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## Putative regulatory sites unraveled by network-embedded thermodynamic analysis of metabolome data

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## Supplement 5: Putative regulatory sites and operational compartmental differences identified for *S. cerevisiae*

Analyzing the *S. cerevisiae* data by NET analysis, several putative active regulatory sites have been identified and also compartmental differences. The following table displays the calculated ranges of feasible Gibbs energy of reaction underlying the drawn conclusions for selected reactions.

Table I: Thermodynamically feasible Gibbs energies of reaction identified as putative regulatory sites or elucidating compartmental differences for the *S. cerevisiae* data

corresponding enzyme	feasible Gibbs energy of reaction [kJ/mol]	
	cytosol	mitochondria
aldehyde dehydrogenase	< -23.9	< -50.1†
asparagine synthase	< -24.3	not present
aspartate transaminase	> 6.8	-21.9 .. 0
dehydroquinase synthase	< -58.8	not present
glycerol 3-phosphate dehydrogenase	< -11.3	< -8.8†
fumerase	-16.6 .. 0	-1.9 .. 0
isocitrate lyase	< -8.4	not present
malate dehydrogenase	12.3 .. 40.9†	-3.2 .. 0
NADH dehydrogenase	< -43.2	< -57.5
phosphofructokinase	< -24.0	not present
phosphogluconolactonase	< -6.1	not present
pyruvate decarboxylase	< -14.8	not present
pyruvate dehydrogenase	not present	< -10.6
pyruvate kinase	< -27.7	not present
serine deaminase	< -43.5	not present

† Reaction not active in the analyzed experiment