

RELATIONSHIP BETWEEN METABOLIC FLUXES AND SEQUENCE-DERIVED PROPERTIES OF ENZYMES

Peteris Zikmanis, Inara Kampenusa
Institute of Microbiology and Biotechnology, University of Latvia, Kronvalda Boulevard 4, LV-1010, Riga, Latvia;
Correspondence should be addressed to Peteris Zikmanis; peteris.zikmanis@lu.lv

Supplementary information 1

Table S1-1. The dataset used in multivariate analysis which comprises metabolic fluxes ^a and numerical vectors representing the average amino acid property ^b for each enzyme sequence.

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1	P_{ave} WV2	P_{ave} WV3	P_{ave} WV4	P_{ave} WV5	P_{ave} WV6	P_{ave} WV7	P_{ave} WV8	P_{ave} WV9	P_{ave} WV10	$(P_{ave} \text{ WV1})^{\gamma^2}$	$(P_{ave} \text{ WV2})^{\gamma^2}$	$(P_{ave} \text{ WV3})^{\gamma^2}$	$(P_{ave} \text{ WV4})^{\gamma^2}$	$(P_{ave} \text{ WV5})^{\gamma^2}$	$(P_{ave} \text{ WV6})^{\gamma^2}$	$(P_{ave} \text{ WV7})^{\gamma^2}$	$(P_{ave} \text{ WV8})^{\gamma^2}$	$(P_{ave} \text{ WV9})^{\gamma^2}$	$(P_{ave} \text{ WV10})^{\gamma^2}$
25	85.99	0.20	-0.06	-0.10	0.19	0.02	0.02	0.02	0.07	-0.01	0.01	0.04	0.00	0.01	0.04	0.00	0.00	0.00	0.00	0.00	2.61E-005
25	85.99	-0.10	0.02	-0.06	0.28	-0.03	0.06	-0.05	0.02	0.02	-0.02	0.01	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00
25	75.19	-0.05	0.04	-0.09	0.27	0.03	0.04	-0.01	0.01	-0.00	0.07	0.00	0.00	0.01	0.07	0.00	0.00	4.82E-005	9.30E-005	8.96E-006	0.01
25	75.19	-0.22	-0.05	-0.01	0.24	-0.01	-0.05	0.01	-0.03	0.01	0.09	0.05	0.00	3.59E-005	0.06	8.03E-005	0.00	0.00	0.00	5.79E-005	0.01
25	75.19	-0.10	0.03	-0.11	0.24	-0.01	0.05	-0.04	0.02	0.02	0.01	0.01	0.00	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.00
25	132.44	-0.03	0.00	-0.15	0.29	0.02	-0.02	0.02	0.08	-0.04	0.04	0.00	1.25E-005	0.02	0.09	0.00	0.00	0.00	0.01	0.00	0.00
25	132.44	-0.07	0.07	-0.11	0.37	-0.02	0.05	0.01	-0.01	0.01	-0.01	0.01	0.00	0.01	0.14	0.00	0.00	8.56E-005	3.04E-005	5.04E-005	3.80E-005
25	132.44	-0.06	-0.00	-0.11	0.28	-0.01	-0.03	-0.00	0.06	0.02	0.05	0.00	4.12E-007	0.01	0.08	5.60E-005	0.00	1.93E-005	0.00	0.00	0.00
25	132.44	-0.00	0.03	-0.11	0.29	-0.01	0.01	-0.01	0.02	-0.01	0.04	1.22E-005	0.00	0.01	0.08	0.00	0.00	0.00	0.00	0.00	0.00
25	125.27	0.04	-0.01	-0.20	0.29	0.03	0.10	0.01	0.05	-0.04	-0.03	0.00	0.00	0.04	0.08	0.00	0.01	6.20E-005	0.00	0.00	0.00
25	80.95	0.06	0.05	-0.13	0.31	-0.01	0.01	-0.04	0.03	-0.02	0.01	0.00	0.00	0.02	0.10	6.31E-005	0.00	0.00	0.00	0.00	5.50E-005
25	132.44	-0.17	0.05	0.00	0.33	-0.06	-0.00	0.01	-0.07	-0.04	-0.01	0.03	0.00	6.91E-006	0.11	0.00	2.34E-005	0.00	0.00	0.00	6.15E-005
25	132.44	-0.08	0.07	-0.15	0.34	0.01	0.04	0.01	-0.03	-0.03	0.04	0.01	0.00	0.02	0.12	2.98E-005	0.00	0.00	0.00	0.00	0.00
25	17.94	0.01	0.04	-0.13	0.26	0.02	0.03	-0.04	0.02	0.02	0.00	4.12E-005	0.00	0.02	0.07	0.00	0.00	0.00	0.00	0.00	4.72E-006
50	88.15	0.20	-0.06	-0.10	0.19	0.02	0.02	0.02	0.07	-0.01	0.01	0.04	0.00	0.01	0.04	0.00	0.00	0.00	0.00	0.00	2.61E-005
50	88.15	-0.10	0.02	-0.06	0.28	-0.03	0.06	-0.05	0.02	0.02	-0.02	0.01	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00
