Electronic Supplementary Material (ESI) for RSC Advances.

Mechanistic Insights of SrtA-LPXTG Blockers targeting the transpeptidase mechanism in *Streptococcus mutans*

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Table S1: Glide docking score and energy value for wild and mutant form LPNTG peptide protein complex

Wild and mutant type LPNTG substrate	Docking Score (Kcal/mol)	Glide Energy (Kcal/mol)
LPNTG (wild)	-10.699	-51.2495
LPNTG-H1 (Mutant)	-5.421	-31.401
LPNTG-H2 (Mutant)	-4.884	-40.228
LPNTG-H3 (Mutant)	-4.126	-38.266
LPNTG-H1_H2 (Mutant)	-3.885	-35.658

Table S2: Extra precision Glide docking score values for peptide blocker compounds with interacting amino acids

Compounds	**XP-d score (Kcal/mol)**	**Glide emodel**	**Glide energy**	**Atomic interaction between LPNTG Peptide and compound**	**Distance (Å)**	**Atomic interaction between protein and compound**	**Distance**
Zn22946756	-5.675	-56.324	-40.0485	[Leu1]=(H1)..OC	1.87	(Ser130C)=O...HN	1.85
Zn28130221	-5.426	-44.575	-31.9506	[Leu1]=(H1)...OC	2.13	(Pro164)=O...HO (Arg192)=H...OH	1.73 1.87
Zn00266826	-5.235	-50.820	-39.8677	[Leu1]= (O)...HO	2.02	(Ser130C)=O...HN	1.89
Zn20577153	-5.037	-54.501	-40.458	[Leu1]=(O)...HN	2.11	(Ser130C)=O...HN	2.27
Zn24294906	-4.295	-46.514	-36.1659	[Leu1]=(H1)...OC	2.20	(Arg192)=H...OC	1.93

Supplementary Figures:

Figure S1: Secondary structure of homology model *S. mutans* SrtA protein.

Figure S2: Structure validation of modeled SrtA protein

Figure S3: Anolea web server represents energy values for each amino acid in a SrtA protein chain.

Figure S4: (A) ProSA-web z-score with respect to residues. The Z-score of the SrtA protein was shown in large black dot and score was found to be -6.22kcal/mol. (**B**) The plot represents the target and template is shown in dark green solid lines and light green solid lines respectively.

Figure S5: Graphs of RMSD C-alpha of complex dynamics of SrtA with native and mutated peptide.

Figure S6: Hydrogen bonding interaction of SrtA bound LPNTG complexes

Figure S7: (A) RMSF of all residues of complex dynamics of SrtA with native and mutated LPNTG substrates. **(B)** Comparison of RMSF of all native an mutated peptide

Figure S8: Funnel based screening protocol followed in this study to screen for Anti-SrtA inhibitors.

Figure S9: RMSF of all residues of complex dynamics of SrtA with native and mutated LPNTG complex with compounds

