

Protein and Ligand Structure Analysis Using MATLAB: Insights for Drug Discovery

Subject : Biology & Research Methodology

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INTRODUCTION

► Protein-Ligand Interactions

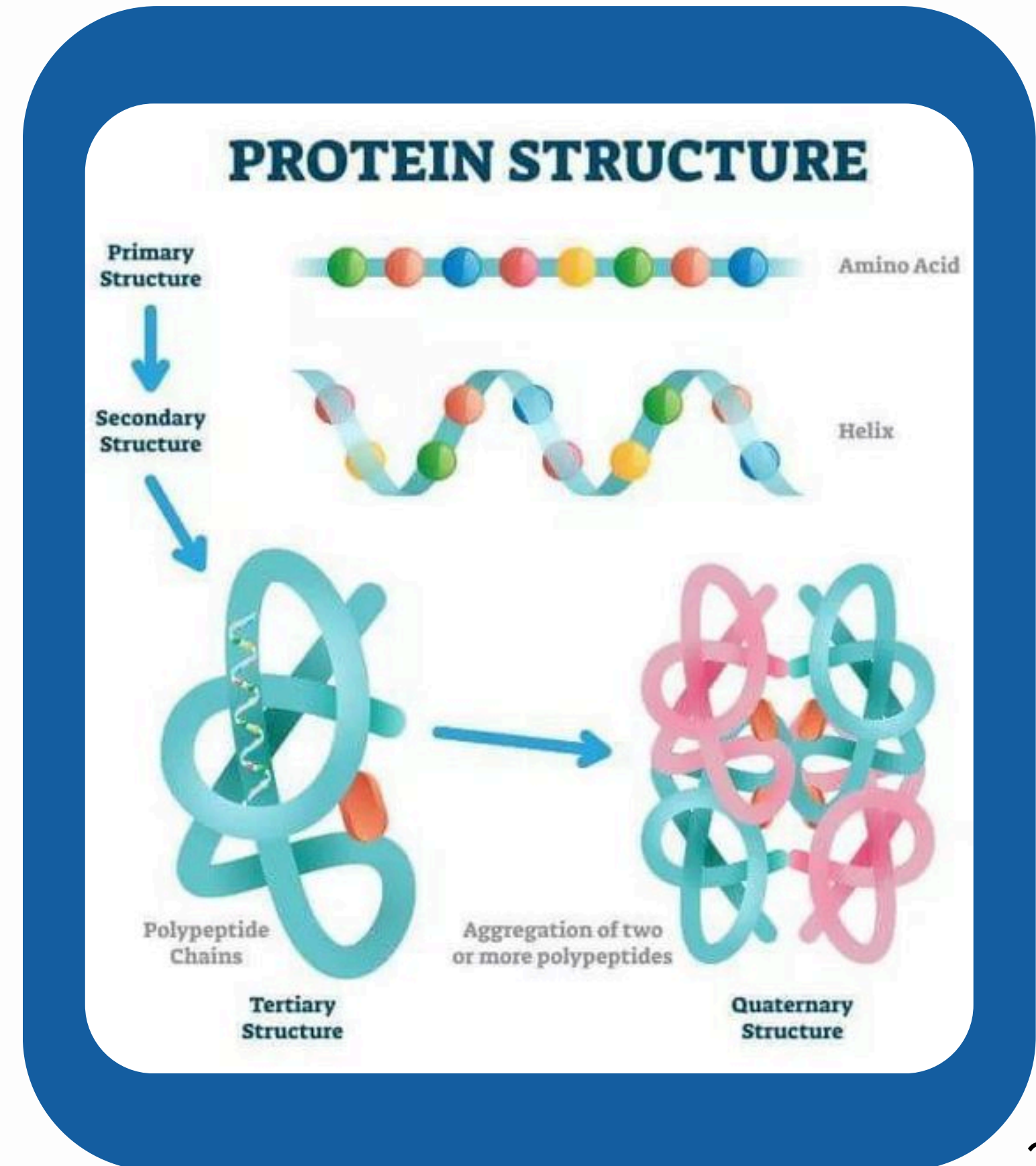
- Protein-ligand interactions are key in drug design, where a drug molecule (ligand) binds to a target protein at a binding site to alter its function.

