System Architecture

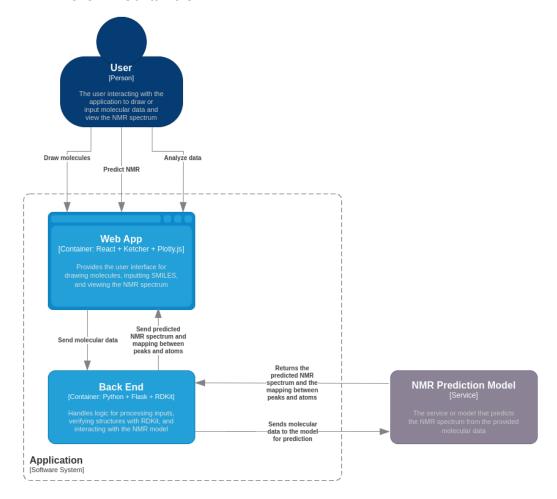
1. Technologies used

- Backend: Python + Flask + RDKit + SciPy + Jcamp + Scikit-Learn
- o Frontend : React + Ketcher + Plotly.js + Mui Material
- o Api : Communication between frontend and backend via API calls
- The system will be based on a client-server architecture with an API between the frontend and the backend. It can be used as a local Desktop App or as a remote Web App.

2. C4 Models

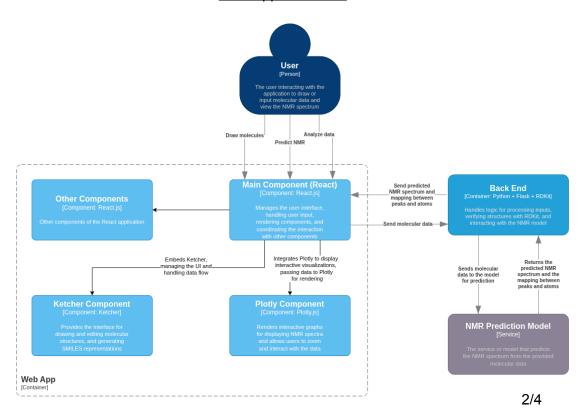
Level 1 - Context User [Person] The user interacting with the application to draw or input molecular data and view the NMR spectrum Creates molecule drawings. Displays the molecular data and the predicted exports in various formats, predicts the NMR spectrum, NMR spectrum to the user analyzes the data Returns the predicted NMR Application spectrum and the **NMR Prediction Model** mapping between [Software System] peaks and atoms The application that processes inputs and communicates with the NMR prediction model to generate and Sends molecular data to the modelfor prediction

■ Level 2 - Containers

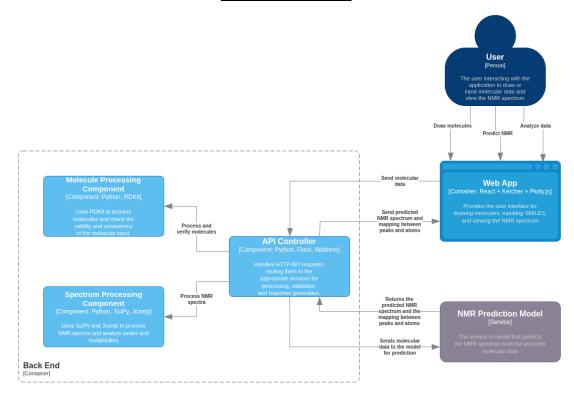


■ Level 3 - Components

Web App Container



Back End Container



3. Sequence diagrams

Predict an NMR Spectrum