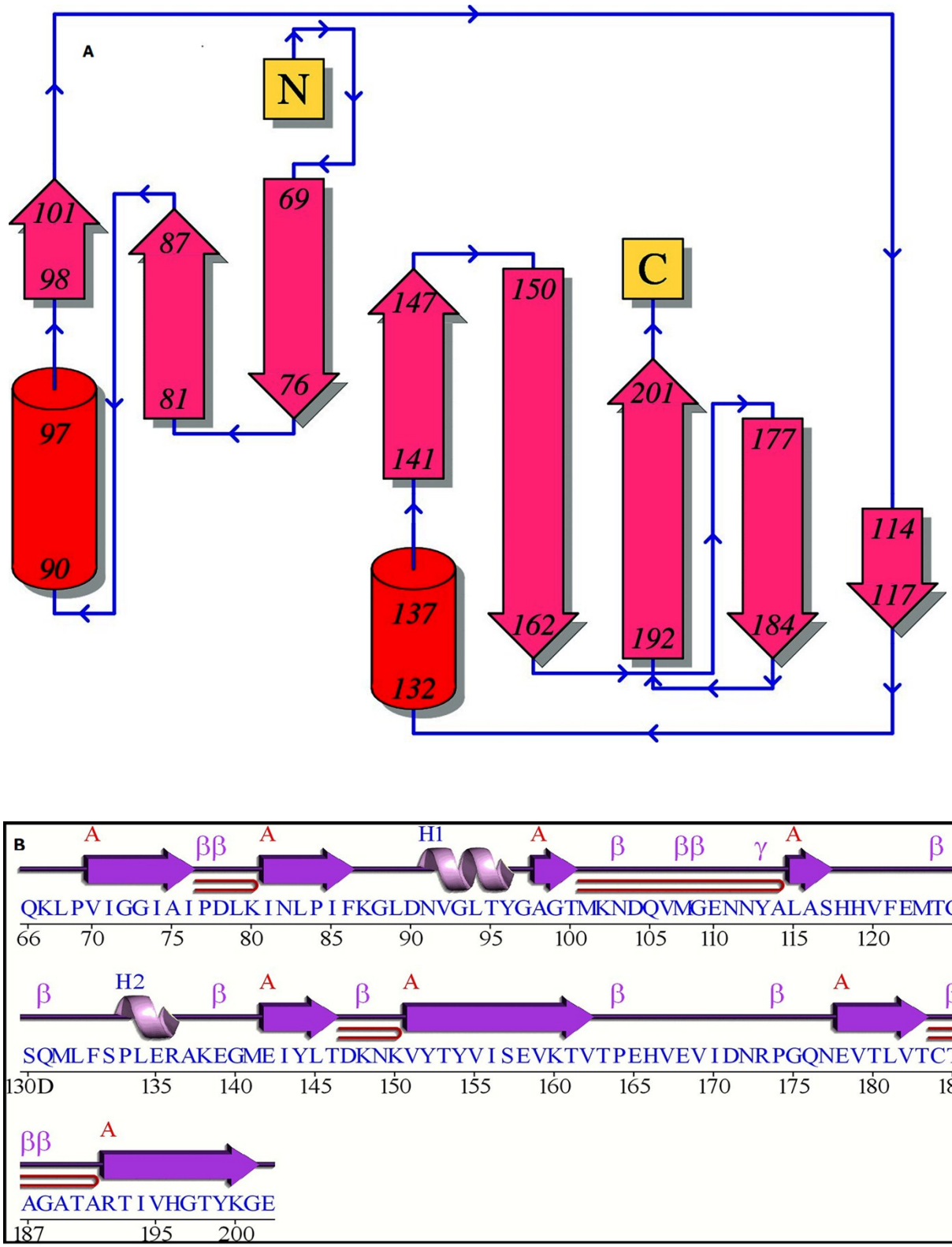

Figure S1 Secondary structure of homology model *S. mutans* SrtA protein.

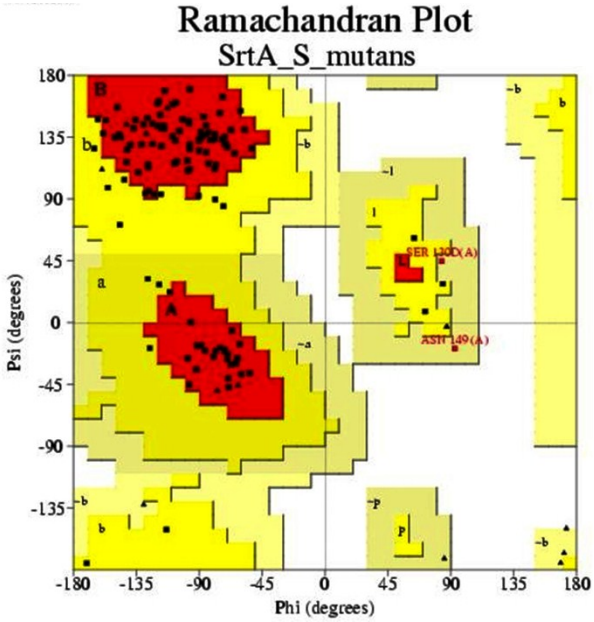

Figure S2: Structure validation of modeled SrtA protein. (Ramachandran plot shows 83.5% of amino acid residue of modeled structure found in favorable region. Red color shows the core region, yellow color shows the allowed region and the white color shows disallowed region.)