► Importance in Drug Discovery

- Understanding these interactions helps design effective, targeted drugs with better binding affinity and fewer side effects.

► Objective

- Use MATLAB to identify active sites and analyze protein-ligand interactions for rational drug design.



Importance of binding sites in Drug discovery

- **Targeted Drug Development**

Binding sites are crucial for designing drugs that interact specifically with a target protein, ensuring precise therapeutic effects

- **Improved Drug Efficacy**

Identifying binding sites allows for the creation of drugs with high binding affinity, leading to stronger therapeutic outcomes.

- **Reducing Side Effects**

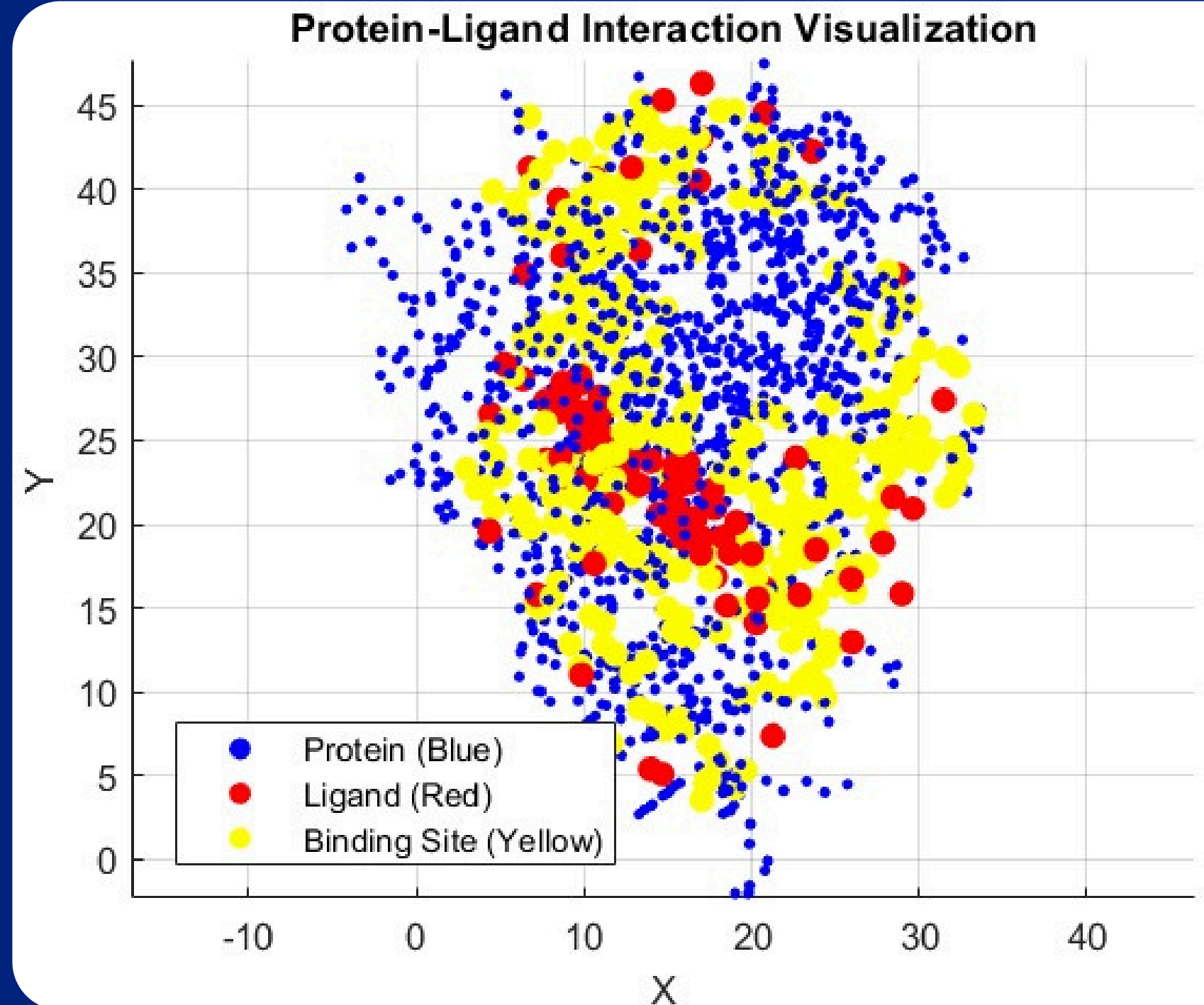
By targeting the correct binding site, drugs can avoid off-target effects, minimizing harmful side effects and increasing drug safety.

