

Figure S1: Electrostatic surfaces of the metabolites and ions at *ZmDHAR* (A, B), *ZmMDHAR* (C, D) and *TaMDHAR* (E, F). In A-D, surfaces of all the metabolites are shown in white, and Al³⁺ in yellow and Mn²⁺ in red. The figure shows that there is no overlap between the metabolites and ions.

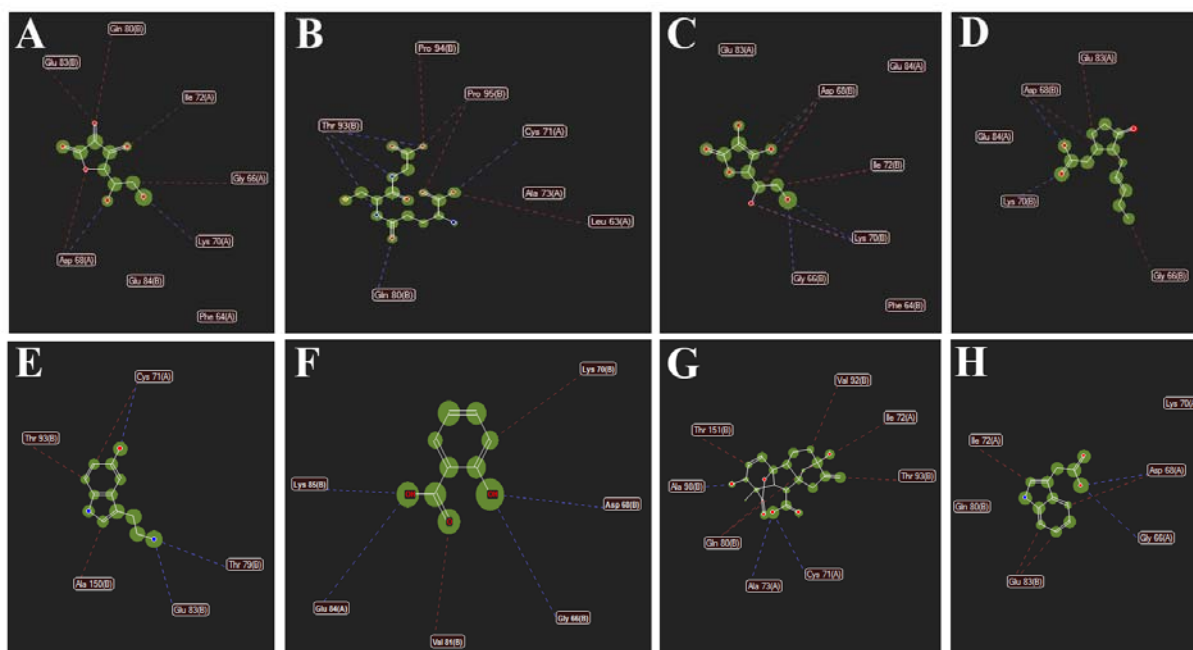


Figure S2: Interactions of different metabolites with the active site amino acid residues of *ZmDHAR* with (A) DHA; (B) GSH; (C) AsA; (D) JA; (E) 5-HT; (F) SA; (G) GA3; (H) IAA. The dotted lines represent hydrogen bonding and steric interactions between the ligands and the amino acid residues shown.