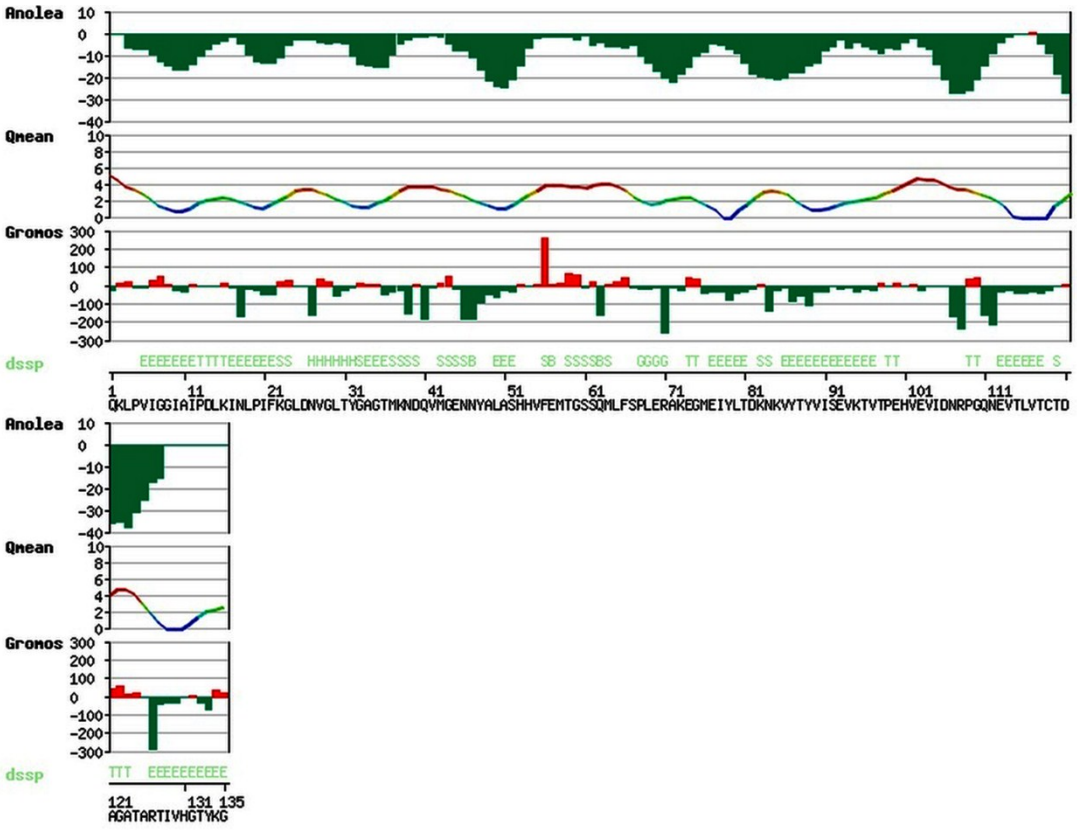

Figure S3: Anolea web server represents energy values for each amino acid in a SrtA protein chain.