- **Rational Drug Design**

Knowledge of binding sites enables structure-based drug design, optimizing drugs for better performance and faster development.

MATLAB simulation of protein - ligand interaction and identification of binding sites

- Visualization of 3D Structures
- Binding Site Identification
- Protein-Ligand Interaction Analysis



HIV-1 protease in complex with inhibitor AHA455

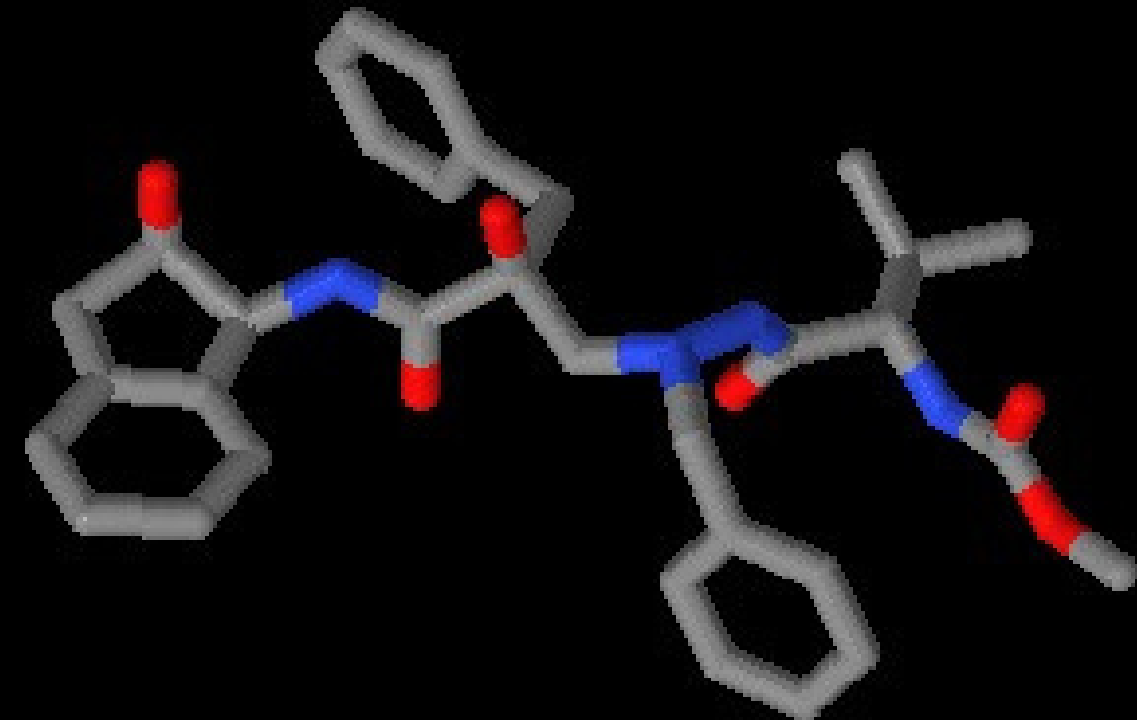
3D model of protein and ligand structures

