

Characterization of *Streptomyces* Species and Validation of Antimicrobial Activity of Their Metabolites Through Molecular Docking

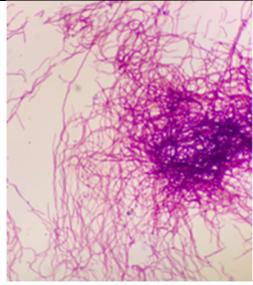
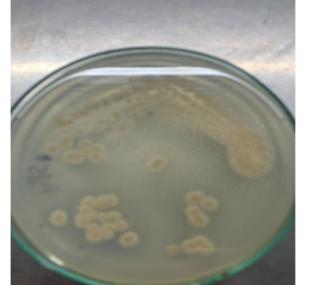
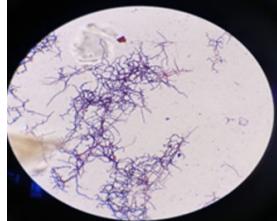
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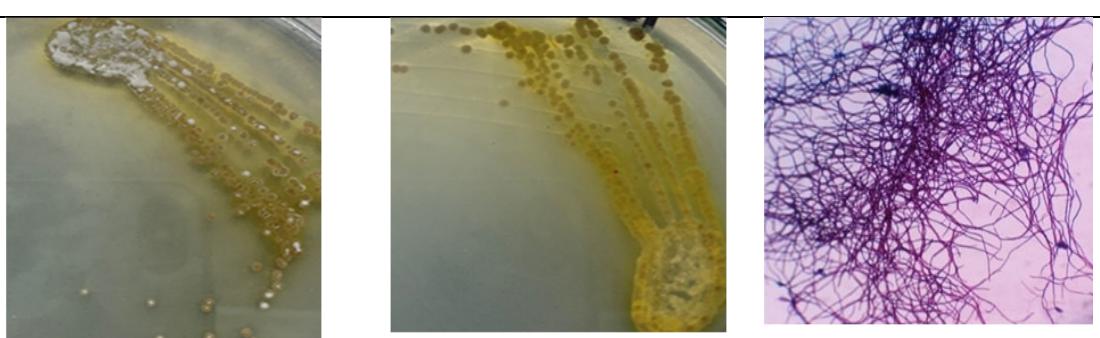
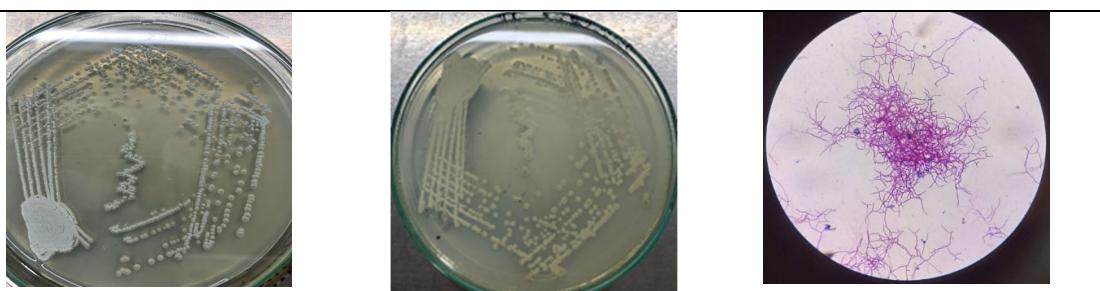
Table S1: Soil profile, total isolated actinomycetes and characterization method

