

# Computational Docking of FtsZ: Survey of Promising Antibiotic Compounds

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## 1. Z-Test Statistical Analysis

$$Z - Score = \frac{(\chi_1 - \chi_2) - (\mu_1 - \mu_2)}{\sqrt{\frac{(\sigma_1)^2}{n_1} + \frac{(\sigma_2)^2}{n_2}}}$$

$\chi$  = sample mean = average of the first few clusters (first 35 to 50 results)

$\mu$  = mean = average of the full data set (usually about 250 results)

$\sigma$  = stdev = standard deviation of the full data set

$n$  = population size = total number of results in the data set

The P-value is calculated as the normal distribution of the Z-score. All calculations done using Google Sheets formulas (AVERAGE, COUNT, STDEV, and NORM.S.DIST). Additional values from the calculations (or simulations) available by request to the corresponding author.

## 2. Free Docking Results

### 2.1. Controls

Ciligin-BP served as a negative control (not expected to bind to FtsZ). PC190723 served as a positive control.

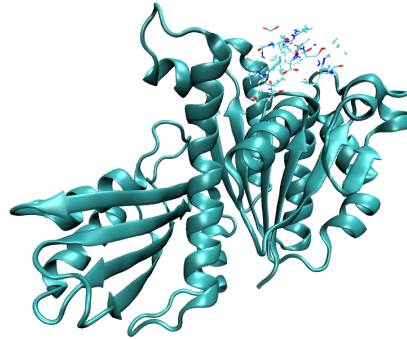


Figure 1: Free docking results of 3wgn protein with Ciligicin-BP ligand.

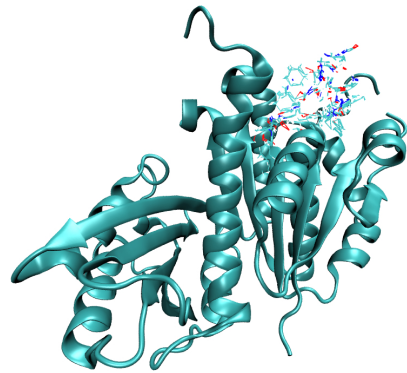


Figure 2: Free docking results of 6umk protein with Ciligicin-BP ligand.

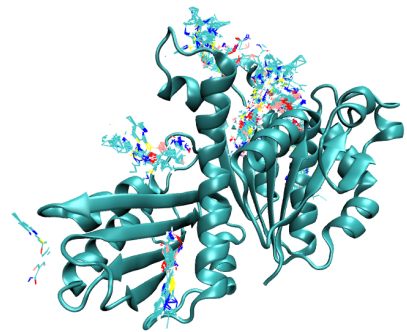


Figure 3: Free docking results of 3wgn protein with PC190723 ligand.

## 2.2. Additional FtsZ Structures Tested

These results were obtained too late to fully analyze for the main text, but similar Average  $\Delta G$  values were observed, along with similar binding sites.

Table 1: Additional FtsZ Species Investigated

PDB Code	Drug Bound	Bacterial Species	Classification	Average $\Delta G$ (kcal/mol)
6unx	Resveratrol	<i>E. coli</i>	Gram-negative	-6.41
2vap	Resveratrol	<i>M. jannaschii</i>	Gram-negative	-6.01
5xdw	Plumbagin	<i>S. aureus</i>	Gram-positive	-5.85
2vaw	TXY436	<i>P. aeruginosa</i>	Gram-negative	-7.33

## 2.3. Experimental Compounds

All other compounds below have their binding energies reported in the main text.

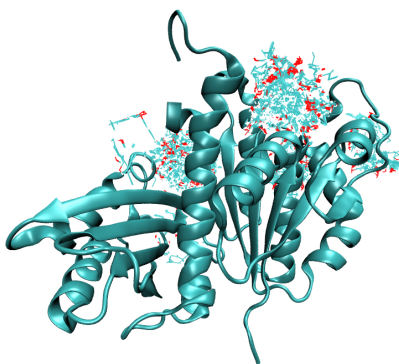


Figure 4: Free docking results of 6unx protein with Chrysopaentin ligand.

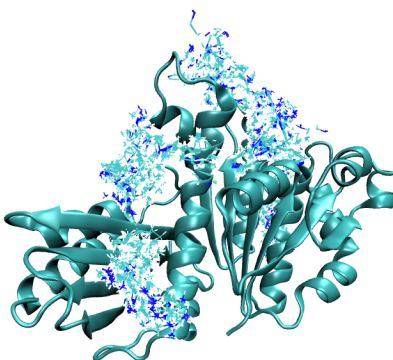


Figure 5: Free docking results of 3wgn protein with compound 12 ligand.

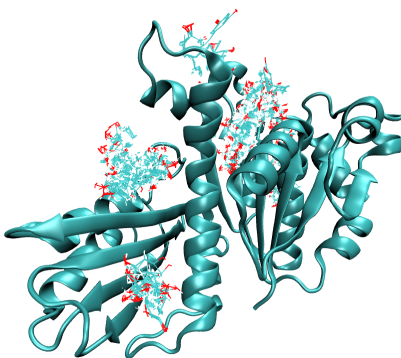


Figure 6: Free docking results of 3wgn protein with resveratrol ligand.

