

Supplementary materials

Searching for new antibacterial compounds against *Staphylococcus aureus*: A computational study on the binding between FtsZ and FtsA

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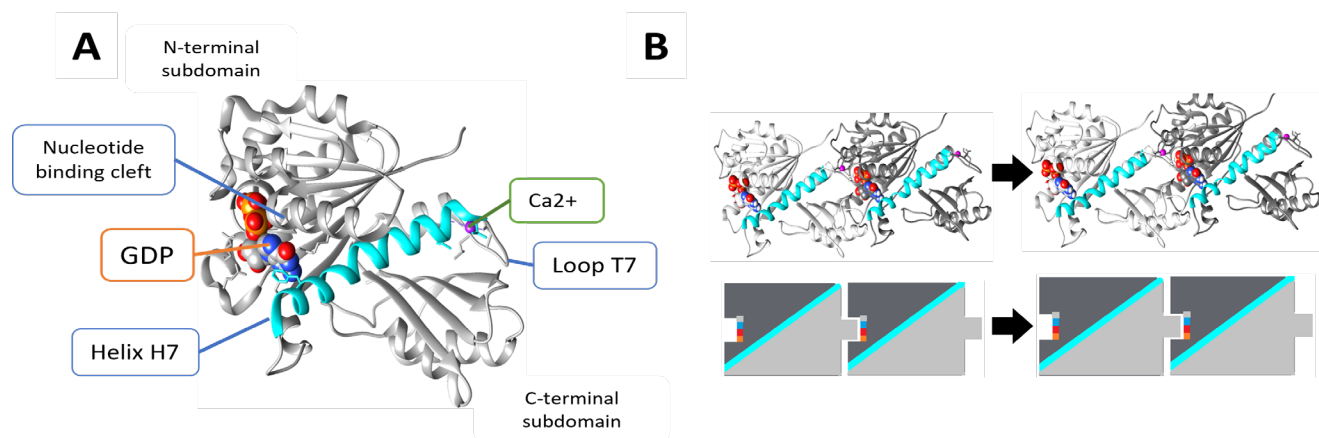


Figure S1. (A) The structure of SaFtsZ (PDB: 3VOA) in light gray shows the N-terminal and C-terminal subdomains indicated with their respective legends. The N-terminal subdomain contains a sphere-shaped molecule that is indicated in the image with the legend GDP (guanosine diphosphate) and is colored in red, yellow, navy blue and gray. The structure colored in cyan blue corresponds to an alpha-helix that separates the two main subdomains (N and C terminals); B) Filamentous units of SaFtsZ that form the head-to-tail binding mode, where the T7 loop indicated in Figure S1A binds to the nucleotide binding site also indicated in Fig. S1A. Therefore, the colorimetry designated for the proteins and their representation in this section is the same as that explained for (A).

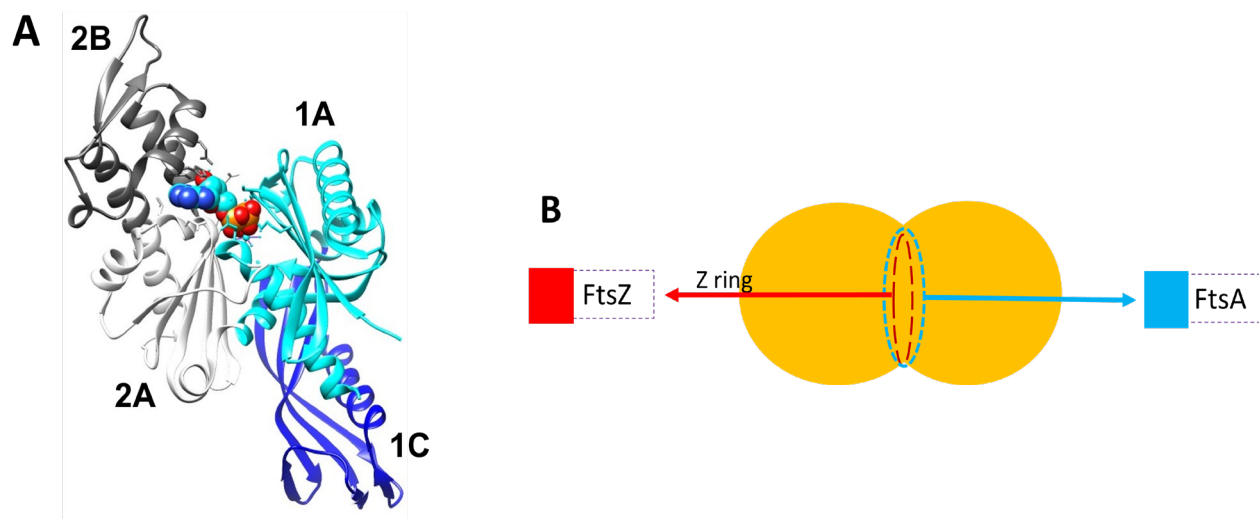


Figure S2. A) Structure of SaFtsA (PDB: 3WT0) where the four subdomains that compose it are distinguished by the following colors: 1A: light blue, 1C: dark blue, 2A: light grey and 2B: dark grey. The molecule in the spherical conformation between the subdomains of the protein, with colors: dark blue, light blue, red and yellow, corresponds to an ATP molecule; B) Formation of the Z ring (ellipse denoted by red dotted lines) at the beginning of the constriction of the bacterial cell by filamentous units of FtsZ, which are in turn anchored to the cytoplasmic membrane when they bind to FtsA units (denoted by an ellipse of blue dotted lines). The yellow spheres represent the cytokinesis of an *S. aureus* cell.



Figure S3. A) Structural alignment of the FtsA structures from *Staphylococcus aureus* (white) and *Thermotoga maritima* (cyan blue). ATP molecules are shown in a sphere-like conformation in red and orange.

(Table S1. Table_FtsZ_Est_Evol_Diverg_Sequences.xlsx).

Table S2. Pharmacophoric candidates gleaned from Pharmit for complex 2, resulting from the molecular docking between FtsA and the CTV segment from the C-terminal helix of FtsZ. The docking score and mRMSD correspond to docking calculations performed with VINA (implemented in Pharmit)

<i>NAME</i>	<i>SCORE</i>	<i>mRMSD</i>
ZINC000095394143	-5.97	1.991
ZINC000096585731	-5.91	1.303
ZINC000409363275	-5.66	1.573
ZINC000033586433	-5.40	1.4095
PubChem-97972478	-3.03	0.510
PubChem-116858227	-3.87	0.633
PubChem-108190517	-3.95	0.735
PubChem-147692426	-3.38	0.778

Table S3. Pharmacophoric candidates gleaned from Pharmit for complex 5, resulting from the molecular docking between FtsA and the CTV segment from the C-terminal helix of FtsZ. The docking score and mRMSD correspond to docking calculations performed with VINA (implemented in Pharmit).

<i>NAME</i>	<i>SCORE</i>	<i>mRMSD</i>
PubChem-164134069	-3.50	1.823
PubChem-91425620	-3.44	0.952
PubChem-164134069	-3.37	0.882
PubChem-89011157	-3.33	0.881