SUPPLEMENTARY DATA

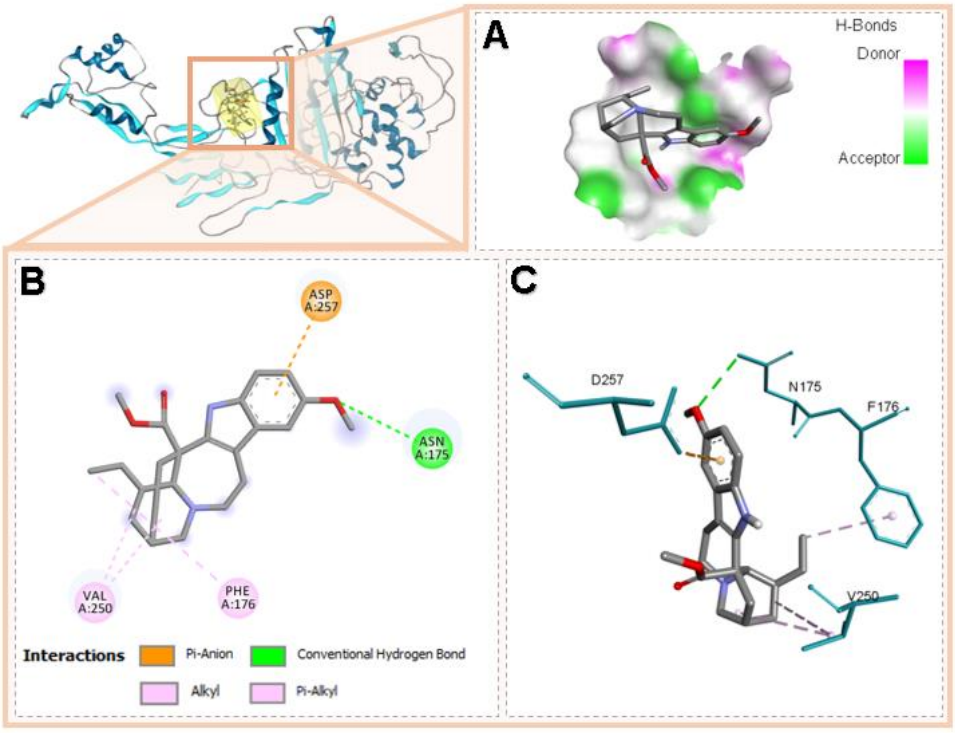

Figure S1. Molecular interactions between PBP1 from *S. aureus* and voacangine. (A) Characterization of the binding site according to the ability to form hydrogen bridges and geometry of the compound at the docking site, (B) 2D plot of the interactions specifying the type of interaction, (C) conformation of the compound during docking and interactions with PBP1 residues in 3D.

