

Flux sampling with simplified poling-based flux balance analysis

Michael John Binns*
Hanyang University
(mbinns@hanyang.ac.kr*)

Metabolic networks are known to contain a certain degree of redundancy in addition to other uncertainties. If enough metabolic fluxes can be measured then the remaining fluxes can be computed through linear optimization to find a set of fluxes which give some maximal yield. However, due to uncertainty and redundancy there will normally be many different solutions giving the same optimal yield. Here, a new method of sampling is presented which is able to identify these different solutions in an iterative manner. This is based on the poling method for generating alternative 3D conformations for molecules. However, here the method has been implemented for generating different fluxes.

This new method has the capability to produce samples with bias identifying the subspace of solutions giving an optimal yield. The method is further improved with the simplification of the poling function to account for the combinatorial nature of the original poling algorithm.

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