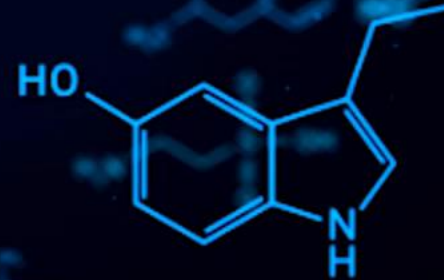


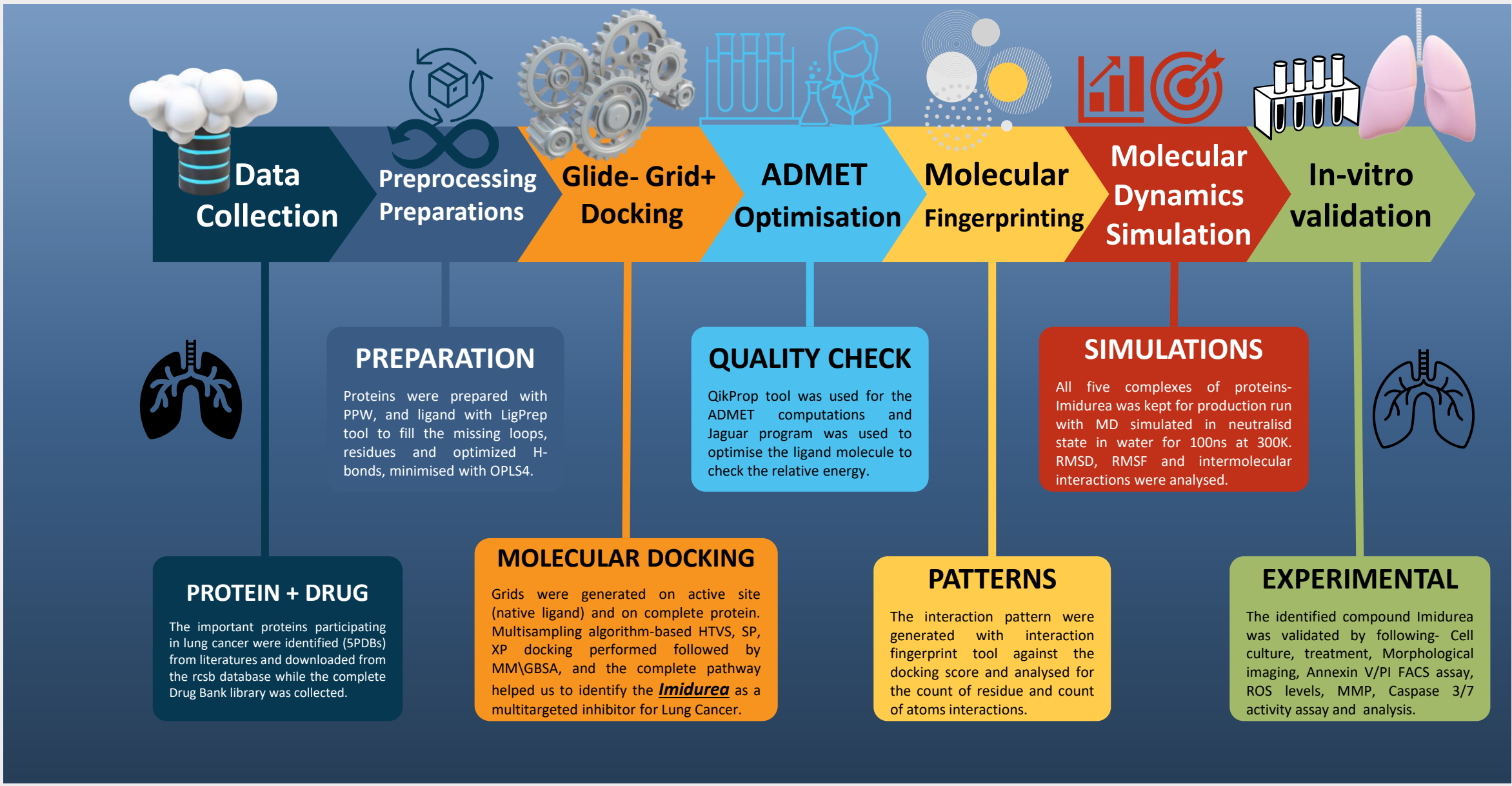
Multialgorithm-based docking reveals Imidazolidinyl urea as a multitargeted inhibitor for Lung Cancer

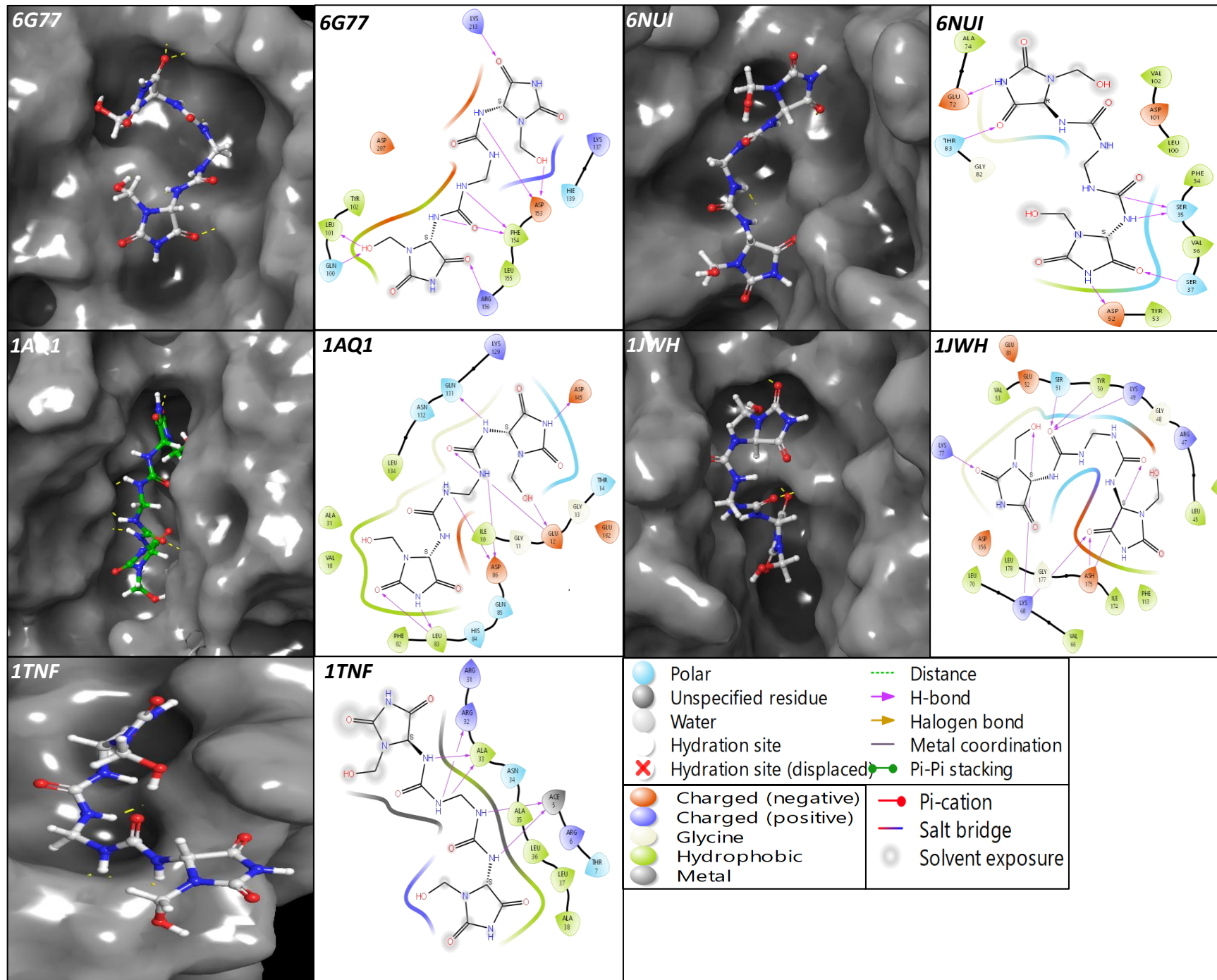


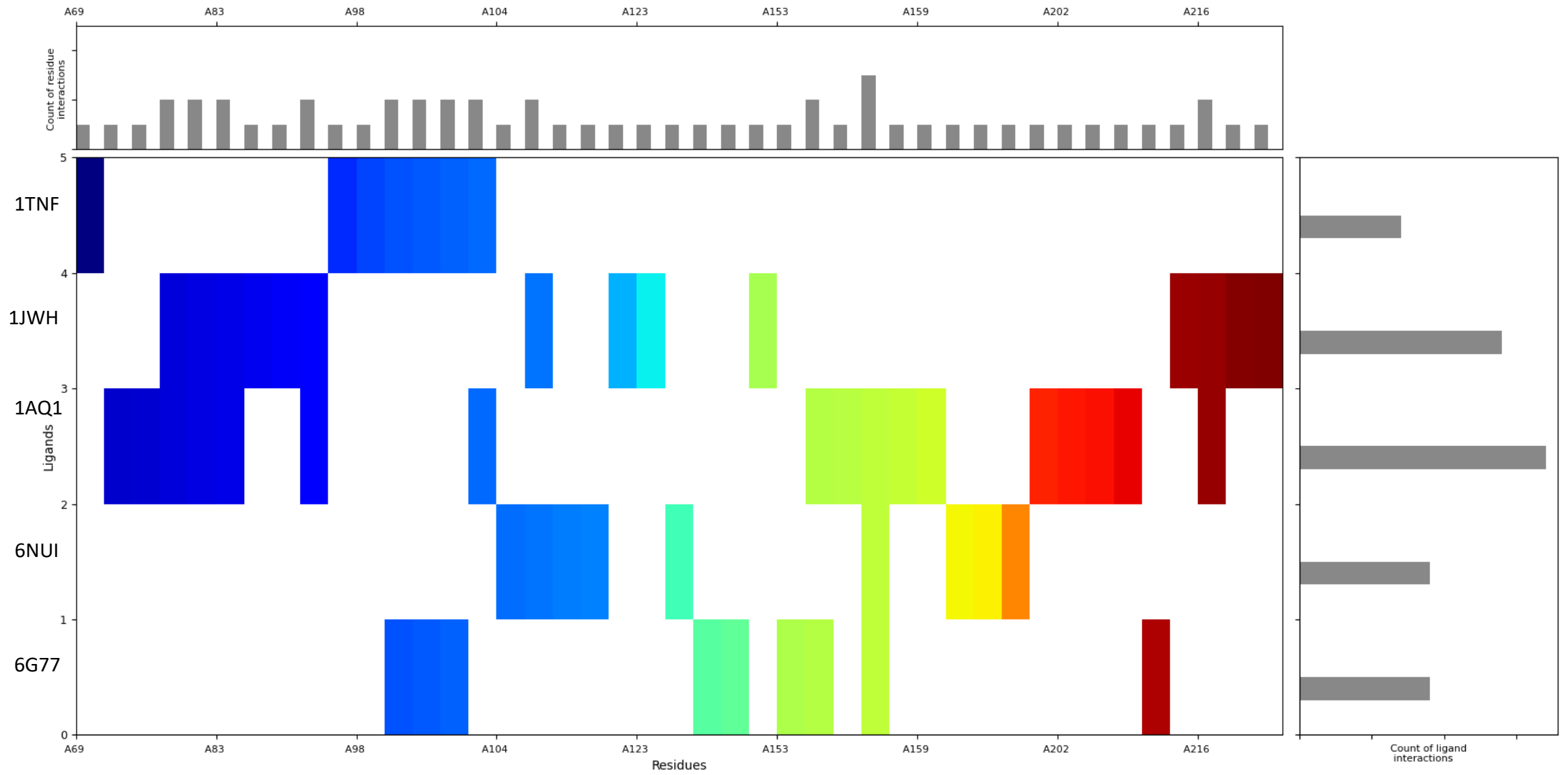
Shaban Ahmad

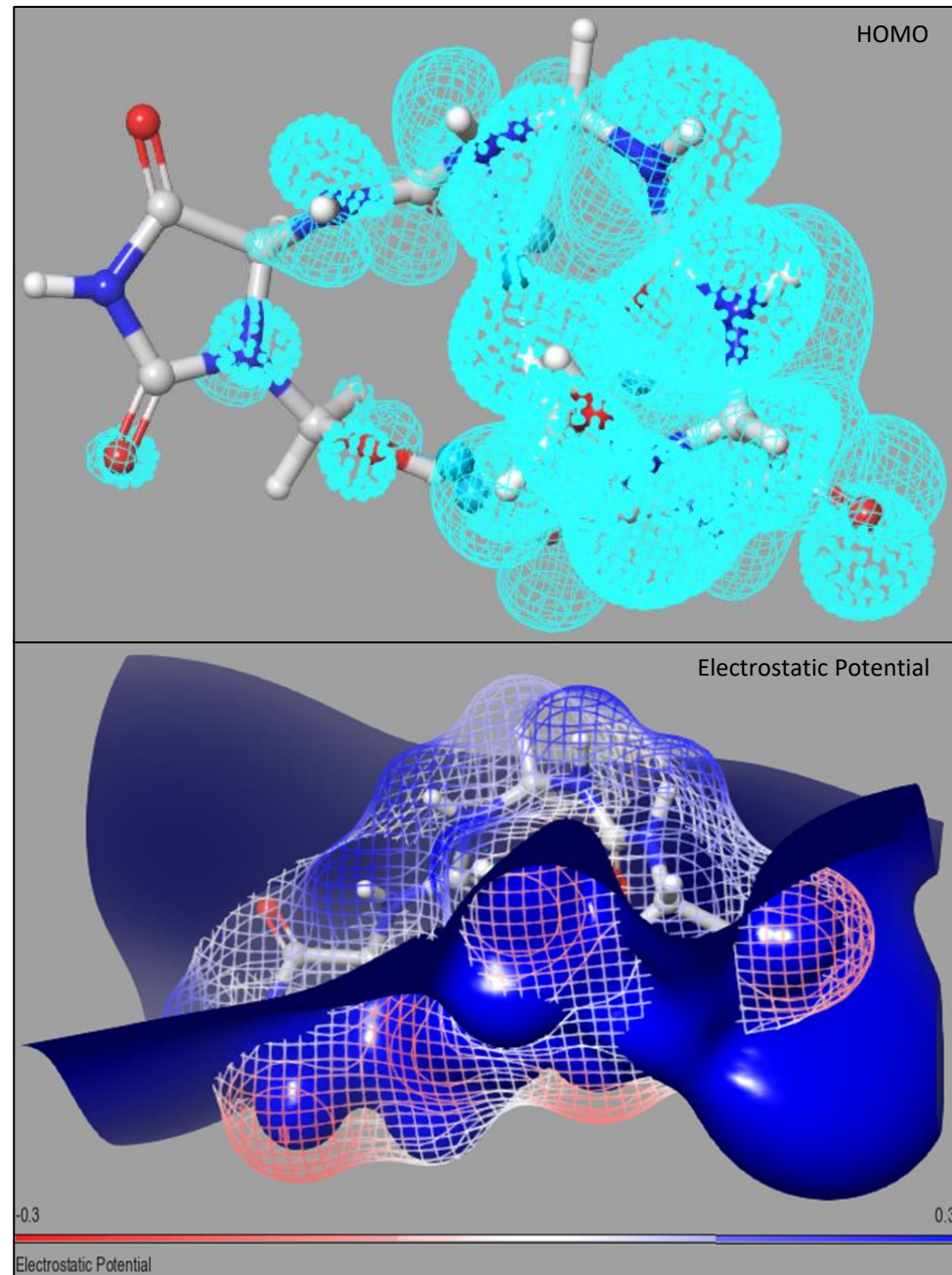
PhD Scholar (Bioinformatics)

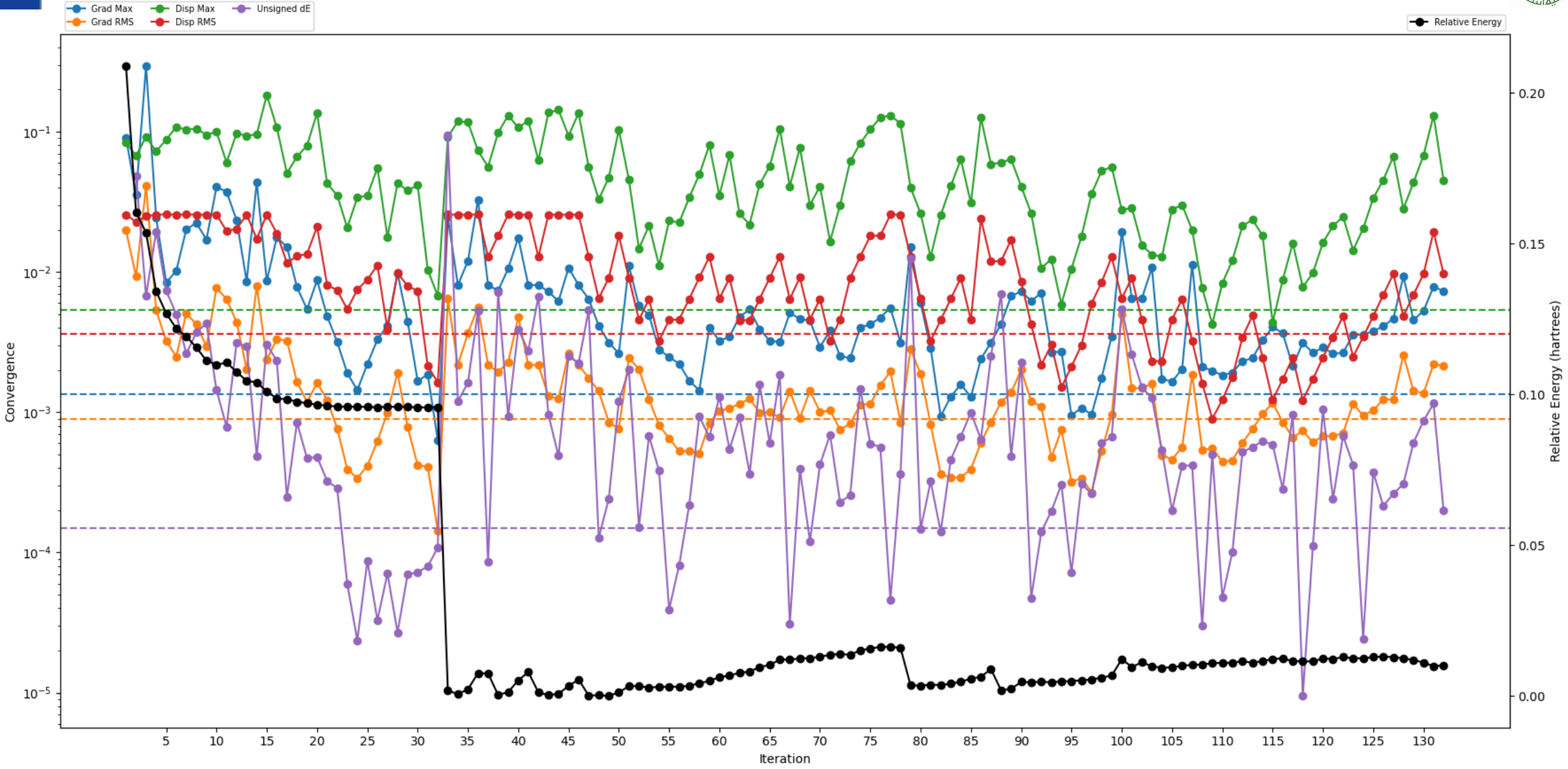
Jamia Millia Islamia University, New Delhi, India.

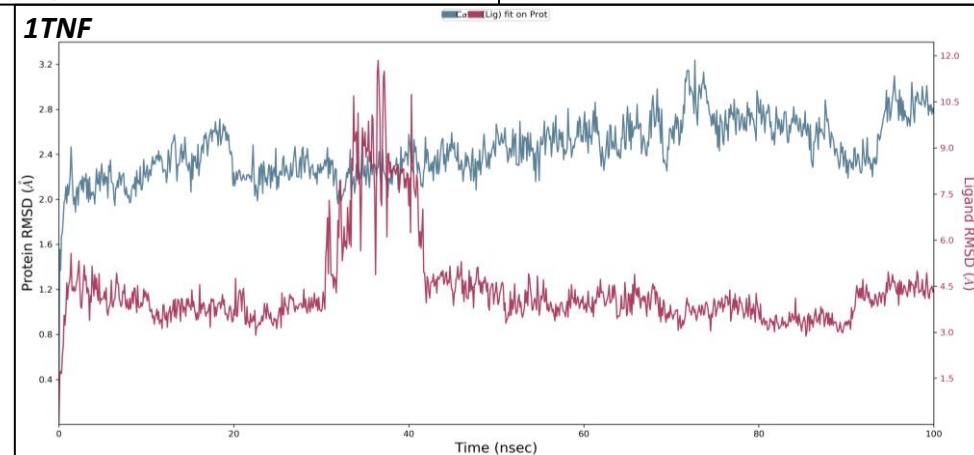
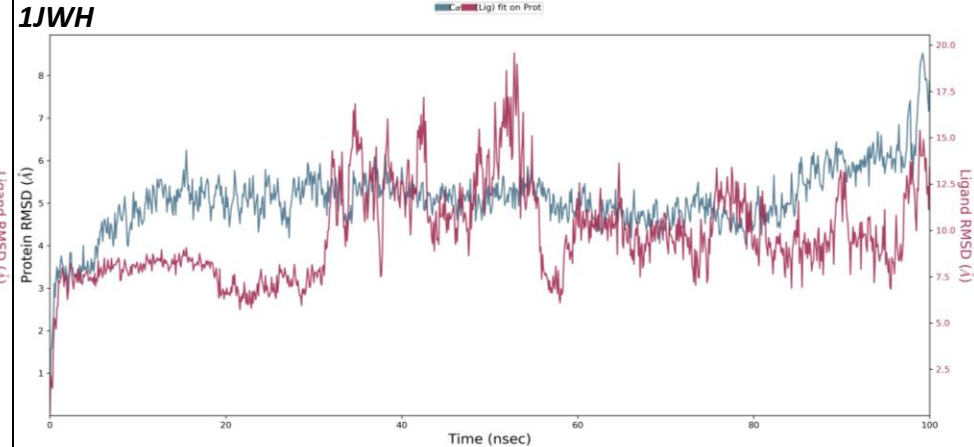
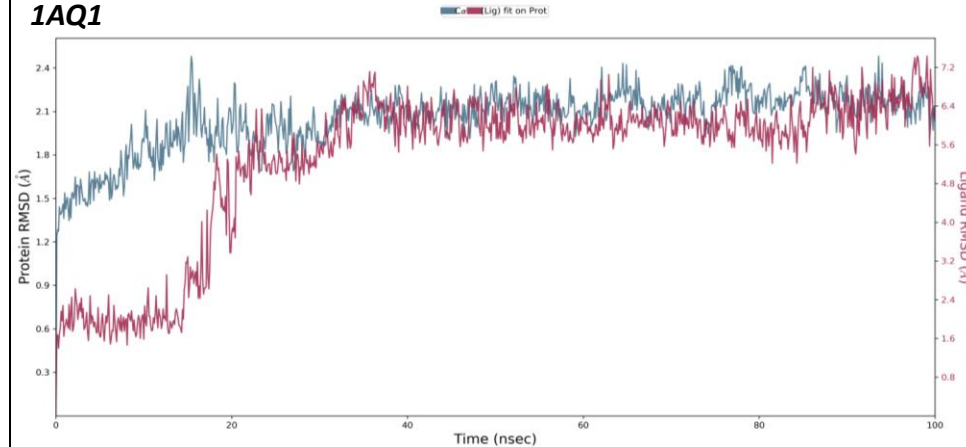
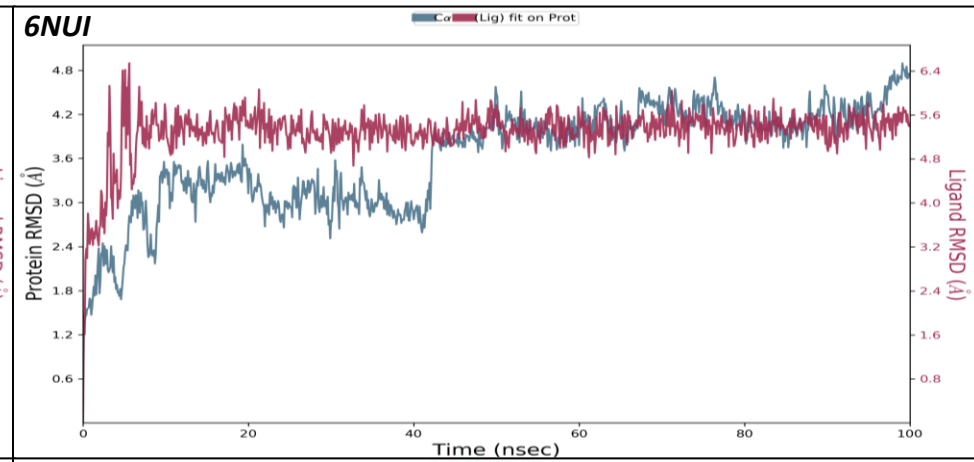
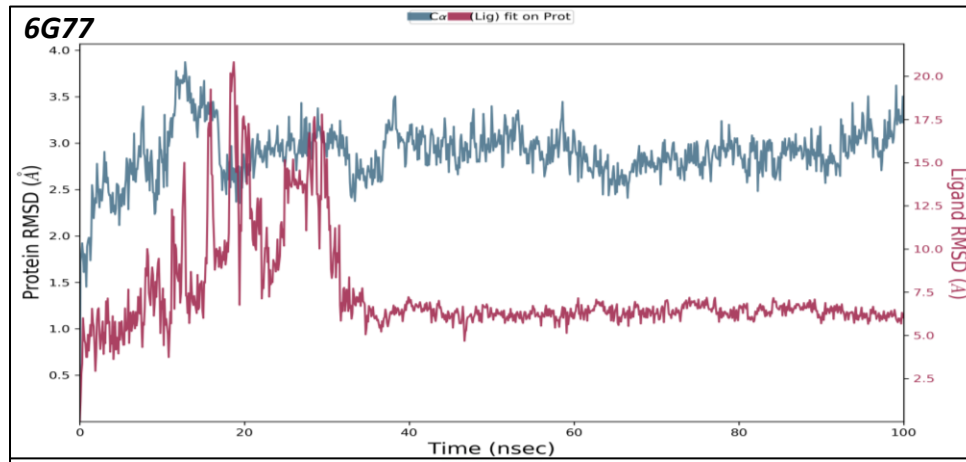


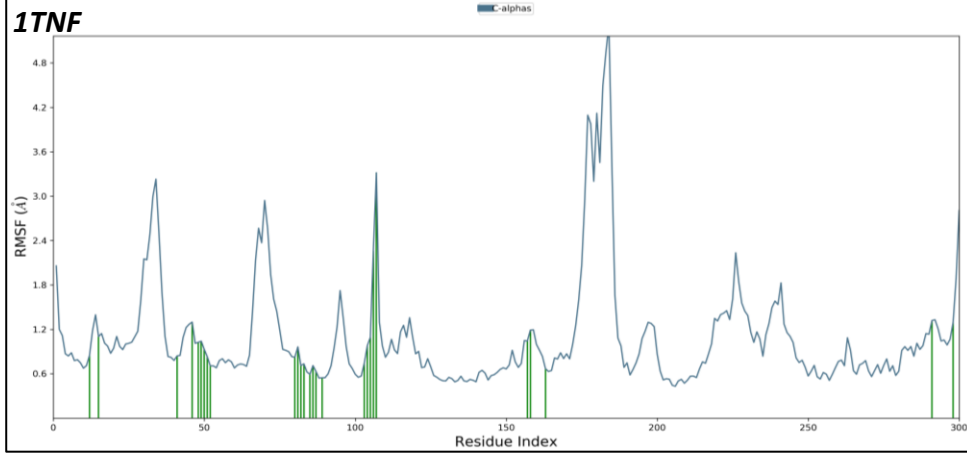
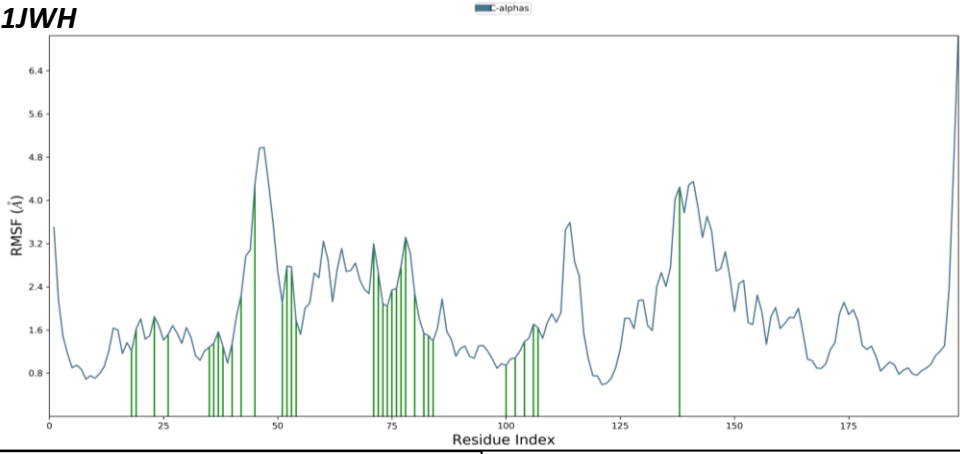
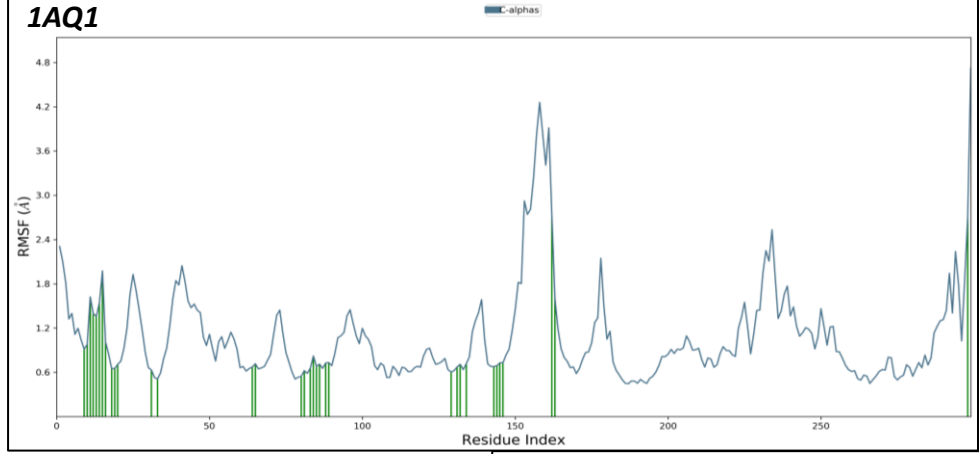
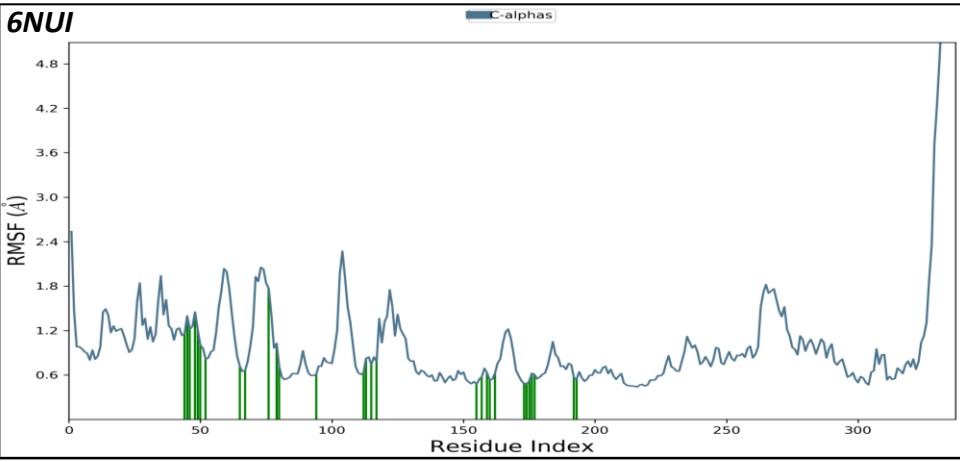
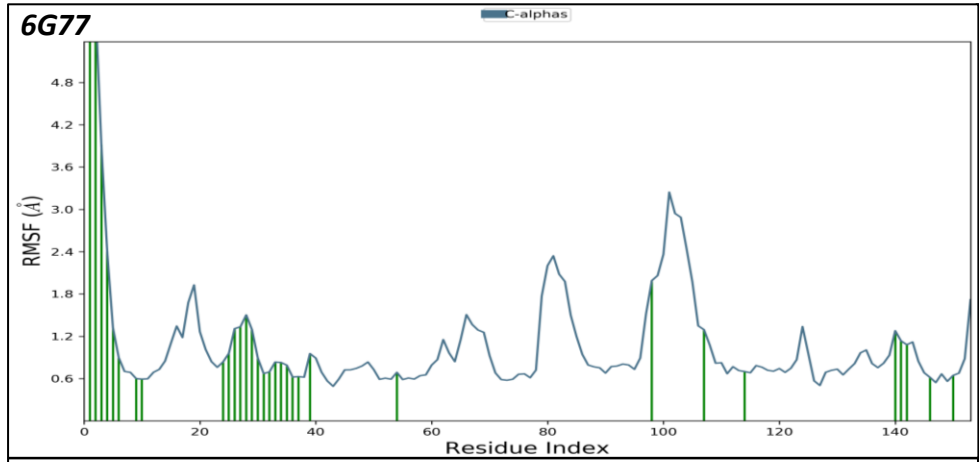


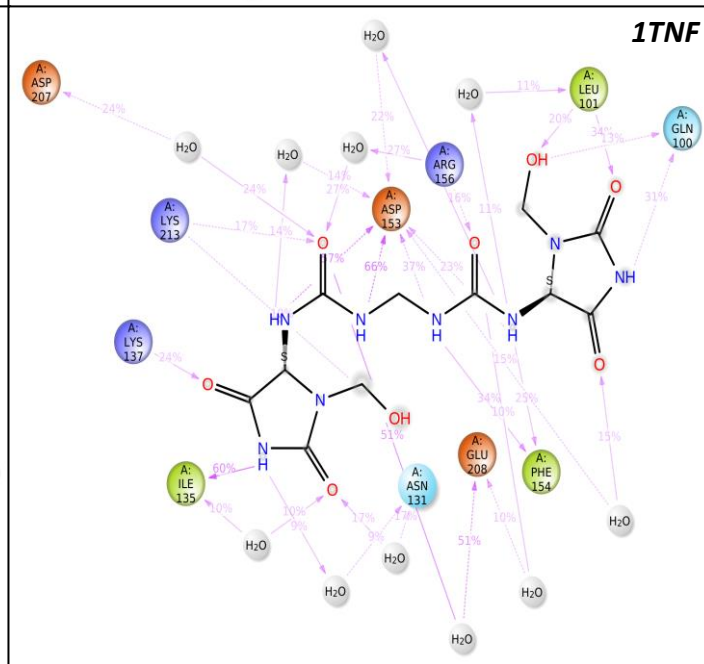
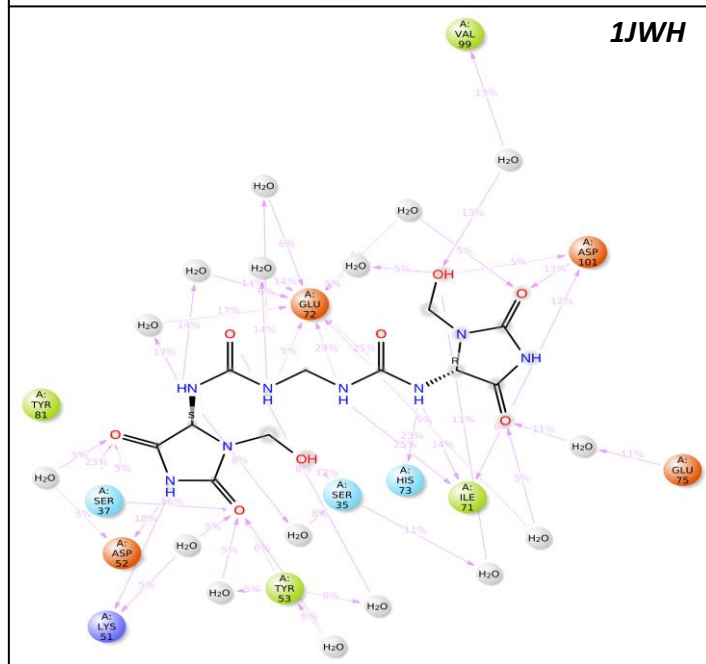
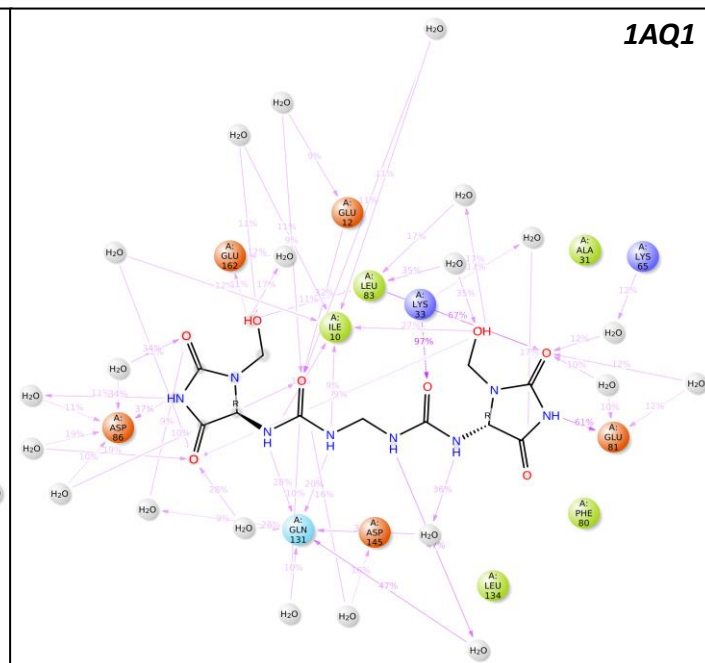
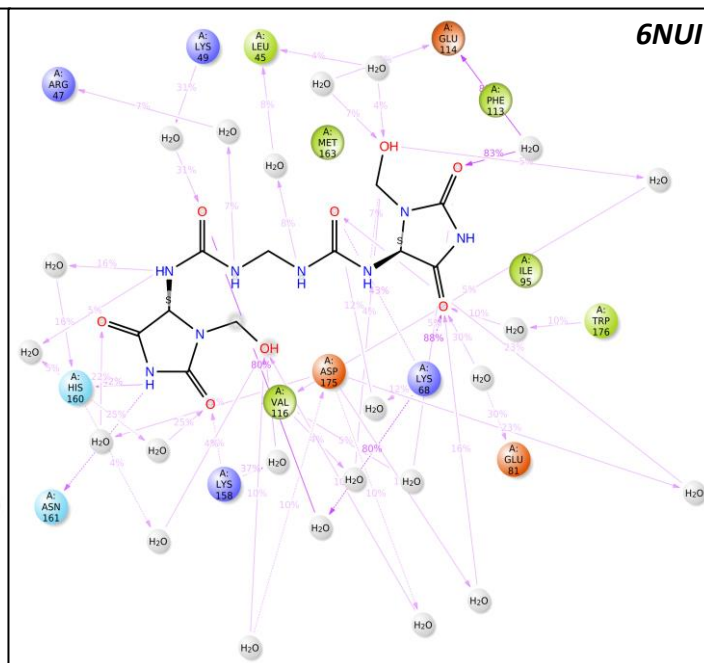
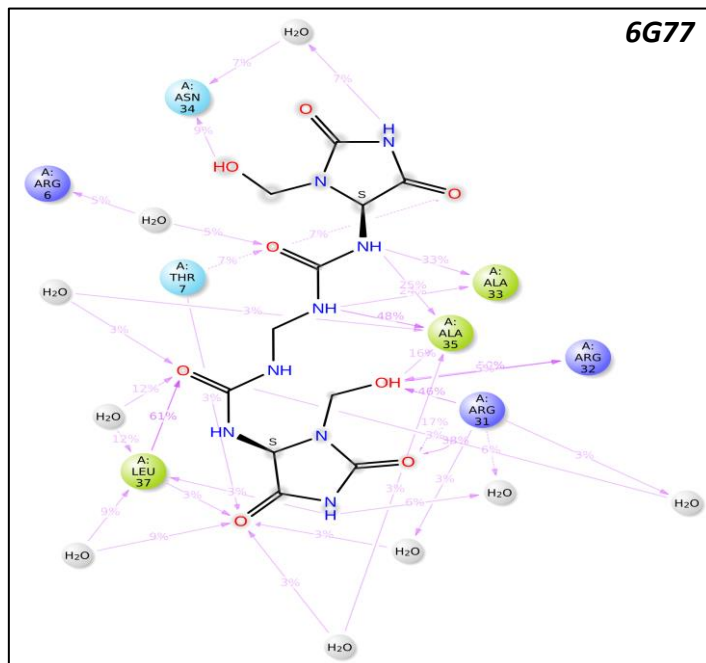




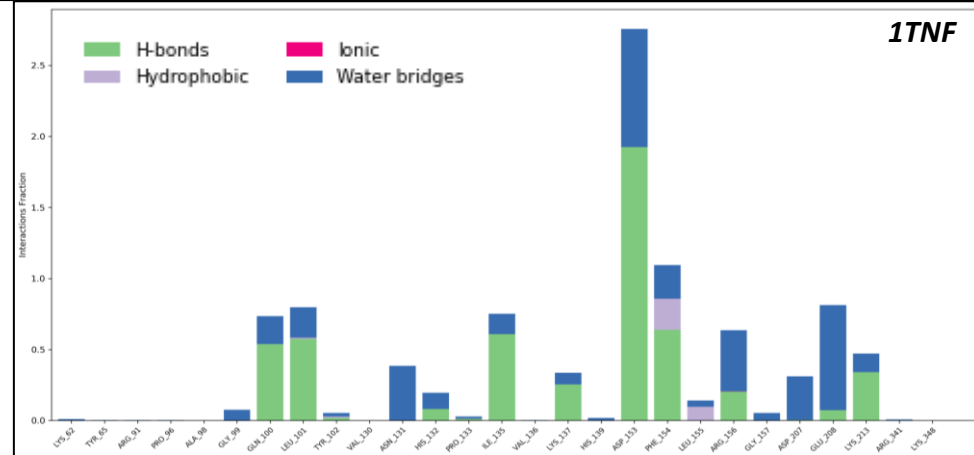
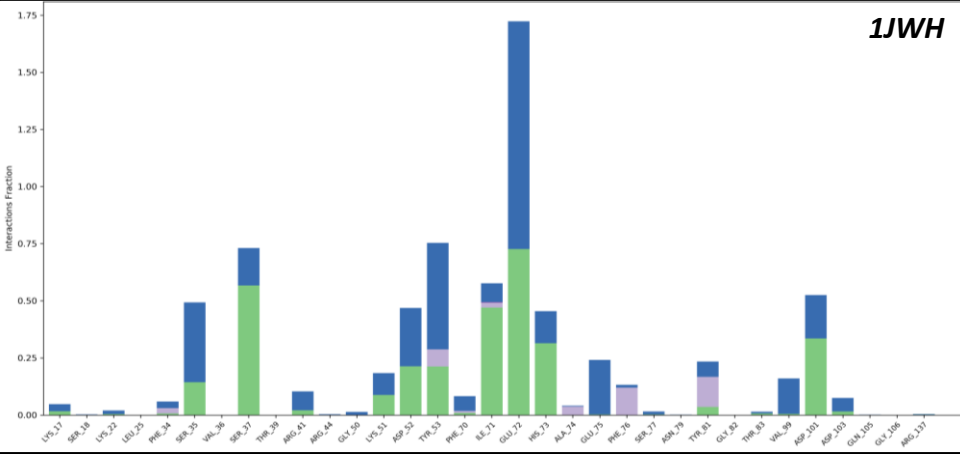
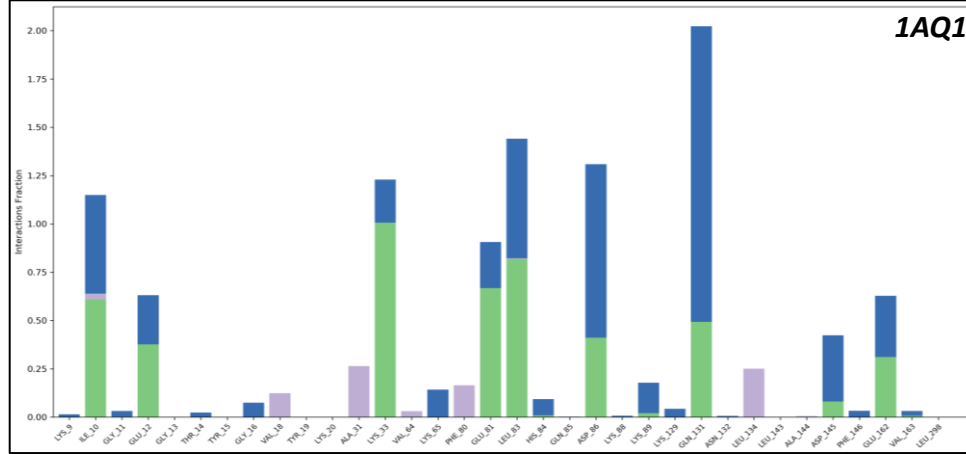
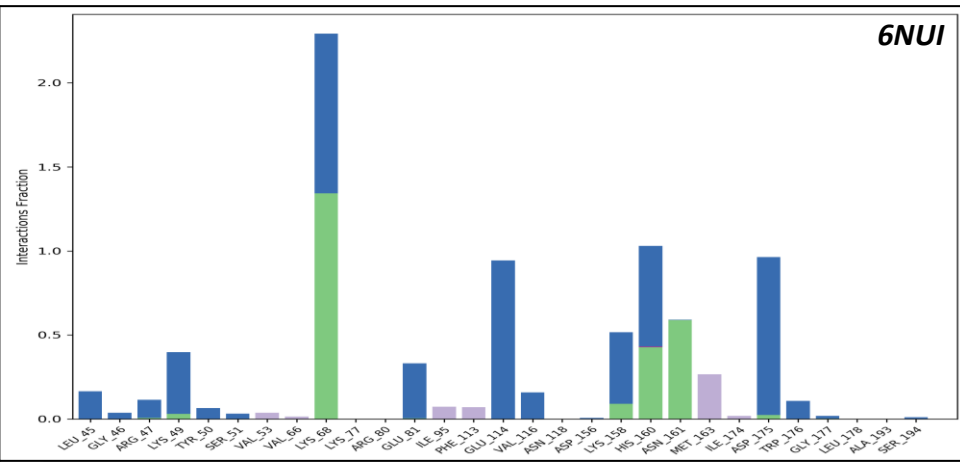
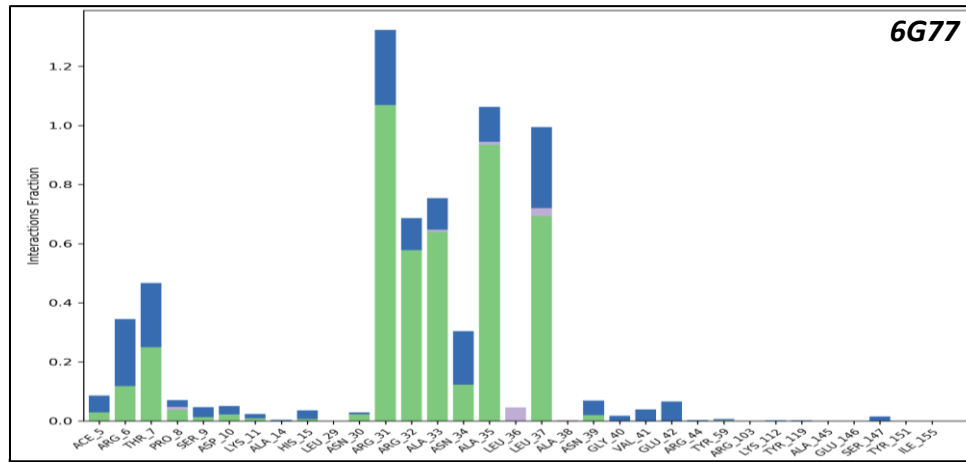


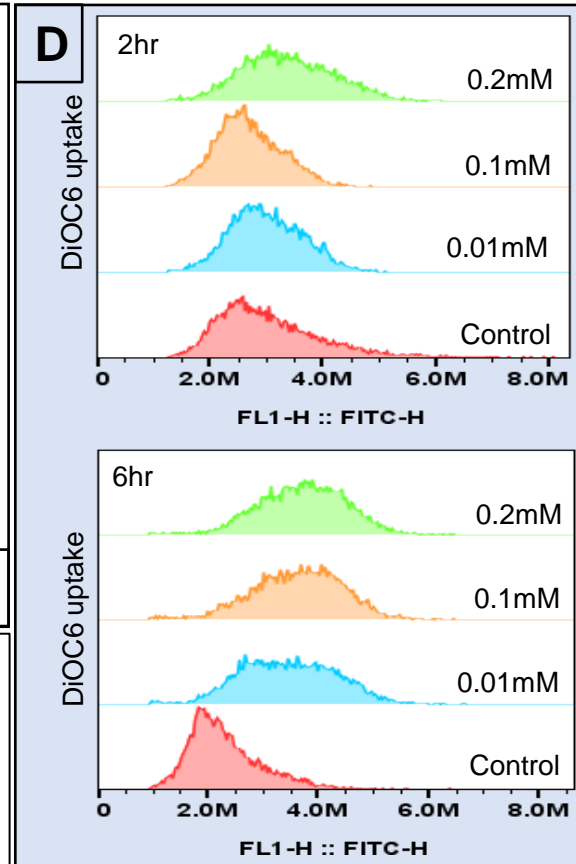
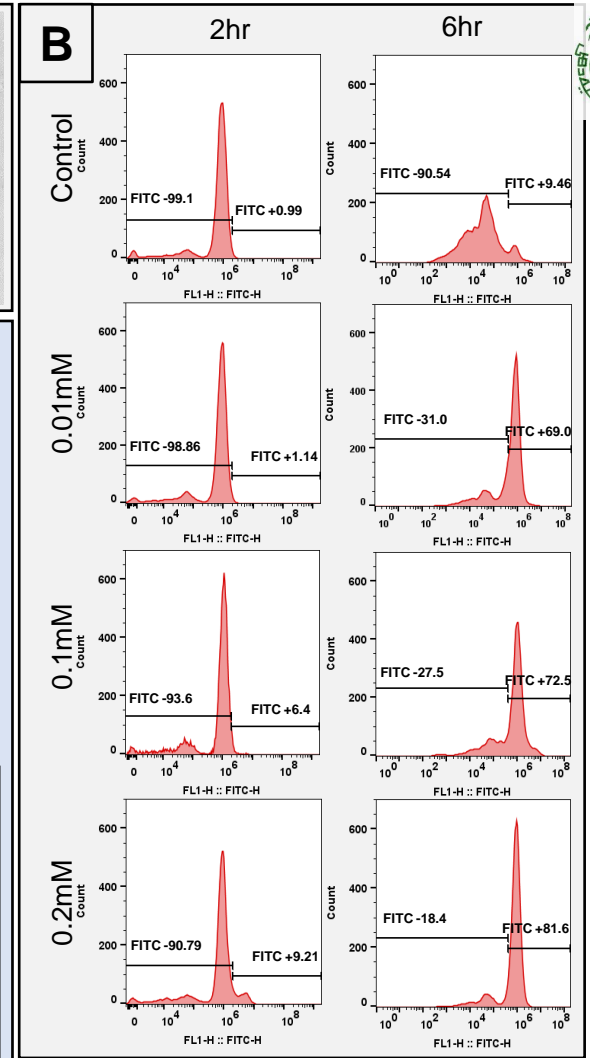
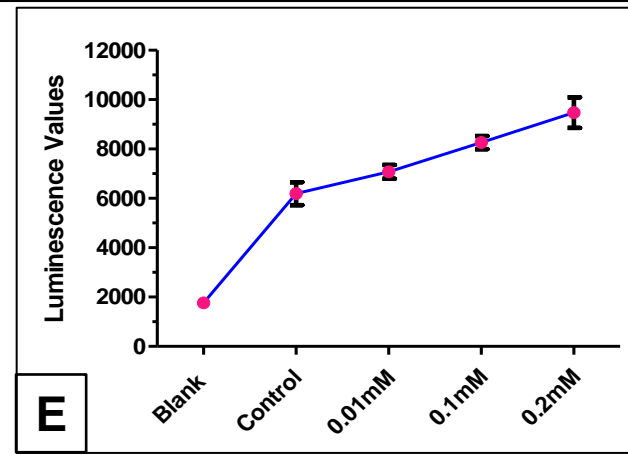
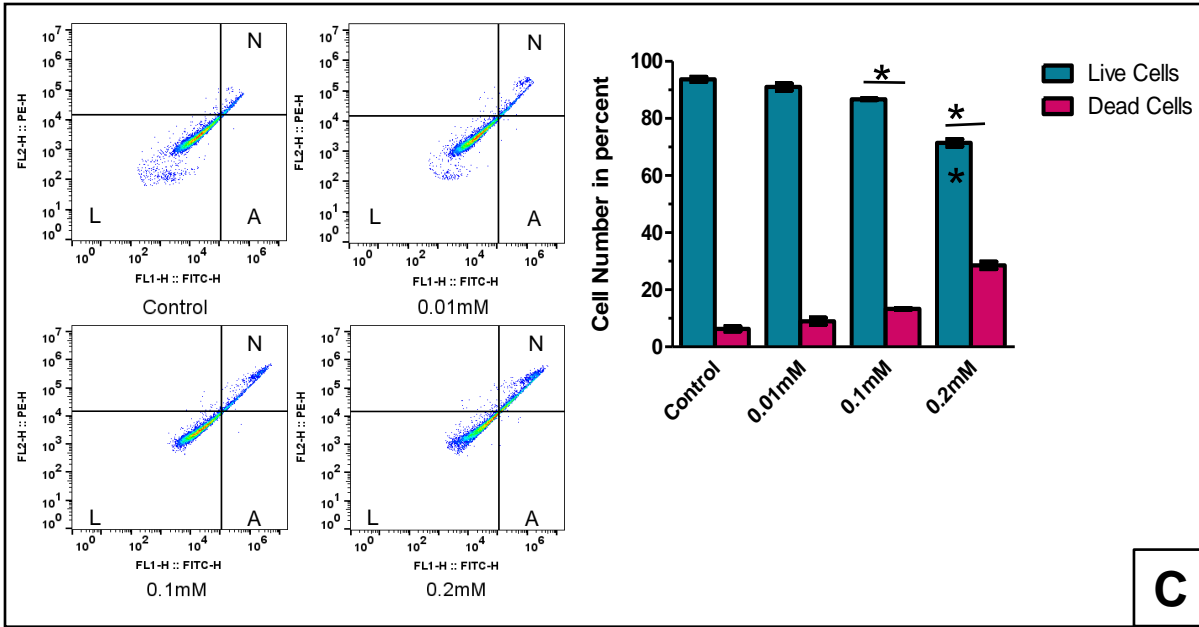
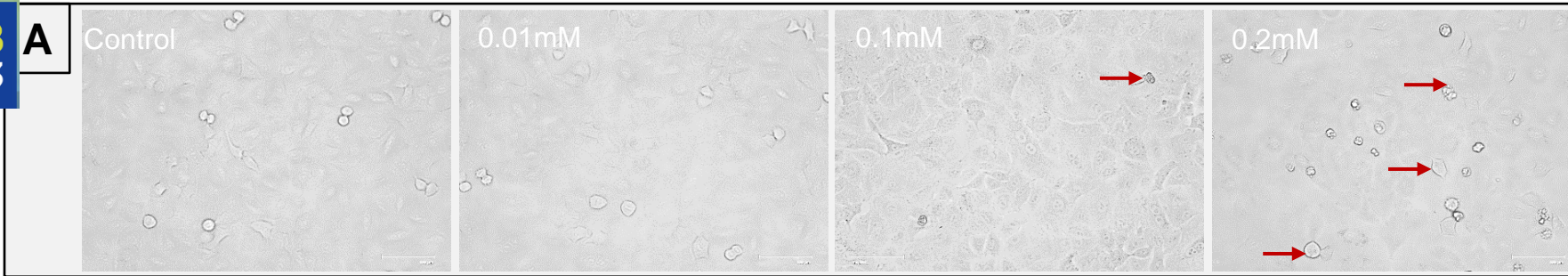






● Charged (negative) ● Hydrophobic ● Water
● Charged (positive) ● Polar ● Solvent exposure





Conclusion

- The food and drug administration has approved almost 100 drugs against SCLC and NSCLC, which are being used actively. However, this is unfortunate; even after so much expenditure, the world frequently faces the drug resistance problem and needs a new drug.
- This study includes multisampling algorithms based on screening, ADMET analysis, interaction pattern analysis and MD simulation for 100ns in the SPC water medium has produced a promising results.
- In this study, we have identified Imidazolidinyl urea as a multitargeted inhibitor against lung cancer, validated with computational methods, and proven as a prominent candidate.
- The identified compound Imidazolidinyl urea has less chance to develop resistance, or it might take a more extended period. It can be experimentally validated and used for the welfare of humankind.
- This study also set an example of how to proceed with multitargeted drug designing or repurposing to cure any prevalent disease and developing resistance.

Thank You