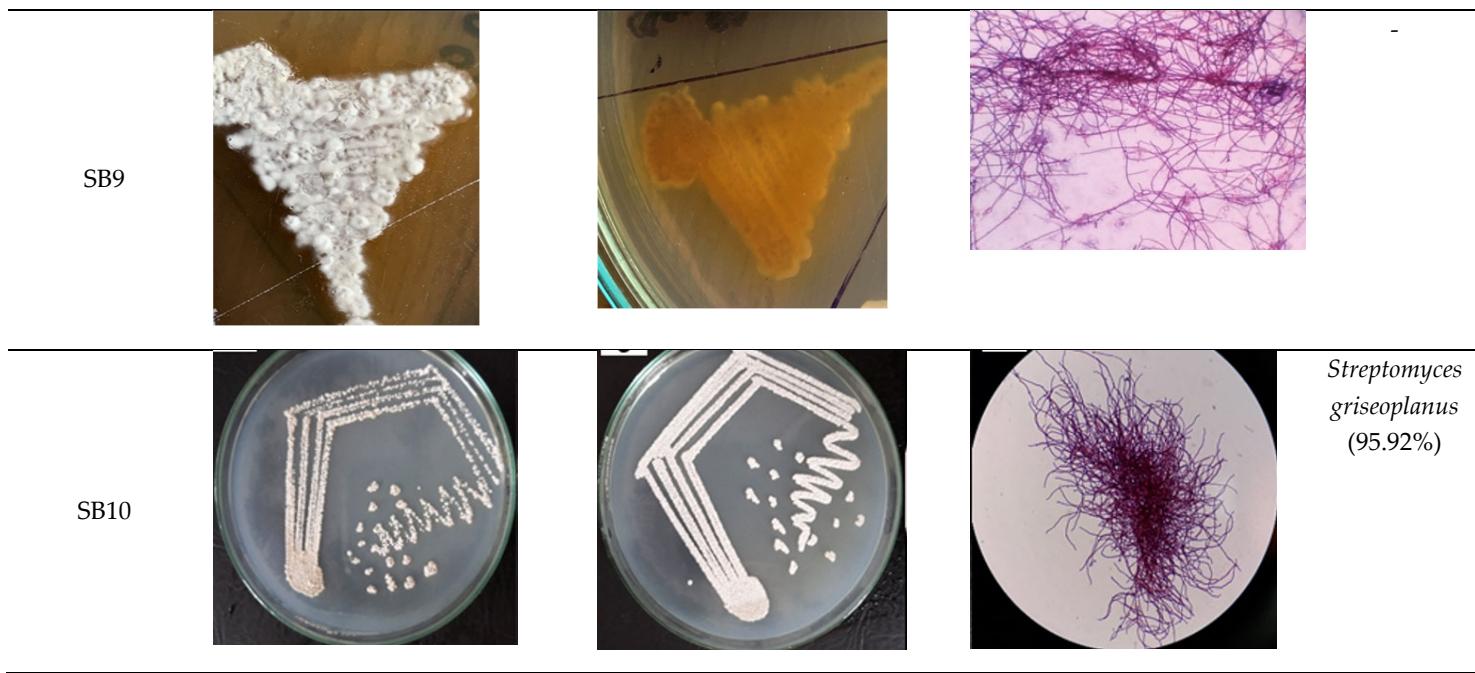
Sample	Soil Profile	Total actinomycetes colonies isolated	Characterization method of isolated strains	Colonies showing antimicrobial activities
SB1	Bare land	3	Culture mycelium, gram staining, and 16S rRNA sequencing	1
SB2	Forest	1	Culture mycelium and gram staining	0
SB3	Forest	3	Culture mycelium, gram staining, and 16S rRNA sequencing	1
SB4	Agriculture land	1	Culture mycelium and gram staining	0
SB5	Forest	0	Culture mycelium and gram staining	0
SB6	Rhizosphere	1	Culture mycelium and gram staining	0
SB7	Hot spring	1	Culture mycelium and gram staining	0
SB8	Rhizosphere	1	Culture mycelium and gram staining	0
SB9	Forest	1	Culture mycelium and gram staining	0
SB10	Bare land	5	Culture mycelium, gram staining, and 16S rRNA sequencing	1

Summary: Total actinomycetes colonies isolated from 10 samples = 17

Table S2: Culture characteristic and gram staining of samples SB1-SB10

Sample	Aerial Mycelium	Substrate Mycelium	Gram staining	#16S rRNA gene Blast search showing highest similarity to
SB1				<i>Streptomyces bungoensis</i> (84.31%)
SB2				
SB3				<i>Streptomyces aureus</i> (95.79%)





**16S rRNA sequencing (partial) is done for those isolates showing greater antimicrobial activities.*

Table S3: Biochemical test of microbial strains

Sample/ Tests	SB1	SB3	SB10
Lipase	+ve	-ve	-ve
Gelatin	+ve	-ve	-ve
Amylase	+ve	-ve	-ve
Nitrate reduction	+ve	-ve	-ve
Sulfur test	+ve	-ve	-ve
Indole	+ve	+ve	-ve
Motility	-ve	-ve	-ve
Urease	-ve	-ve	+ve
Catalase	-ve	-ve	-ve
MR	-ve	-ve	-ve
VP	-ve	-ve	-ve

