

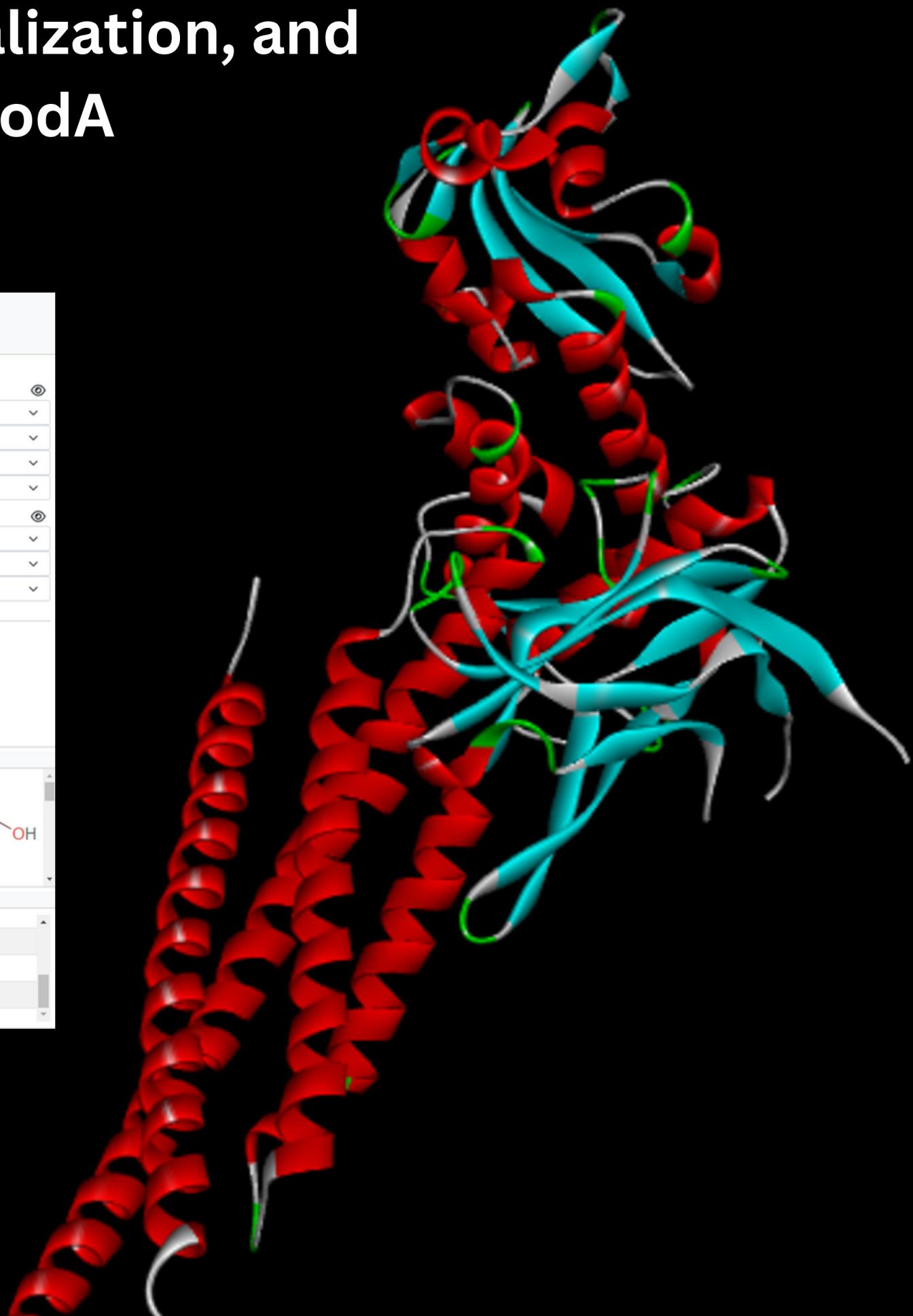
Automating PubChem Data Retrieval, Reaction Visualization, and Fragment-Based Lead Optimization in MolModA

