

RELATIONSHIP BETWEEN METABOLIC FLUXES AND SEQUENCE-DERIVED PROPERTIES OF ENZYMES

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Supplementary information 3

Table S3. Elements and the statistical indices for multiple linear regression model which links the values of metabolic fluxes and the average AA properties of the yeast *Saccharomyces cerevisiae* enzyme sequences expressed according to the AAindex scales.

Dependent ^a variable	Parameters ^b	Regression coefficient (standardized value)	S.E.	t value	P value	R ² , % R ² _{adj} , %	VIF ^c
	<i>constant</i>	43.4234	6.193	7.01	0.0000	71.95 68.08	
metabolic	<i>P_{ave}WV5-1</i>	-3.2314 (-0.6118)	0.626	-5.16	0.0000		1.45
flux	<i>P_{ave}WV8-1</i>	8.0585 (0.3406)	2.842	2.84	0.0082		1.49
	<i>P_{ave}VW10-1</i>	-11.5014 (-1.0396)	1.828	-6.29	0.0000		2.82
	<i>P_{ave}WV10-3</i>	28.6417 (1.2986)	3.607	7.94	0.0000		2.76

^a represent the values of metabolic fluxes for HXT, HKX, GPI, ALD, PFK, TIM, GAPDH, PGK, PGM, ENOL, PK, PDC, ADH, GPD, ATPase, AK and α,α -trehalose-phosphate synthase (Q00764) as specified in the “Material and Methods” and listed in Stanford *et al.*, 2013 [25] for both the standard model built without regulatory information and the model with an integrated regulatory information.

^b elements of multiple linear regression which represent the average AA property of the yeast *Saccharomyces cerevisiae* enzyme sequences and the constant (intercept) of equation, specified (Stanford *et al.*, 2013 [25]) as follows:

P_{ave}WV5-1 (BUNA790101) represents α -NH chemical shifts (Bundi-Wuthrich, 1979);

P_{ave}WV8-1 (QIAN880117) represents weights for β -sheet at the window position of _3 (Qian-Sejnowski, 1988);

P_{ave}VW10-1 (MAXF760103) represents normalized frequency of zeta R (Maxfield-Scheraga, 1976);

P_{ave}WV10-3 (WERD780102) represents free energy change of epsilon(i) to epsilon(ex) (Wertz-Scheraga, 1978).

In brackets: the AA index accession numbers.

^c the variance inflation factor which indicates the impact of collinearity between the independent variables (Kock and Lynn, 2012 [22]).

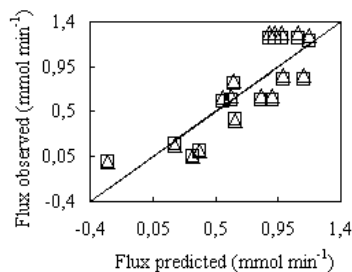


Fig. S3 The linear plot for the metabolic fluxes of the yeast *Saccharomyces cerevisiae* glycolysis pathway estimated by kinetic models (Stanford *et al.*, 2013 [25]) against those predicted by linear regression model (Table S3). (□) – The standard model; (Δ) – The model with regulatory information. R=0.848, Kendall's τ = 0.642, Spearman's ρ = 0.831.