-ve: represents a negative result, +ve: represents a positive result

Table S4: Cultural and physiological characteristics of microbial strains

Characteristics		Microbial Strains		
		SB1	SB3	SB10
pH tolerance:	5	++	+	++
	7	+++	+++	++
	9	+++	+++	+
	11	+++	+++	+
NaCl tolerance:	1%	+++	+++	+++
	3%	+++	+	+
	5%	+	-	+
	7%	-	-	-
Growth on:	ISP1	+++	+++	+++
	ISP2	++	++	++
	ISP3	+++	++	++
	ISP4	+++	+++	+++
	ISP5	+++	+++	+++

3+, 2+, +, and – represents strong growth, moderate growth, poor growth, and no growth respectively

Table S5: The binding energies of target proteins with potent compounds

Target proteins (PDB ID)	N6,N6-Dimethyladenosine	Cyclo(L-		Albumycin	Cyclo(D-		Cyclo(L-	
		Leu-L-	Pro)		Ala-L-	Pro)	Tyr-L-	Leu)
1J1J	-8.1		-7.6	-7.5	-6.8	-7.8		
6J33	-6.9		-5.8	-6.2	-5.4	-7.7		
3TTZ	-6.2		-6.5	-6.3	-5.6	-7.1		
3SRW	-7.7		-7.1	-6.8	-6.4	-7.8		
4UMW	-4.9		-6.6	-4.4	-5.3	-6.5		
3UDI	-6.7		-5.9	-5.7	-5.2	-7.3		
7KRK	-6.0		-5.6	-5.7	-4.9	-6.5		

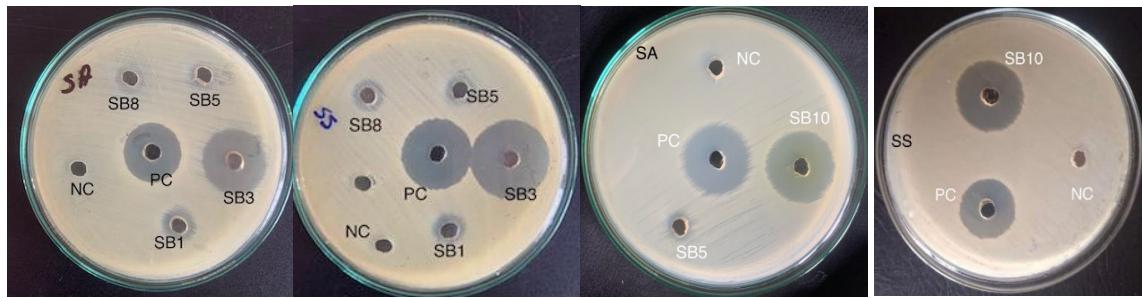


Figure S1: Zone of inhibition exhibited by SB1, SB3, and SB10 against *S. aureus* and *S. sonnei*.

