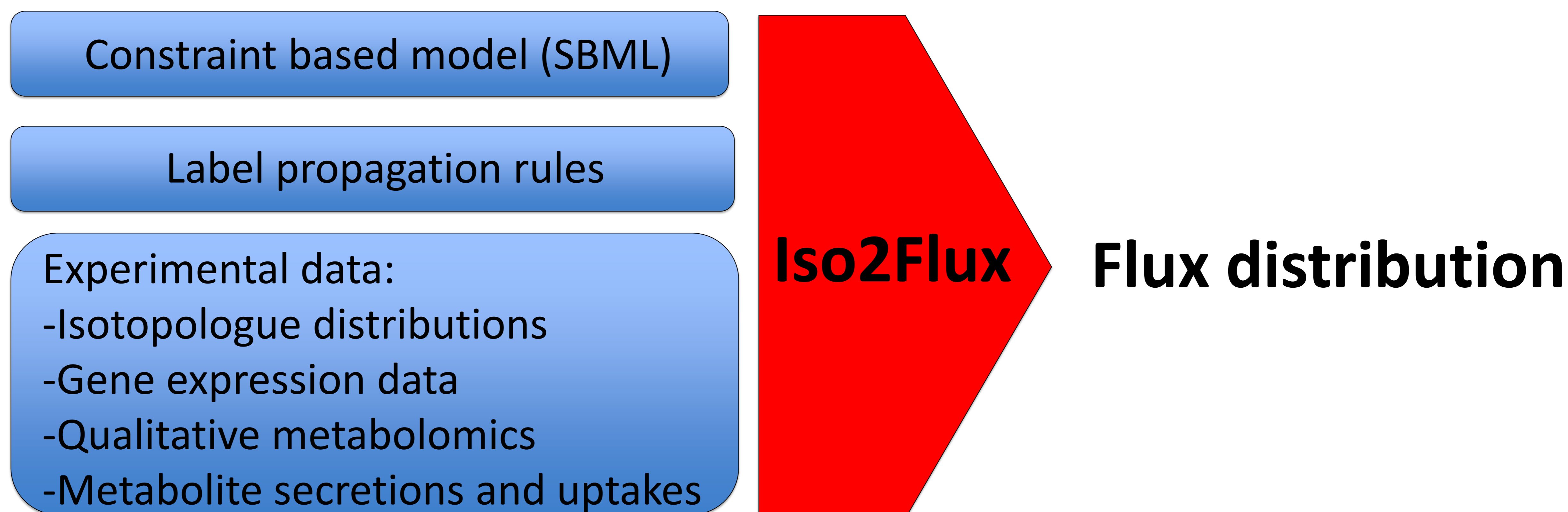


Iso2Flux: A new software for ¹³C fluxomics developed in the framework of PhenoMeNal