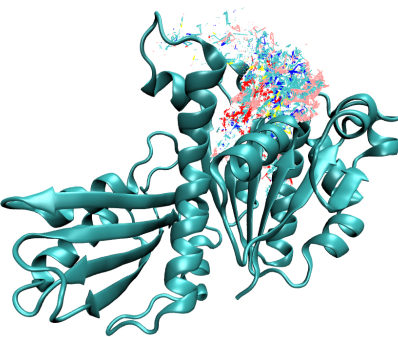


Figure 7: Free docking results of 3wgn protein with TXA709 ligand.

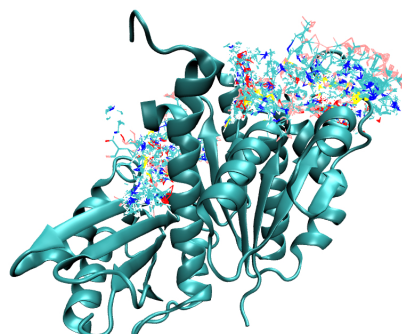


Figure 8: Free docking results of 6umk protein with TXA709 ligand.

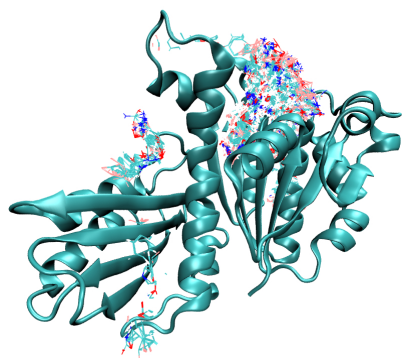


Figure 9: Free docking results of 3wgn protein with TXA6101 ligand.

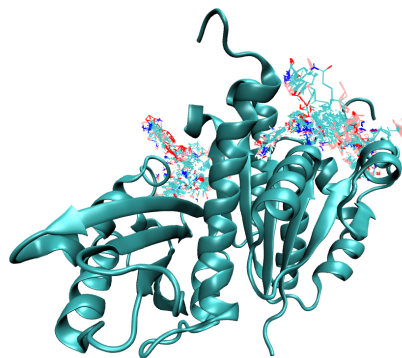


Figure 10: Free docking results of 6umk protein with TXA6101 ligand.

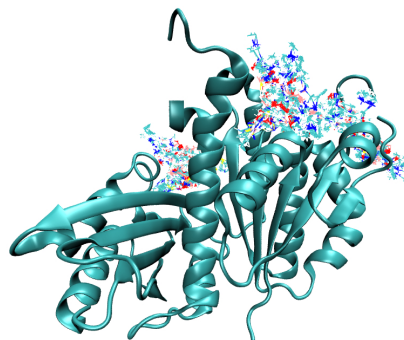


Figure 11: Free docking results of 6umk protein with TXY436 ligand.

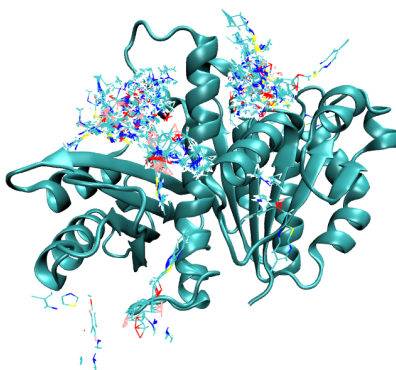


Figure 12: Free docking results of 2vam protein with TXY436 ligand.

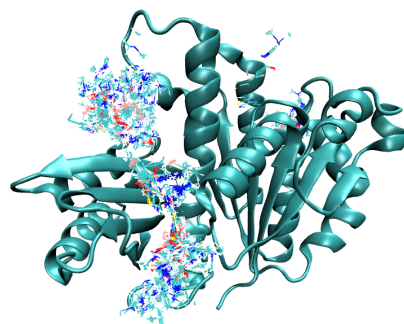


Figure 13: Free docking results of 2vxy protein with TXY436 ligand.

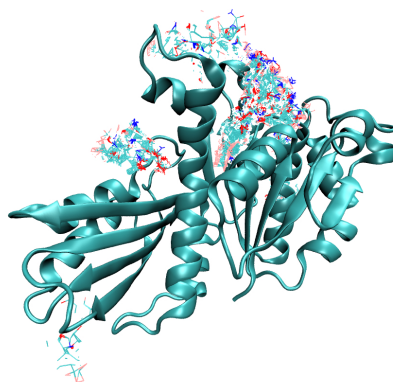


Figure 14: Free docking results of 3wgn protein with TXY6129 ligand.

