

## Summary

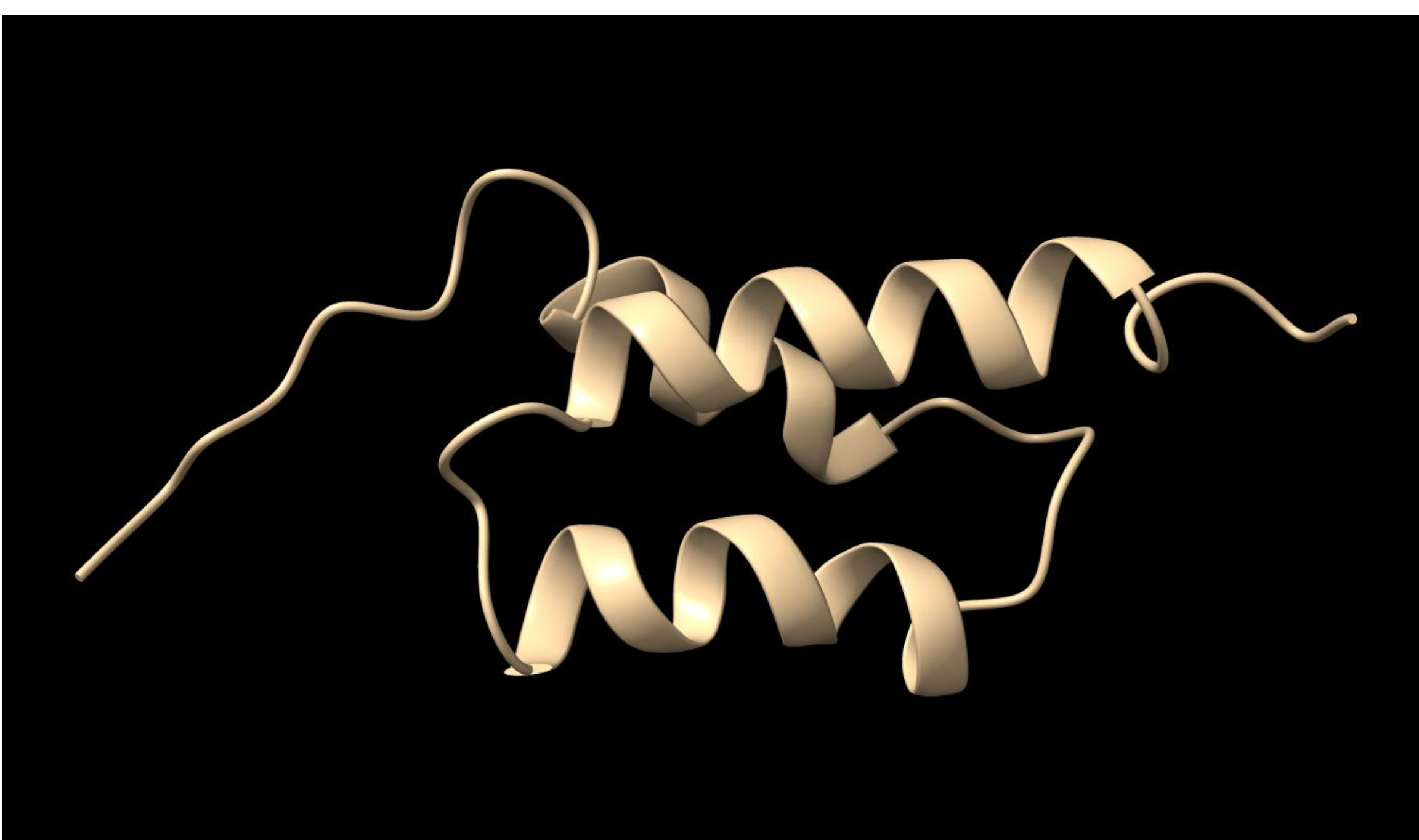
- Foodborne pathogens are different types of biological agents that can cause a foodborne illness events
  - Pathogens can be parasites, bacterial, or viral
- Staphylococcus Aureus is a foodborne illness that causes boils on the skin and can lead to pneumonia and other bodily infections
- Protein A is on the surface of 90% of all S. Aureus and prevents it from being destroyed

## Motivation

This project studies the stability between different DNA aptamers and Protein A that is present on the pathogen called Staphylococcus Aureus. The results from this will help with the diagnosis and treatment for people who have contracted S. Aureus.