50	77.35	-0.05	0.04	-0.09	0.27	0.03	0.04	-0.01	0.01	-0.00	0.07	0.00	0.00	0.01	0.07	0.00	0.00	4.82E-005	9.30E-005	8.96E-006	0.01
50	77.35	-0.22	-0.05	-0.01	0.24	-0.01	-0.05	0.01	-0.03	0.01	0.09	0.05	0.00	3.59E-005	0.06	8.03E-005	0.00	0.00	0.00	5.79E-005	0.01
50	77.35	-0.10	0.03	-0.11	0.24	-0.01	0.05	-0.04	0.02	0.02	0.01	0.01	0.00	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.00
50	136.50	-0.03	0.00	-0.15	0.29	0.02	-0.02	0.02	0.08	-0.04	0.04	0.00	1.25E-005	0.02	0.09	0.00	0.00	0.00	0.01	0.00	0.00
50	136.50	-0.07	0.07	-0.11	0.37	-0.02	0.05	0.01	-0.01	0.01	-0.01	0.01	0.00	0.01	0.14	0.00	0.00	8.56E-005	3.04E-005	5.04E-005	3.80E-005
50	136.50	-0.06	-0.00	-0.11	0.28	-0.01	-0.03	-0.00	0.06	0.02	0.05	0.00	4.12E-007	0.01	0.08	5.60E-005	0.00	1.93E-005	0.00	0.00	0.00
50	136.50	-0.00	0.03	-0.11	0.29	-0.01	0.01	-0.01	0.02	-0.01	0.04	1.22E-005	0.00	0.01	0.08	0.00	0.00	0.00	0.00	0.00	0.00
50	129.22	0.04	-0.01	-0.20	0.29	0.03	0.10	0.01	0.05	-0.04	-0.03	0.00	0.00	0.04	0.08	0.00	0.01	6.20E-005	0.00	0.00	0.00
50	84.53	0.06	0.05	-0.13	0.31	-0.01	0.01	-0.04	0.03	-0.02	0.01	0.00	0.00	0.02	0.10	6.31E-005	0.00	0.00	0.00	0.00	5.50E-005
50	136.50	-0.17	0.05	0.00	0.33	-0.06	-0.00	0.01	-0.07	-0.04	-0.01	0.03	0.00	6.91E-006	0.11	0.00	2.34E-005	0.00	0.00	0.00	6.15E-005
50	136.50	-0.08	0.07	-0.15	0.34	0.01	0.04	0.01	-0.03	-0.03	0.04	0.01	0.00	0.02	0.12	2.98E-005	0.00	0.00	0.00	0.00	0.00
50	18.20	0.01	0.04	-0.13	0.26	0.02	0.03	-0.04	0.02	0.02	0.00	4.12E-005	0.00	0.02	0.07	0.00	0.00	0.00	0.00	0.00	4.72E-006
100	89.27	0.20	-0.06	-0.10	0.19	0.02	0.02	0.02	0.07	-0.01	0.01	0.04	0.00	0.01	0.04	0.00	0.00	0.00	0.00	0.00	2.61E-005
100	89.27	-0.10	0.02	-0.06	0.28	-0.03	0.06	-0.05	0.02	0.02	-0.02	0.01	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00
100	78.47	-0.05	0.04	-0.09	0.27	0.03	0.04	-0.01	0.01	-0.00	0.07	0.00	0.00	0.01	0.07	0.00	0.00	4.82E-005	9.30E-005	8.96E-006	0.01
100	78.47	-0.22	-0.05	-0.01	0.24	-0.01	-0.05	0.01	-0.03	0.01	0.09	0.05	0.00	3.59E-005	0.06	8.03E-005	0.00	0.00	0.00	5.79E-005	0.01
100	78.47	-0.10	0.03	-0.11	0.24	-0.01	0.05	-0.04	0.02	0.02	0.01	0.01	0.00	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.00
100	138.59	-0.03	0.00	-0.15	0.29	0.02	-0.02	0.02	0.08	-0.04	0.04	0.00	1.25E-005	0.02	0.09	0.00	0.00	0.00	0.01	0.00	0.00
100	138.59	-0.07	0.07	-0.11	0.37	-0.02	0.05	0.01	-0.01	0.01	-0.01	0.01	0.00	0.01	0.14	0.00	0.00	8.56E-005	3.04E-005	5.04E-005	3.80E-005
100	138.59	-0.06	-0.00	-0.11	0.28	-0.01	-0.03	-0.00	0.06	0.02	0.05	0.00	4.12E-007	0.01	0.08	5.60E-005	0.00	1.93E-005	0.00	0.00	0.00
100	138.59	-0.00	0.03	-0.11	0.29	-0.01	0.01	-0.01	0.02	-0.01	0.04	1.22E-005	0.00	0.01	0.08	0.00	0.00	0.00	0.00	0.00	0.00
100	131.25	0.04	-0.01	-0.20	0.29	0.03	0.10	0.01	0.05	-0.04	-0.03	0.00	0.00	0.04	0.08	0.00	0.01	6.20E-005	0.00	0.00	0.00
100	86.38	0.06	0.05	-0.13	0.31	-0.01	0.01	-0.04	0.03	-0.02	0.01	0.00	0.00	0.02	0.10	6.31E-005	0.00	0.00	0.00	0.00	5.50E-005
100	138.59	-0.17	0.05	0.00	0.33	-0.06	-0.00	0.01	-0.07	-0.04	-0.01	0.03	0.00	6.91E-006	0.11	0.00	2.34E-005	0.00	0.00	0.00	6.15E-005
100	138.59	-0.08	0.07	-0.15	0.34	0.01	0.04	0.01	-0.03	-0.03	0.04	0.01	0.00	0.02	0.12	2.98E-005	0.00	0.00	0.00	0.00	0.00

