Reproducing Our Computational Analyses

System and Environment

All calculations and analyses were performed on **Windows (64-bit)** using **Anaconda 3** with the following specifications:

- **Conda version**: 24.11.3
- **Conda-build version**: 24.9.0
- **Python version**: 3.12.7.final.0
- **Solver**: libmamba (default)

Virtual packages:
```
__archspec=1=haswell
__conda=24.11.3=0
__cuda=10.1=0
__win=0=0
```

We used the open-source packages **CobraPy** (for Flux Balance Analysis) and **eQuilibrator** (for thermodynamic calculations

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Required Files

Create a folder on your computer and place the following files inside:

```
custom_plot_functions.py
equilibrator_custom_functions.py
equilibrator_custom_functions_my.py
input C13 data.xlsx
input physiologic data during labeling.xlsx
input_data_bioreactor.csv
input_MW_values.csv
input_kinetic_parameters_database.csv
input_metabolite_ranges_default.csv
input_proteomics.xlsx
script_01_processing_proteomic_and_physiology_data.ipynb
script_02_FBA_stoichiometric_model_maker.ipynb
script_03_plotting_labeling_data.ipynb
script_04_FBA_metabolic_fluxes_labeling.ipynb
script_05_MDF_metabolic_fluxes_labeling.ipynb
script_06_FBA_pathway_maker.ipynb
script_07_MDF_pathways.ipynb
script_08_FBA_generating_file_for_ECM.ipynb
script_09_ECM_calculations.ipynb
```

Option 1: Using the Predefined Environment File (Recommended)

To ensure all software dependencies are correctly installed, use the environment file we created.

Steps:

1. **Download** the file `cobra_and_equilibrator.yml` and place it in an easy-to-find folder.
2. **Open** the **Anaconda Prompt**.
3. **Navigate** to the folder where the `.yml` file is located. For example:
   ```
   cd path\to\your\folder
   ```
4. **Create the environment** by running: