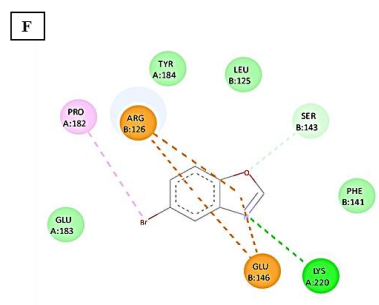
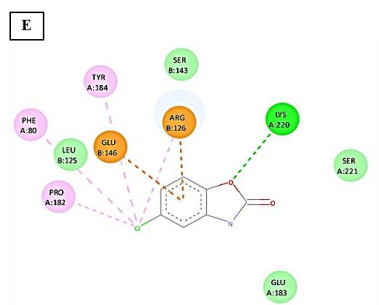
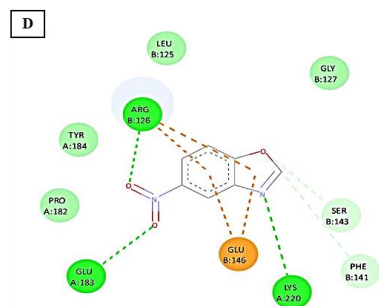
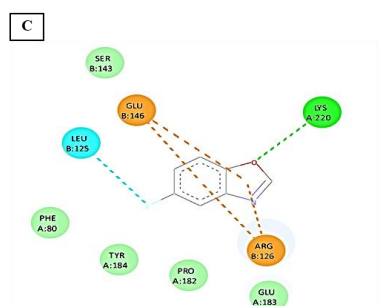
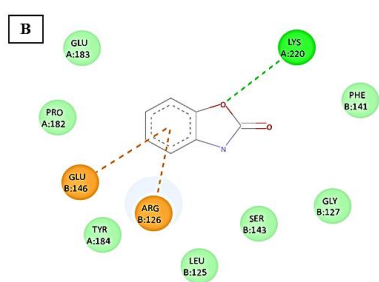
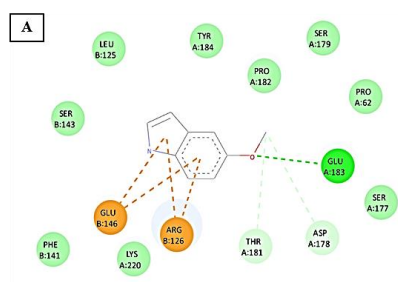



