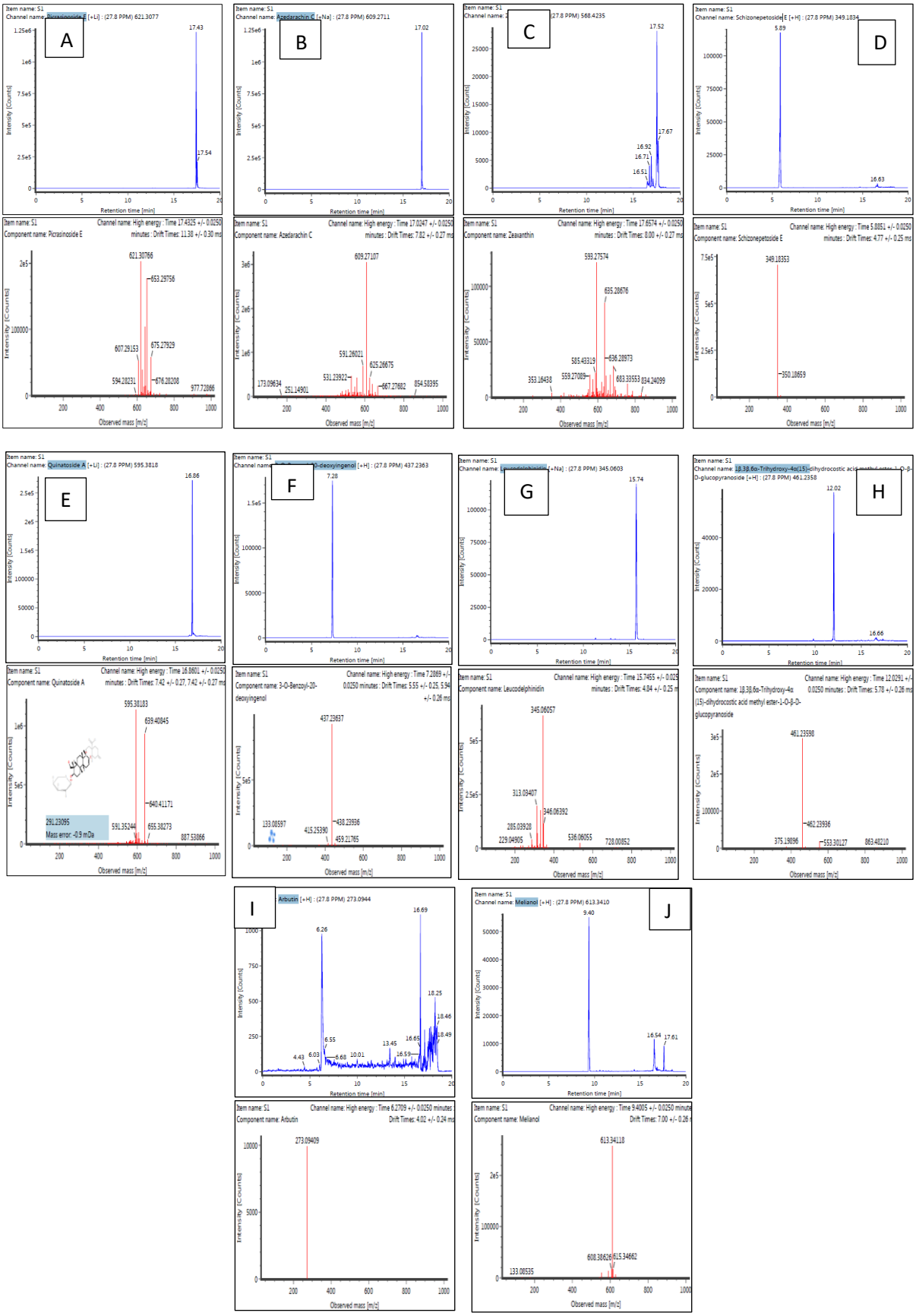
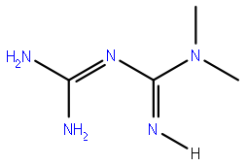
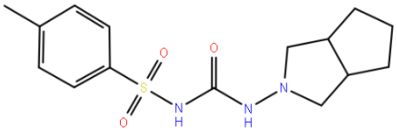