PROTEIN



HIV-1 protease

LIGAND



AHA455

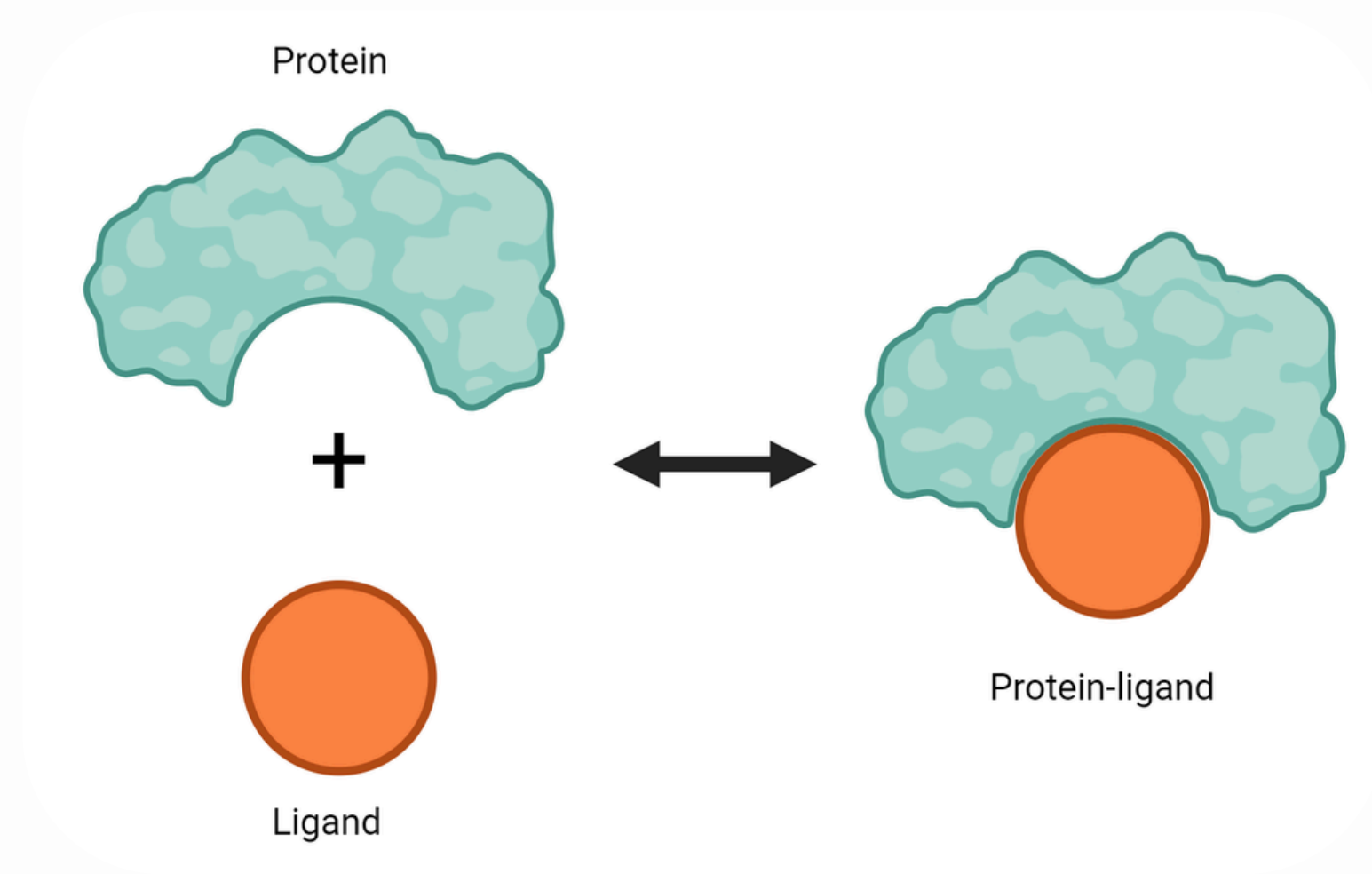
Active site identification and importance

- **Active Site:** Specific protein region where a ligand binds and reactions occur.
- **Importance in Drug Design:**
 - Precision: Enables targeted action on proteins, enhancing drug effectiveness.
 - Binding Affinity: Supports strong ligand attachment for potent drug response.
- **Optimizing Specificity:** Reduces off-target effects, improving drug safety.
- **Protein Function Insight:** Understanding active sites helps clarify protein roles, aiding drug discovery.

