

molvizpy

May 2024

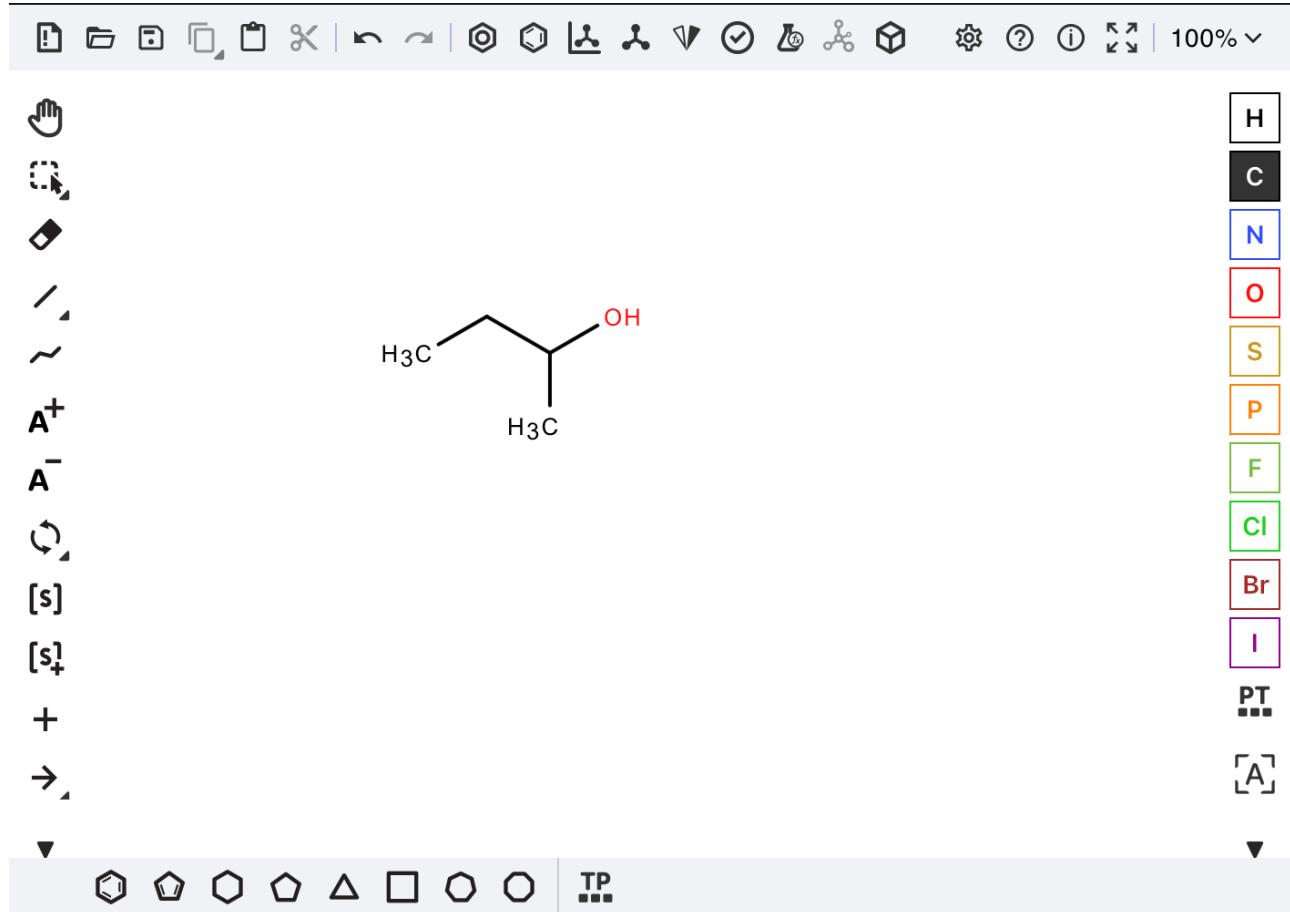
We are showcasing our python package/app, molvizpy, which helps in viewing molecules in 3D and find their symmetry group:

