Component specification

Software components:

1. Graphical User Interface (GUI)
    - Description: Provides a user-friendly interface for researchers to interact with the software package, facilitating ease of navigation and operation.
2. File Import Function
    - Description: Allows users to import data from .csv and .xlsx files seamlessly into the system for processing.
3. Data Selection Function
    - Description: Enables users to select specific data fields such as Name, Concentration, and other relevant metrics for analysis.
4. Regulation Analysis Function
    - Description: Implements statistical analysis (e.g., t-test) to identify down-regulators and up-regulators from the dataset, assisting researchers in pinpointing key metabolites.
5. Data Output Function
    - Description: Generates formatted output data that can be easily exported or utilized in further analysis.
6. Clipboard Function
    - Description: Provides a clipboard feature for users to copy and paste data directly into MetaboAnalyst or other platforms.
7. Metabolite Separation Function
    - Description: Facilitates the separation of different metabolites within the dataset for more focused analysis.
8. Metabolite Identification Function
    - Description: Identifies metabolites and converts their names into PubChem IDs, linking to an extensive database for further research.

Interactions to Accomplish Use Cases

1. Use Case 1: Metabolite Selection
    - The researcher utilizes the Graphical User Interface (GUI) to import raw data files (.csv or .xlsx).
    - They select relevant parameters such as Name and Concentration using the Data Selection Function.
    - The researcher then uses the Metabolite Separation Function to filter specific metabolites of interest.
    - Finally, the Data Output Function generates a formatted list of metabolites, which can be copied using the Clipboard Function for further analysis.
2. **Use Case 2: Regulation Analysis**
    - The researcher accesses the GUI to import their experimental data.
    - They select the relevant variables for analysis, including concentrations of potential regulators, through the Data Selection Function.
    - The researcher initiates the Regulation Analysis Function, which uses a t-test to identify down-regulators and up-regulators in the dataset.
    - The results are displayed in the output area, where the researcher can utilize the Clipboard Function to copy the findings directly to MetaboAnalyst or other platforms.

Preliminary Plan

- 11/13: Complete the development of basic functions that yield a usable output compatible with MetaboAnalyst.
- 11/20: Finalize testing of the GUI and ensure all import and selection functions are operational.
- 11/27: Implement the regulation analysis and output functions, ensuring accurate data processing.
- 12/1: Conduct final reviews and testing, addressing any issues, and prepare for project completion.