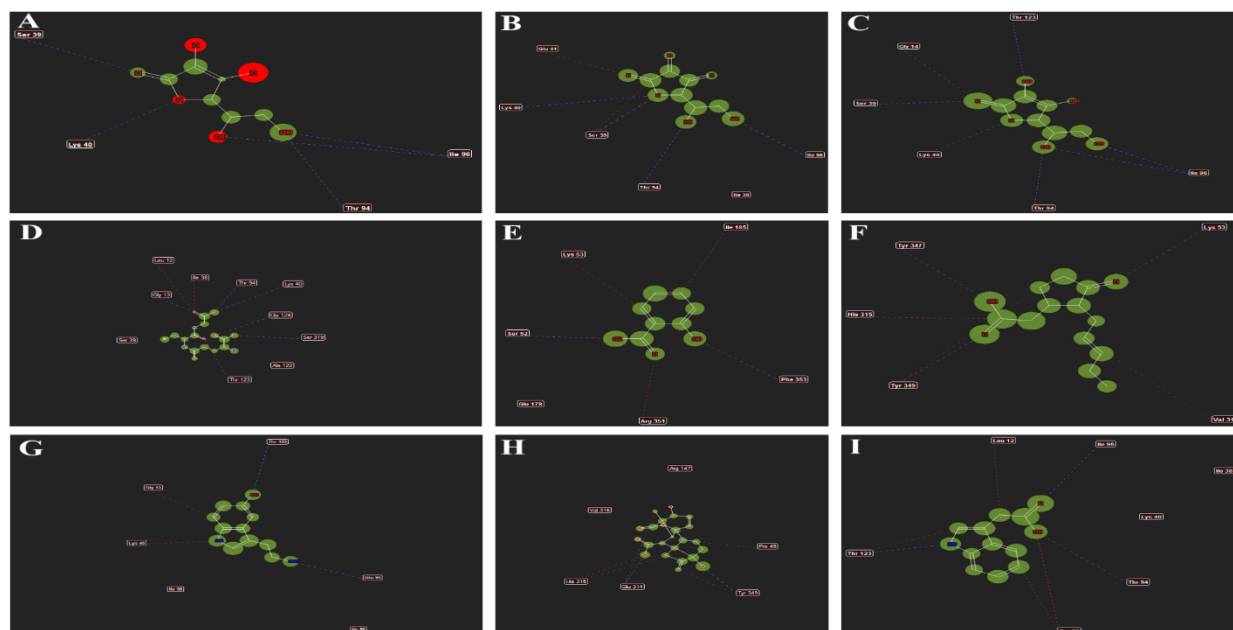


Figure S3: Interactions of different metabolites (A) MDHA; (B) DHA; (C) AsA; (D) GSH; (E) SA; (F) JA; (G) 5-HT; (H) GA3; (I) IAA with different amino acids of the active site of *ZmMDHAR*. Amino acids shown are the ones with which the metabolites form hydrogen bonds and steric interactions.

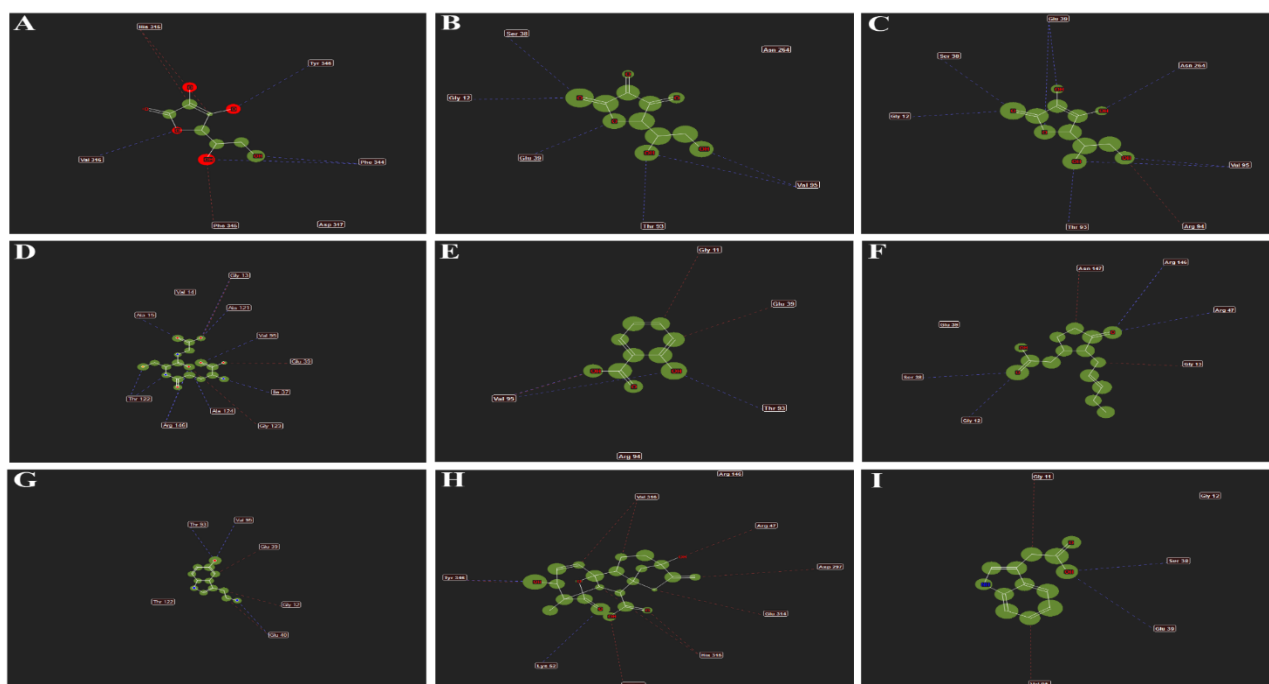


Figure S4: Interactions of the metabolites (A) MDHA; (B) DHA; (C) AsA; (D) GSH; (E) SA; (F) JA; (G) 5-HT; (H) GA3; (I) IAA with the active site residues of *TaMDHAR*. Amino acids shown are the ones with which the metabolites form hydrogen bonds and stearic interactions.