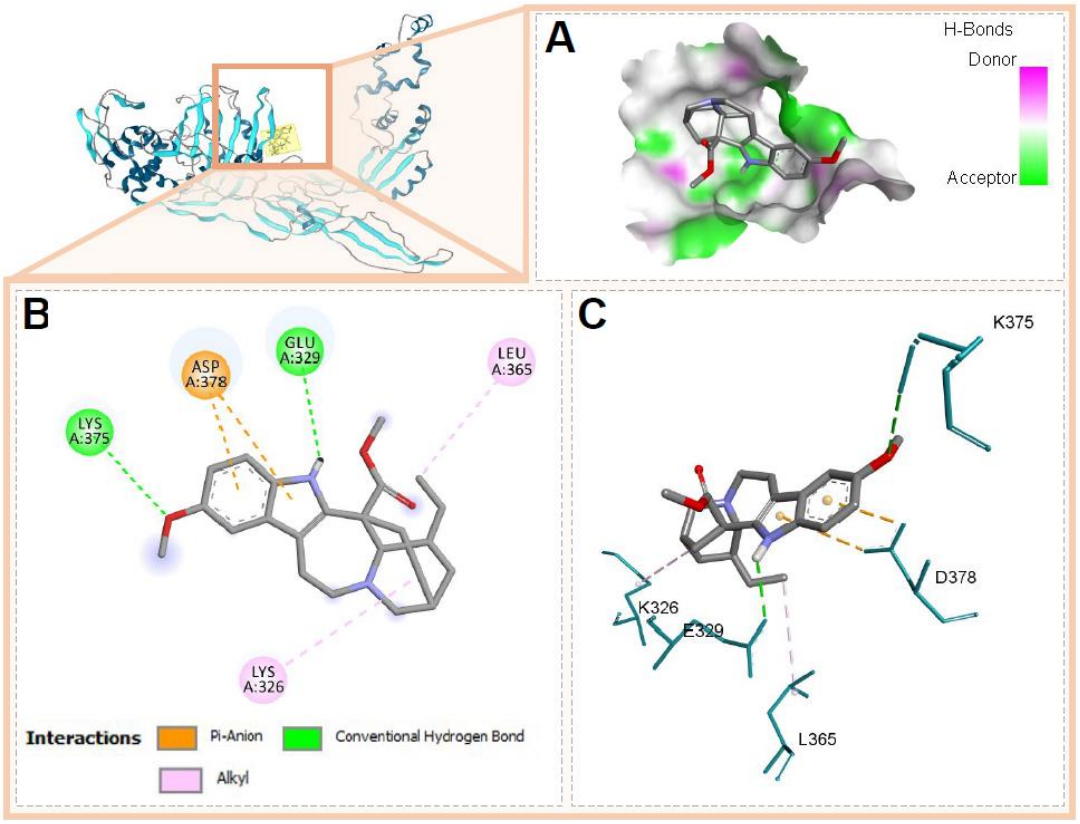

Figure S2. Molecular interactions between PBP3 from *S. aureus* and voacangine. (A) Characterization of the binding site according to the ability to form hydrogen bridges and geometry of the compound at the docking site, (B) 2D plot of the interactions specifying the type of interaction, (C) conformation of the compound during docking and interactions with PBP3 residues in 3D.

