

## **Supplementary Materials**

**Novel Insights into the Antibacterial, Antifungal, and Antibiofilm Activity of Pyrroloquinoline quinone (PQQ); *in vitro*, *in silico* and Shotgun Proteomic Studies**

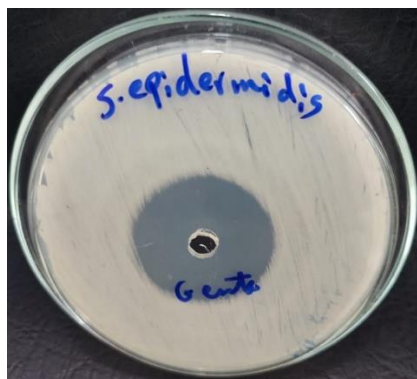


(A)

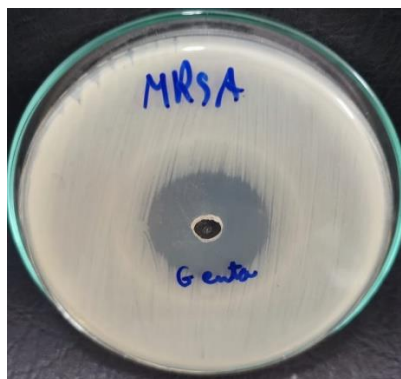


(B)

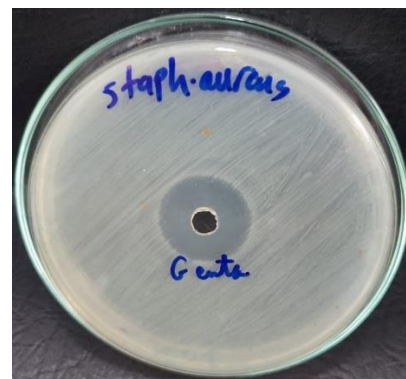
**Figure S1.** (A-B) Growth inhibition zones of *Penicillium marneffei* (A) and *Trichophyton rubrum* (B) after treatment with Ketoconazole.



(A)

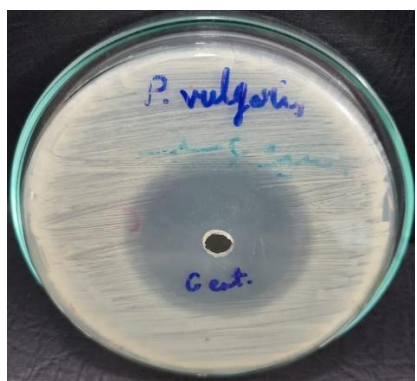


(B)

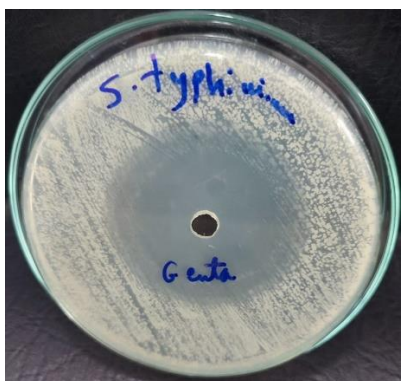


(C)

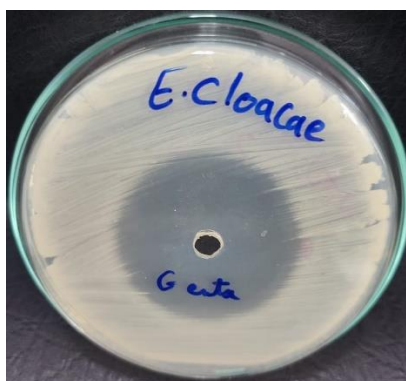
**Figure S2.** (A-C) Growth inhibition zones of *Staphylococcus epidermidis* (A), Methicillin-Resistant *Staphylococcus aureus* (MRSA) (B), and *Staphylococcus aureus* (C) after treatment with Gentamycin.