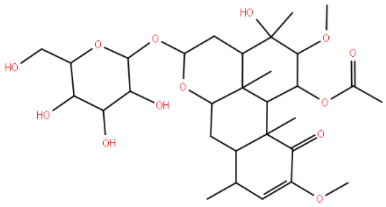
Figure S1: LC chromatogram and mass spectra of CILEx for high-intensity compounds identified and vertically arranged as (**A**) Picrasinoside E; (**B**) Azedarachin C; (**C**) Zeaxanthin; (**D**) Quinatoside A; (**E**) 3-*O*-Benzoyl-20- deoxyingenol; (**F**) Leucodelphinidin; (**G**) Schizonepetoside E; (**H**) 1β,3β,6α-Trihydroxy-4α(15)-dihydrocostic acid methyl ester-1-*O*-β-Dglucopyranoside; (**I**) Melianol; (**J**) Arbutin.



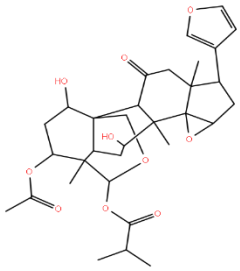
Metformin



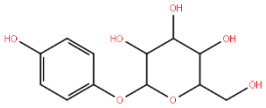
Gliclazide



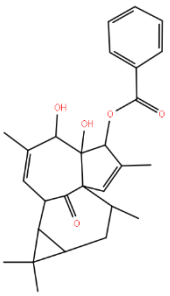
Picrasonide_E



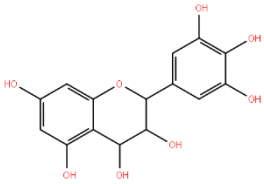
Azedarachin C



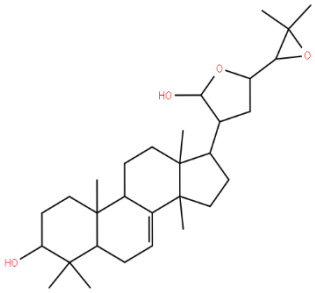
Arbutin



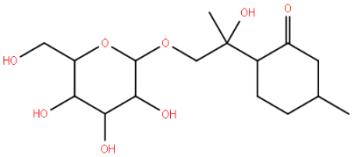
3-O-Benzoyl-2-O-deoxyingenol



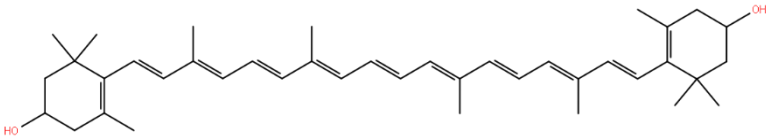
Leucodelphinidin



Melianol



Schizonepetoside E



Zeaxanthin

Figure S2: list of chemical structures of the ligand molecules available in PubChem.