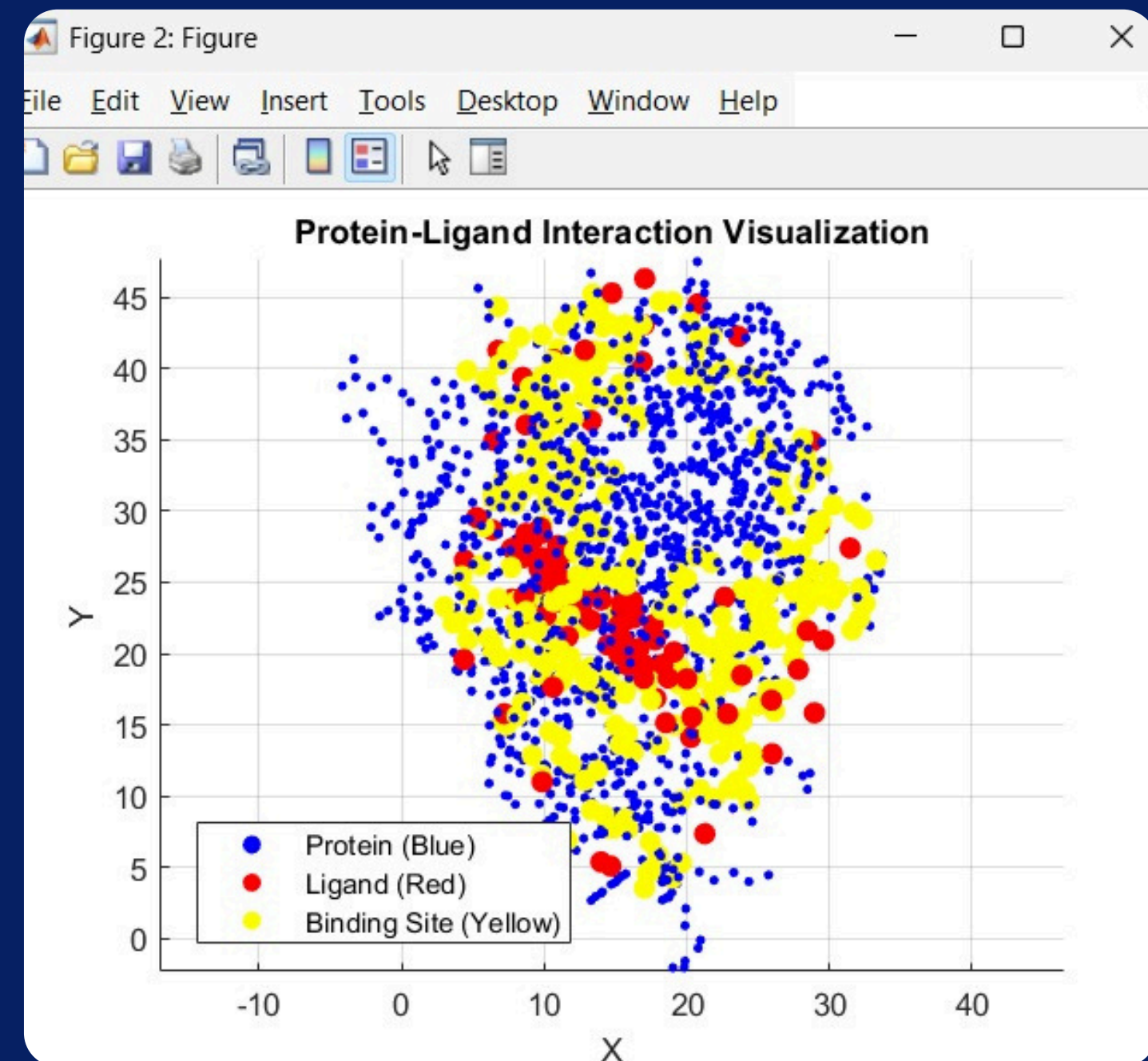