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1	P_{ave} WV2	P_{ave} WV3	P_{ave} WV4	P_{ave} WV5	P_{ave} WV6	P_{ave} WV7	P_{ave} WV8	P_{ave} WV9	P_{ave} WV10	$(P_{ave} \text{ WV1})^{\wedge 2}$	$(P_{ave} \text{ WV2})^{\wedge 2}$	$(P_{ave} \text{ WV3})^{\wedge 2}$	$(P_{ave} \text{ WV4})^{\wedge 2}$	$(P_{ave} \text{ WV5})^{\wedge 2}$	$(P_{ave} \text{ WV6})^{\wedge 2}$	$(P_{ave} \text{ WV7})^{\wedge 2}$	$(P_{ave} \text{ WV8})^{\wedge 2}$	$(P_{ave} \text{ WV9})^{\wedge 2}$	$(P_{ave} \text{ WV10})^{\wedge 2}$
100	18.34	0.01	0.04	-0.13	0.26	0.02	0.03	-0.04	0.02	0.02	0.00	4.12E-005	0.00	0.02	0.07	0.00	0.00	0.00	0.00	0.00	4.72E-006

^a estimated by the Teusink's kinetic model as described in Material and Methods;
^b in accordance with 10 VARIMAX-derived scales (Georgiev, 2009 [18]) which represent generalized numerical scores for physical-chemical and structural features of amino acids.

Table S1-2. The dataset used in multivariate analysis which comprises metabolic fluxes ^a and numerical vectors representing the average amino acid property ^b for each enzyme sequence.

