SUPPLEMENTARY MATERIAL I

Finding free fluxes in the metabolic networks

Metabolic networks were mathematically modeled by steady state flux balance equations around metabolites. Reversible fluxes were modeled by two different fluxes – a forward flux and a backward flux. The reversibility 'r' of a reaction is defined as

$$r = \frac{v_f}{v_b},$$

where v_f is the forward flux and v_b the backward flux.

The number of free fluxes f in a metabolic network with m metabolites and n net fluxes of which p are measured is given by $f = n - m - p$. The free fluxes in a metabolic network were chosen such that the matrix S_c was invertible

$$S_c.v_c + S_m.v_m = 0$$

$$v_c = (S_c^{-1}).S_m.v_m,$$

here v_m and v_c are the measured and estimated fluxes respectively.

Several sets of free fluxes exist and they can be transformed into each other. Free fluxes and reversibilities are the parameters of the mathematical model that have to be estimated by fitting experimental measurements to the model.