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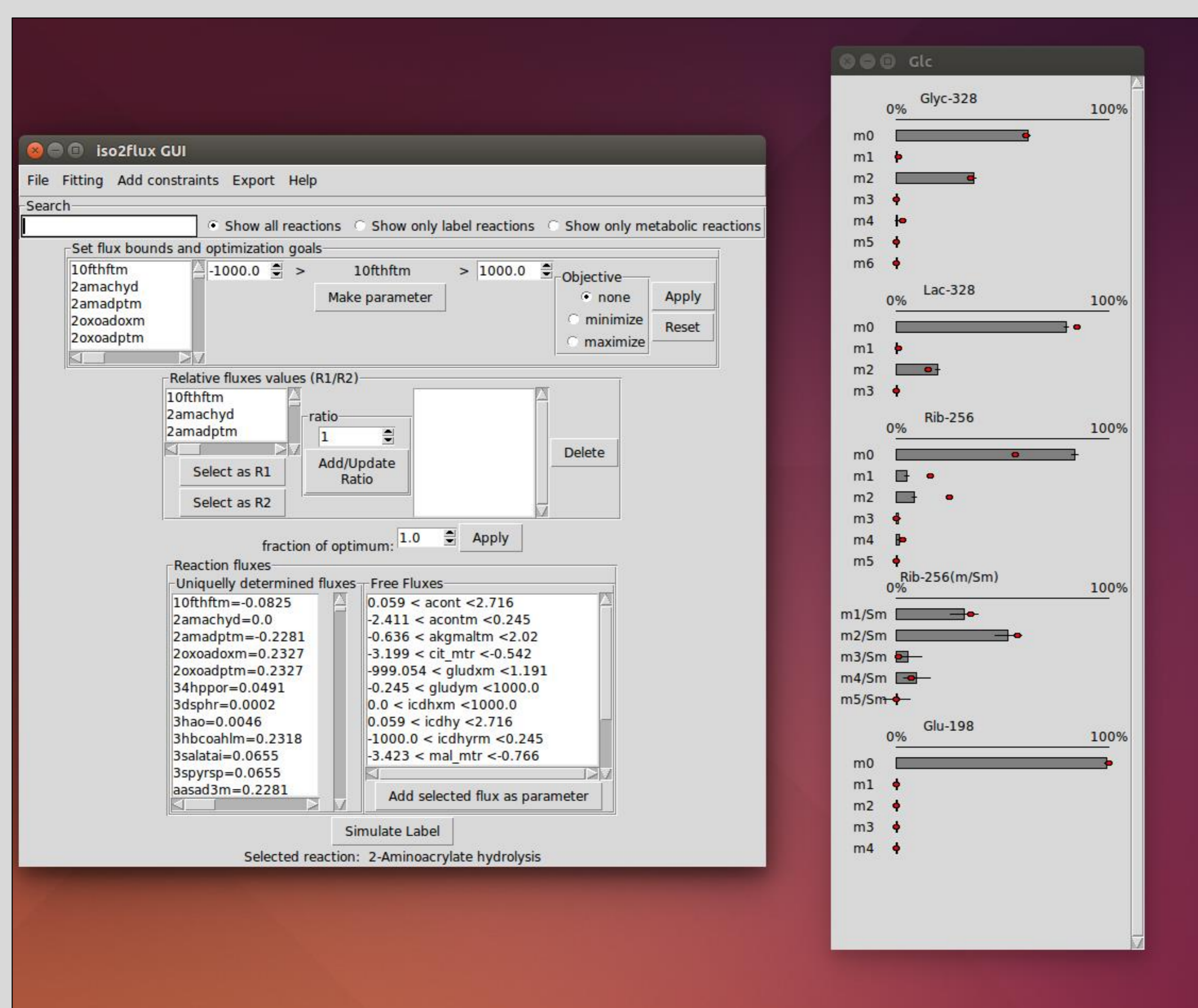
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We present Iso2Flux a new software capable of ¹³C assisted fluxomics. Iso2Flux has been optimized for maximal performance thanks to the automatic conversion of the isotopomer propagation model to EMU (Elementary Metabolite Units) balances, the pruning of infeasible isotopologues and the automatic compilation of the generated models into C modules. In addition to isotopologues measurements, Iso2Flux is capable of integrating a wide array of experimental data (metabolites secretions and uptakes, gene expression and metabolomics) to identify the steady state metabolic flux distribution that is most consistent with experimental measurements. Additionally, Iso2Flux, which is developed in python and based on the COBRAPy package, allows seamless integration with genome scale metabolic models. Moreover, Iso2Flux has been designed as a flexible tool that can be operated both through the command line and a graphical user interface. Iso2Flux is being integrated in the workflow for fluxomics of the PhenoMeNal project (EC-654241) which aims to build e-infrastructures for metabolomics data (<http://phenomenal-h2020.eu/home/>).