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1	P_{ave} WV2	P_{ave} WV3	P_{ave} WV4	P_{ave} WV5	P_{ave} WV6	P_{ave} WV7	P_{ave} WV8	P_{ave} WV9	P_{ave} WV10	$(P_{ave} \text{ WV1})^{\wedge 2}$	$(P_{ave} \text{ WV2})^{\wedge 2}$	$(P_{ave} \text{ WV3})^{\wedge 2}$	$(P_{ave} \text{ WV4})^{\wedge 2}$	$(P_{ave} \text{ WV5})^{\wedge 2}$	$(P_{ave} \text{ WV6})^{\wedge 2}$	$(P_{ave} \text{ WV7})^{\wedge 2}$	$(P_{ave} \text{ WV8})^{\wedge 2}$	$(P_{ave} \text{ WV9})^{\wedge 2}$	$(P_{ave} \text{ WV10})^{\wedge 2}$
25	0.84	20.09	-5.87	-9.85	19.15	1.64	3.87	1.56	6.93	-1.10	0.51	405.66	34.44	104.19	366.91	2.68	26.78	3.83	40.91	1.21	0.48
25	49.36	-9.75	2.10	-5.61	28.44	-3.18	5.59	-4.90	1.72	2.10	-2.10	95.03	4.42	31.46	809.06	10.09	31.29	23.97	2.96	4.42	4.40
25	28.58	-4.88	3.73	-8.79	26.64	3.46	3.76	-0.69	0.96	-0.30	7.23	23.81	13.94	77.31	709.47	11.95	14.13	0.48	0.93	0.09	52.27
25	28.58	-21.96	-5.43	-0.60	23.99	-0.90	-4.83	1.43	-3.30	0.76	8.75	482.11	29.54	0.36	575.31	0.80	23.33	2.04	10.91	0.58	76.56
25	28.58	-9.68	3.35	-10.89	23.67	-1.14	4.95	-3.85	1.54	2.14	1.10	93.70	11.22	118.51	560.48	1.31	24.54	14.79	2.38	4.56	1.21
25	24.27	-6.01	4.08	-12.24	33.83	4.30	3.52	-1.30	2.96	-1.45	2.43	36.09	16.67	149.81	1144.47	18.52	12.36	1.69	8.75	2.11	5.90
25	52.85	-3.50	0.35	-15.43	29.19	1.75	-2.40	1.77	7.59	-3.80	4.34	12.24	0.13	238.16	851.93	3.07	5.74	3.14	57.61	14.41	18.83
25	52.85	-7.43	6.91	-10.65	37.25	-1.55	4.75	0.93	-0.55	0.71	-0.62	55.26	47.75	113.52	1387.26	2.41	22.58	0.86	0.30	0.50	0.38
25	52.85	-5.93	-0.06	-11.28	28.26	-0.75	-3.02	-0.44	6.44	1.65	5.44	35.11	0.00	127.27	798.65	0.56	9.13	0.19	41.50	2.72	29.58
25	52.85	-0.35	2.64	-11.10	29.12	-1.32	1.33	-1.03	1.85	-1.32	4.20	0.12	6.98	123.16	848.14	1.74	1.77	1.06	3.42	1.74	17.67
25	48.54	3.63	-1.37	-20.07	28.59	2.61	10.28	0.79	5.02	-4.16	-3.36	13.20	1.88	402.82	817.43	6.81	105.67	0.62	25.24	17.28	11.32
25	6.98	5.63	4.56	-13.44	31.18	-0.79	1.31	-3.53	3.21	-2.12	0.74	31.67	20.81	180.75	972.18	0.63	1.73	12.49	10.28	4.51	0.55
25	0	-15.60	7.22	-12.60	26.79	-8	5.60	-0.25	-1.05	-2.26	-0.08	243.45	52.16	158.85	717.96	64	31.32	0.06	1.10	5.13	0.01
25	20.78	-6.66	2.03	0.74	26.41	1.46	1.43	-4.46	-1.30	5.58	4.65	44.32	4.14	0.55	697.27	2.13	2.05	19.87	1.70	31.17	21.67
25	4.31	0.64	3.78	-12.84	25.91	2.31	3.46	-3.82	1.70	1.69	0.22	0.41	14.27	164.90	671.32	5.35	11.94	14.60	2.88	2.84	0.05
50	0.84	20.09	-5.87	-9.85	19.15	1.64	3.87	1.56	6.93	-1.10	0.51	405.66	34.44	104.19	366.91	2.68	26.78	3.83	40.91	1.21	0.48
50	49.38	-9.75	2.10	-5.61	28.44	-3.18	5.59	-4.90	1.72	2.10	-2.10	95.03	4.42	31.46	809.06	10.09	31.29	23.97	2.96	4.42	4.40
50	28.60	-4.88	3.73	-8.79	26.64	3.46	3.76	-0.69	0.96	-0.30	7.23	23.81	13.94	77.31	709.47	11.95	14.13	0.48	0.93	0.09	52.27
50	28.60	-21.96	-5.43	-0.60	23.99	-0.90	-4.83	1.43	-3.30	0.76	8.75	482.11	29.54	0.36	575.31	0.80	23.33	2.04	10.91	0.58	76.56
50	28.60	-9.68	3.35	-10.89	23.67	-1.14	4.95	-3.85	1.54	2.14	1.10	93.70	11.22	118.51	560.48	1.31	24.54	14.79	2.38	4.56	1.21
50	24.28	-6.01	4.08	-12.24	33.83	4.30	3.52	-1.30	2.96	-1.45	2.43	36.09	16.67	149.81	1144.47	18.52	12.36	1.69	8.75	2.11	5.90
50	52.88	-3.50	0.35	-15.43	29.19	1.75	-2.40	1.77	7.59	-3.80	4.34	12.24	0.13	238.16	851.93	3.07	5.74	3.14	57.61	14.41	18.83
50	52.88	-7.43	6.91	-10.65	37.25	-1.55	4.75	0.93	-0.55	0.71	-0.62	55.26	47.75	113.52	1387.26	2.41	22.58	0.86	0.30	0.50	0.38
50	52.88	-5.93	-0.06	-11.28	28.26	-0.75	-3.02	-0.44	6.44	1.65	5.44	35.11	0.00	127.27	798.65	0.56	9.13	0.19	41.50	2.72	29.58
50	52.88	-0.35	2.64	-11.10	29.12	-1.32	1.33	-1.03	1.85	-1.32	4.20	0.12	6.98	123.16	848.14	1.74	1.77	1.06	3.42	1.74	17.67
50	48.56	3.63	-1.37	-20.07	28.59	2.61	10.28	0.79	5.02	-4.16	-3.36	13.20	1.88	402.82	817.43	6.81	105.67	0.62	25.24	17.28	11.32
50	6.98	5.63	4.56	-13.44	31.18	-0.79	1.31	-3.53	3.21	-2.12	0.74	31.67	20.81	180.75	972.18	0.63	1.73	12.49	10.28	4.51	0.55
50	0	-15.60	7.22	-12.60	26.79	-8	5.60	-0.25	-1.05	-2.26	-0.08	243.45	52.16	158.85	717.96	64	31.32	0.06	1.10	5.13	0.01
50	20.79	-6.66	2.03	0.74	26.41	1.46	1.43	-4.46	-1.30	5.58	4.65	44.32	4.14	0.55	697.27	2.13	2.05	19.87	1.70	31.17	21.67
50	4.32	0.64	3.78	-12.84	25.91	2.31	3.46	-3.82	1.70	1.69	0.22	0.41	14.27	164.90	671.32	5.35	11.94	14.60	2.88	2.84	0.05
100	0.84	20.09	-5.87	-9.85	19.15	1.64	3.87	1.56	6.93	-1.10	0.51	405.66	34.44	104.19	366.91	2.68	26.78	3.83	40.91	1.21	0.48
100	49.39	-9.75	2.10	-5.61	28.44	-3.18	5.59	-4.90	1.72	2.10	-2.10	95.03	4.42	31.46	809.06	10.09	31.29	23.97	2.96	4.42	4.40
100	28.60	-4.88	3.73	-8.79	26.64	3.46	3.76	-0.69	0.96	-0.30	7.23	23.81	13.94	77.31	709.47	11.95	14.13	0.48	0.93	0.09	52.27
100	28.60	-21.96	-5.43	-0.60	23.99	-0.90	-4.83	1.43	-3.30	0.76	8.75	482.11	29.54	0.36	575.31	0.80	23.33	2.04	10.91	0.58	76.56
100	28.60	-9.68	3.35	-10.89	23.67	-1.14	4.95	-3.85	1.54	2.14	1.10	93.70	11.22	118.51	560.48	1.31	24.54	14.79	2.38	4.56	1.21
100	24.28	-6.01	4.08	-12.24	33.83	4.30	3.52	-1.30	2.96	-1.45	2.43	36.09	16.67	149.81	1144.47	18.52	12.36	1.69	8.75	2.11	5.90
100	52.88	-3.50	0.35	-15.43	29.19	1.75	-2.40	1.77	7.59	-3.80	4.34	12.24	0.13	238.16	851.93	3.07	5.74	3.14	57.61	14.41	18.83
100	52.88	-7.43	6.91	-10.65	37.25	-1.55	4.75	0.93	-0.55	0.71	-0.62	55.26	47.75	113.52	1387.26	2.41	22.58	0.86	0.30	0.50	0.38
100	52.88	-5.93	-0.06	-11.28	28.26	-0.75	-3.02	-0.44	6.44	1.65	5.44	35.11	0.00	127.27	798.65	0.56	9.13	0.19	41.50	2.72	29.58
100	52.88	-0.35	2.64	-11.10	29.12	-1.32	1.33	-1.03	1.85	-1.32	4.20	0.12	6.98	123.16	848.14	1.74	1.77	1.06	3.42	1.74	17.67
100	48.56	3.63	-1.37	-20.07	28.59	2.61	10.28	0.79	5.02	-4.16	-3.36	13.20	1.88	402.82	817.43	6.81	105.67	0.62	25.24	17.28	11.32