(A)

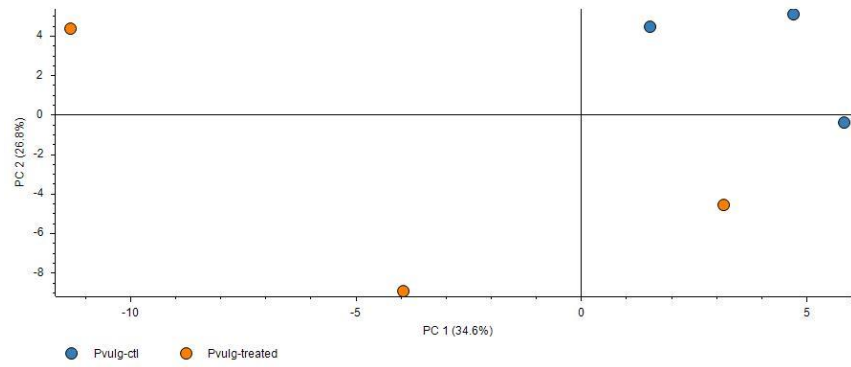


(B)

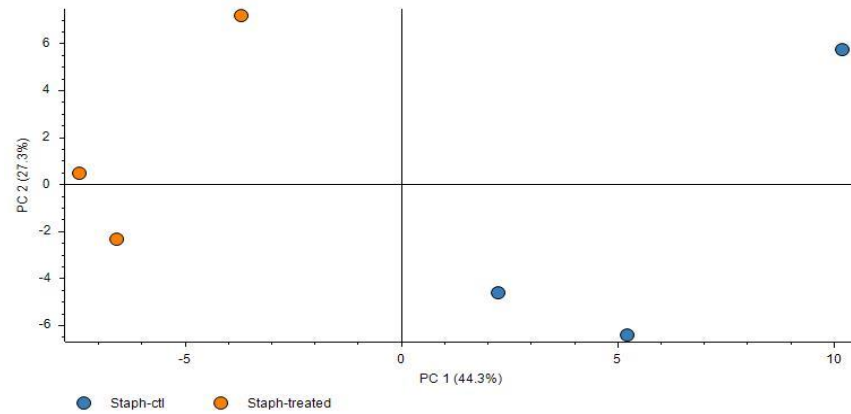


(C)

**Figure S3.** (A-C) Growth inhibition zones of *Proteus vulgaris* (A), *Salmonella typhimurium* (B), and *Enterobacter cloacae* (C) after treatment with Gentamycin.

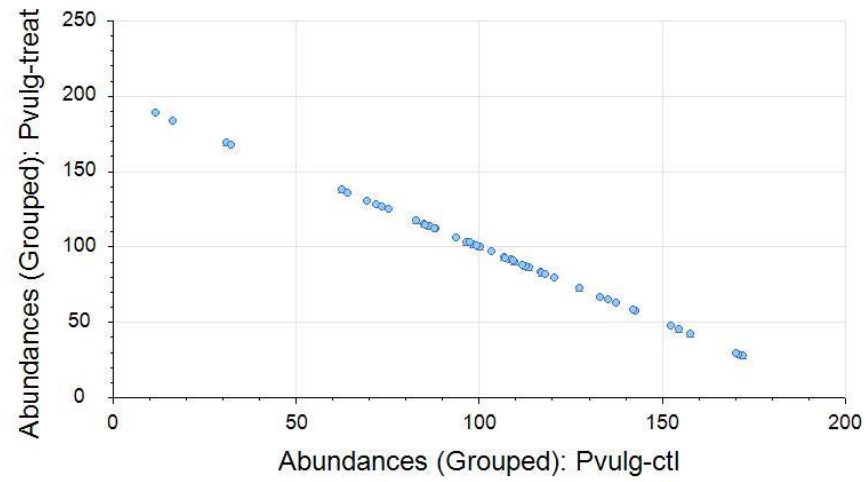


(A)

