**FASIMU: flexible software for flux-balance batch computation in large metabolic networks**

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**Summary**

Flux-balance analysis (FBA) based on linear optimization is widely used to compute metabolic fluxes in large metabolic networks and gains more importance in network curation and structural analysis which requires a computational tool flexible enough to select from the wide variety of FBA algorithms and able to handle batch series.

We present FASIMU, a command line oriented software for the computation of flux distributions using a variety of most common FBA algorithms, including the first available implementation of (i) weighted flux minimization, (ii) flux maximization for partially inhibited enzymes, and (iii) the concentration based thermodynamic feasibility constraint. It allows batch computation with varying objectives and constraints suited for network pruning, leak analysis, flux-variability analysis, and systematic probing of metabolic objectives for network curation controlled by an intuitive description file. Input and output supports SBML. FASIMU can work with free (lp_solve and GLPK) or commercial solvers (CPLEX, LINDO). Plugins have been developed to visualize calculated flux distributions in Cytoscape (FluxViz) and BINA (faBiNA).

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**References:**


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**Data flow in FASIMU**

**Objective:** • Flux minimization [5]  
• Fitness maximization [6]  
• Biomass maximization [7]  
• Network prediction by expression profiles [8]  
**Constraints:** • Thermodynamic constraint based on metabolite concentrations [9]  
• Constraining individual fluxes [10]  

**Implemented methods**

- Flux-variability analysis [12]  
- Minimal functional flux modes [2]  
- Network pruning [11]  
- Leak analysis: similar to [11][3]  

**Software layout**

- Runs on LINUX, Windows, MAC, UNIX  
- Requires bash, gawk  
- Requires external solver (CPLEX, LINDO, GLPK, lp_solve)  
- External network visualization helpful (BiNA, Cytoscape, CellWorkAnalyzer, or SBW)  
- Easily available, open sources (GPL)  

**Example script**

One line per simulation, organized in columns

1. name  
2. objective  
3. constraints  
4. objective

**Simulation definition**

- Can be based on freely available software  
- Freely available, open source (GPL)  
- External network visualization helpful  
- Requires external solver (CPLEX, LINDO, GLPK, lp solve)  
- Runs on LINUX, Windows, MAC, UNIX

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**References:**