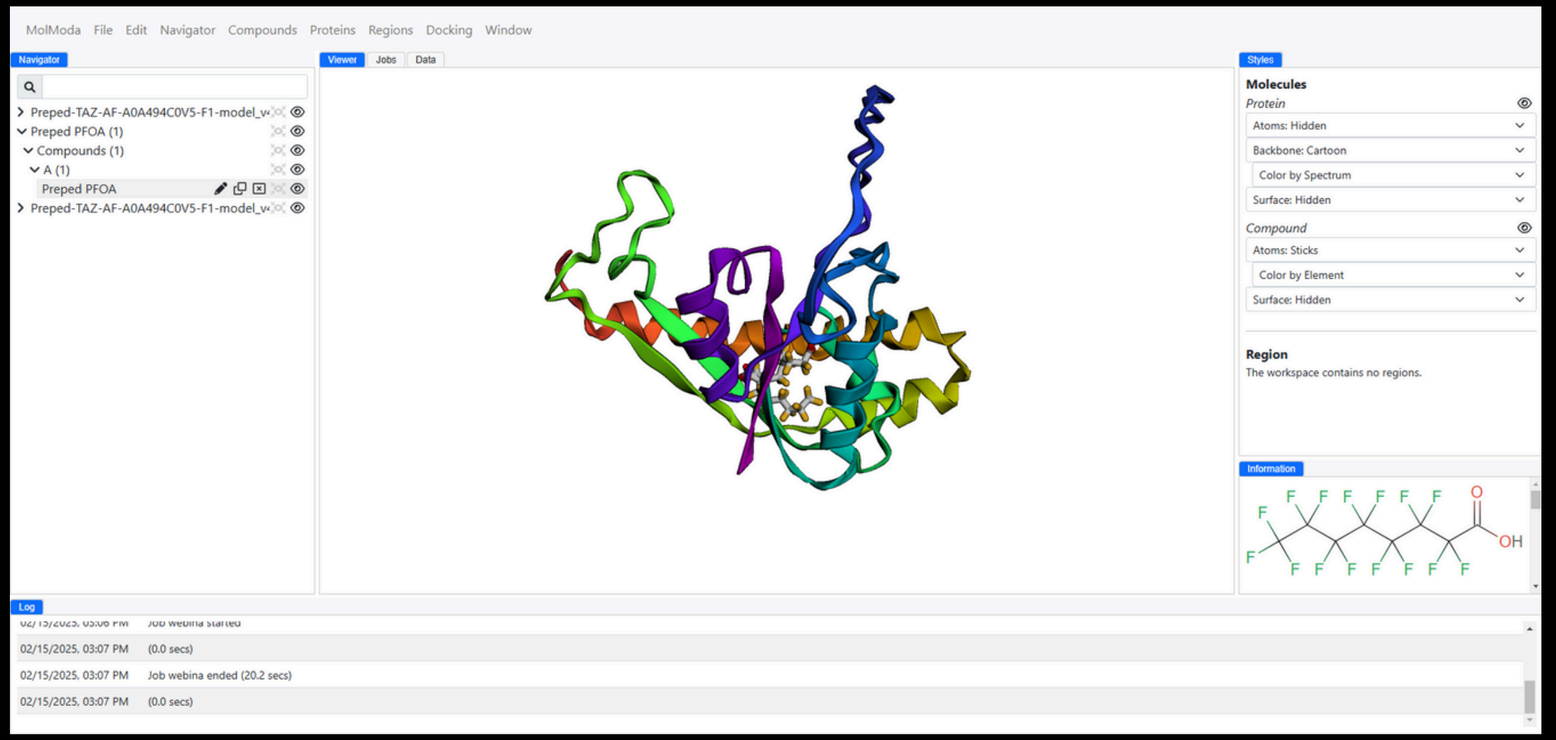
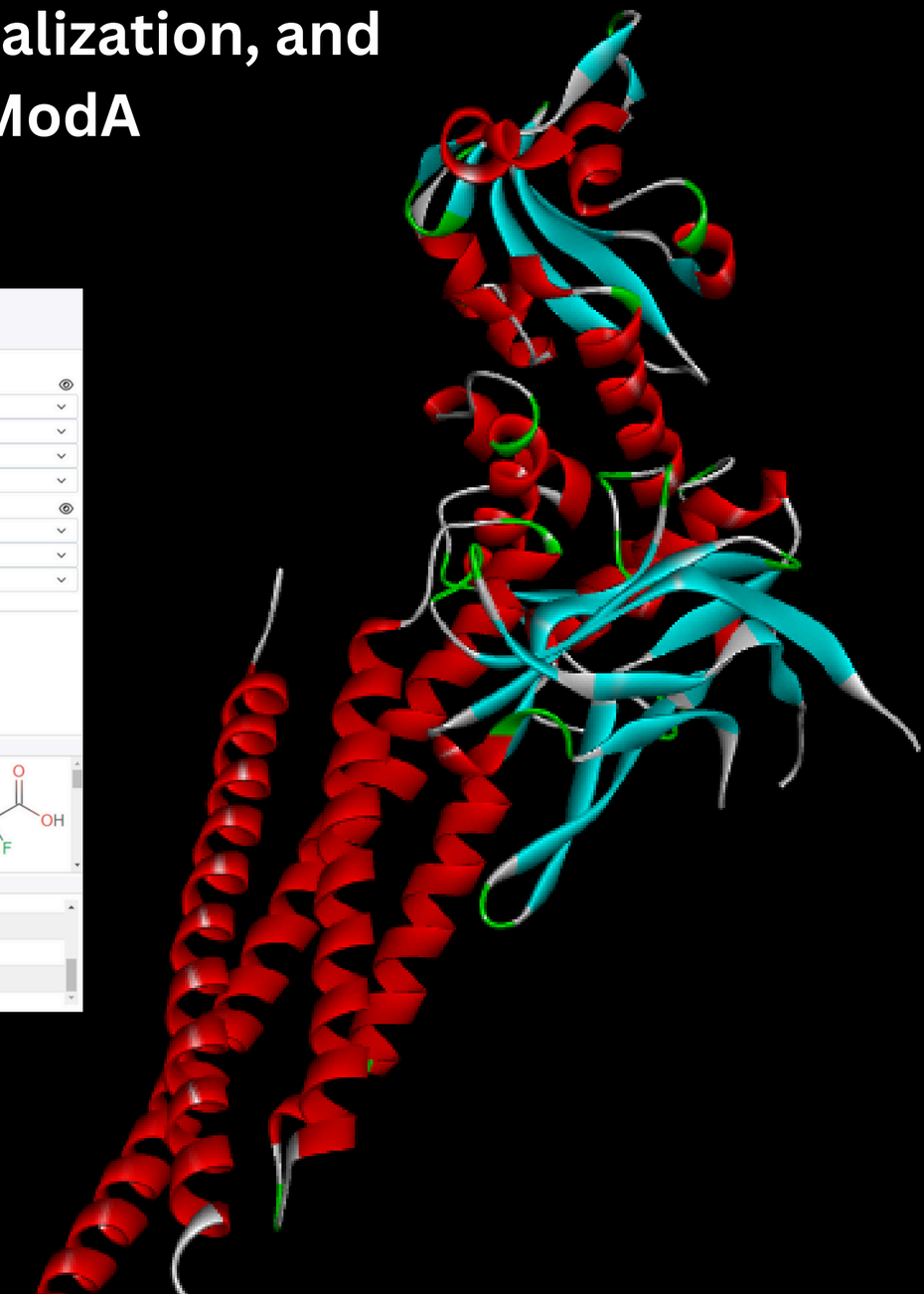
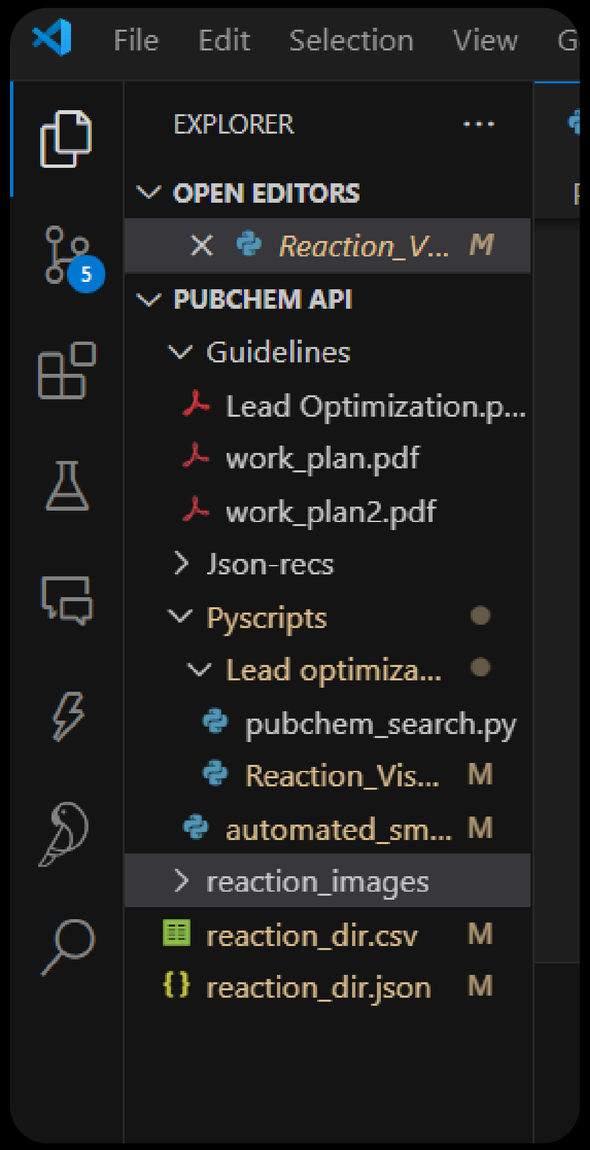
Automating PubChem Data Retrieval, Reaction Visualization, and Fragment-Based Lead Optimization in MolModA



MolModA





AIM: This project incorporates new features into MolModa by automating molecular data retrieval, reaction visualization, and fragment-based lead optimization, making it a more efficient tool for molecular docking and drug discovery

- **PubChem API Integration**: Enables users to retrieve molecular properties of input compounds within MolModa.
- **Reaction Visualization**: Generates labeled images of chemically tractable reactions, allowing users to select and apply transformations to their molecules.
- **Reactive Fragment Database**: Provides a library of commercially available small molecules (<150 Da) with reactive moieties, helping users grow lead compounds with valid chemical transformations.