Electronic Supplementary Material (ESI) for Molecular BioSystems.

Structural Elucidation of SrtA enzyme in *Enterococcus faecalis: An Emphasis on* Screening of Potential Inhibitors against the Biofilm Formation

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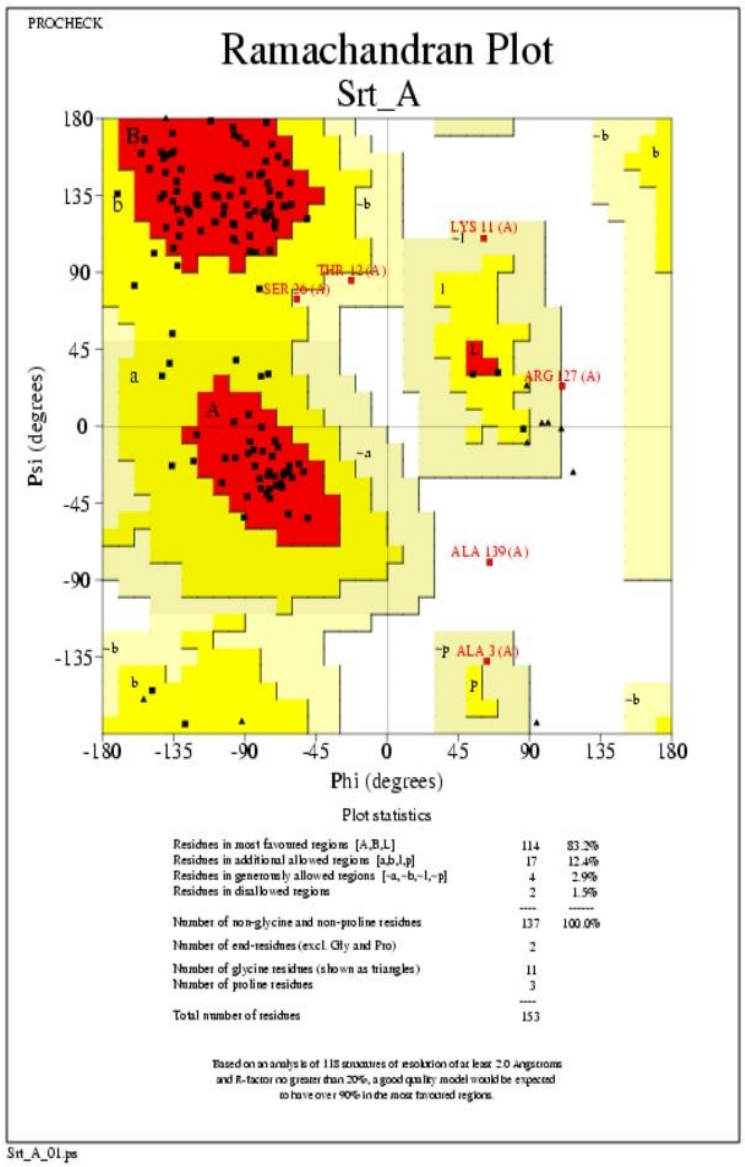