## Research Question

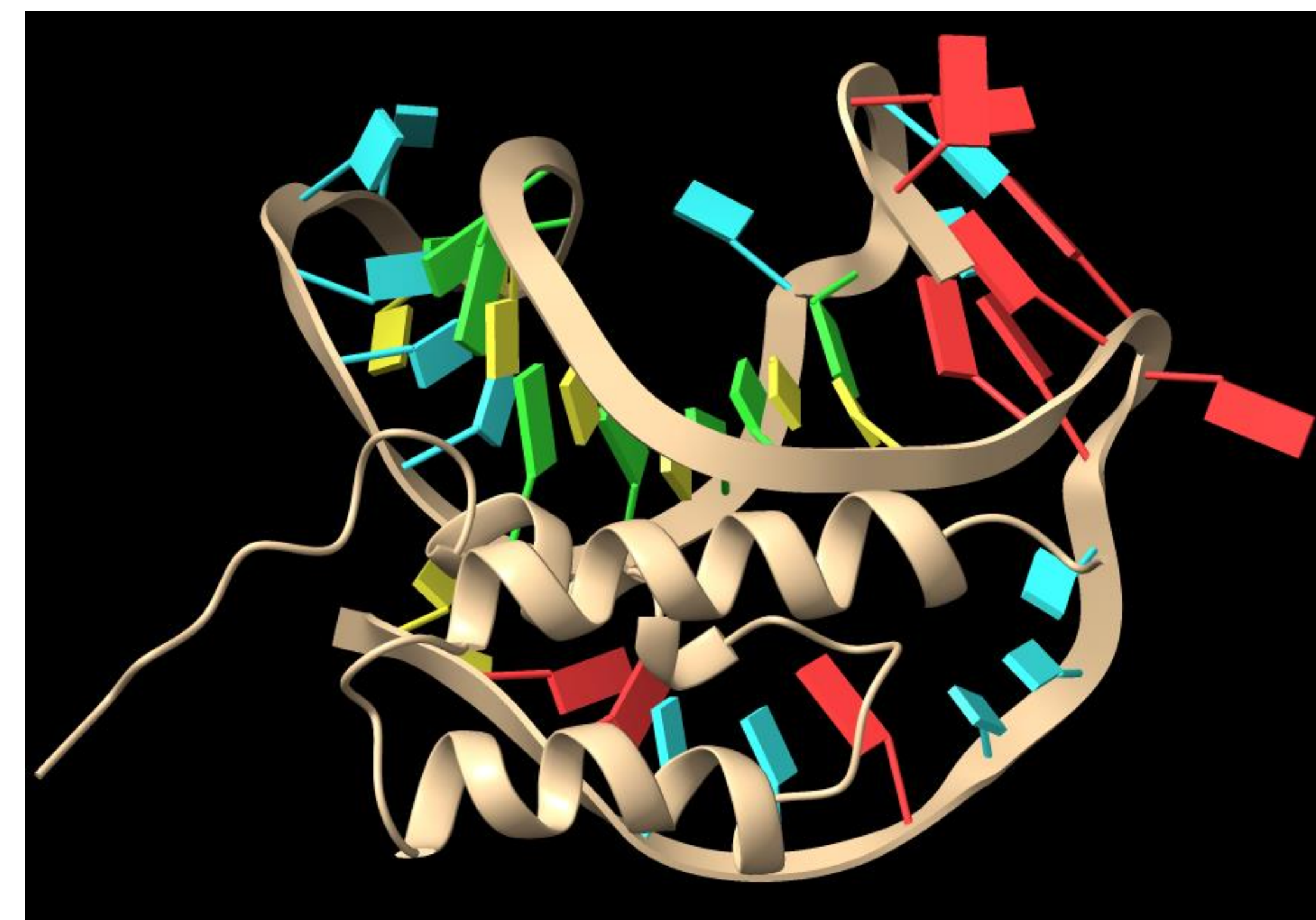
Which aptamer has the highest binding stability with Protein A