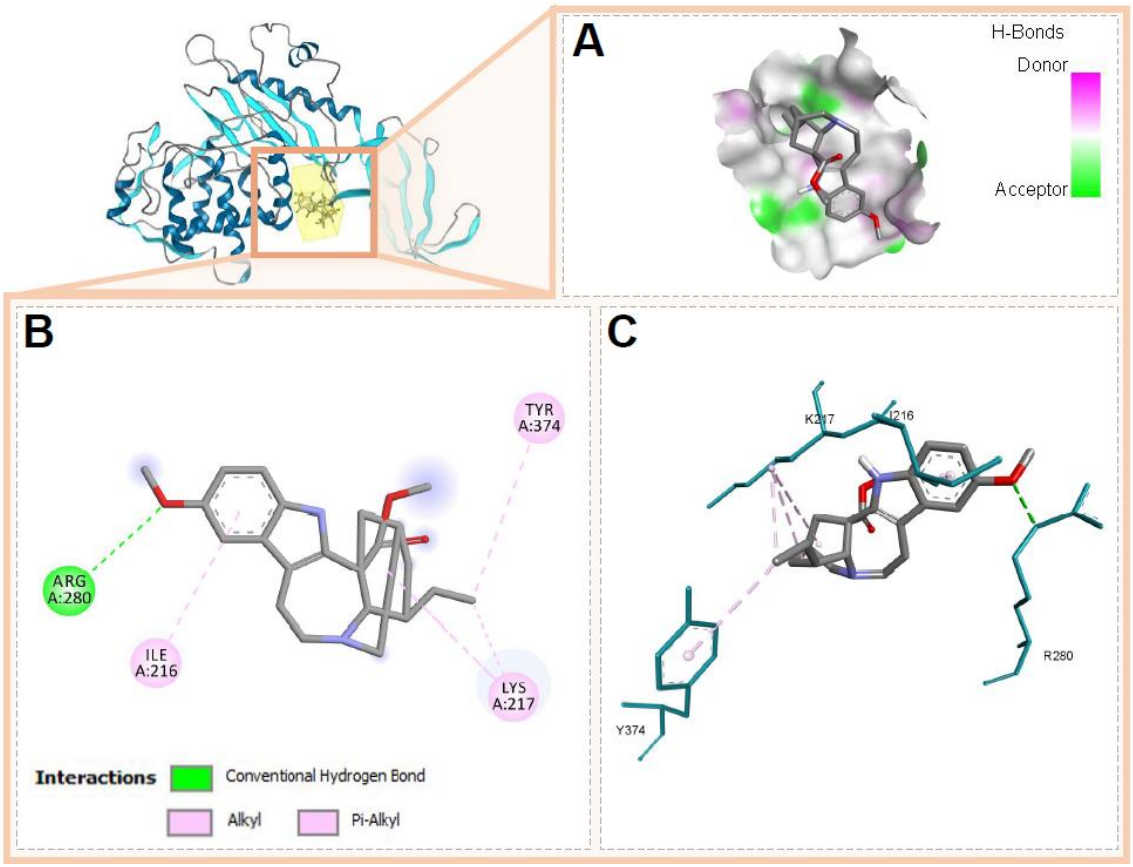

Figure S3. Molecular interactions between PBP4 from *S. aureus* and voacangine. (A) Characterization of the binding site according to the ability to form hydrogen bridges and geometry of the compound at the docking site, (B) 2D plot of the interactions specifying the type of interaction, (C) conformation of the compound during docking and interactions with PBP4 residues in 3D.