The screenshot shows the MolVizPy web application. At the top, the title "MolVizPy" is displayed. Below it, there are two tabs: "General molecules" (which is selected) and "Proteins". A dropdown menu titled "Choose an identifier" is open, showing the option "Name" selected. In the text input field, the word "ethanol" is typed. Below the input field, there is a note: "Note: the app will prioritize the above's box so if you want to use the drawing option, make sure nothing is in the text box." To the right of the input field is a drawing toolbar with various chemical symbols and a periodic table of elements (H, C, N, O, S, P, F, Cl, Br, I). At the bottom of the interface is a large drawing canvas.

You can input a chemical identifier (SMILES, InChi, InChiKey, CID) or the name of a molecule:

A close-up screenshot of the "Choose an identifier" dropdown menu. The "Name" option is currently selected and highlighted in grey. Other options listed include "SMILES", "InChi", "InChiKey", and "CID".

Alternatively, you can also directly draw the molecule in the Ketcher box:

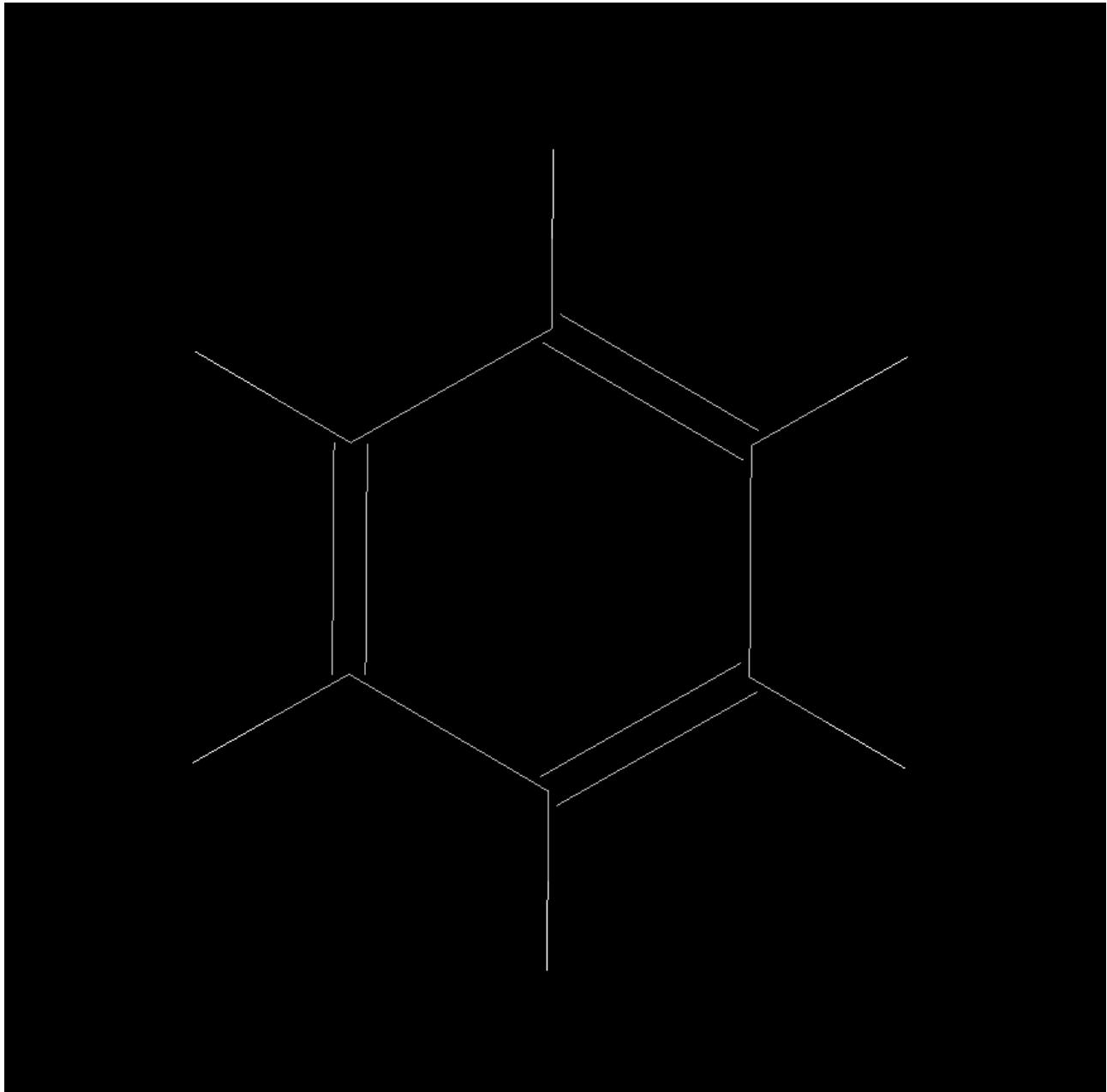


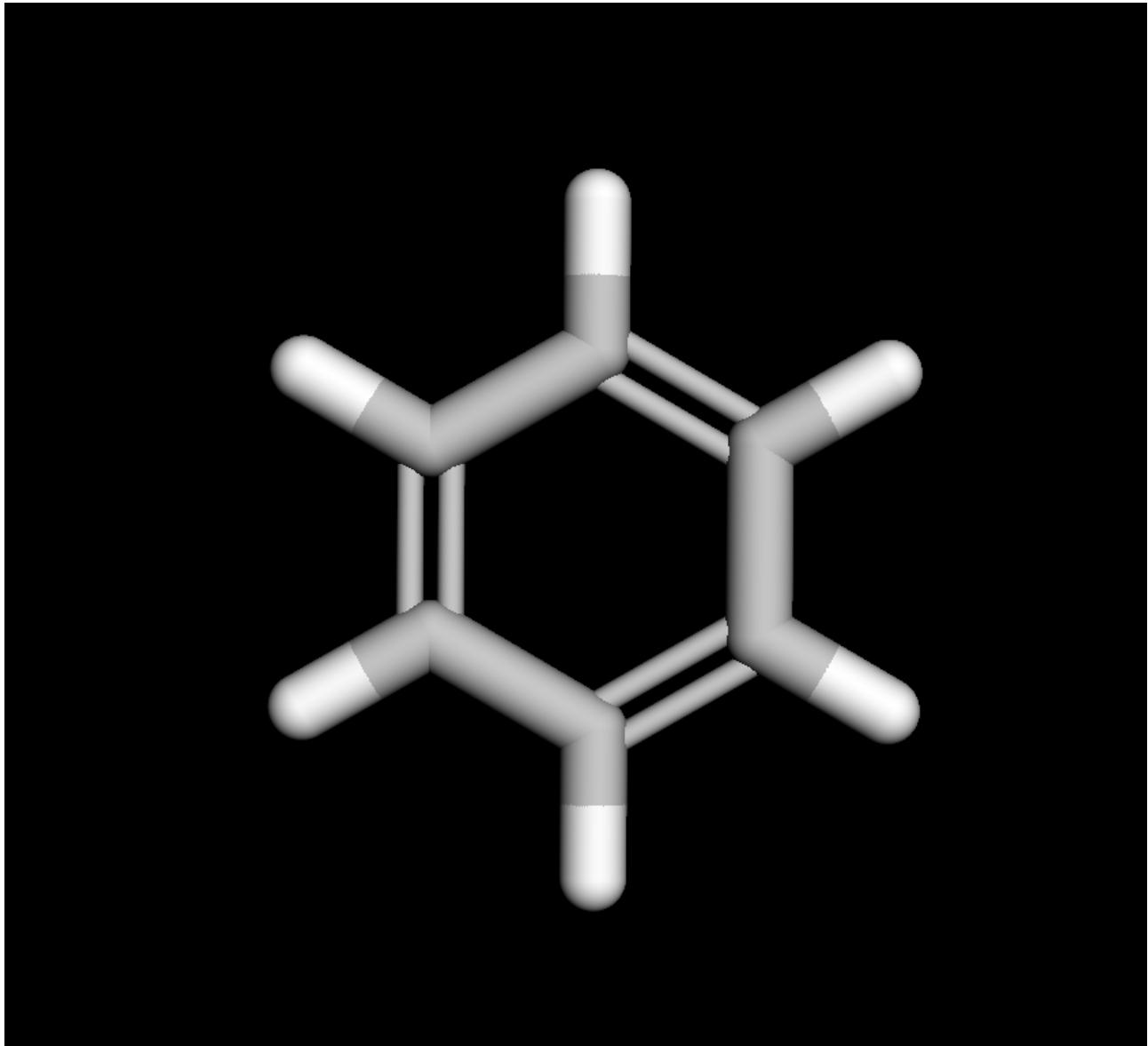
Note however that if there is a chemical identifier, the app will use that instead of the ketcher box. To use a drawn molecule, the chemical identifier box must be empty.

