

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

<sup>a</sup> represent the values of metabolic fluxes for HXT, HXK, GPI, ALD, PFK, TIM, GAPDH, PGK, PGM, ENOL, PK, PDC, ADH, GPD, ATPase, AK and  $\alpha,\alpha$ -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.

<sup>b</sup> 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  $\alpha$ -NH chemical shifts (Bundi-Wuthrich, 1979);

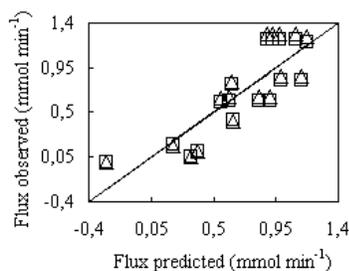
$P_{ave}WV8-1$  (QIAN880117) represents weights for  $\beta$ -sheet at the window position of \_3 (Qian-Sejnowski, 1988);

$P_{ave}VW10-1$  (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.

<sup>c</sup> 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  $\tau = 0.642$ , Spearman's  $\rho = 0.831$ .