

RELATIONSHIP BETWEEN METABOLIC FLUXES AND SEQUENCE-DERIVED PROPERTIES OF ENZYMES

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Supplementary information 2

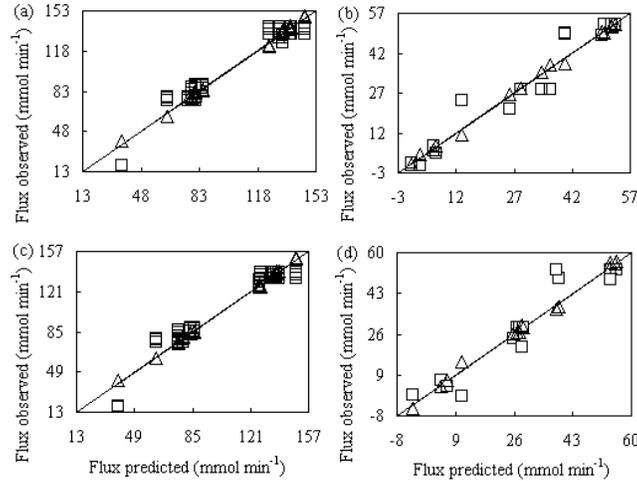


Fig. S2 The linear plots (a, b, c, and d) for the metabolic fluxes of the yeast *Saccharomyces cerevisiae* glycolysis pathway estimated by kinetic models against those predicted by linear regression models I-IV, respectively, (\square) and by the leave-one-out cross-validation (LOOCV) of the models (Δ) (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	<i>p</i> -value
I	metabolic flux (Teusink's ^a model)	$P_{ave}VW7, P_{ave}VW5, (P_{ave}VW1)^2,$ $(P_{ave}VW5)^2, (P_{ave}VW2)^2, P_{ave}VW6,$ $P_{ave}VW1$	model	48821.70	7	6974.53	82.81	0.0000
			residual	2863.50	34	84.22		
			total	51685.20	41			
II	metabolic flux (Hynne's model)	$(P_{ave}VW2)^2, P_{ave}VW7, P_{ave}VW1,$ $(P_{ave}VW1)^2, (P_{ave}VW5)^2, P_{ave}VW5,$ $P_{ave}VW6, (P_{ave}VW3)^2$	model	16603.00	8	2075.37	73.09	0.0000
			residual	1022.26	36	28.40		
			total	17625.20	44			
III	metabolic flux (Teusink's model)	$(P_{ave}VW7-1)^2, P_{ave}VW2-3, (P_{ave}VW5-1)^2,$ $(P_{ave}VW1-1)^2, P_{ave}VW3-1$	model	48594.00	5	9718.80	113.18	0.0000
			residual	3091.21	36	85.87		
			total	51685.20	41			
IV	metabolic flux (Hynne's model)	$(P_{ave}VW1-1)^2, P_{ave}VW1-3, P_{ave}VW2-1,$ $(P_{ave}VW5-1)^2, (P_{ave}VW7-1)^2,$ $P_{ave}VW6-1, P_{ave}VW3-1$	model	15907.30	7	2272.47	48.94	0.0000
			residual	1717.95	37	46.43		
			total	17625.20	44	17625.20		

^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
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