Figure S1. Ramachandran plot values of Modeled SrtA structure

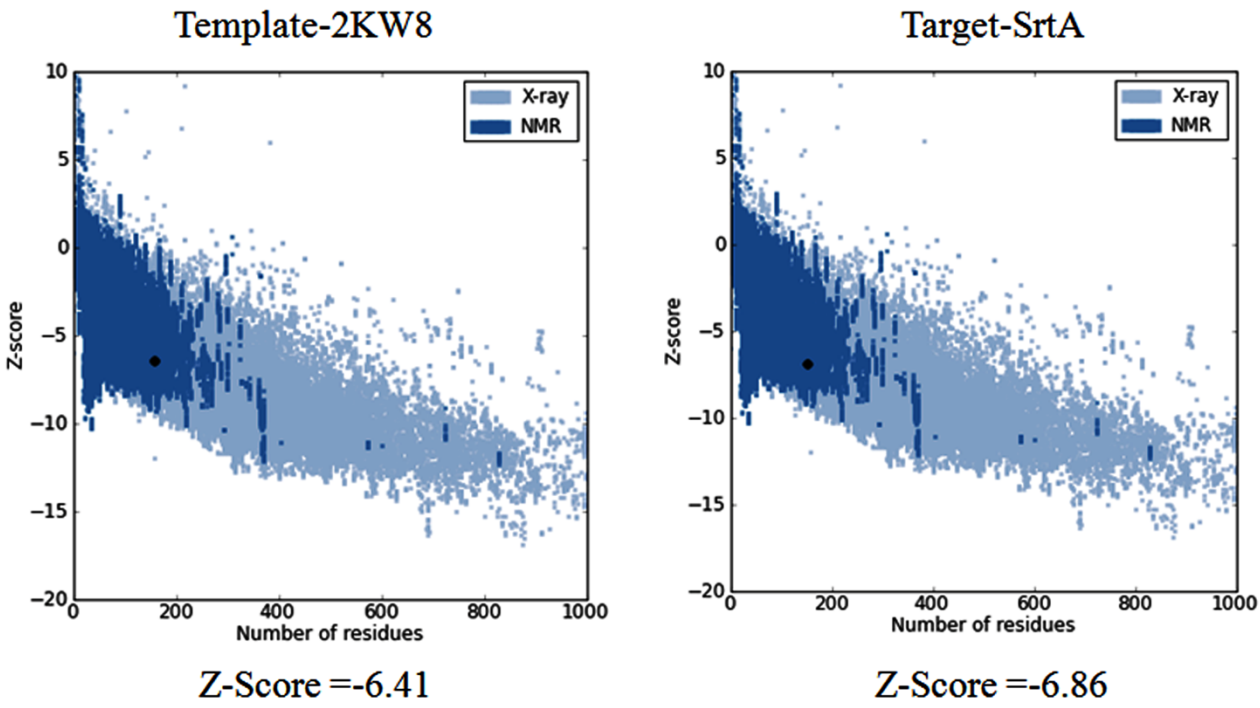

Figure S2. This plot that contained the Z score of ProSA analysis indicated that the overall interaction energy of the model was -6.86kcal/mol and template was -6.41 kcal/mol