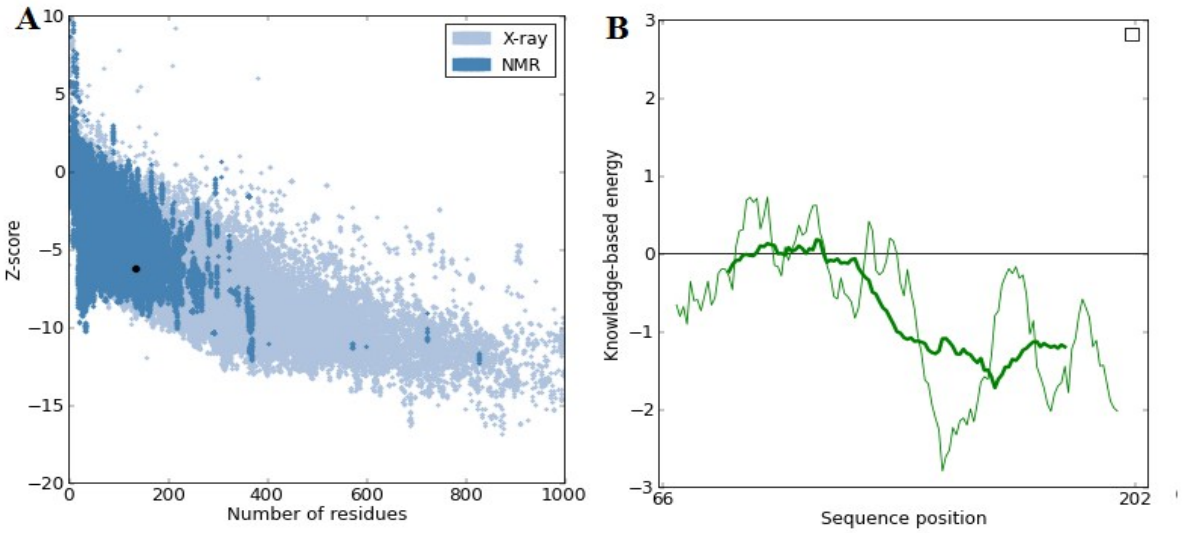

Figure S4 (A): ProSA-web z-score with respect to residues. The Z-score of the SrtA protein was shown in large black dot and score was found to be -6.22kcal/mol. (**B**) The plot represents the target and template is shown in dark green solid lines and light green solid lines respectively.