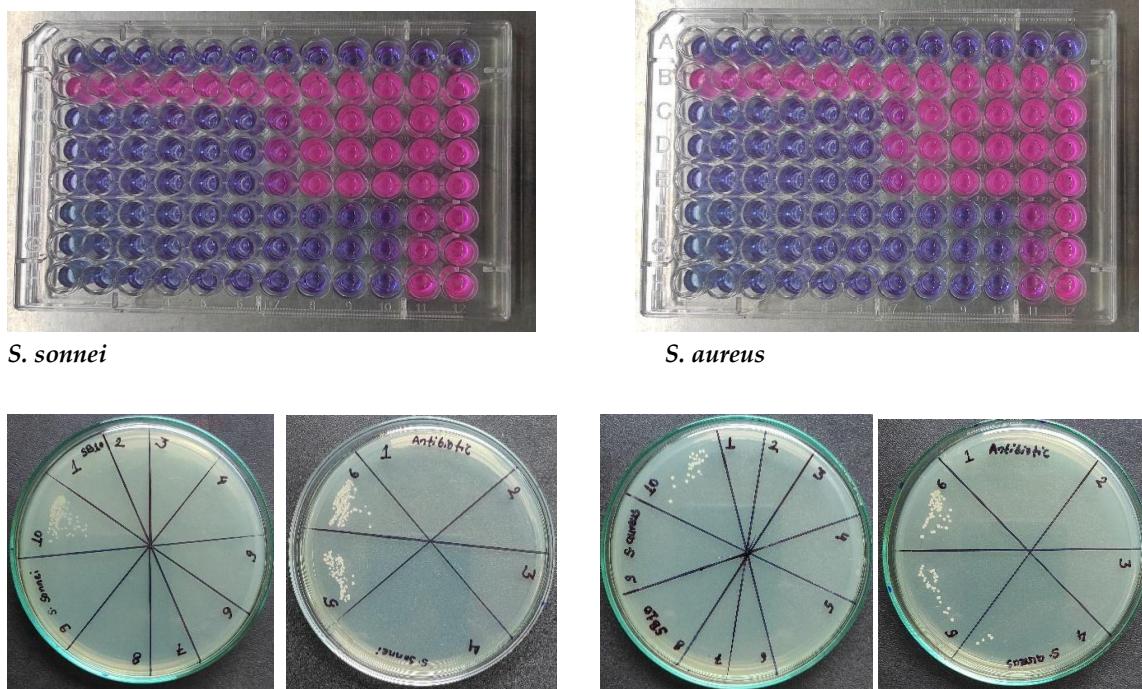


Figure S2: Determination of MICs and MBCs of the extract SB10 against *S. sonnei* and *S. aureus*

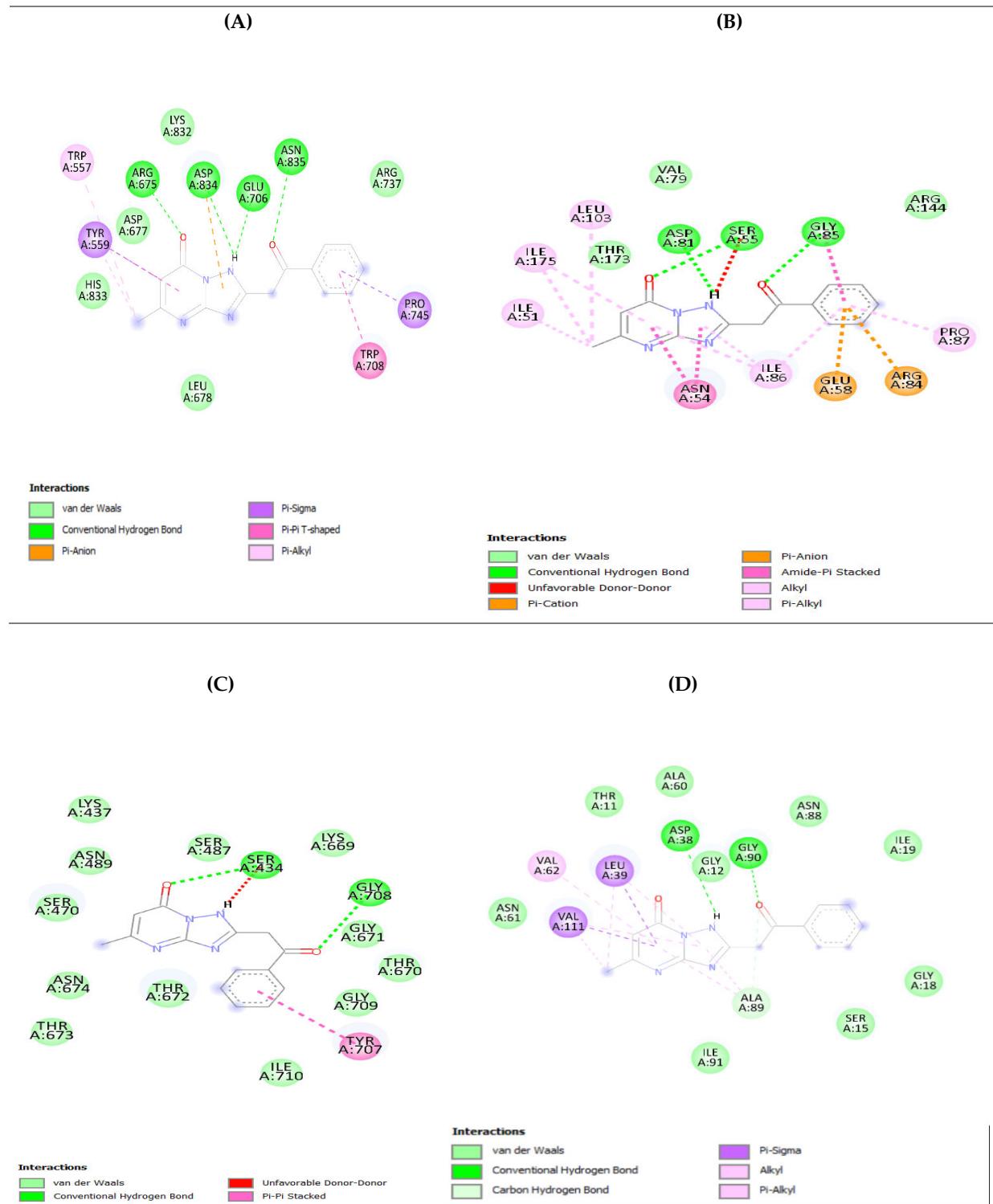


Figure S3: (A), (B), (C), and (D) represent 2D structures of essramycin with target proteins: PulA from *Klebsiella pneumonia* (6J33), Topoisomerase ATPase inhibitor (3TTZ), *A. baumannii* PBP1a (3UDI), and Putative FabG from *A. baumannii* (7KRK) respectively.