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1	P_{ave} WV2	P_{ave} WV3	P_{ave} WV4	P_{ave} WV5	P_{ave} WV6	P_{ave} WV7	P_{ave} WV8	P_{ave} WV9	P_{ave} WV10	$(P_{ave}^{WV1})^2$	$(P_{ave}^{WV2})^2$	$(P_{ave}^{WV3})^2$	$(P_{ave}^{WV4})^2$	$(P_{ave}^{WV5})^2$	$(P_{ave}^{WV6})^2$	$(P_{ave}^{WV7})^2$	$(P_{ave}^{WV8})^2$	$(P_{ave}^{WV9})^2$	$(P_{ave}^{WV10})^2$
100	6.98	5.63	4.56	-13.44	31.18	-0.79	1.31	-3.53	3.21	-2.12	0.74	31.67	20.81	180.75	972.18	0.63	1.73	12.49	10.28	4.51	0.55
100	-5.68E-014	-15.60	7.22	-12.60	26.79	-8	5.60	-0.25	-1.05	-2.26	-0.08	243.45	52.16	158.85	717.96	64	31.32	0.06	1.10	5.13	0.01
100	20.79	-6.66	2.03	0.74	26.41	1.46	1.43	-4.46	-1.30	5.58	4.65	44.32	4.14	0.55	697.27	2.13	2.05	19.87	1.70	31.17	21.67
100	4.32	0.64	3.78	-12.84	25.91	2.31	3.46	-3.82	1.70	1.69	0.22	0.41	14.27	164.90	671.32	5.35	11.94	14.60	2.88	2.84	0.05

^a estimated by the Hynne's kinetic model as described in Material and Methods;
^b in accordance with 10 VARIMAX-derived scales (Georgiev, 2009 [18]) which represent generalized numerical scores for physical-chemical and structural features of amino acids.

Table S1-3. The dataset used in multivariate analysis which comprises metabolic fluxes ^a and numerical vectors representing the average amino acid property ^b for each enzyme sequence.