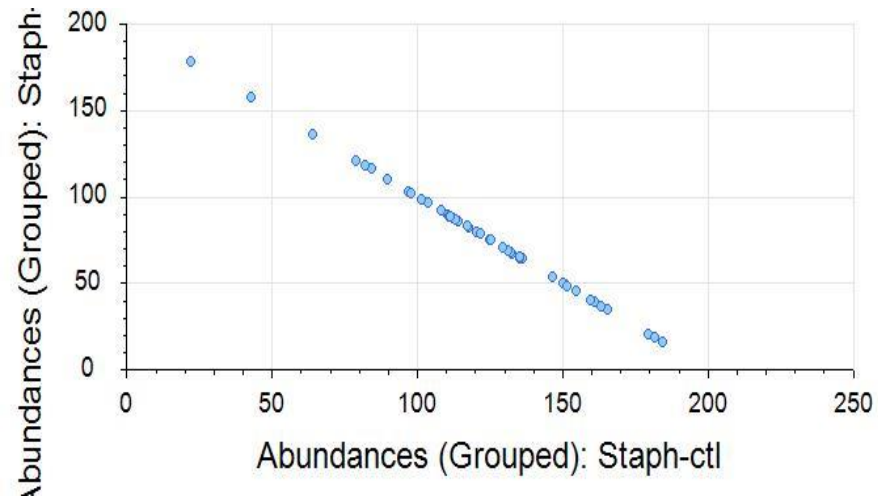


(B)

**Figure S4:** Principal component analysis (PCA) between treated and control groups for *Proteus vulgaris* (A) and *Staphylococcus epidermidis* (B).