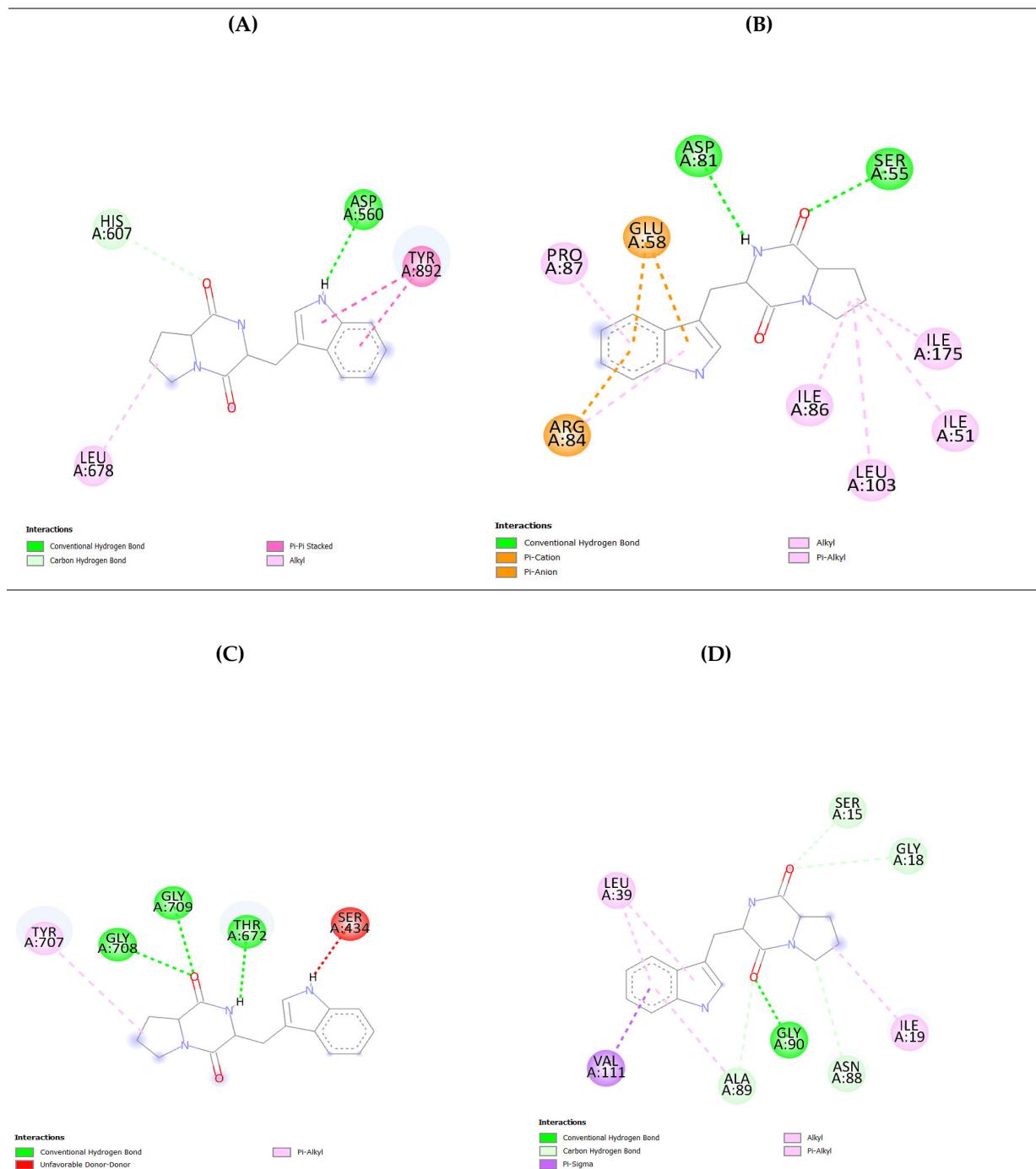