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave}^{WV1-1}	P_{ave}^{WV1-2}	P_{ave}^{WV1-3}	$(P_{ave}^{WV1-1})^2$	$(P_{ave}^{WV1-2})^2$	$(P_{ave}^{WV1-3})^2$	P_{ave}^{WV2-1}	P_{ave}^{WV2-2}	P_{ave}^{WV2-3}	$(P_{ave}^{WV2-1})^2$	$(P_{ave}^{WV2-2})^2$	$(P_{ave}^{WV2-3})^2$	P_{ave}^{WV3-1}	P_{ave}^{WV3-2}	P_{ave}^{WV3-3}	$(P_{ave}^{WV3-1})^2$	$(P_{ave}^{WV3-2})^2$	$(P_{ave}^{WV3-3})^2$	P_{ave}^{WV5-1}	P_{ave}^{WV5-2}	P_{ave}^{WV5-3}	$(P_{ave}^{WV5-1})^2$	$(P_{ave}^{WV5-2})^2$	$(P_{ave}^{WV5-3})^2$	P_{ave}^{WV6-1}	P_{ave}^{WV6-2}	P_{ave}^{WV6-3}	$(P_{ave}^{WV6-1})^2$	$(P_{ave}^{WV6-2})^2$	$(P_{ave}^{WV6-3})^2$	P_{ave}^{WV7-1}	P_{ave}^{WV7-2}	P_{ave}^{WV7-3}	$(P_{ave}^{WV7-1})^2$	$(P_{ave}^{WV7-2})^2$	$(P_{ave}^{WV7-3})^2$
25	85.99	10.30	33.63	0.75	106.15	1130.78	0.56	0.98	0.99	0.99	0.97	0.97	0.99	143.74	138.34	3.30	20660.76	19137.84	10.89	8.02	1.56	0.96	64.28	2.44	0.93	0.99	11.68	1.21	0.99	136.45	1.47	0.00	5.96	1.05	1.00E-006	35.52	1.09
25	85.99	-15.80	7.82	0.72	249.55	61.20	0.52	1.02	1.03	1.04	1.03	1.06	1.07	142.46	137.45	3.25	20295.82	18892.31	10.55	7.92	1.72	1.04	62.79	2.95	1.07	1.01	11.19	1.18	1.02	125.29	1.40	-0.03	5.96	1.04	0.00	35.55	1.09
25	75.19	-9.69	11.13	0.72	93.80	123.88	0.52	1.02	1.03	1.04	1.04	1.06	1.08	141.89	136.94	3.21	20132.26	18752.29	10.32	8.12	1.42	0.99	65.96	2.01	0.99	1.01	11.25	1.21	1.03	126.55	1.46	-0.02	5.94	1.06	0.00	35.29	1.13
25	75.19	-25.82	-2.95	0.71	666.52	8.68	0.50	0.99	1.00	0.99	0.97	1.00	0.98	144.43	138.74	3.36	20860.80	19248.18	11.29	7.86	1.81	1.04	61.72	3.26	1.08	0.97	11.60	1.19	0.93	134.59	1.42	0.01	6.08	1.10	6.40E-005	36.93	1.22
25	75.19	-14.64	7.29	0.72	214.45	53.17	0.52	1.02	1.03	1.04	1.04	1.07	1.08	141.39	135.89	3.17	19991.67	18465.66	10.07	7.98	1.63	1.02	63.70	2.66	1.04	1.03	11.17	1.19	1.05	124.80	1.41	-0.03	5.94	1.05	0.00	35.32	1.11
25	132.44	-8.11	10.02	0.72	65.76	100.46	0.52	1.00	1.01	1.01	1.00	1.02	1.03	138.11	133.47	3.03	19075.73	17814.16	9.18	7.99	1.53	1.00	63.88	2.34	1.00	0.98	11.43	1.10	0.95	130.62	1.20	0.01	6.04	1.06	3.60E-005	36.47	1.12
25	132.44	-12.91	7.83	0.72	166.75	61.25	0.52	1.03	1.04	1.05	1.06	1.08	1.11	138.53	134.52	3.05	19191.12	18096.73	9.33	8.01	1.57	1.03	64.18	2.47	1.05	1.01	11.02	1.14	1.03	121.39	1.29	0	6.06	1.07	0	36.77	1.14
25	132.44	-10.64	9.26	0.72	113.17	85.67	0.52	1.01	1.02	1.02	1.01	1.03	1.04	140.57	135.74	3.14	19760.88	18423.99	9.84	7.94	1.67	1.02	63.07	2.78	1.04	0.97	11.67	1.12	0.94	136.24	1.26	0.00	6.05	1.06	4.00E-006	36.58	1.12
25	132.44	-6.03	14.37	0.73	36.39	206.50	0.53	1.01	1.02	1.03	1.03	1.04	1.06	140.22	135.50	3.12	19660.75	18360.71	9.76	7.95	1.62	1.01	63.17	2.62	1.02	0.98	11.33	1.15	0.97	128.27	1.33	-0.02	5.94	1.05	0.00	35.24	1.09
25	125.27	-3.21	16.31	0.73	10.30	265.95	0.53	0.99	1.00	1.00	0.99	1.01	1.01	135.68	130.95	2.92	18410.12	17148.37	8.55	8.03	1.52	0.99	64.49	2.32	0.97	1.06	10.79	1.21	1.13	116.47	1.47	-0.01	5.98	1.04	0.00	35.79	1.07