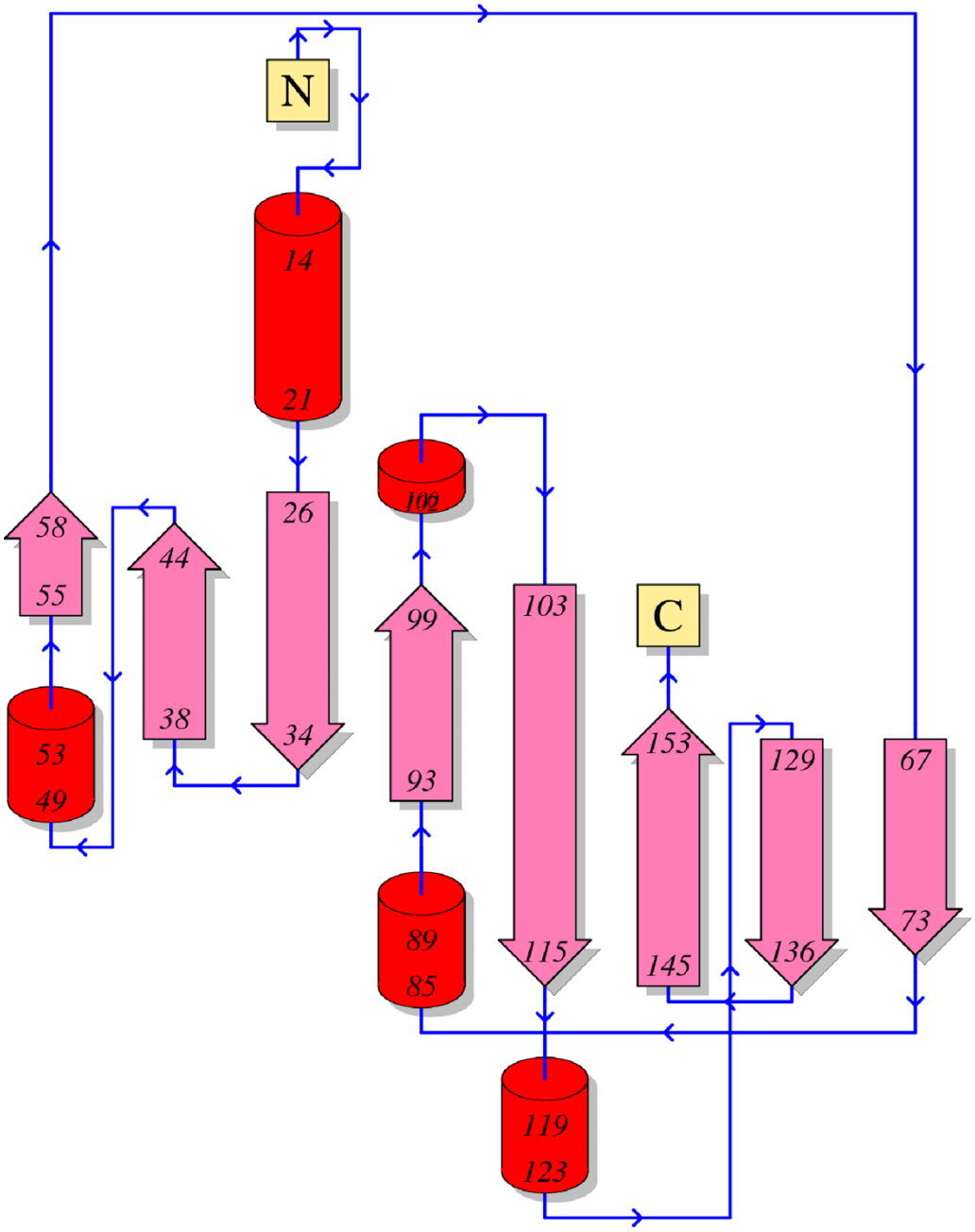

Figure S3. Protein topology of SrtA, which clearly explains the protein alignments from N-terminal to C-terminal