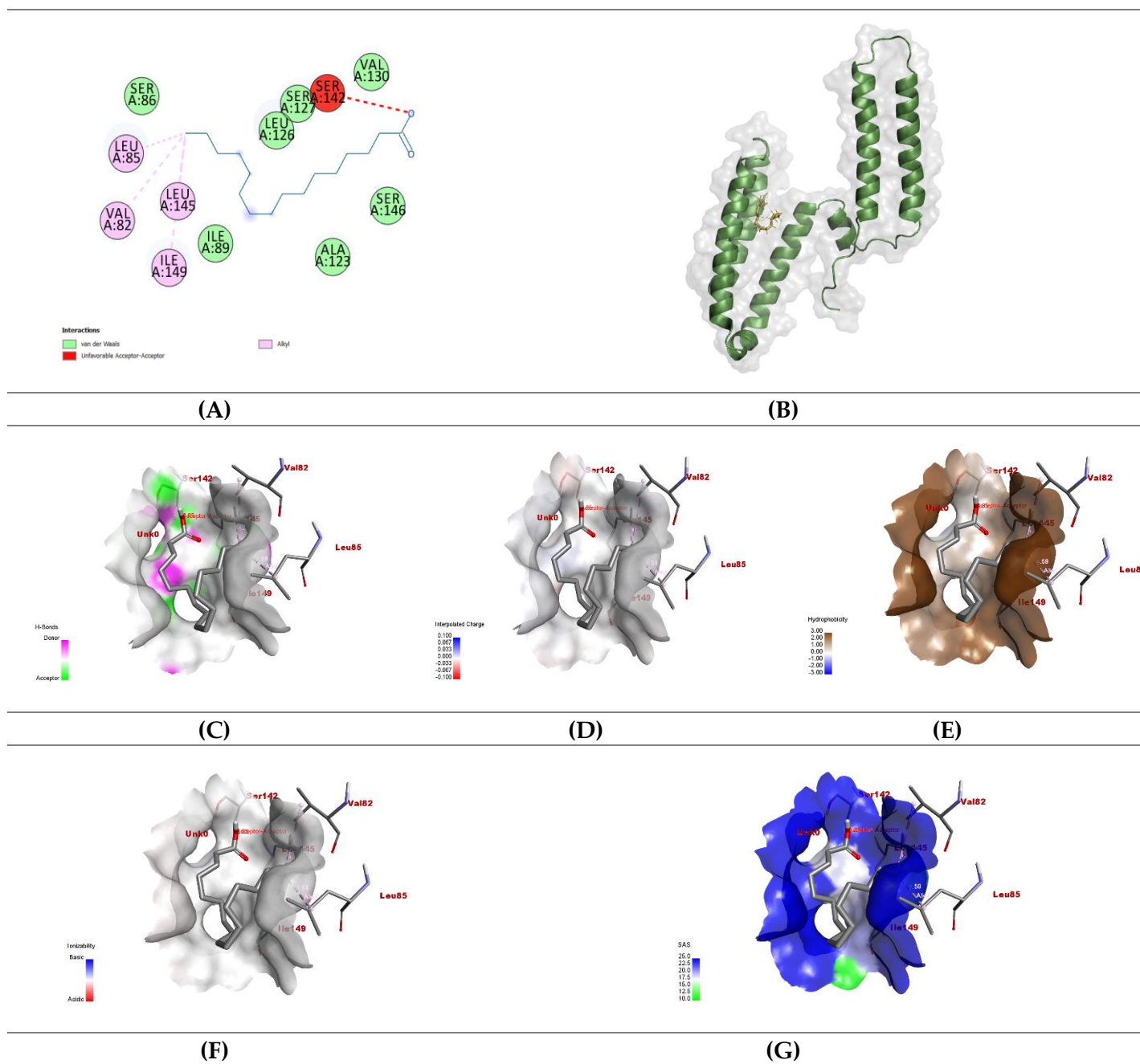


(A)