25	80.95	0.15	19.61	0.73	0.02	384.36	0.54	1.02	1.03	1.04	1.05	1.05	1.09	139.44	135.03	3.09	19443.65	18232.10	9.56	8.01	1.55	1.00	64.11	2.40	1.01	0.97	11.31	1.14	0.94	128.02	1.29	-0.04	5.90	1.03	0.00	34.77	1.07
25	132.44	-22.98	1.13	0.71	528.26	1.27	0.50	1.03	1.04	1.05	1.06	1.08	1.09	143.55	138.85	3.29	20605.20	19278.66	10.85	7.82	1.85	1.06	61.14	3.42	1.13	0.97	11.21	1.11	0.94	125.70	1.24	0.01	6.14	1.09	0.00	37.65	1.19
25	132.44	-11.57	6.71	0.72	133.77	44.98	0.52	1.03	1.04	1.06	1.06	1.09	1.12	137.68	133.28	2.98	18954.54	17763.56	8.90	8.09	1.49	1.02	65.50	2.22	1.04	1.01	10.85	1.15	1.02	117.62	1.32	-0.01	6.03	1.08	0.00	36.41	1.16
25	17.94	-5.24	16.95	0.73	27.43	287.30	0.53	1.02	1.03	1.04	1.04	1.06	1.07	140.23	135.40	3.15	19665.01	18333.08	9.92	8.05	1.52	1.00	64.83	2.31	0.99	1.01	11.25	1.18	1.01	126.55	1.40	-0.04	5.91	1.04	0.00	34.91	1.08
50	88.15	10.30	33.63	0.75	106.15	1130.78	0.56	0.98	0.99	0.99	0.97	0.97	0.99	143.74	138.34	3.30	20660.76	19137.84	10.89	8.02	1.56	0.96	64.28	2.44	0.93	0.99	11.68	1.21	0.99	136.45	1.47	0.00	5.96	1.05	1.00E-006	35.52	1.09
50	88.15	-15.80	7.82	0.72	249.55	61.20	0.52	1.02	1.03	1.04	1.03	1.06	1.07	142.46	137.45	3.25	20295.82	18892.31	10.55	7.92	1.72	1.04	62.79	2.95	1.07	1.01	11.19	1.18	1.02	125.29	1.40	-0.03	5.96	1.04	0.00	35.55	1.09
50	77.35	-9.69	11.13	0.72	93.80	123.88	0.52	1.02	1.03	1.04	1.04	1.06	1.08	141.89	136.94	3.21	20132.26	18752.29	10.32	8.12	1.42	0.99	65.96	2.01	0.99	1.01	11.25	1.21	1.03	126.55	1.46	-0.02	5.94	1.06	0.00	35.29	1.13
50	77.35	-25.82	-2.95	0.71	666.52	8.68	0.50	0.99	1.00	0.99	0.97	1.00	0.98	144.43	138.74	3.36	20860.80	19248.18	11.29	7.86	1.81	1.04	61.72	3.26	1.08	0.97	11.60	1.19	0.93	134.59	1.42	0.01	6.08	1.10	6.40E-005	36.93	1.22
50	77.35	-14.64	7.29	0.72	214.45	53.17	0.52	1.02	1.03	1.04	1.04	1.07	1.08	141.39	135.89	3.17	19991.67	18465.66	10.07	7.98	1.63	1.02	63.70	2.66	1.04	1.03	11.17	1.19	1.05	124.80	1.41	-0.03	5.94	1.05	0.00	35.32	1.11
50	136.50	-8.11	10.02	0.72	65.76	100.46	0.52	1.00	1.01	1.01	1.00	1.02	1.03	138.11	133.47	3.03	19075.73	17814.16	9.18	7.99	1.53	1.00	63.88	2.34	1.00	0.98	11.43	1.10	0.95	130.62	1.20	0.01	6.04	1.06	3.60E-005	36.47	1.12
50	136.50	-12.91	7.83	0.72	166.75	61.25	0.52	1.03	1.04	1.05	1.06	1.08	1.11	138.53	134.52	3.05	19191.12	18096.73	9.33	8.01	1.57	1.03	64.18	2.47	1.05	1.01	11.02	1.14	1.03	121.39	1.29	0	6.06	1.07	0	36.77	1.14
50	136.50	-10.64	9.26	0.72	113.17	85.67	0.52	1.01	1.02	1.02	1.01	1.03	1.04	140.57	135.74	3.14	19760.88	18423.99	9.84	7.94	1.67	1.02	63.07	2.78	1.04	0.97	11.67	1.12	0.94	136.24	1.26	0.00	6.05	1.06	4.00E-006	36.58	1.12
50	136.50	-6.03	14.37	0.73	36.39	206.50	0.53	1.01	1.02	1.03	1.03	1.04	1.06	140.22	135.50	3.12	19660.75	18360.71	9.76	7.95	1.62	1.01	63.17	2.62	1.02	0.98	11.33	1.15	0.97	128.27	1.33	-0.02	5.94	1.05	0.00	35.24	1.09
50	129.22	-3.21	16.31	0.73	10.30	265.95	0.53	0.99	1.00	1.00	0.99	1.01	1.01	135.68	130.95	2.92	18410.12	17148.37	8.55	8.03	1.52	0.99	64.49	2.32	0.97	1.06	10.79	1.21	1.13	116							