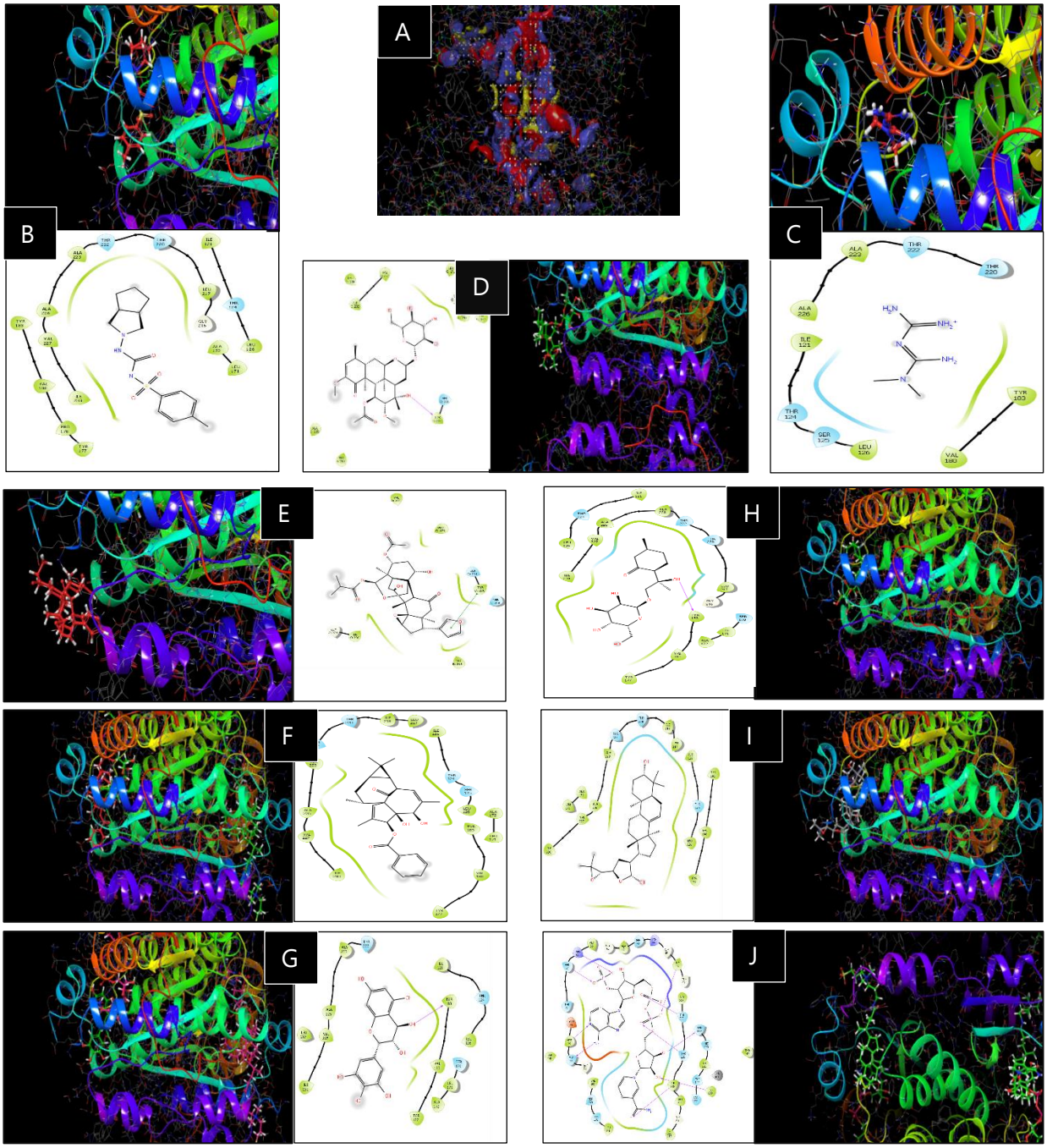


Figure S3: Interactions based on **A**. site map of seven ligands **D**. Picrasonide E; **E.** Azedarachin C; **F.** 3-*O*-Benzoyl-20-deoxyingenol; **G.** Leucodelphinidin; H. Schizonepetoside E; **I.** Melianol; and **J.** Arbutin with the receptor **IXU9**. Schizonepetosie showed the highest docking score (−8.145) compared with the reference antidiabetic drugs B. Gliclazide and C. Metformin.

