

## VIRTUAL SCREENING OF DATABASES ASSOCIATED WITH MULTICOMPONENT REACTIONS TO OBTAIN POTENTIAL FTSZ INHIBITORS OF *Staphylococcus aureus*

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In 2019, it was estimated that 1.3 million deaths worldwide were associated with antibiotic resistance. Among the major resistant pathogens, methicillin-resistant *Staphylococcus aureus* (MRSA) was estimated to cause more than 100,000 deaths.<sup>1</sup> MRSA is a type of Gram-positive bacteria that has exhibited resistance to glycopeptides, as well as daptomycin, linezolid, and vancomycin. This resistance is attributable to mutations and single nucleotide polymorphisms (SNPs).<sup>2</sup>

A notable drug target that has gained relevance is the protein Filamenting temperature-sensitive mutant Z (FtsZ), which plays a crucial role in bacterial reproduction and infection. The inhibition of FtsZ assembly has been demonstrated to impede the process of peptidoglycan septum formation during cell division, thereby promoting cell lysis.<sup>3</sup>

In the present study, we obtained databases related to scaffolds associated with multicomponent reactions. The molecules were subjected to virtual screening using molecular docking tools, specifically targeting the interdomain of the *S. aureus* FtsZ protein (PDB: 3VOB), utilizing AutoDock 4.2, Vina, and GOLD. Molecules that demonstrated optimal scores and binding affinities were then analyzed and selected for the synthesis of potential inhibitors of the *S. aureus* FtsZ protein.

### References

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