Supplementary Materials

Table S1. Source of Peptides.

Peptide name	Peptide Source	Peptides Sequence
VS-9	Fresh garlic	VKLRSLLCS
F3-C	Laba garlic	AVDRAV
TP-1	horseshoe crab	MKKLVIALCLMMVLAVMVEEAEAKWCFRVCYRG ICYRRCRGKRNEVRQYRDRGYDVRAIPEETFFTRQ DEDEDDDEE

Table S2. The quality of a predicted protein structure.

Protein name	Score *	Clash Score	R** Favored	R** Outliers	Rotamer Outliers	C-Beta Deviations	Bad Bonds	Bad Angles
LasR	0.60	0.27	98.31%	0.42%	0.00%	1	0 / 1918	11 / 2599
Bamp	0.90	0.83	97.20%	0.31%	0.36%	6	0 / 2484	19 / 3396
SrtA	1.06	1.20	96.57%	0.00%	0.55%	2	1 / 1689	10 / 2275

* MolProbity Score; ** Ramachandran

Table S3: Protein structure refinement using GalaxyRefine

A: LasR quorum sensing protein.

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotamers	Rama favored
Initial	1.0000	0.000	0.908	1.6	0.0	98.3
MODEL 1	0.9979	0.242	1.417	7.6	0.5	99.2
MODEL 2	0.9948	0.248	1.667	10.2	1.5	99.2
MODEL 3	0.9958	0.250	1.636	9.4	1.5	99.2
MODEL 4	0.9958	0.247	1.417	7.6	0.0	99.2
MODEL 5	0.9969	0.242	1.454	8.4	0.5	99.2

B: Biofilm-associated surface protein (Baps)

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotamers	Rama favored
Initial	1.0000	0.000	1.095	1.9	0.4	97.2
MODEL 1	0.9738	0.347	1.510	9.7	0.0	99.7
MODEL 2	0.9838	0.308	1.468	8.7	0.4	100.0
MODEL 3	0.9815	0.325	1.518	9.9	0.0	99.7
MODEL 4	0.9722	0.347	1.485	9.1	0.4	99.7
MODEL 5	0.9799	0.333	1.449	8.3	0.0	99.7

C: sortase A form Staphylococcus *aureus*

Model	GDT-HA	RMSD	MolProbity	Clash score	Poor rotamers	Rama favored
Initial	1.0000	0.000	1.470	4.8	0.5	96.6
MODEL 1	0.9830	0.318	1.637	8.8	1.6	98.5
MODEL 2	0.9951	0.280	1.759	12.1	1.6	98.5
MODEL 3	0.9915	0.279	1.650	9.1	1.6	98.5
MODEL 4	0.9867	0.289	1.887	10.9	2.7	98.5
MODEL 5	0.9927	0.279	1.729	11.2	1.6	98.5