

RELATIONSHIP BETWEEN METABOLIC FLUXES AND SEQUENCE-DERIVED PROPERTIES OF ENZYMES

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Supplementary information 2

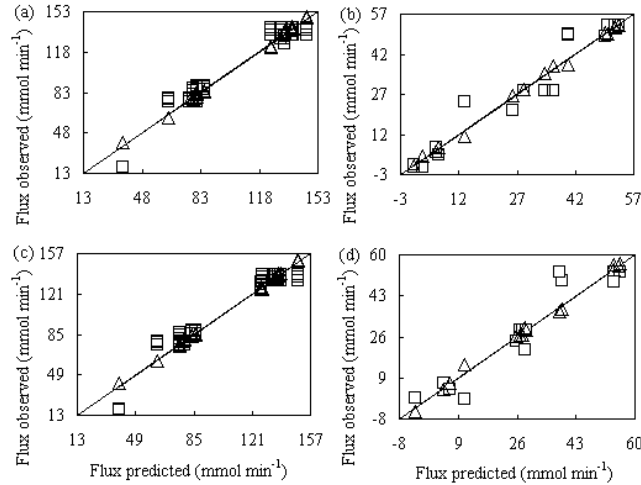


Fig. S2 The linear plots (a, b, c, and d) for the metabolic fluxes of the yeast *Saccharomyces cerevisiae* glycolysis pathway estimated by kinetic models against those predicted by linear regression models I-IV, respectively, (\square) and by the leave-one-out cross-validation (LOOCV) of the models (Δ) (Table 2, Table 3) with the R^2_{adj} values of 91.69, 91.46, 91.95 and 85.61 percent, respectively.

Table S2-1. The variance analysis of the regression models. Multiple linear regression models linking the values of metabolic fluxes and the average AA properties of the yeast *Saccharomyces cerevisiae* enzyme sequences.

Model	dependent	Variables independent ^a	Variance source	Sum of squares	Df	Mean square	F-ratio	p-value
I	metabolic flux (Teusink's ^a model)	$P_{ave}VW7, P_{ave}VW5, (P_{ave}VW1)^{1/2}, (P_{ave}VW5)^{1/2}, (P_{ave}VW2)^{1/2}, P_{ave}VW6, P_{ave}VW1$	model residual total	48821.70 2863.50 51685.20	7 34 41	6974.53 84.22	82.81	0.0000
II	metabolic flux (Hynne's model)	$(P_{ave}VW2)^{1/2}, P_{ave}VW7, P_{ave}VW1, (P_{ave}VW1)^{1/2}, (P_{ave}VW5)^{1/2}, P_{ave}VW5, P_{ave}VW6, (P_{ave}VW3)^{1/2}$	model residual total	16603.00 1022.26 17625.20	8 36 44	2075.37 28.40	73.09	0.0000
III	metabolic flux (Teusink's model)	$(P_{ave}VW7-1)^{1/2}, P_{ave}VW2-3, (P_{ave}VW5-1)^{1/2}, (P_{ave}VW1-1)^{1/2}, P_{ave}VW3-1$	model residual total	48594.00 3091.21 51685.20	5 36 41	9718.80 85.87	113.18	0.0000
IV	metabolic flux (Hynne's model)	$(P_{ave}VW1-1)^{1/2}, P_{ave}VW1-3, P_{ave}VW2-1, (P_{ave}VW5-1)^{1/2}, (P_{ave}VW7-1)^{1/2}, P_{ave}VW6-1, P_{ave}VW3-1$	model residual total	15907.30 1717.95 17625.20	7 37 44	2272.47 46.43	48.94	0.0000

^a as specified in the Table 1

Table S2-2. Standard errors and confidence intervals for the linear regression models.

Model	\pm S.E. ^b , mmol min ⁻¹	\pm CI ^b , mmol min ⁻¹	
		95%	99%
I	9.177	18.650	25.039
II	5.329	10.808	14.492
III	9.266	18.792	25.199
IV	6.814	13.806	18.503

^a the standard error of the estimate for the regression model

^b the confidence interval for predicted values of a linear regression model