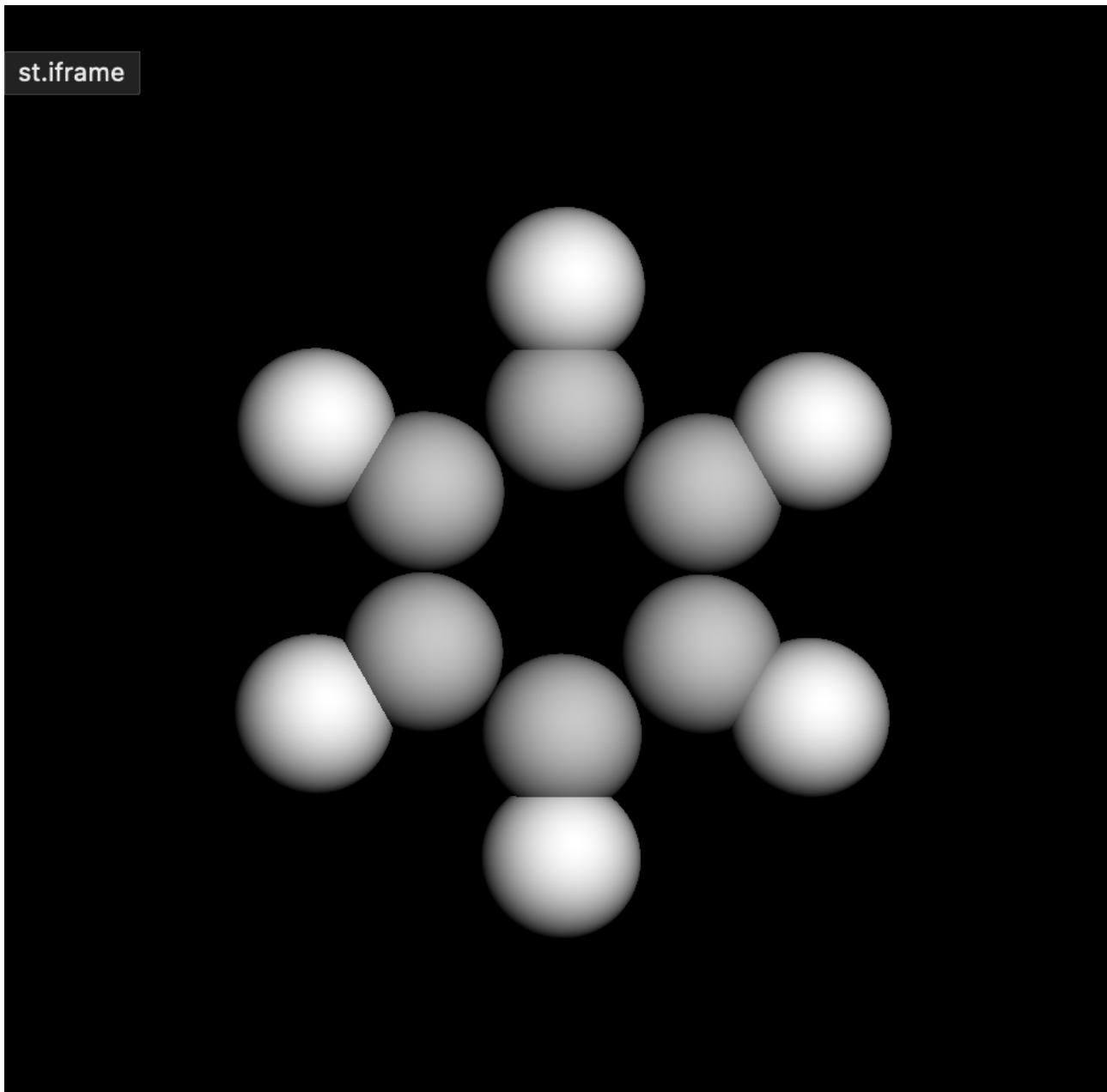
The point group of the molecule can then be calculated from a single button. This was a challenging function as the SDF files we originally used were all in 2D giving the wrong point groups. We then however fixed this by taking the 3D SDF files from pubchem.