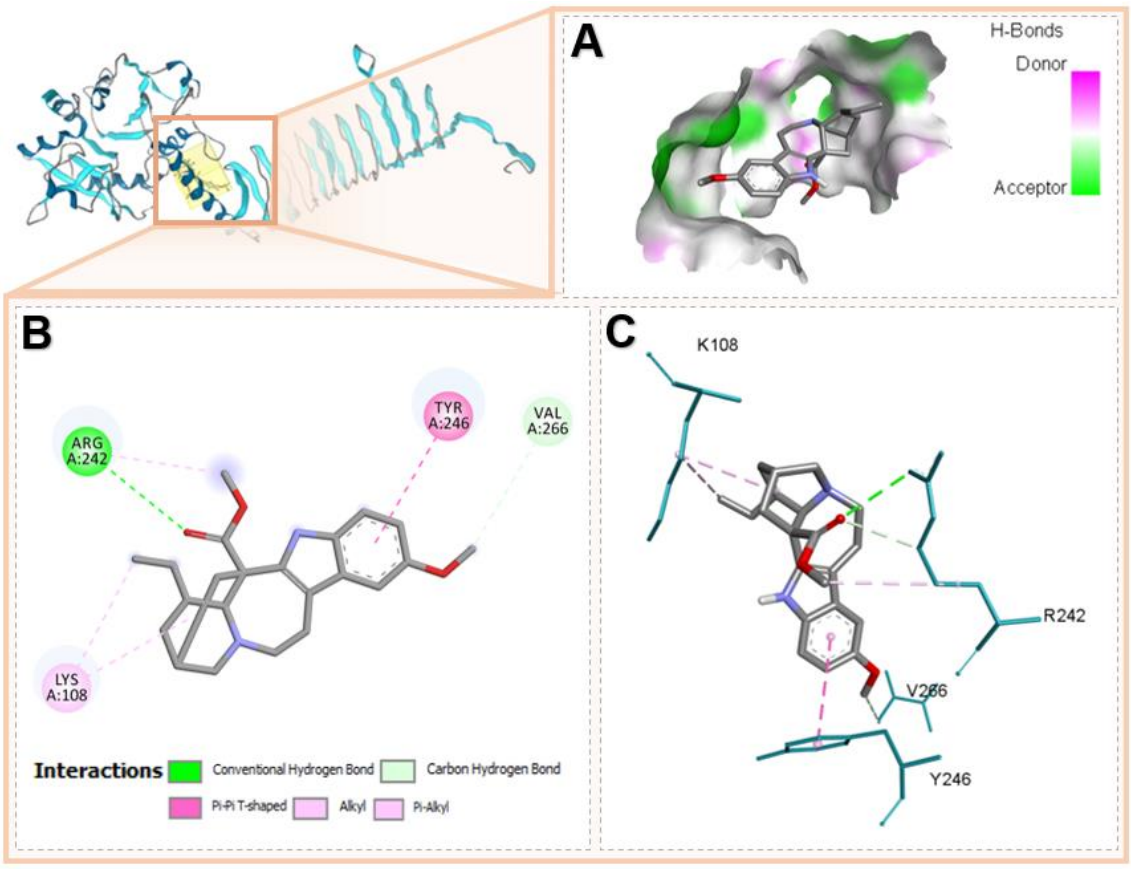

Figure S4. Molecular interactions between GlmU from *S. aureus* and voacangine. (A) Characterization of the binding site according to the ability to form hydrogen bridges and geometry of the compound at the docking site, (B) 2D plot of the interactions specifying the type of interaction, (C) conformation of the compound during docking and interactions with GlmU residues in 3D.

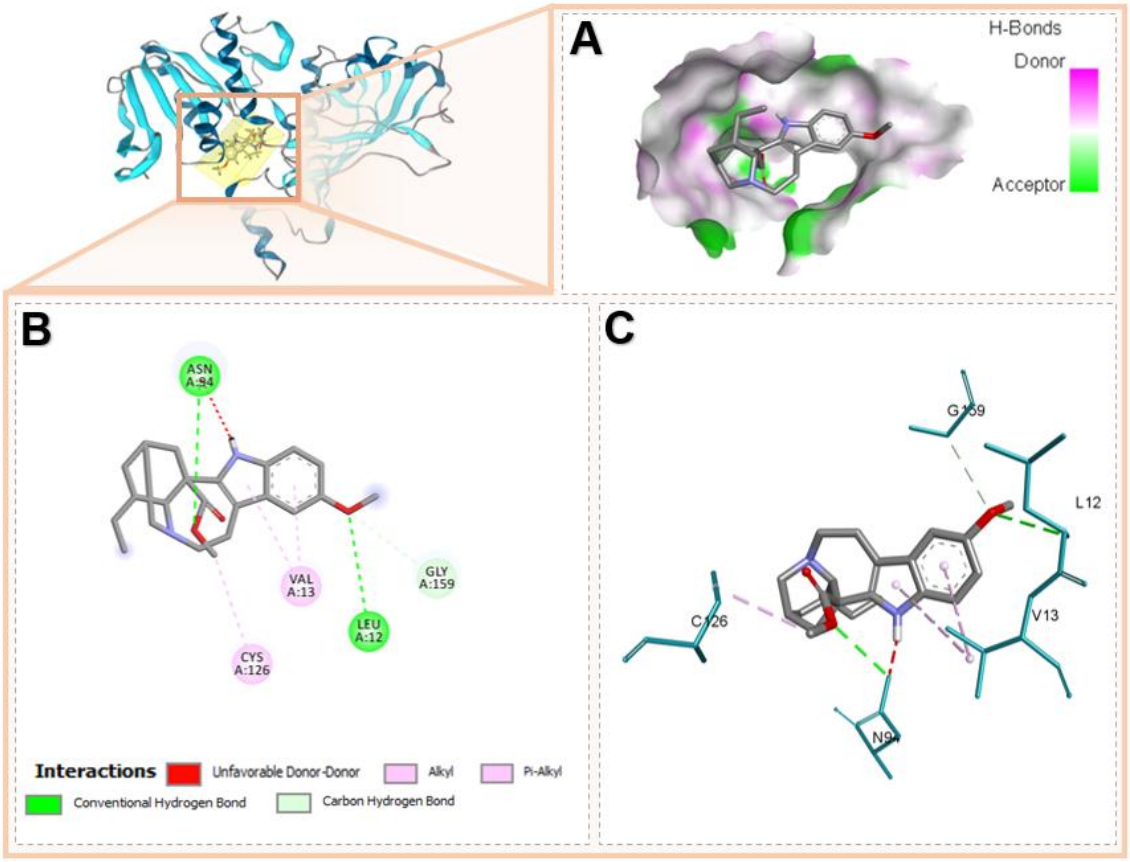

Figure S5. Molecular interactions between ASADH from *S. aureus* and voacangine. (A) Characterization of the binding site according to the ability to form hydrogen bridges and geometry of the compound at the docking site, (B) 2D plot of the interactions specifying the type of interaction, (C) conformation of the compound during docking and interactions with ASADH residues in 3D.