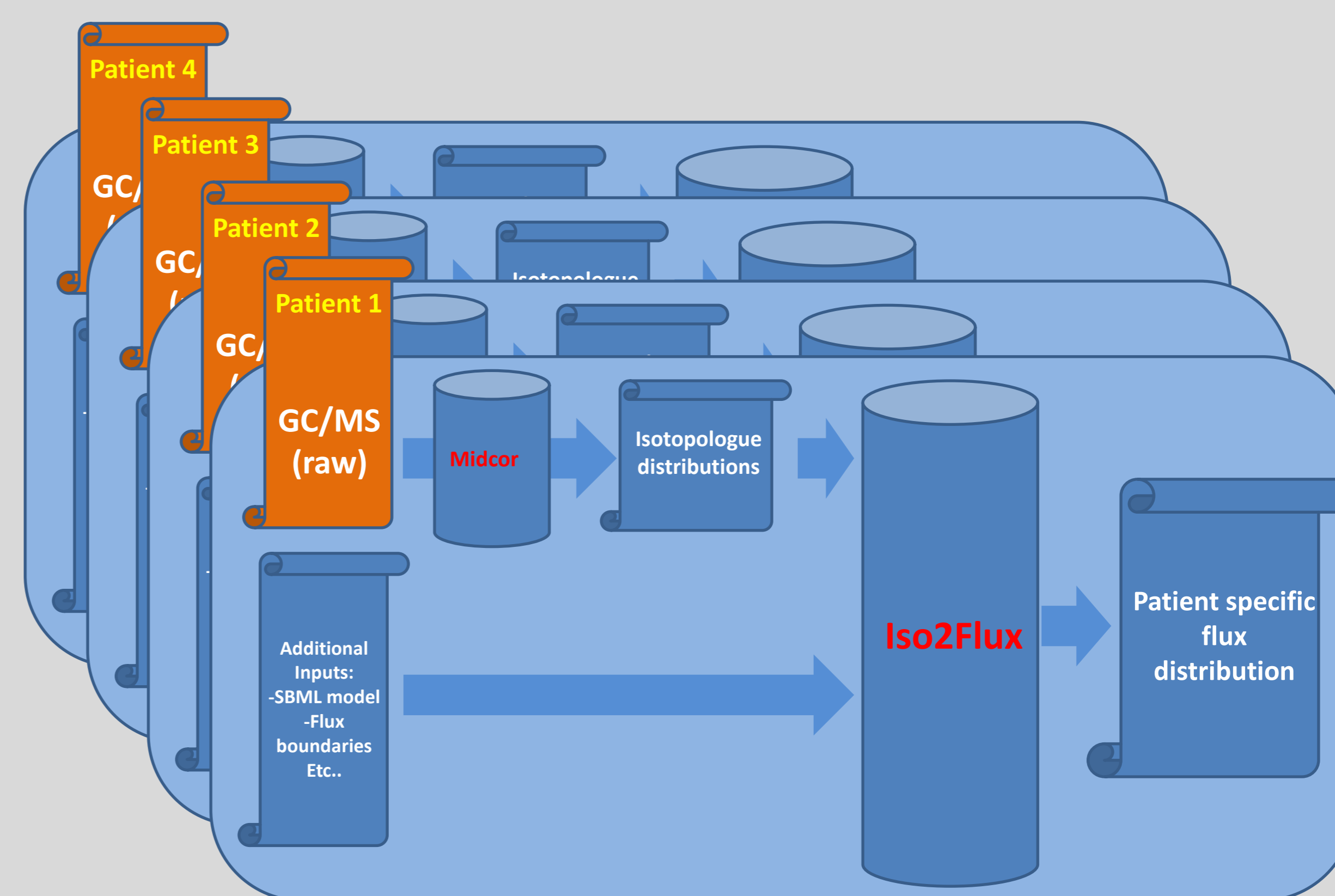
Using Iso2Flux

Standalone



Iso2Flux can be installed and run as a standalone program. It can be operated either through an intuitive graphical interface (shown above) or as a command line program. Additionally Iso2Flux can also function as a python package allowing its functions to be integrated into any python script. Iso2Flux can be run on any operating system that supports python.

Fluxomics Workflow



Iso2Flux will also be usable as part of the fluxomics workflow of the PhenoMeNal project. With this aim, a dockerfile for Iso2Flux has been uploaded to the GitHub repository of PhenoMeNal allowing to automatically build a docker image capable of running Iso2Flux. A Galaxy wrapper for this docker image, which is currently being developed, will be used to integrate Iso2Flux into the fluxomics workflow of PhenoMeNal. Specifically, Iso2Flux will be using the output of Midcor, an R-tool for experimental ¹³C data correction for natural isotope enrichment, as well as additional inputs to generate a set of metabolic flux predictions. Once completed, the fluxomics workflow of PhenoMeNal will allow to read patient data from repositories like MetaboLights (www.ebi.ac.uk/metabolights) and estimate patient specific metabolic flux distributions.

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