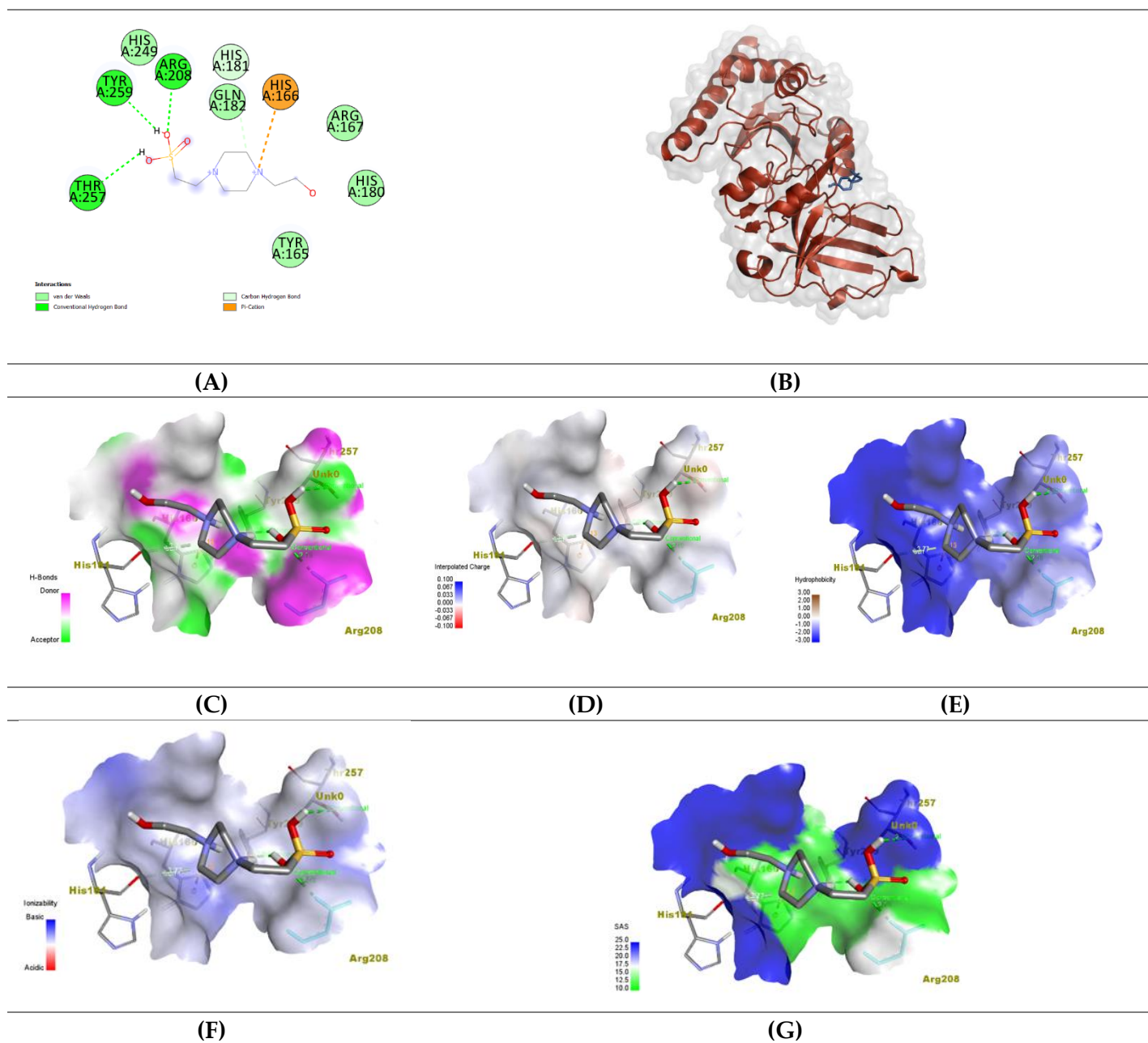


(B)

**Figure S5:** Scatter plot showing the correlation of the protein abundances between the treated and control groups in *Proteus vulgaris* (A) and *Staphylococcus epidermidis* (B).