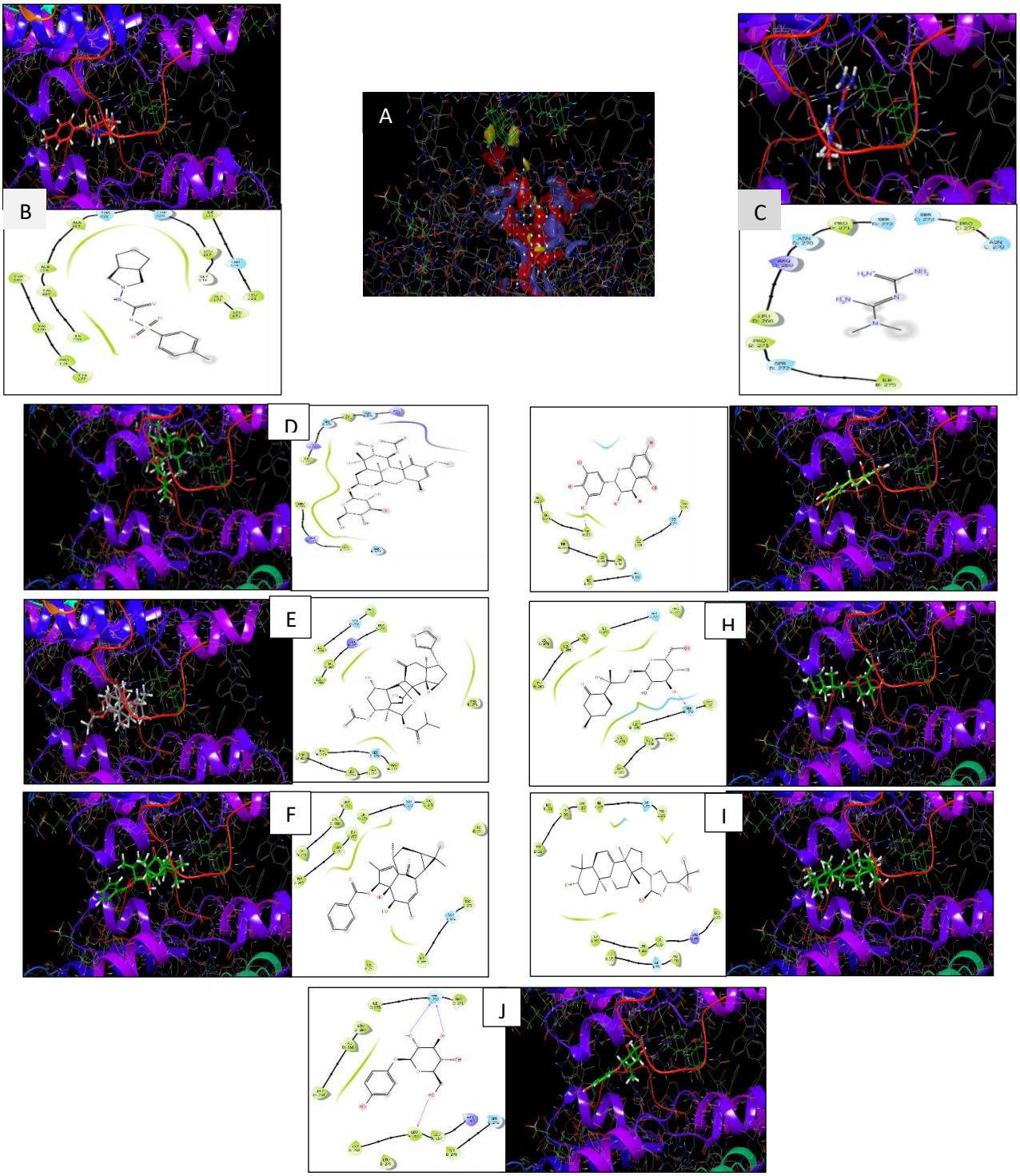


Figure S4: Interactions based on **A**. site map of seven ligands **D**. Picrasonide_E; **E.** Azedarachin C; **F.** 3-*O*-Benzoyl-20-deoxyingenol; G. Leucodelphinidin; H. Schizonepetoside E; **I.** Melianol; and **J.** Arbutin with the receptor **IXU7**. Melianol showed the highest docking score (−8.475) compared with the reference antidiabetic drugs B. Gliclazide and C. Metformin. The 3D protein binding has been presented with respective amino acid grooves for ligand interaction.