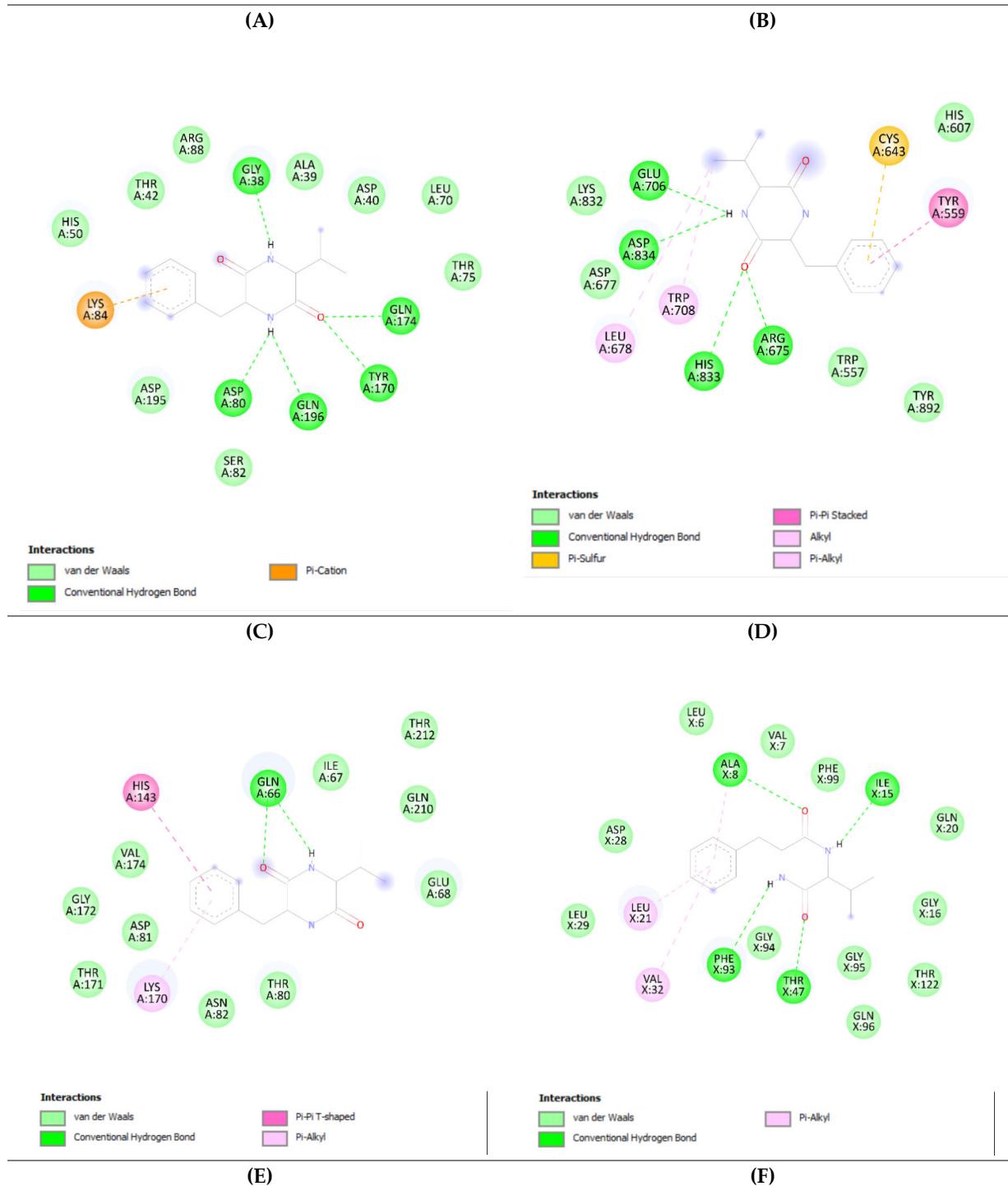


