

Interactive Metabolic Pathway Visualization for Optimization of Energy Flux

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The goal of this project is to gain new insights into the photosynthetic eukaryote *Phaeodactylum tricornutum* using a systems biology approach. To analyze and contextualize the omics data and predictive metabolic models developed for the project, new interactive, data-rich, web-based visualizations are being developed. The Escher pathway visualization tool (<https://escher.github.io>) will be used as a starting point, and it will be extended to represent compartmentalization in the diatom, to visualize ¹³C isotope tracing data, to visualize time series data, and to give non-computational users the ability to explore and modify models.

To meet the visualization and data analysis needs of genome-scale models (GEMs), such as the diatom reconstruction, we developed Escher (<https://escher.github.io>), a web application for visualizing data on biological pathway maps. Through this project, a new version of Escher is being developed that improves the performance, reliability, and extensibility of the metabolic pathway maps. The new version includes visual representation of cellular compartments, and it is the basis of three visualization applications that will enable systems-level optimization of *Phaeodactylum tricornutum*.

First, a new visualization package called Escher-Trace has been developed through a collaboration with Prof. Christian Metallo's research group at UCSD. Escher-Trace makes ¹³C isotope tracing data more accessible by improving data presentation and streamlining analysis. Users can upload containing isotope tracing data in common file formats (JSON, CSV) to visualize them on the Escher metabolic map. Once loaded, users can automatically generate publication quality graphs of mass isotopomer distribution, metabolite abundance, mole percent enrichment, and kinetic labeling and abundance. Escher-trace corrects for natural isotope abundance of ¹³C labeled datasets and provides full control over data normalization and sample/condition grouping. Next, Escher-Trace will be incorporated with the metabolic pathway map of *Phaeodactylum tricornutum* to analyze new ¹³C tracing datasets.

Second, we are developing methods for time-series visualization on the Escher map, particularly for gene expression data. The resulting map will allow animated playback of datasets through time with precise controls and the ability to export publication-ready figures.

Finally, a web-based collaboration platform is under development that will allow non-computational users to expand metabolic models with new heterologous pathways. This platform will take advantage of Escher and the interactive flux simulator Escher-FBA (<https://sbrg.github.io/escher-fba>) for rapid prototyping of new diatom strain designs.

Supported by DE-SC0018344, Biological and Environmental Research