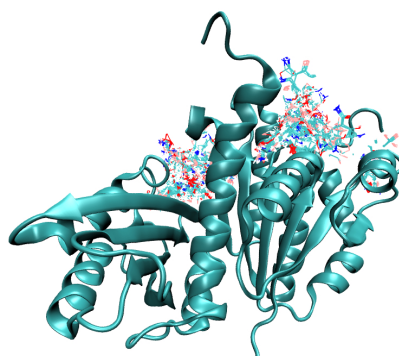


Figure 15: Free docking results of 6umk protein with TXY6129 ligand.

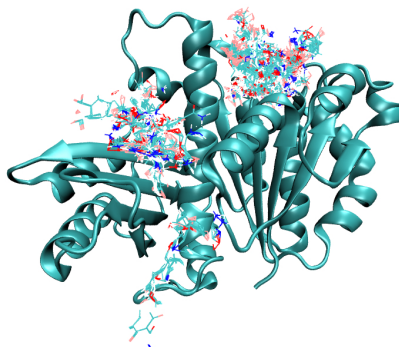


Figure 16: Free docking results of 2vam protein with compound 1 ligand.

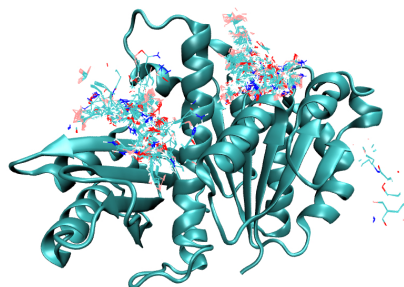


Figure 17: Free docking results of 2vam protein with compound 2 ligand.

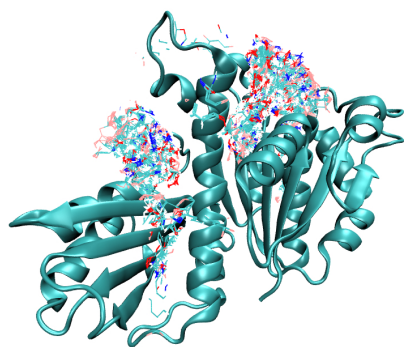


Figure 18: Free docking results of 3vo8 protein with compound 1 ligand.

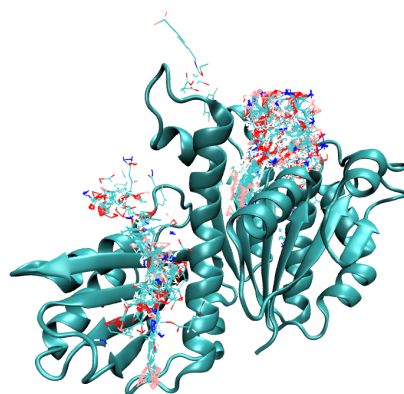


Figure 19: Free docking results of 3vo8 protein with compound 2 ligand.



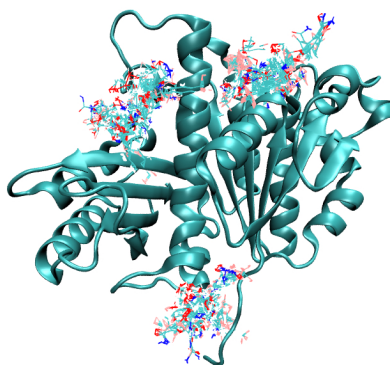


Figure 20: Free docking results of 5zue protein with compound 1 ligand.

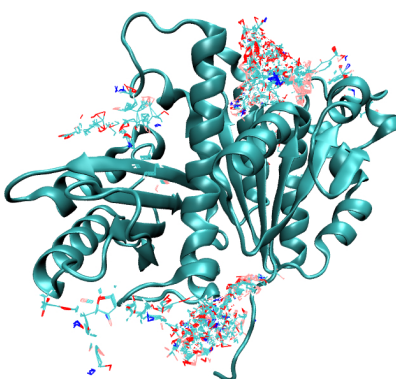


Figure 21: Free docking results of 5zue protein with compound 2 ligand.

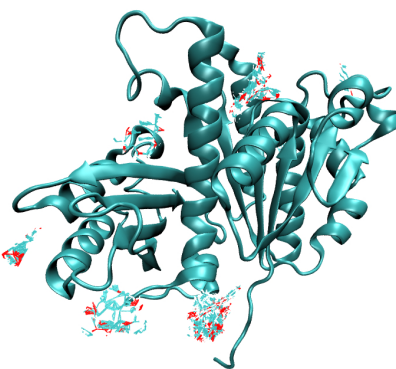


Figure 22: Free docking results of 5zue protein with plumbagin ligand.

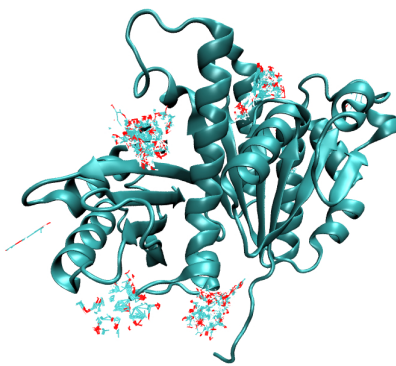


Figure 23: Free docking results of 5zue protein with scopoletin ligand.