Title: A shiny app for determining the labeling duration for a two-sample experiment

A screenshot of a computer

AI-generated content may be incorrect.

Figure A)

A screenshot of a computer

AI-generated content may be incorrect.

Figure B)

This application is designed to assist researchers in planning stable isotope labeling experiments by estimating the optimal labeling duration for a given peptide, based on key experimental parameters. The tool offers two modes of input, illustrated in Figure A and Figure B.

In Figure A, the application takes a single expected turnover rate along with the peptide sequence, body water enrichment (BWE), and ΔI₀ (the smallest detectable change in isotopic enrichment). The user can also specify the maximum labeling duration using a slider. Based on these inputs, the tool simulates the labeling curve over time and identifies the time window during which the isotopic signal (I₀(t)) falls between the theoretical upper and lower bounds, shown as red and black dashed lines, respectively. This interval—visually represented as a green shaded region on the plot—corresponds to the recommended minimum and maximum labeling durations for that peptide and condition.

In Figure B, the application allows the user to input a range of turnover rates (e.g., slowest and fastest expected rates), which is useful when turnover is uncertain or varies among conditions. The labeling curves are then simulated for both the lower and upper turnover rates, shown in black and blue points respectively. The valid labeling window is determined by the intersection of these simulations with the detection thresholds, and is again shown as a shaded region in the plot. This mode provides a more conservative estimate by accommodating uncertainty in turnover dynamics.

In both modes, the output includes a graphical plot and a text summary indicating the minimum and maximum labeling durations (in days) recommended for reliable detection of label incorporation. These tools help guide the design of time-course experiments by identifying the most informative sampling windows, minimizing unnecessary sampling while maximizing detection power.