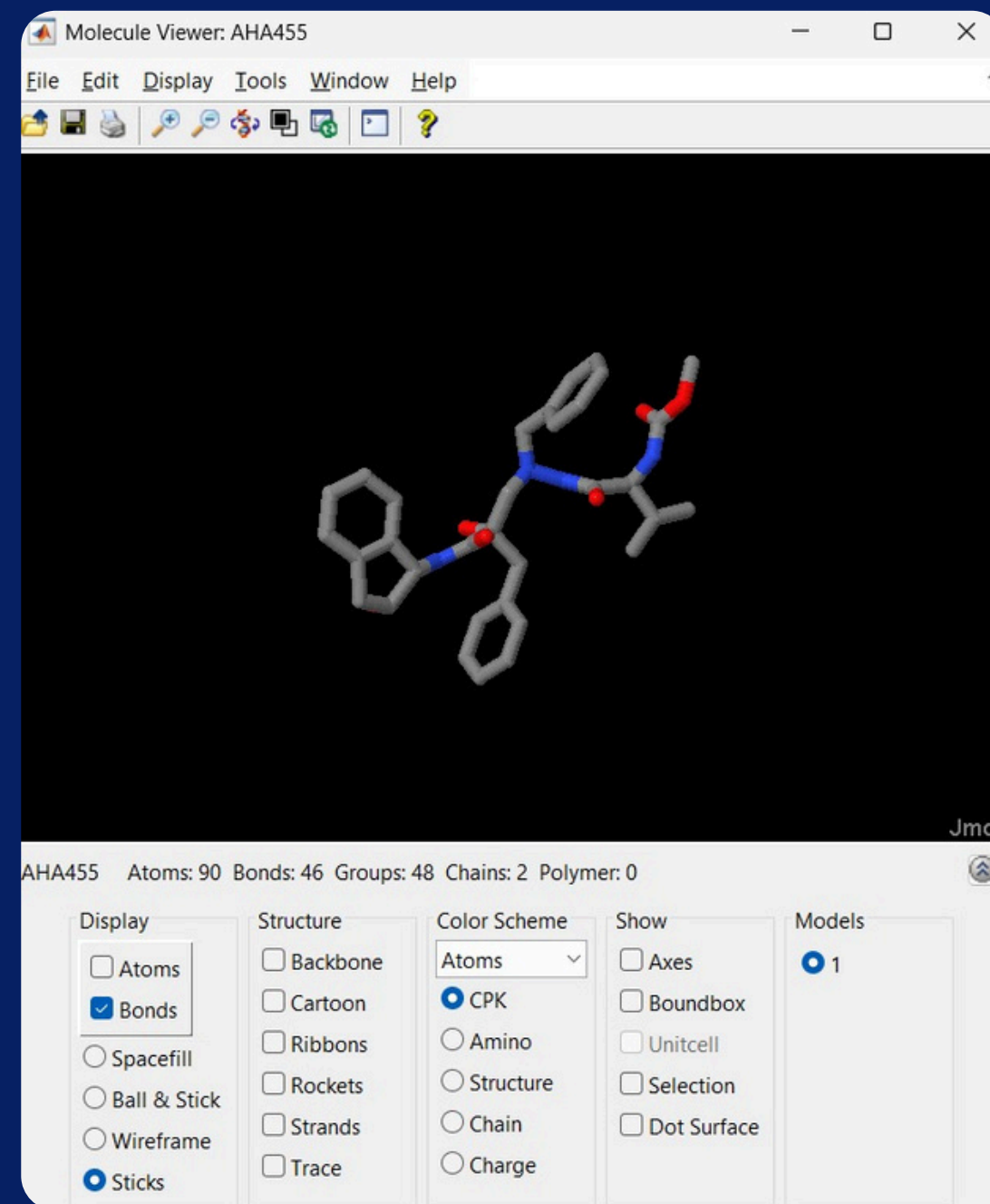