Figure S4: (A), (B), (C), and (D) represent 2D structures of brevianamide F with target proteins: PulA from *Klebsiella pneumoniae* (6J33), Topoisomerase ATPase inhibitor (3TTZ), *A. baumannii* PBP1a (3UDI), and Putative FabG from *A. baumannii* (7KRK) respectively.



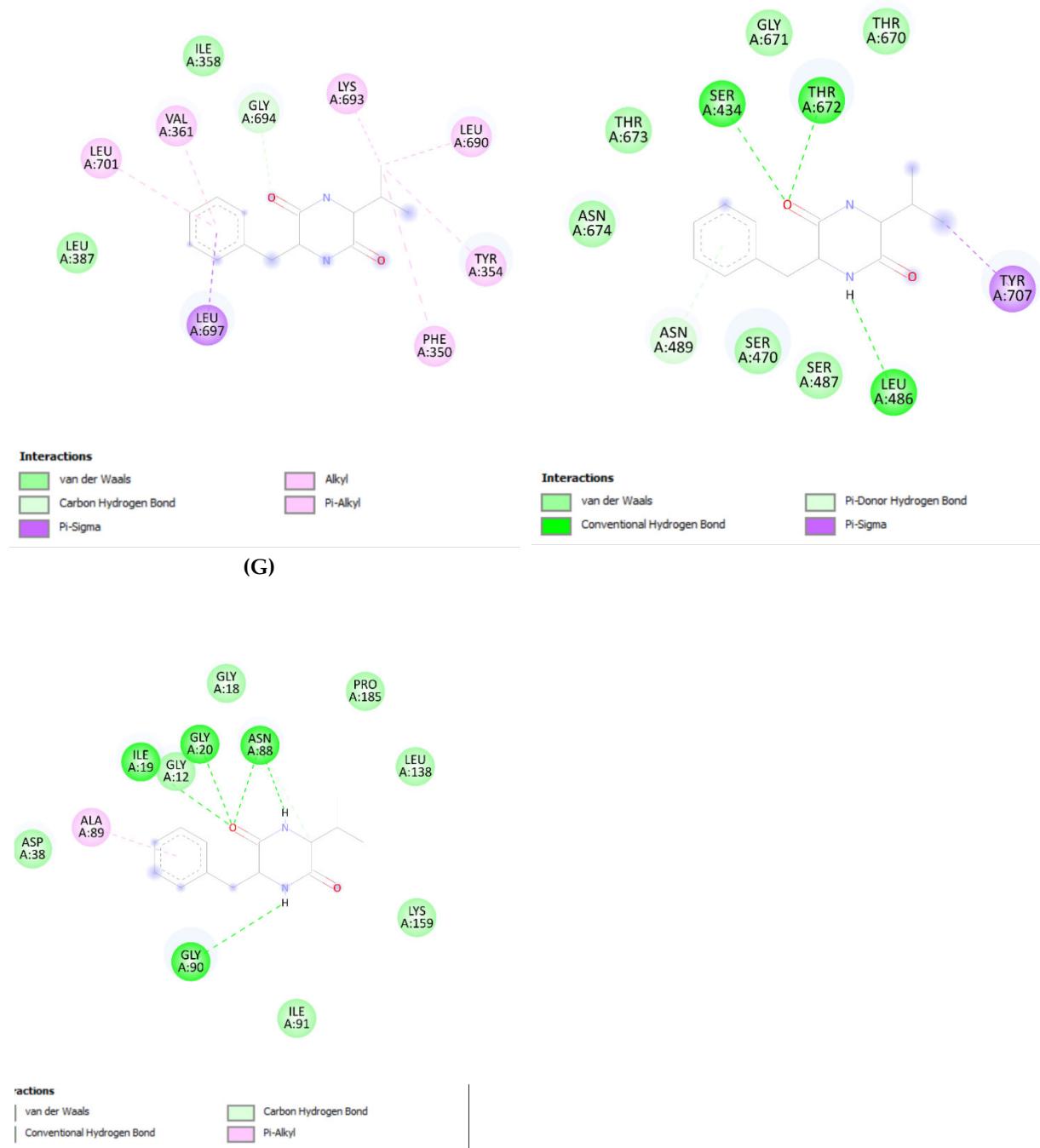
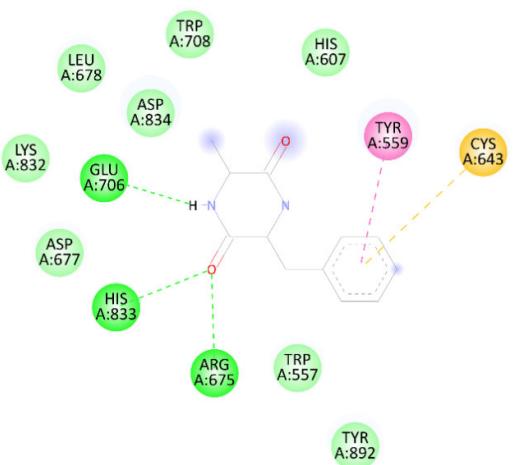
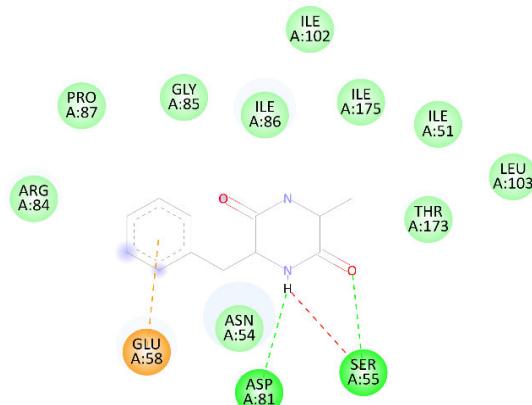