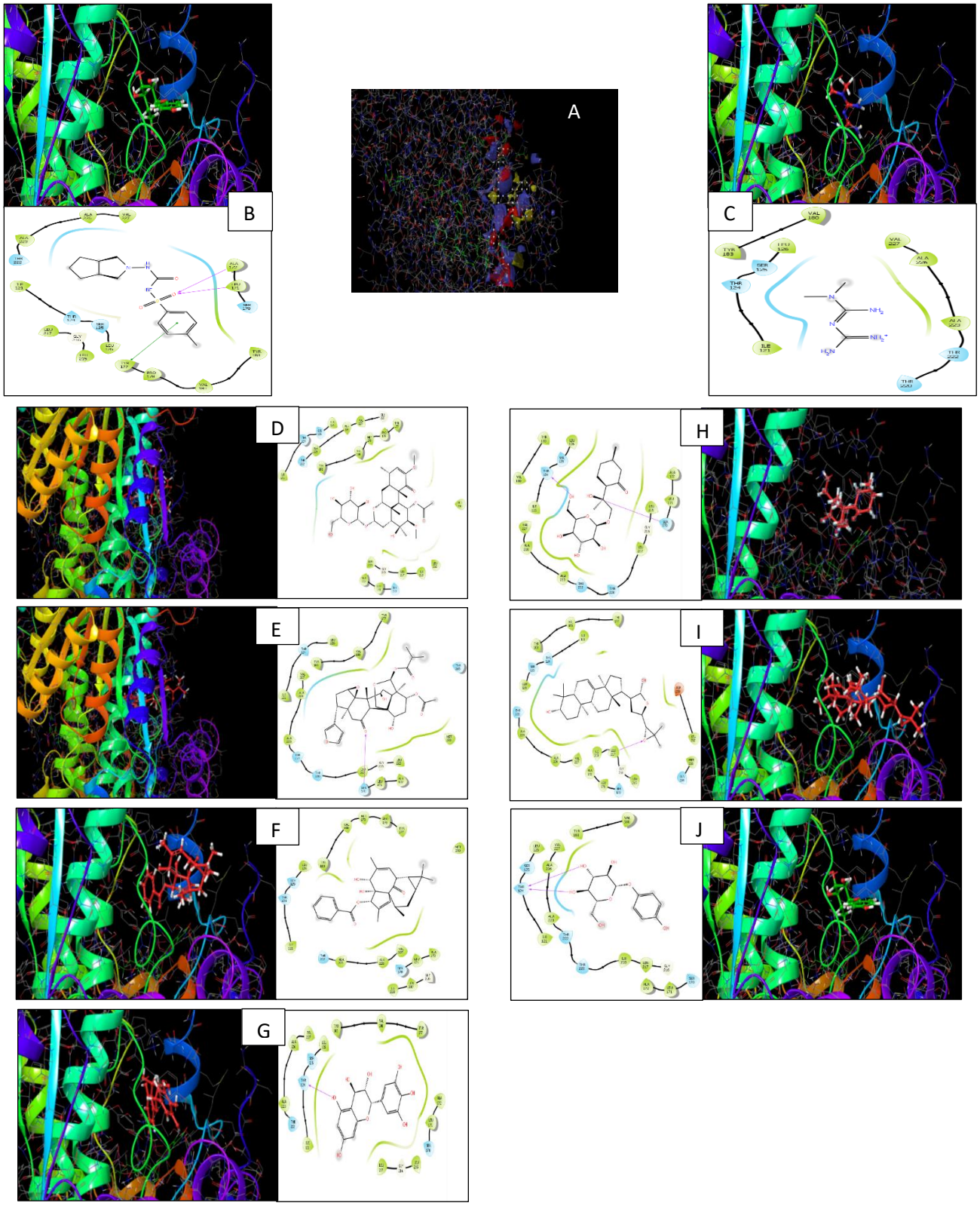


Figure S5: Interactions based on **A**. site map of seven ligands B. Gliclazide; C. Metformin; **D**. Picrasonide E; **E.** Azedarachin C; **F.** 3-*O*-Benzoyl-20-deoxyingenol; G. Leucodelphinidin; H. Schizonepetoside E; **I.** Melianol; and **J.** Arbutin with the receptor **2BEL**. Melianol showed the highest docking score (−8.995) compared with the reference antidiabetic drugs B. Gliclazide and C. Metformin. The 3D protein binding has been presented with respective amino acid grooves for ligand interaction.