SUPPLEMENTARY MATERIAL

2D INTERACTIONS OF ALL LIGANDS AND TARGET CLOCK PROTEINS

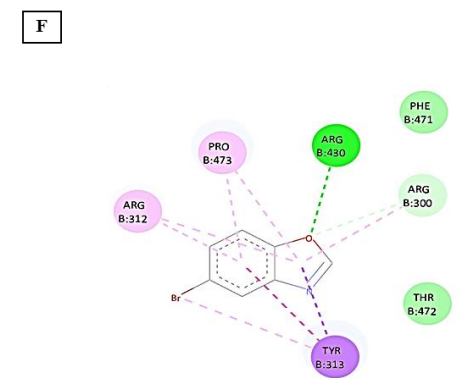
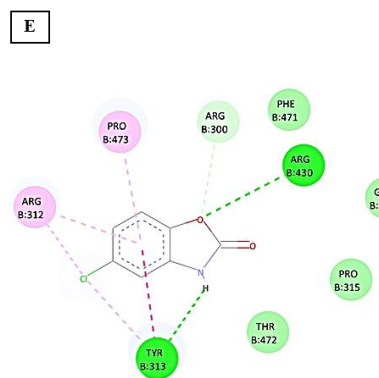
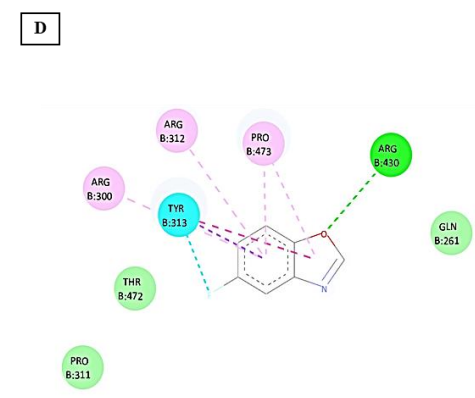
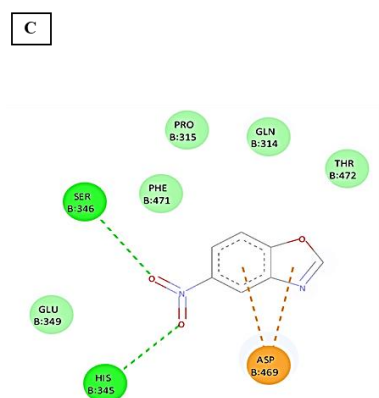
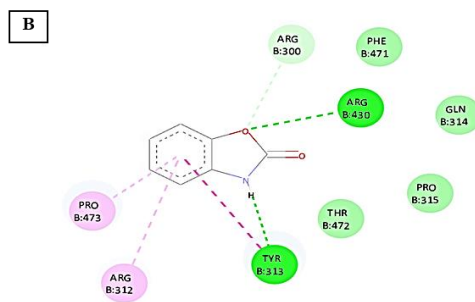
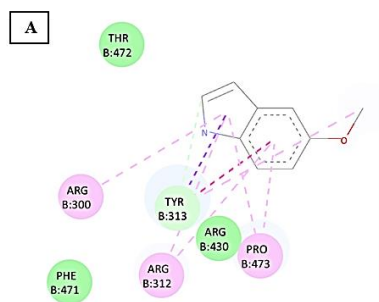
2D interactions of ligands in the active binding region of CLOCK: Bmal1 Dimer. Interacting amino acid residues of CLOCK: Bmal1 and complexes with 5-Methoxyindole (A), 2-(3H)-Benzoxazolone (B), 5-Nitro-2-Benzoxazolone (C), 5-Fluoro-2-Benzoxazolone (D), 5-Chloro-2-Benzoxazolone (E), and 5-Bromo-2-Benzoxazolone (F). The types of interactions are illustrated with different colors (Dark Green: Conventional Hydrogen Bonds, Light Green: Carbon-Hydrogen Bonds, Orange: Pi-Anion/Cation Bonds, Blue: Halogen (Fluorine), Pink: Pi-Alkyl/Alkyl).



Interactions

	van der Waals		Pi-Anion
	Conventional Hydrogen Bond		Alkyl
	Carbon Hydrogen Bond		Pi-Alkyl
	Pi-Cation		
	Halogen (Fluorine)		

2D interactions of ligands in the active binding region of Per1. Interacting amino acid residues of Per1 and complexes with 5-Methoxyindole (A), 2-(3H)-Benzoxazolone (B), 5-Nitro-2-Benzoxazolone (C), 5-Fluoro-2-Benzoxazolone (D), 5-Chloro-2-Benzoxazolone (E), and 5-Bromo-2-Benzoxazolone (F). The types of interactions are illustrated with different colors (Dark Green: Conventional Hydrogen Bonds, Light Green: Carbon-Hydrogen Bonds, Orange: Pi-Anion, Blue: Halogen (Fluorine), Purple: Pi-Sigma, Light Pink: Pi-Alkyl, Dark Pink: Pi-Pi T-shaped).