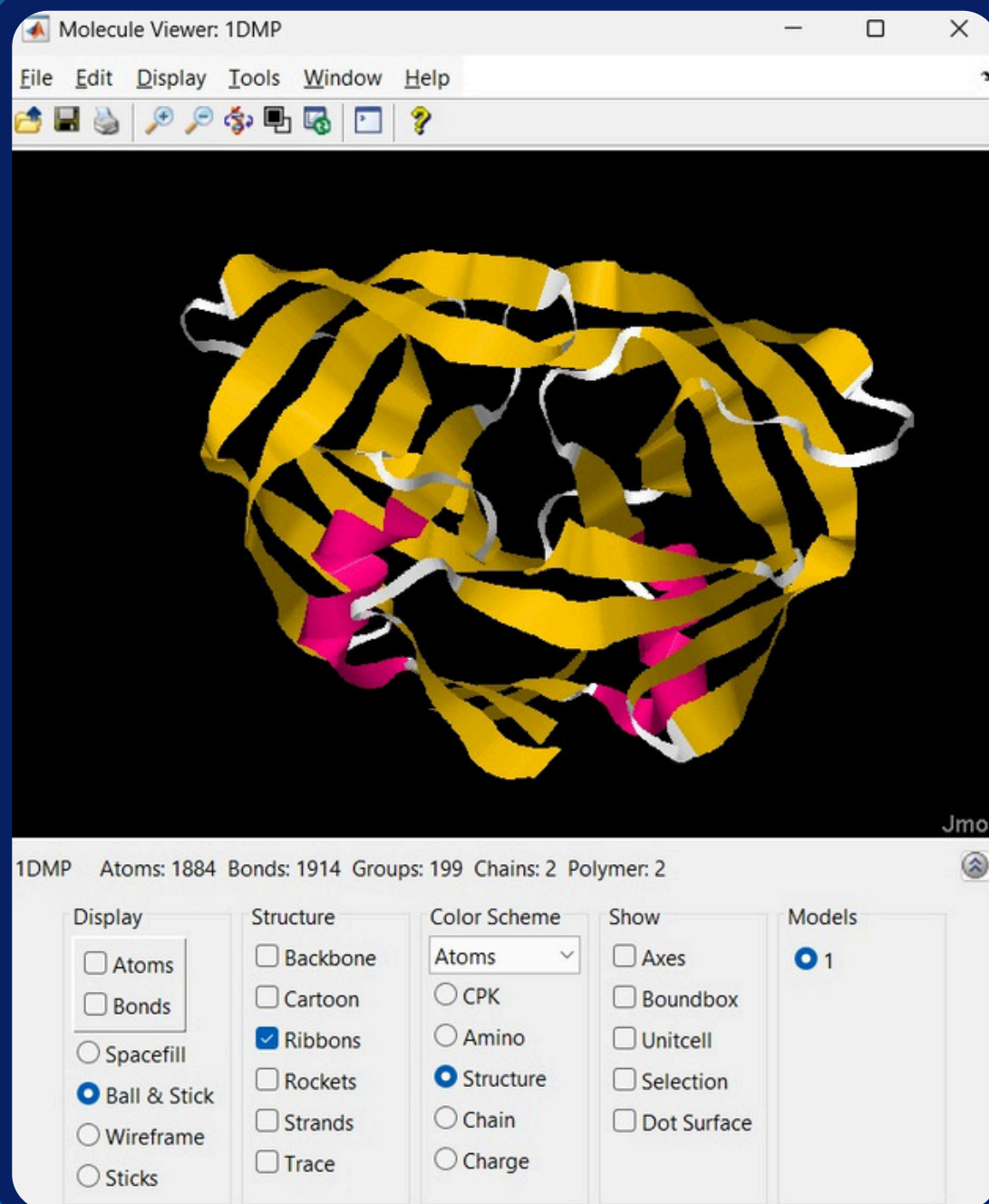