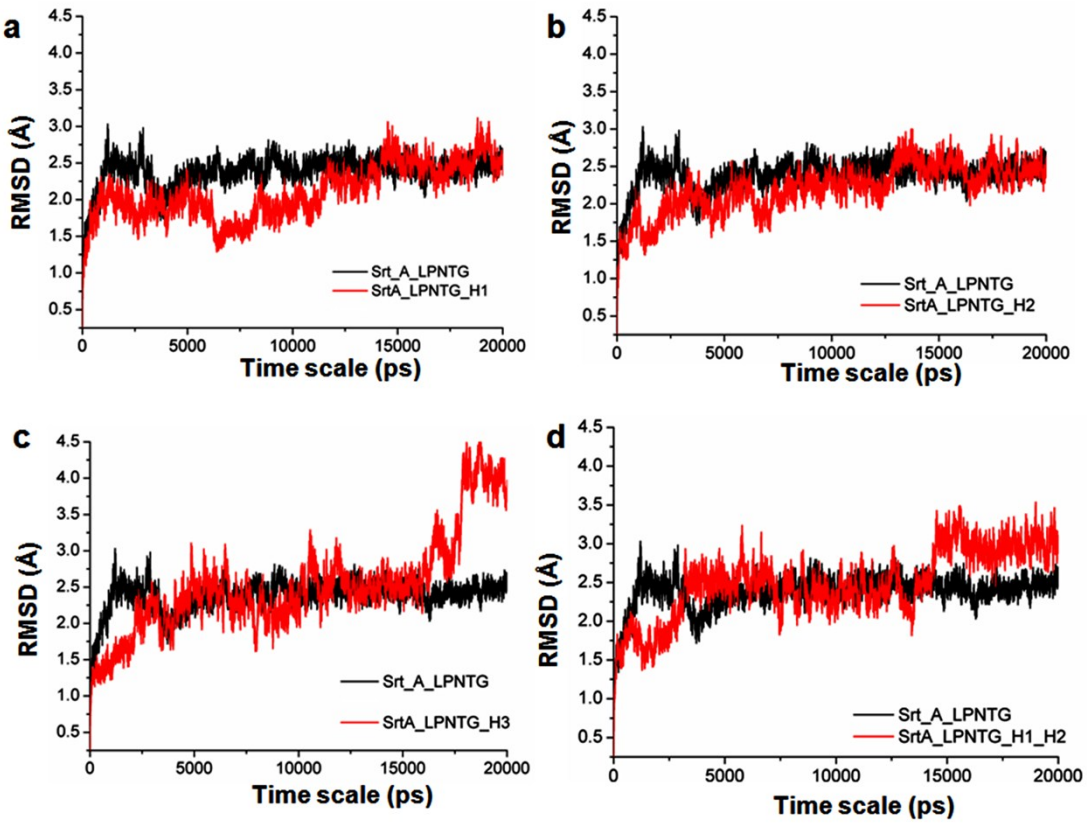

Figure S5: Graphs of RMSD C-alpha of complex dynamics of SrtA with native and mutated peptide.