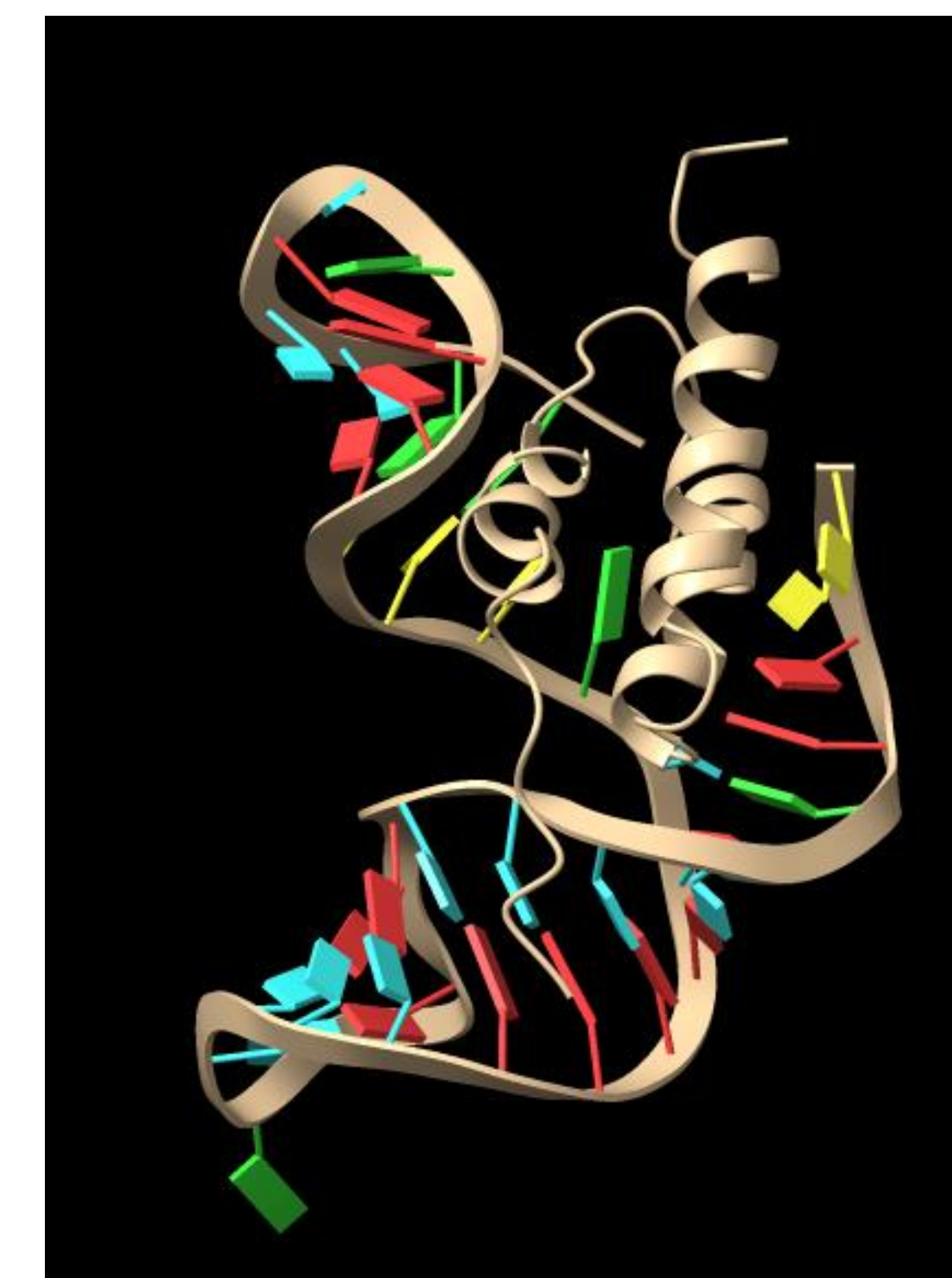
Protein A from PDB

## Methods & Materials

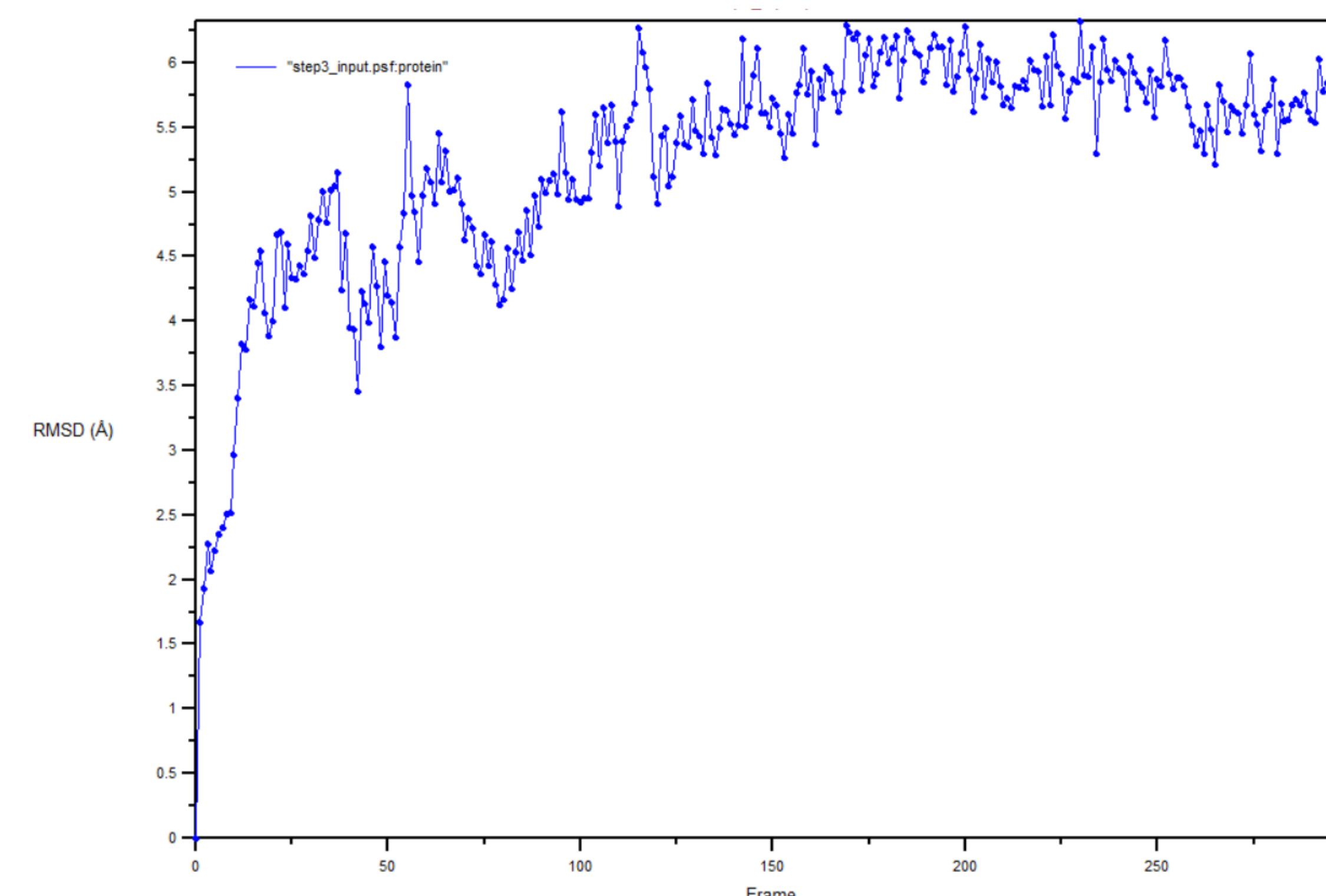
- Download the 1bdd.pdf file from the PDB database
- Used github and intellij IDEA to find different aptamers
- Hdock helped with the docking of each of the aptamers with Protein A
- UTC's SIM center helped with putting each of the docked molecules in a solution box
- Then VMD helped with finding and graphing the RMSD analysis