The screenshot shows the Molvizpy interface after calculating the point group. A button labeled "Get Molecule Point Group" is visible. Below it, a message box displays the text "Point group of benzene is d6h".

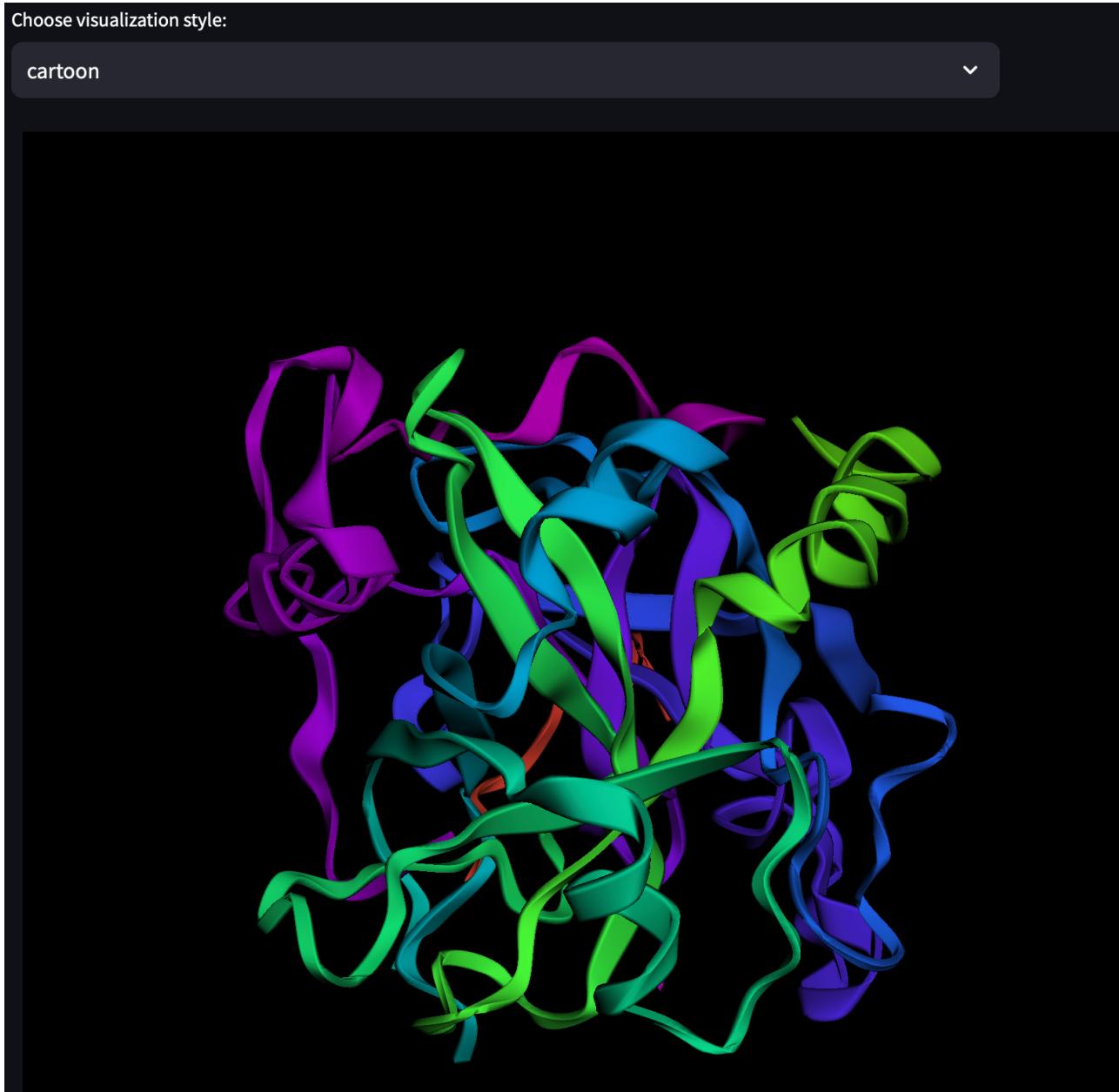
You can then visualize this molecule in a 3D viewer. You have the selection of line, stick and sphere, each with parameters that can be changed. This uses an SDF file to be able to visualize even large molecules