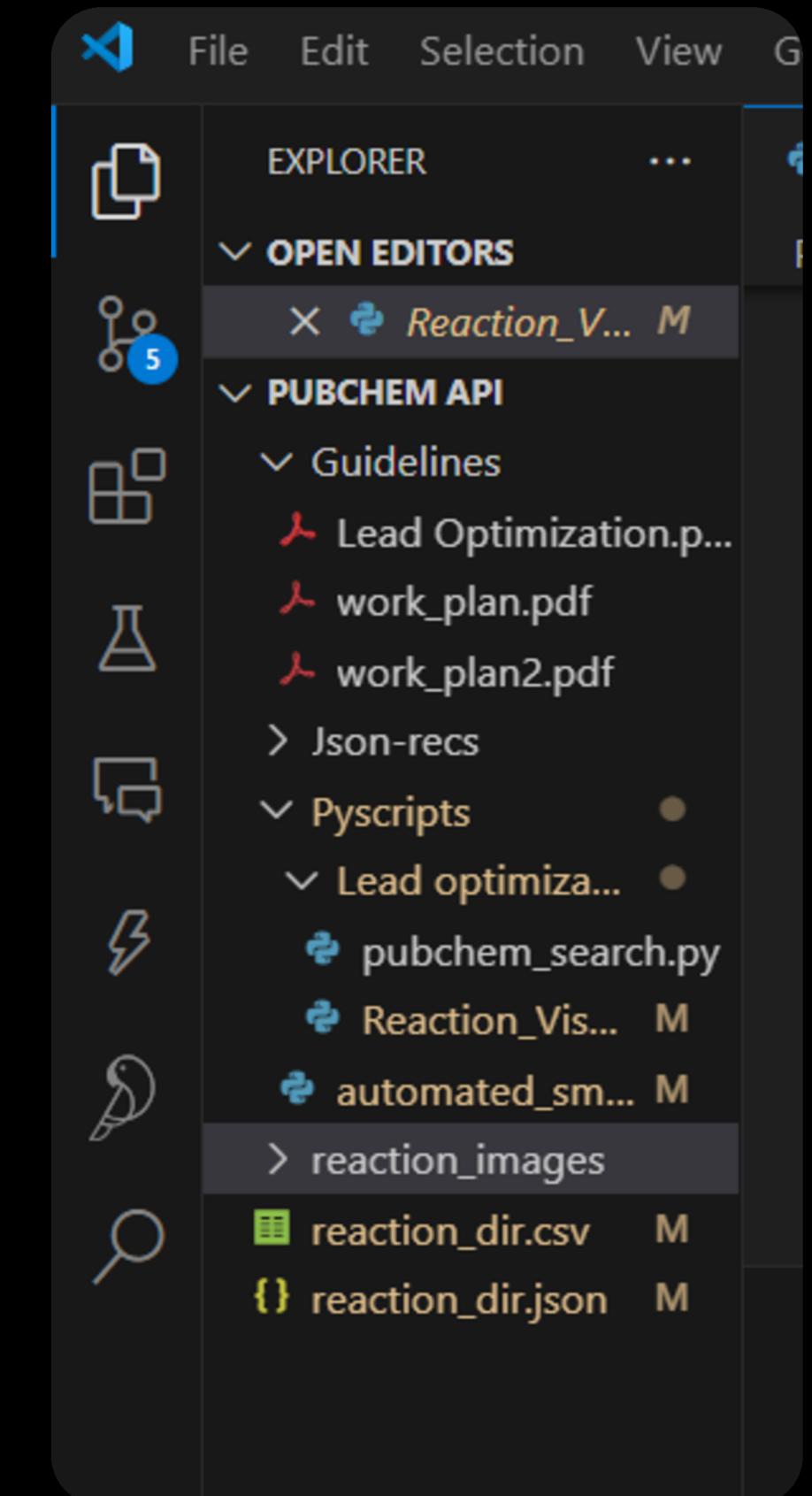
The screenshot shows the MolModA software interface. The main window displays a 3D ribbon model of a protein-ligand complex. The protein backbone is shown in red, while the ligand is represented by colored sticks (green, blue, purple). To the left of the viewer is a navigation panel with a search bar and a tree view of project files. The tree view includes entries like 'Preped-TAZ-AF-A0A494C0V5-F1-model_v2', 'Preped PFOA (1)', 'Compounds (1)', and 'A (1)'. Below the navigation panel is a log window showing the following entries:

- 02/15/2025, 03:07 PM Job webina started
- 02/15/2025, 03:07 PM (0.0 secs)
- 02/15/2025, 03:07 PM Job webina ended (20.2 secs)
- 02/15/2025, 03:07 PM (0.0 secs)

On the right side of the viewer are several panels: 'Styles' (containing settings for 'Protein' and 'Compound'), 'Region' (noting 'The workspace contains no regions.'), and 'Information' (displaying the chemical structure of PFOA: FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)O).

MolModA





AIM: Integrating the scripts with MolModA automates the retrieval of molecules from Pubchem and their properties and enables application fragment-growing strategies for lead optimization. Users will input starting molecules, and the MolModa plugin will add fragments based on chemically feasible reactions.

- **PubChem API Integration:** Enables users to retrieve molecular properties of input compounds within MolModa.
- **Reaction Visualization:** Create an RDKit-based script to generate simple images representing a set of chemically tractable reactions (sourced from a GitHub repository).
- **Reactive Fragment Database:** Develop a Python script to query PubChem for small molecules (<150 Da) containing reactive moieties that can participate in the listed reactions.