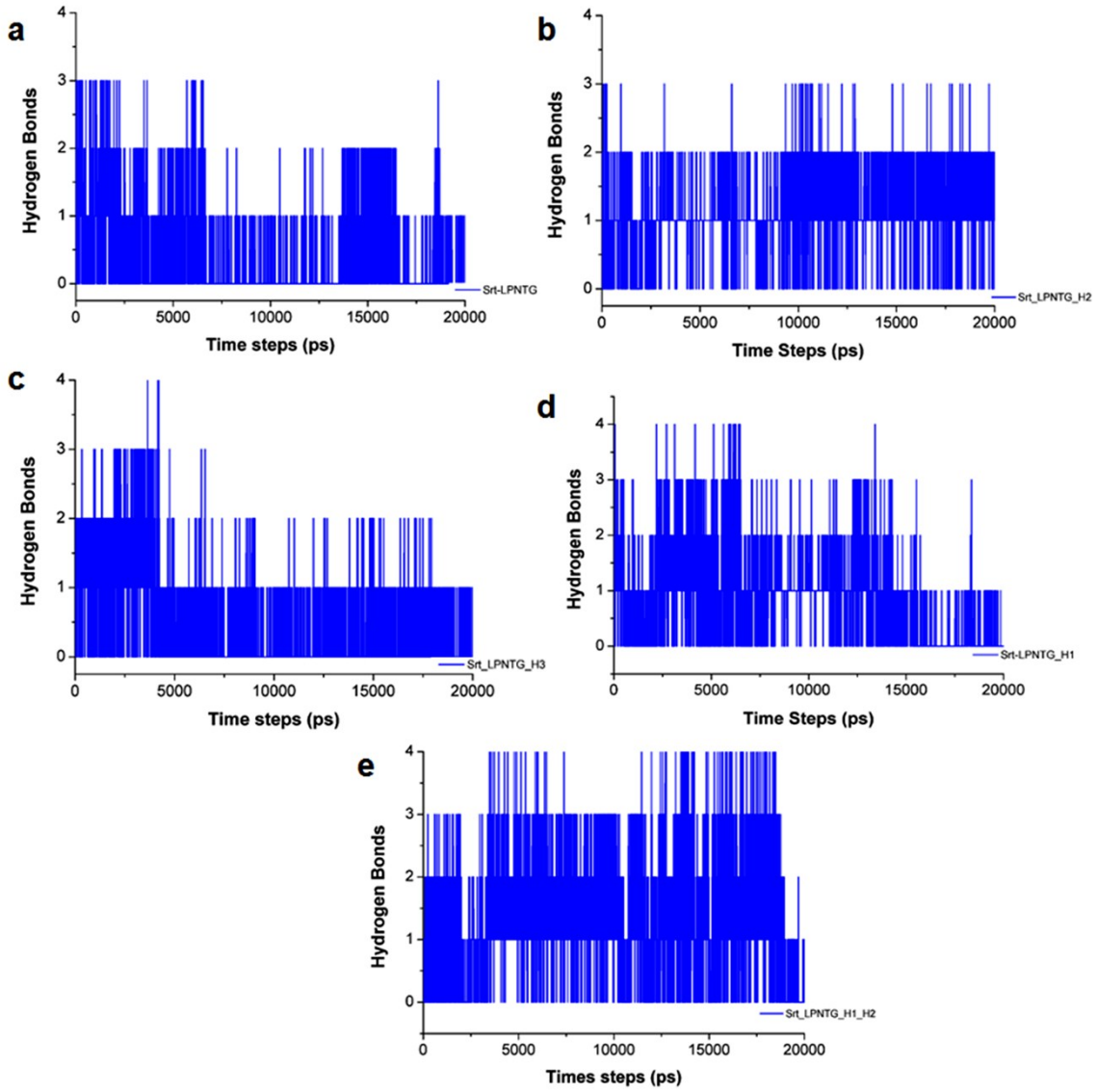

Figure S6: Hydrogen bonding interaction of SrtA bound LPNTG complexes

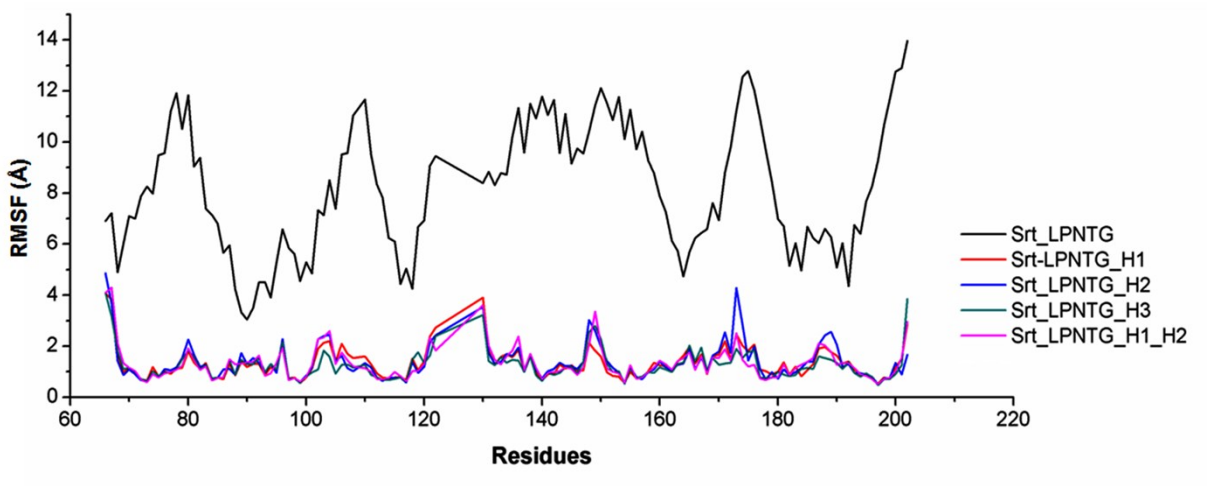

Figure S7: (A) RMSF of all residues of complex dynamics of SrtA with native and mutated LPNTG substrates.