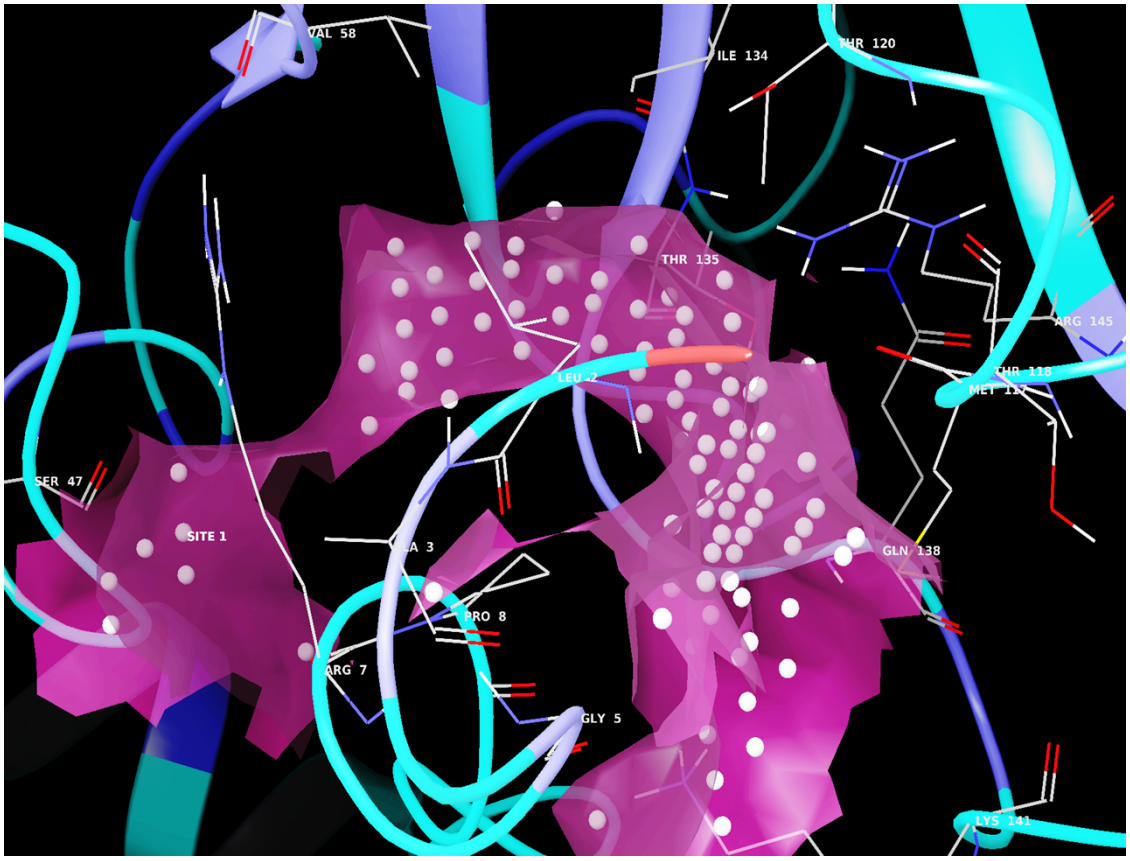

Figure S4: Predicted active site pocket in SrtA structure of *E. faecalis* showing the predicted active site residues of Ser1, Leu2, Ala3, Gln5, Arg7, Pro8, Asp46, Ser47, MET117, THR118, THR120, Ile134, THR135, GLN138, lys141, and ARG145