Figure S5: (A), (B), (C), (D), (E), (F), and (G) represents 2D structures of cyclo(L-Val-L-Phe) with target proteins: *S. aureus* TyrRS (1JJ1), PulA from *Klebsiella pneumonia* (6J33), Topoisomerase ATPase inhibitor (3TTZ), *S. aureus* Dihydrofolate Reductase (3SRW), Zinc transporting PIB-type ATPase in E2.PI state (4UMW), *A. baumannii* PBP1a (3UDI), and Putative FabG from *A. baumannii* (7KRK), respectively.

(A)



(B)

**Interactions**

- [Green] van der Waals
- [Green] Conventional Hydrogen Bond

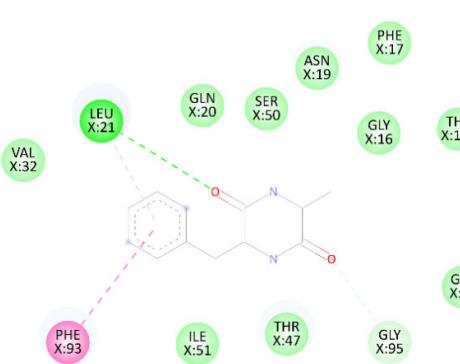
- [Yellow] Pi-Sulfur
- [Pink] Pi-Pi Stacked

Interactions

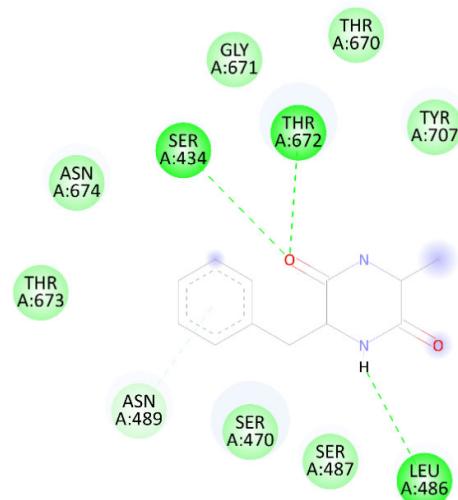
- [Green] van der Waals
- [Green] Conventional Hydrogen Bond

- [Red] Unfavorable Donor-Donor
- [Orange] Pi-Anion

(C)



(D)

**Interactions**

- [Green] van der Waals
- [Green] Conventional Hydrogen Bond
- [Light Blue] Carbon Hydrogen Bond

- [Pink] Pi-Pi Stacked
- [Light Blue] Pi-Alkyl

- [Green] van der Waals
- [Green] Conventional Hydrogen Bond

- [Light Blue] Pi-Donor Hydrogen Bond

(E)

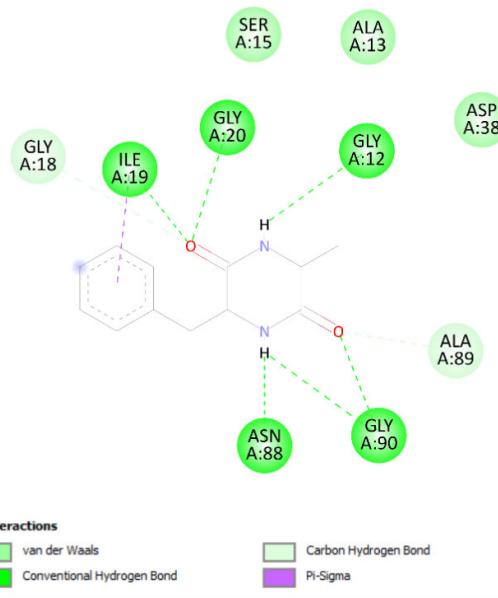


Figure S6: (A), (B), (C), (D), and (E) represent 2D structures of cyclo(L-Phe-L-Ala) with target proteins: PulA from Klebsiella pneumonia (6J33), Topoisomerase ATPase inhibitor (3TTZ), *S.aureus* Dihydrofolate Reductase (3SRW), *A. baumannii* PBP1a (3UDI), and Putative FabG from *A. baumannii* (7KRK), respectively.