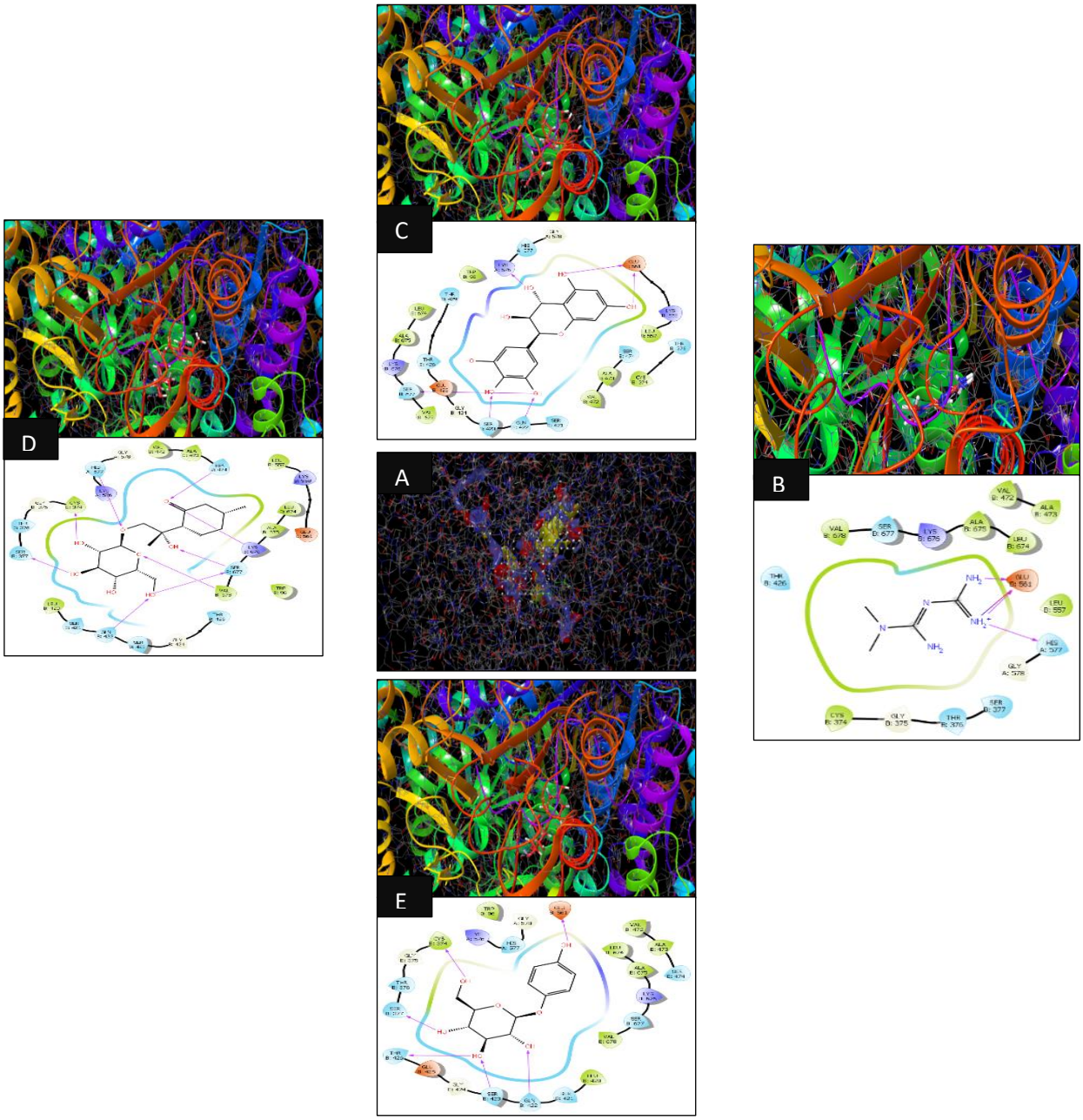


Figure S6: Interactions based on **A**. site map of three ligands **C**. Leucodelphinidin; D. Schizonepetoside E; and **E.** Arbutin with the receptor **GR4F**. Arbutin showed the highest docking score (−7.492) compared with the reference antidiabetic drug B. Metformin. The 3D protein binding has been presented with respective amino acid grooves for ligand interaction.