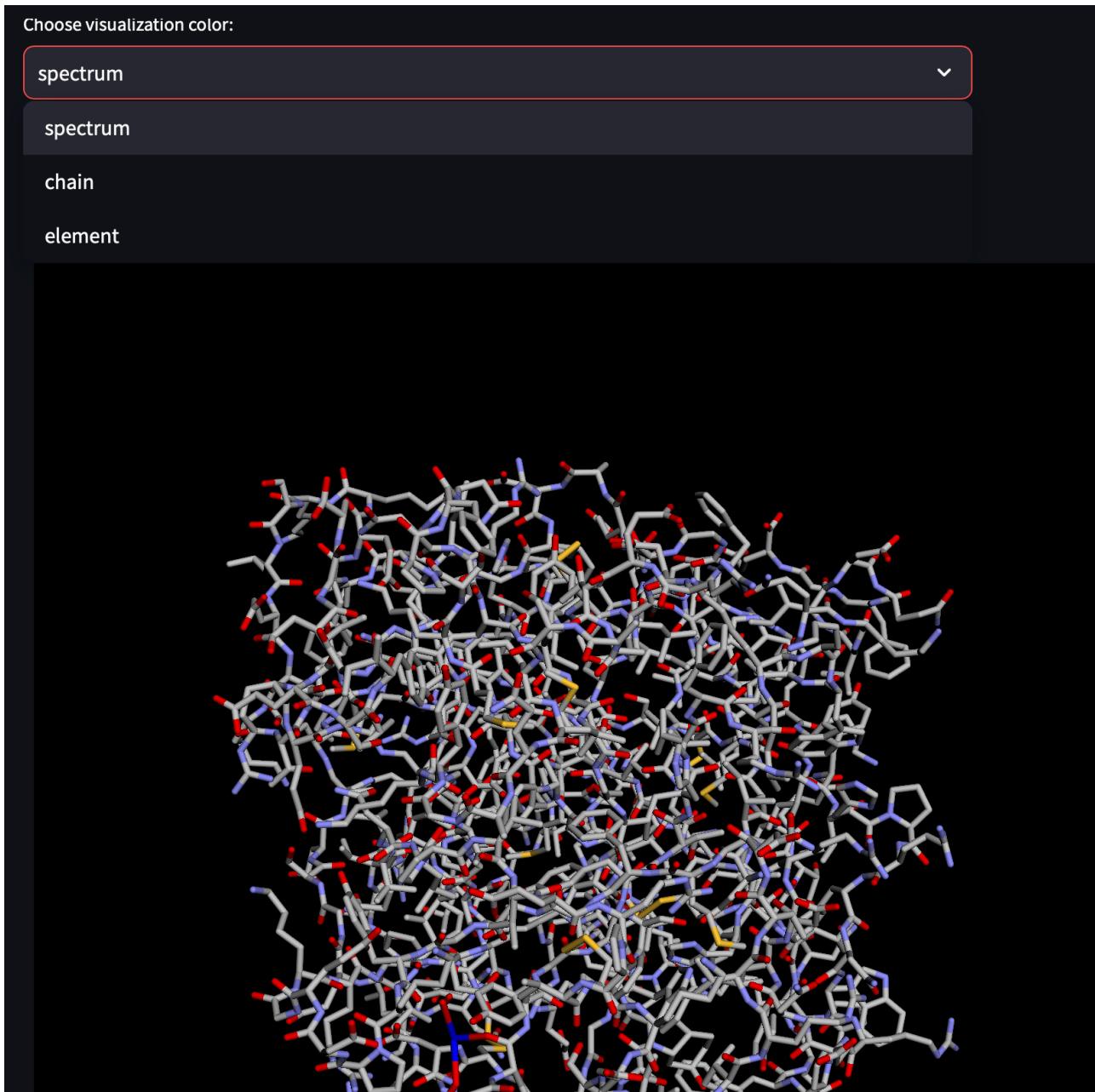


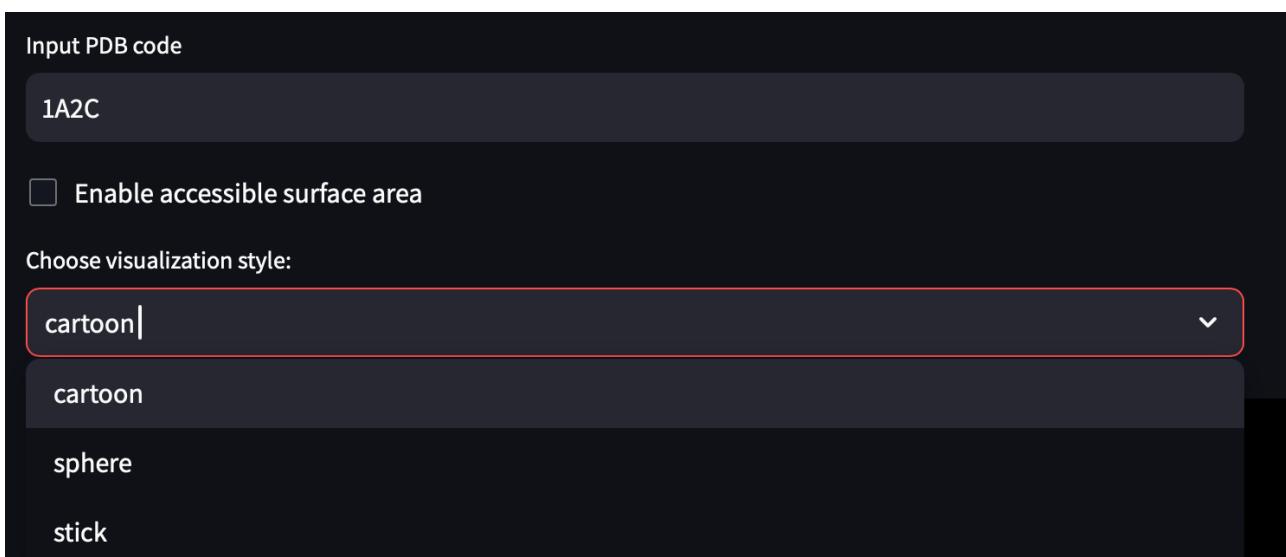
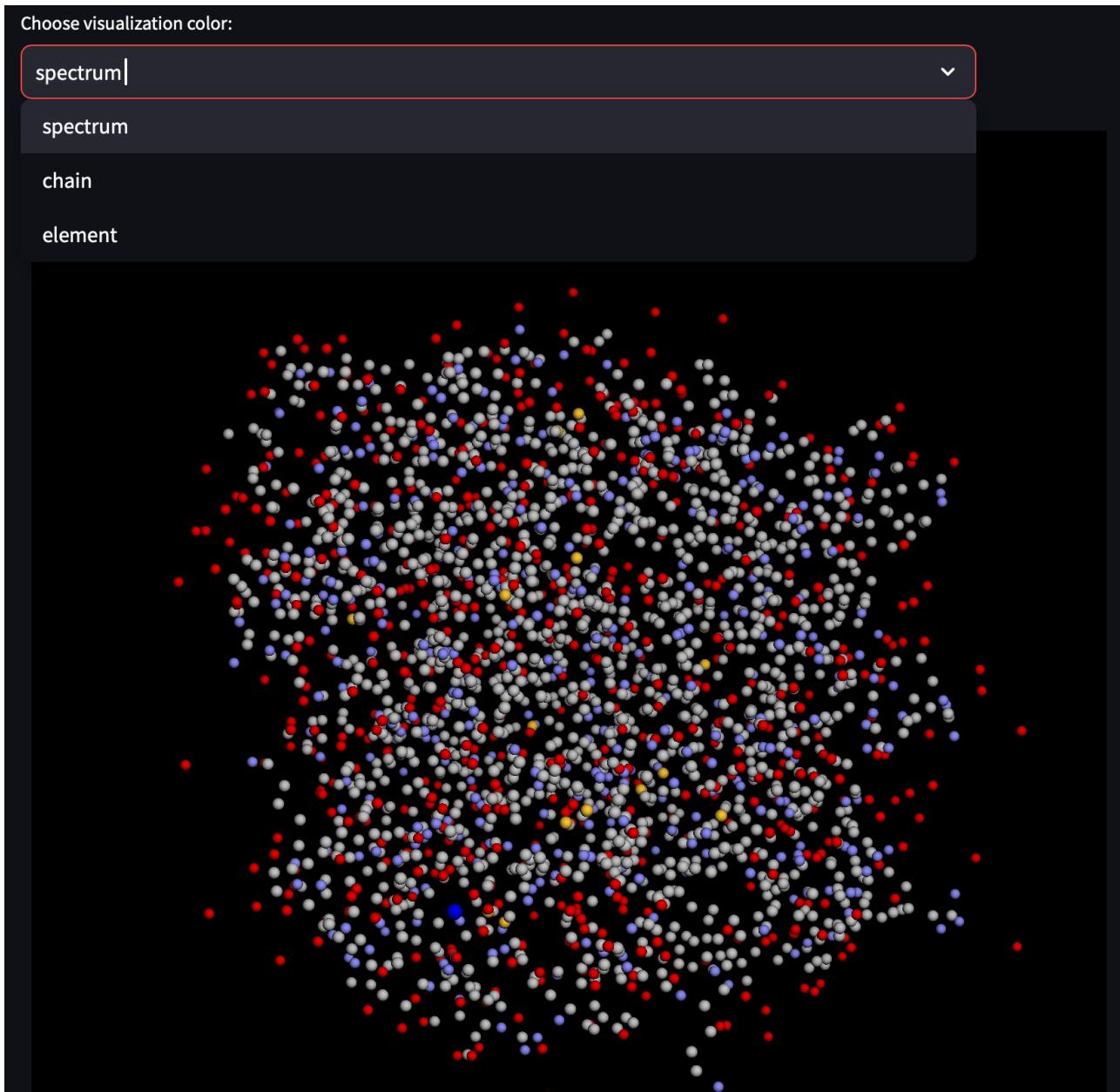




A protein viewer also exists on a second tab, where a cartoon structure is available, as well as a stick or sphere representation:







Originally this viewer was supposed to be able to select different chains in a protein and change how they could be visualized. This however proved too challenging and because of time constraints, was decided to not be done.

The viewer is also able to show the ASA of the protein with a checkbox, which the opacity can be changed with a slider:



This about shows all the functionality of the app, other functions were created such as the view2D function (more information in the notebook), where there was substructure matching. However this was not included since we had the ketcher input which served the same purpose. All the functions that we used in the project can be found in the notebook.