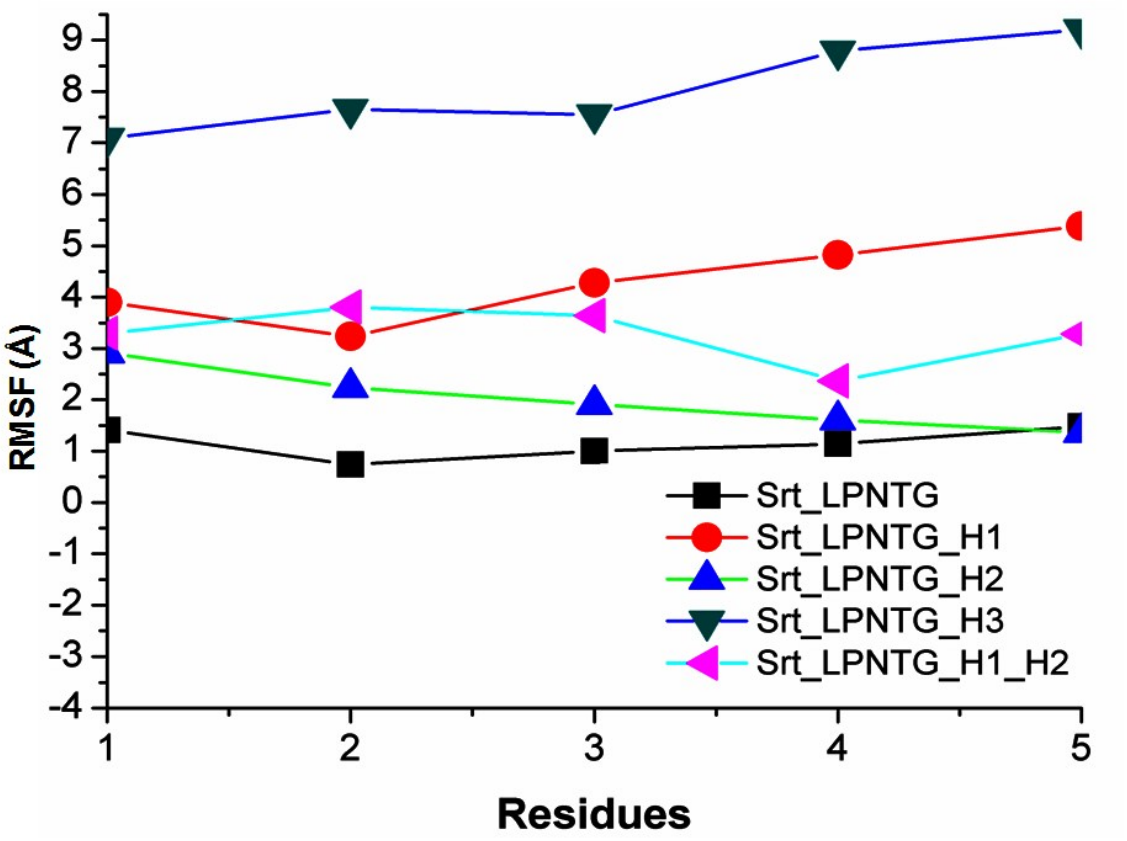

Figure S7: (B) Comparison of RMSF of all native an mutated peptide

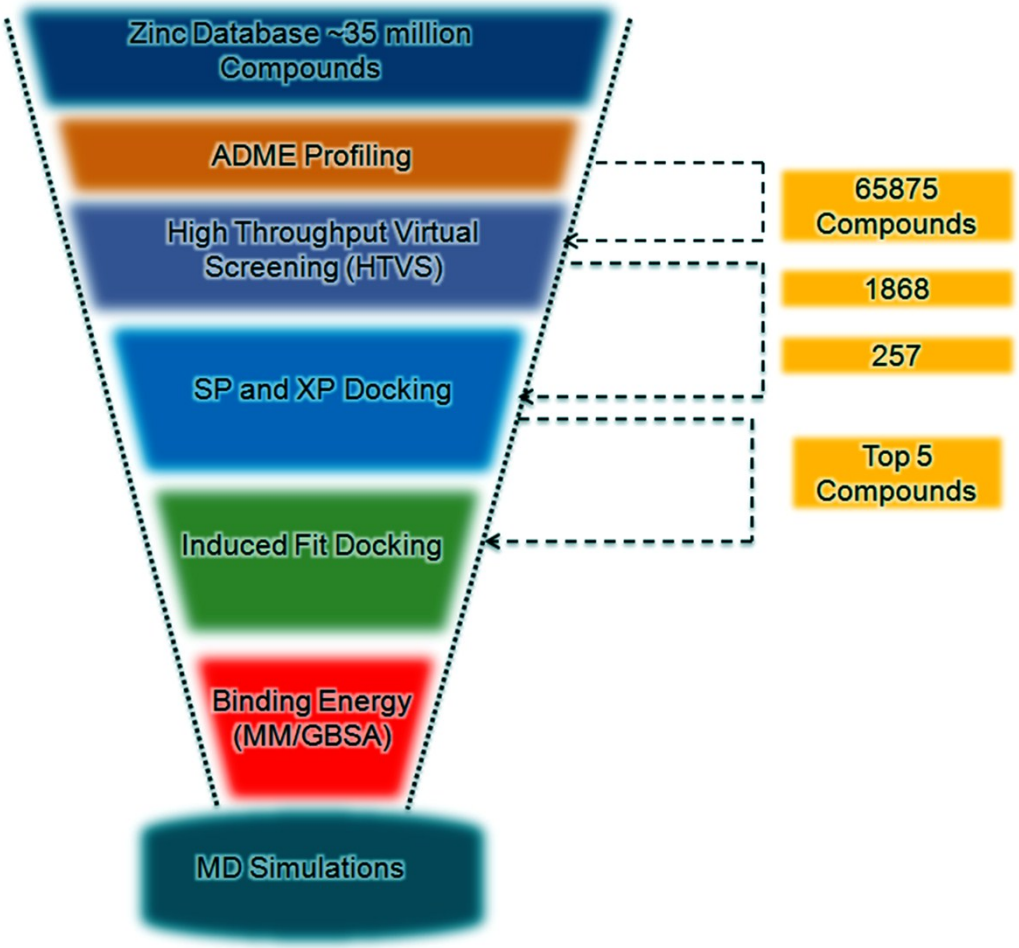

Figure S8: Funnel based screening protocol followed