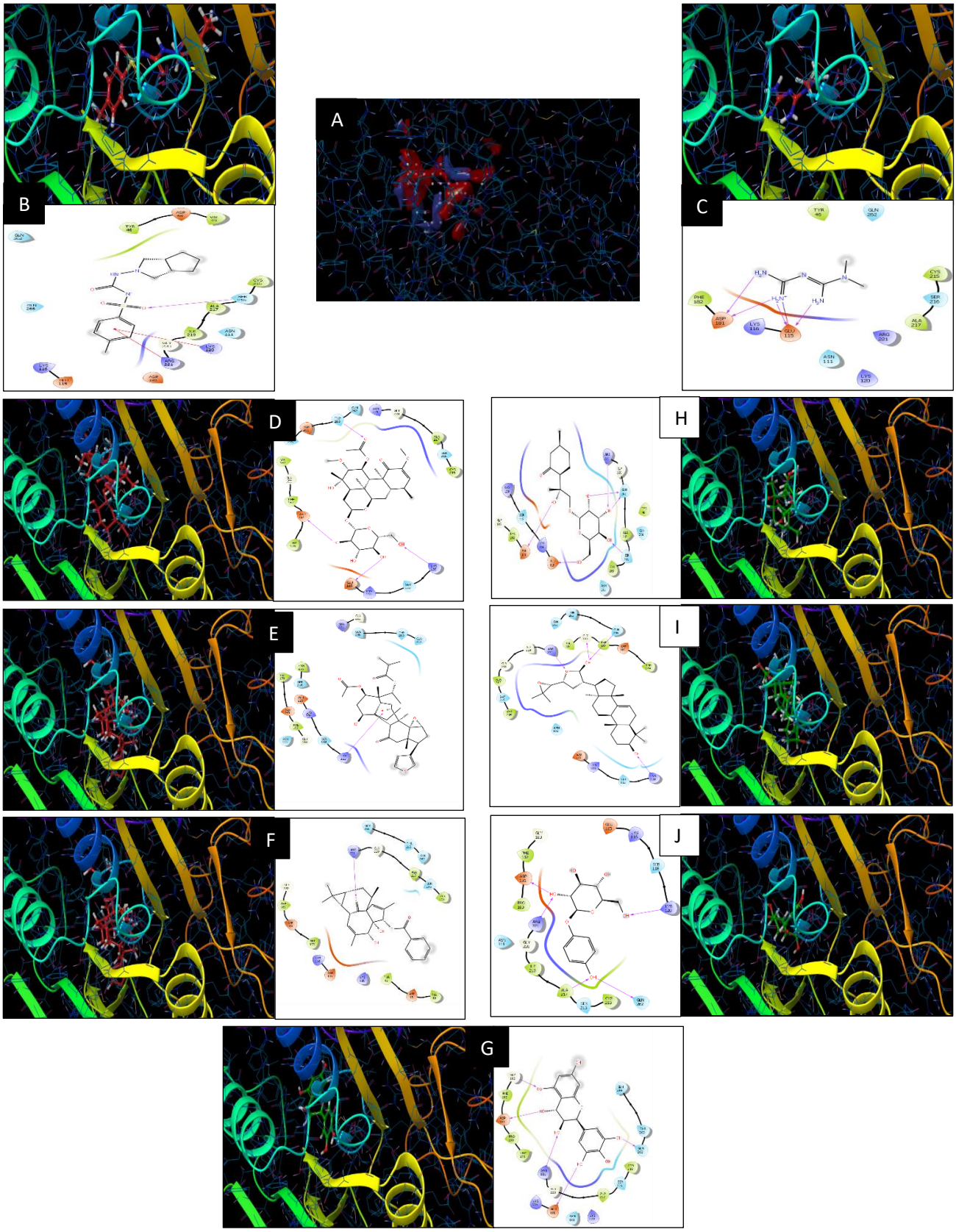
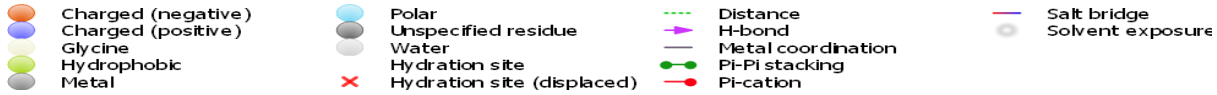


Figure S7: Interactions based on **A**. site map of seven ligands B. Gliclazide; C. Metformin; **D**. Picrasonide E; **E.** Azedarachin C; **F.** 3-*O*-Benzoyl-20-deoxyingenol; G. Leucodelphinidin; H. Schizonepetoside E; **I.** Melianol; and **J.** Arbutin with the receptor **3A5J**. 3-*O*-Benzoyl-20-deoxyingenol showed the highest docking score (−6.123) compared with the reference antidiabetic drugs B. Gliclazide and C. Metformin. The 3D protein binding has been presented with respective amino acid grooves for ligand interaction.


Charged (negative)
Charged (positive)
Glycine
Hydrophobic
Metal
Polar
Unspecified residue
Water
Hydration site
Hydration site (displaced)
Distance
H-bond
Metal coordination
Pi-Pi stacking
Pi-cation
Salt bridge
Solvent exposure