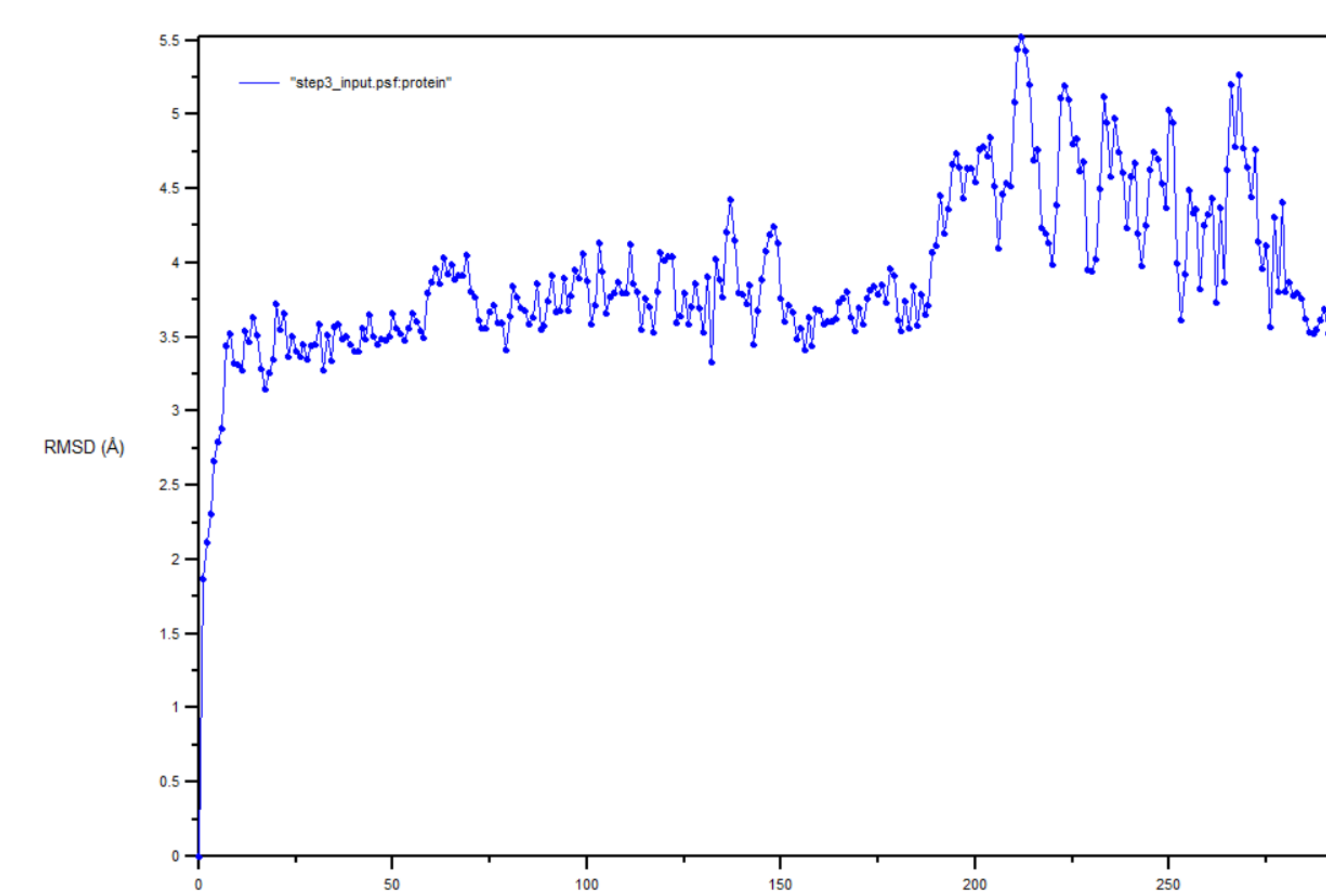
Docking between the 1st aptamer and Protein A  
 Free energy = -4.0



Docking between the 5<sup>th</sup> aptamer and Protein A  
 Free energy = -8.0



RMSD chart of the binding between aptamer 1 and protein A



RMSD chart of the binding between aptamer 4 and protein A

## Conclusion

- Protein A is a good protein to use when trying to detect S. Aureus
- The RMSD charts need to have less fluctuation to show the stability
  - Beginning of aptamer 5 RMSD chart shows minimal fluctuation
- The higher the free energy indicates greater stability
  - RMSD charts of aptamer 1 vs. aptamer 5
- Future studies will help us find the best aptamer

## Acknowledgements

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## References

Foster T. Staphylococcus. In: Baron S, editor. Medical Microbiology. 4th edition. Galveston (TX): University of Texas Medical Branch at Galveston; 1996. Chapter 12. Available from: <https://www.ncbi.nlm.nih.gov/books/NBK8448/>