Ligand binding and interactions

- **Ligand Binding:** Ligands attach to specific protein sites to initiate a biological response.
- **Key Interactions:**
 - Hydrogen Bonds: Stabilize ligand-protein complex.
 - Hydrophobic Interactions: Favor nonpolar regions.
 - Ionic Bonds: Strengthen binding via electrostatic attraction.
- **Importance in Drug Design:**
 - Binding Affinity: Strong interactions improve drug effectiveness.
 - Specificity: Targeted binding reduces side effects.
- **Drug Optimization:** Visualizing interactions helps refine drug structure for enhanced potency and safety



Simulation Results



Application to drug discovery

▶ Accelerating Drug Development

- Simulation of binding sites helps identify promising drug candidates early, reducing time and costs in drug development.

▶ Structure-Based Drug Design

- Protein-ligand interaction insights allow for designing drugs with higher affinity and specificity, improving therapeutic effectiveness.

▶ Minimizing Side Effects

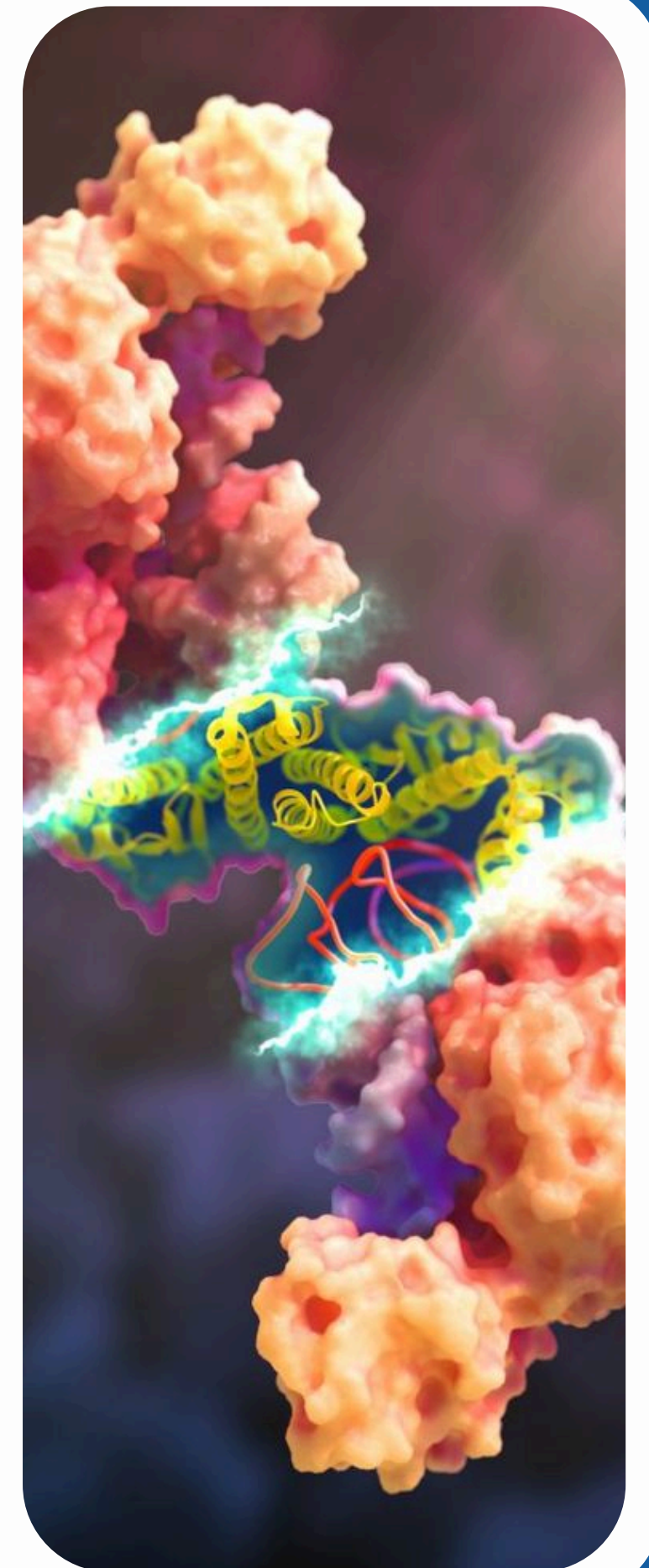
- Understanding binding interactions helps design drugs that target only specific proteins, lowering the risk of off-target effects and side effects.

▶ Personalized Medicine

- By analyzing binding sites, drugs can be customized for individuals based on unique protein structures, supporting personalized treatment approaches

Conclusion

- **Protein-Ligand Interactions:** Understanding these interactions and identifying binding sites are crucial steps in targeted drug design.
- **MATLAB's Contribution:** The simulation offers a powerful tool for visualizing protein-ligand binding and analyzing interactions, which supports rational drug discovery.
- **Benefits to Drug Development:**
 - Accelerates drug discovery processes.
 - Reduces development costs.
 - Improves drug efficacy and safety through precise targeting.
- **Future Potential:** Enhanced computational methods will further drive personalized medicine and expand effective treatments for various conditions.



A person wearing VR goggles is shown in profile, interacting with a futuristic digital interface. The interface features glowing blue lines, circular data visualizations, and various icons. The person is wearing a white lab coat. The background is dark and filled with more digital elements.

THANK YOU