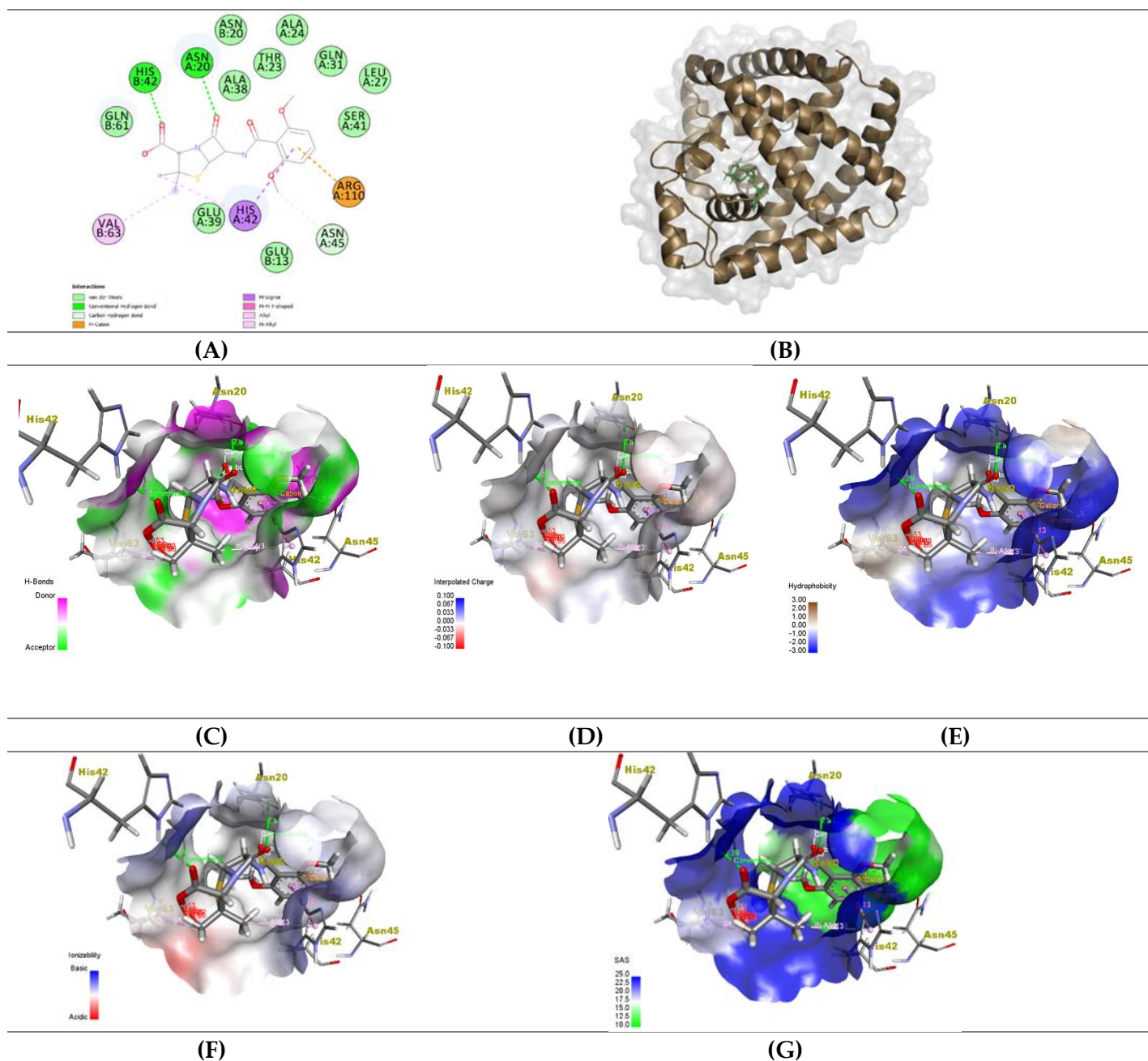


**Figure S6.** (A) 2D chemical interaction of palmitic acid with the ligand binding domain of the Mp1p receptor. (B) The ribbon demonstrates the palmitic acid and Mp1p receptor docked complex (binding energy -4.9 kmol/cal). (C) Surface view showing the hydrogen bond interaction. (D) Interpolated charges. (E) Hydrophobicity. (F) Ionizability. (G) SAS interactions of the docked complex.