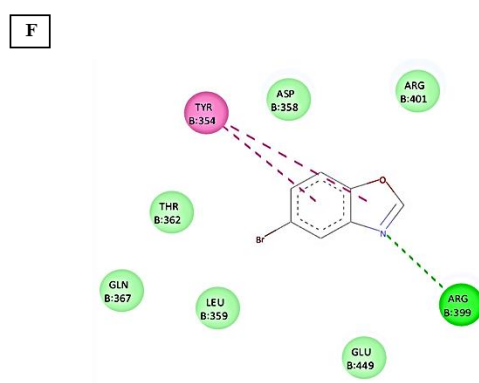
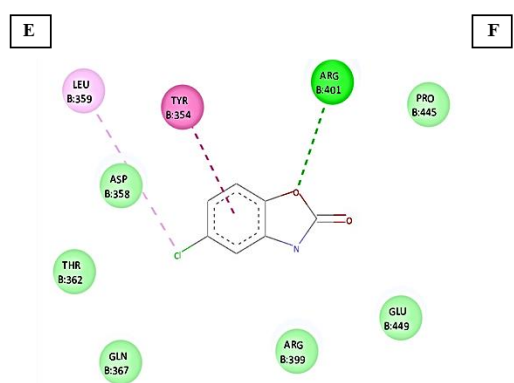
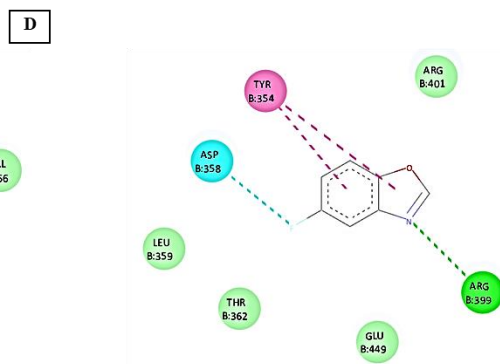
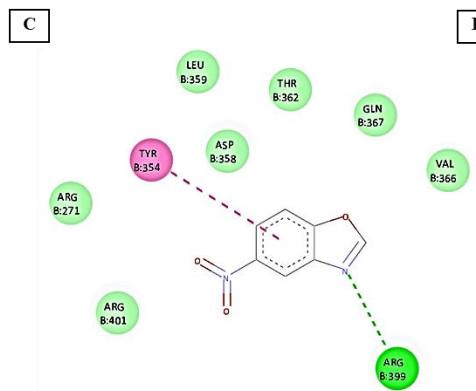
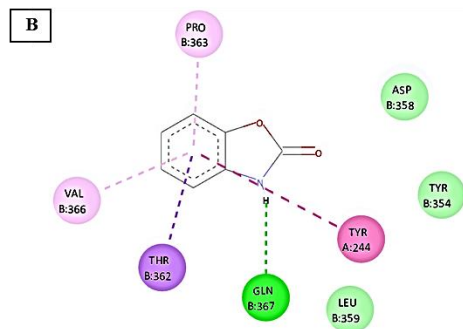
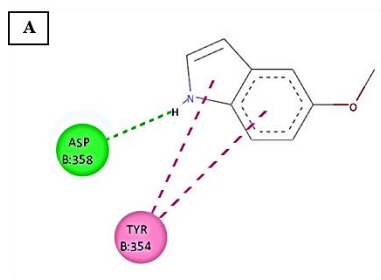


Interactions








	van der Waals
	Conventional Hydrogen Bond
	Carbon Hydrogen Bond
	Halogen (Fluorine)

	Pi-Sigma
	Pi-Pi T-shaped
	Pi-Alkyl
	Pi-Anion

2D interactions of ligands in the active binding region of Per2. Interacting amino acid residues of Per2 and complexes with 5-Methoxyindole (A), 2-(3H)-Benzoxazolone (B), 5-Nitro-2-Benzoxazolone (C), 5-Fluoro-2-Benzoxazolone (D), 5-Chloro-2-Benzoxazolone (E), and 5-Bromo-2-Benzoxazolone (F). The types of interactions are illustrated with different colors (Dark Green: Conventional Hydrogen Bonds, Light Green: Pi-Donor Hydrogen Bonds, Blue: Halogen (Fluorine), Purple: Pi-Sigma, Light Pink: Pi-Alkyl, Dark Pink: Pi-Pi T-shaped).



Interactions

	van der Waals		Pi-Sigma
	Conventional Hydrogen Bond		Pi-Alkyl
	Pi-Donor Hydrogen Bond		
	Halogen (Fluorine)		
	Pi-Pi T-shaped		

2D interactions of ligands in the active binding region of Cry2. Interacting amino acid residues of Cry2 and complexes with 5-Methoxyindole (A), 2-(3H)-Benzoxazolone (B), 5-Nitro-2-Benzoxazolone (C), 5-Fluoro-2-Benzoxazolone (D), 5-Chloro-2-Benzoxazolone (E), and 5-Bromo-2-Benzoxazolone (F). The types of interactions are illustrated with different colors (Dark Green: Conventional Hydrogen Bonds, Light Green: Carbon-Hydrogen Bonds, Orange: Pi-Sulfur, Pink: Pi-Alkyl, Purple: Pi-Sigma).