in this study to screen for Anti-SrtA inhibitors.

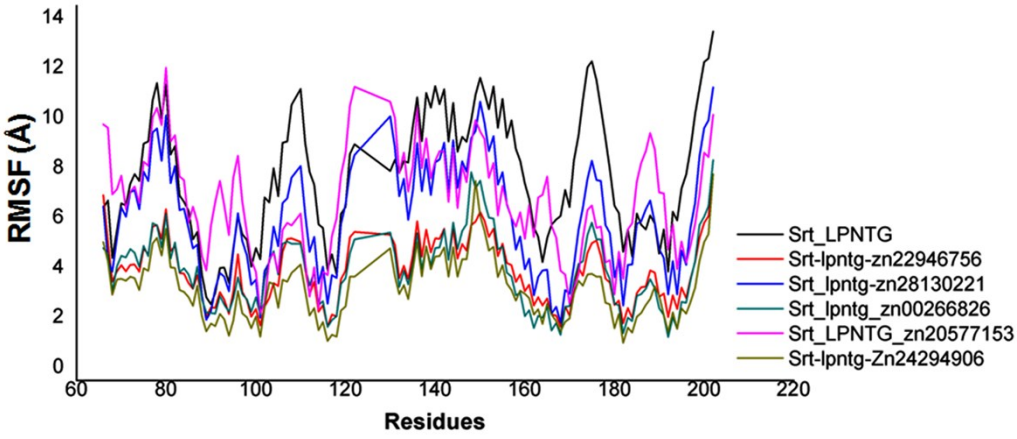

Figure S9: RMSF of all residues of complex dynamics of SrtA with native and mutated LPNTG complex with compounds.