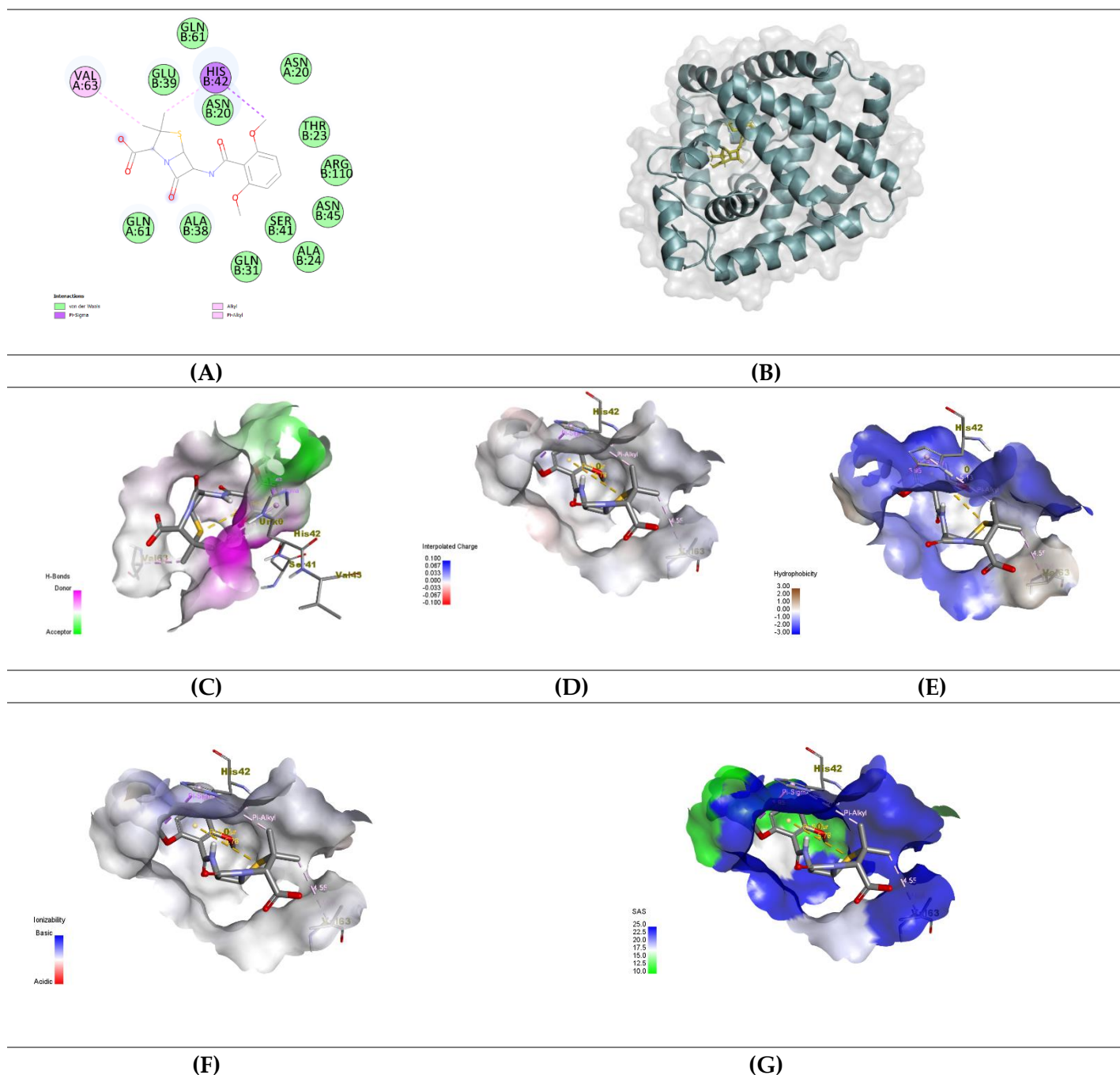


**Figure S7.** (A) 2D chemical interaction of the endonuclease with EPE. (B) The ribbon demonstrates the endonuclease with EPE docked complex (binding energy -5.2 kcal/mol). (C) Surface view showing the hydrogen bond interaction. (D) Interpolated charges. (E) Hydrophobicity. (F) Ionizability. (G) SAS interactions of the docked complex.





**Figure S8.** (A) 2D diagram showed the chemical interactions between TcaR (chain A) and methicillin. (B) The ribbon demonstrates the TcaR (chain A) and methicillin docked complex (binding energy -7.5 kcal/mol). (C) Surface view showed the hydrogen bond interaction. (D) Interpolated charges. (E) Hydrophobicity. (F) Ionizability. (G) SAS interactions of the docked complex.



**Figure S9.** (A) 2D diagram showing the chemical interactions between chain B of TcaR and methicillin. (B) The ribbon demonstrates the chain B of TcaR and methicillin docked complex (binding energy -7.6 kJ/mol). (C) Surface view showing the hydrogen bond interaction. (D) Interpolated charges. (E) Hydrophobicity. (F) Ionizability. (G) SAS interactions of the docked complex.



**Table S1:** The antifungal activity of the ketoconazole as minimum inhibitory concentration (MIC) in µg/mL toward the examined fungal strains using the diffusion agar technique.

Fungal strain	Ketoconazole	
	MIC	MFC
<i>Syncephalastrum racemosum</i> RCMB 016001 (1)	0.05	Cidal
<i>Penicillium marneffeii</i> (RCMB 001022)	0.35	Cidal
<i>Candida lipolytica</i> RCMB 005007(1)	2	Cidal
<i>Trichophyton rubrum</i> (RCMB 025002)	1	Cidal

**Table S2:** The antibacterial activity of the gentamycin as minimum inhibitory concentration (MIC) in µg/mL toward the examined bacterial strains using the diffusion agar technique.

Bacterial strain	Gentamycin	
	MIC	MBC
<i>Staphylococcus aureus</i> ATCC 25923	1	Cidal
<i>Staphylococcus epidermidis</i> RCMB 009 (2)	0.8	Cidal
<i>Micrococcus sp.</i> RCMB 028 (1)	1.5	Cidal
<i>Methicillin-Resistant Staphylococcus aureus</i> (MRSA) ATCC 4330	4	Cidal
<i>Enterobacter cloacae</i> RCMB 001 (1) ATCC 23355	60	Cidal
<i>Salmonella typhimurium</i> RCMB 006 (1) ATCC 14028	0.5	Cidal
<i>Proteus vulgaris</i> RCMB 004 (1) ATCC 13315	3	Cidal
<i>Serratia marcescens</i> 007001	2	Cidal