Web App to Extract Features for AI-based Drug Development

The aim of this project is to perform feature extraction using a smile library in Python for drug molecules. The project includes two methods for feature extraction: the first method involves using natural language processing (NLP) to retrieve features, while the second method involves using the Morgan fingerprint method. The project includes a web interface that allows users to upload a CSV file containing information related to drug smiles. The uploaded data is transferred to Python dataframes, which are then sent through a custom Flask API to the smile package for feature extraction. The results are then converted back from JSON to dataframes and then converted to CSV format to generate a downloadable link. Additionally, the data is passed to HTML using the tohtml function. Finally, on the frontend side, the application provides an option to visualize the data generated using Plotly and download the data using a download button.

Technology/Language	Purpose
Python	Main programming language used for feature extraction and data manipulation
Smile Library	Library used for feature extraction
Flask	Micro web framework used for developing the API
HTML	Markup language used for designing the web interface
CSS	Style sheet language used for styling the web interface
JavaScript	Scripting language used for client-side web development
Plotly	Library used for data visualization
JSON	Data interchange format used for sending and receiving data

Overall, this project provides a simple and efficient way for drug researchers and professionals to extract features from drug molecules. The project's web interface and data visualization features make it user-friendly and easy to use. Additionally, the use of Python and various libraries and frameworks ensures the project's flexibility and scalability for future development.