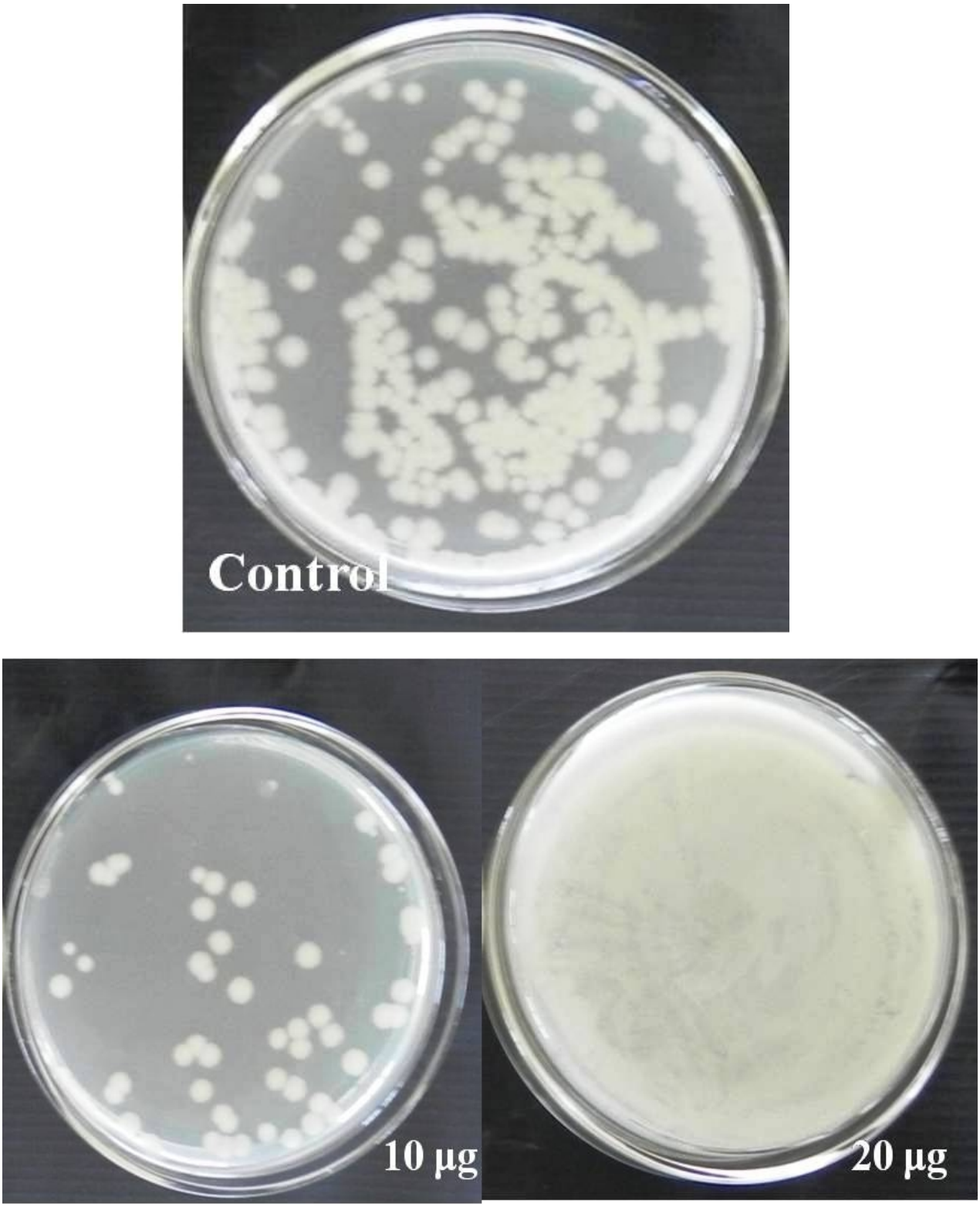

Figure S4. Plates showing 52 colonies were grown in 10 µg/mL of esomeprazole in LB

S. No	Model Name (Best five)	Dope Score
1	**TvLDH.B99990001**	-30481.58211
2	TvLDH.B99990002	-29003.167969
3	TvLDH.B99990003	-28726.529297
4	TvLDH.B99990004	-29056.332031
5	TvLDH.B99990005	-29234.333984

Table S1. Scoring values of different models through DOPE score in MODELLER

S.No	Name of the drug	Code no
1	Esomeprazole	**E7906**
2	Amoxicillin	**A8523**
3	Cefixime	**18588**
4	Glipizide	**G117**
5	Enalapril	75847-73-3
6	Amphicillin	**A9393**
7	Chloramphenical	**TC204 (Himedia)**
8	Amlodipine	**-----**
9	Losartan	**61188**
10	Cephalaxin	**MD014 (Himedia)**

Table S2: product number for experimental studies

Ligand Name	Docking Score (Kcal/mol)	Docking Energy (Kcal/mol)	Binding Energy (Kcal/mol)	H- bonds
Amoxicillin	-10.104	-57.451	-63.485	6
Cefixime	-10.535	-84.019	-73.341	10
Esomeprazole	-8.956	-51.877	-68.45	3
Cephalaxin	-8.897	-62.272	-59.577	5
Losartran	-7.521	-48.389	-43.574	3
Olmesartan	-7.312	-49.277	-53.315	3
Docetaxel	-6.707	-54.776	-54.885	2
Remikiren	-6.540	-51.121	-58.411	3
Ticagrelor	-6.428	-50.558	-63.412	2
Glimepiride	-6.275	-48.57	-52.82	4
Ritonavir	-6.266	-44.128	-54.817	3
Saprisartan	-6.186	-53.733	-45.005	1
Terlipressin	-6.161	-58.635	-47.41	1
Fosamprenavir	-6.047	-54.212	-49.873	2
Valganciclovir	-5.598	-42.730	-50.900	3

Table S3: Docking score values of screened compounds.