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1-1	P_{ave} WV1-2	P_{ave} WV1-3	$(P_{ave}$ WV1-1) ⁻²	$(P_{ave}$ WV1-2) ⁻²	$(P_{ave}$ WV1-3) ⁻²	P_{ave} WV2-1	P_{ave} WV2-2	P_{ave} WV2-3	$(P_{ave}$ WV2-1) ⁻²	$(P_{ave}$ WV2-2) ⁻²	$(P_{ave}$ WV2-3) ⁻²	P_{ave} WV3-1	P_{ave} WV3-2	P_{ave} WV3-3	$(P_{ave}$ WV3-1) ⁻²	$(P_{ave}$ WV3-2) ⁻²	$(P_{ave}$ WV3-3) ⁻²	P_{ave} WV5-1	P_{ave} WV5-2	P_{ave} WV5-3	$(P_{ave}$ WV5-1) ⁻²	$(P_{ave}$ WV5-2) ⁻²	$(P_{ave}$ WV5-3) ⁻²	P_{ave} WV6-1	P_{ave} WV6-2	P_{ave} WV6-3	$(P_{ave}$ WV6-1) ⁻²	$(P_{ave}$ WV6-2) ⁻²	$(P_{ave}$ WV6-3) ⁻²	P_{ave} WV7-1	P_{ave} WV7-2	P_{ave} WV7-3	$(P_{ave}$ WV7-1) ⁻²	$(P_{ave}$ WV7-2) ⁻²	$(P_{ave}$ WV7-3) ⁻²
100	86.38	0.15	19.61	0.73	0.02	384.36	0.54	1.02	1.03	1.04	1.05	1.05	1.09	139.44	135.03	3.09	19443.65	18232.10	9.56	8.01	1.55	1.00	64.11	2.40	1.01	0.97	11.31	1.14	0.94	128.02	1.29	-0.04	5.90	1.03	0.00	34.77	1.07
100	138.59	-22.98	1.13	0.71	528.26	1.27	0.50	1.03	1.04	1.05	1.06	1.08	1.09	143.55	138.85	3.29	20605.20	19278.66	10.85	7.82	1.85	1.06	61.14	3.42	1.13	0.97	11.21	1.11	0.94	125.70	1.24	0.01	6.14	1.09	0.00	37.65	1.19
100	138.59	-11.57	6.71	0.72	133.77	44.98	0.52	1.03	1.04	1.06	1.06	1.09	1.12	137.68	133.28	2.98	18954.54	17763.56	8.90	8.09	1.49	1.02	65.50	2.22	1.04	1.01	10.85	1.15	1.02	117.62	1.32	-0.01	6.03	1.08	0.00	36.41	1.16
100	18.34	-5.24	16.95	0.73	27.43	287.30	0.53	1.02	1.03	1.04	1.04	1.06	1.07	140.23	135.40	3.15	19665.01	18333.08	9.92	8.05	1.52	1.00	64.83	2.31	0.99	1.01	11.25	1.18	1.01	126.55	1.40	-0.04	5.91	1.04	0.00	34.91	1.08

^a estimated by the Teusink's kinetic model as described in Material and Methods;
^b in accordance with 10 VARIMAX-derived scales (Georgiev, 2009 [18]) which represent generalized numerical scores for physical-chemical and structural features of amino acids.

Table S1-4. The dataset used in multivariate analysis which comprises metabolic fluxes ^a and numerical vectors representing the average amino acid property ^b for each enzyme sequence.

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1-1	P_{ave} WV1-2	P_{ave} WV1-3	$(P_{ave}$ WV1-1) ²	$(P_{ave}$ WV1-2) ²	$(P_{ave}$ WV1-3) ²	P_{ave} WV2-1	P_{ave} WV2-2	P_{ave} WV2-3	$(P_{ave}$ WV2-1) ²	$(P_{ave}$ WV2-2) ²	$(P_{ave}$ WV2-3) ²	P_{ave} WV3-1	P_{ave} WV3-2	P_{ave} WV3-3	$(P_{ave}$ WV3-1) ²	$(P_{ave}$ WV3-2) ²	$(P_{ave}$ WV3-3) ²	P_{ave} WV5-1	P_{ave} WV5-2	P_{ave} WV5-3	$(P_{ave}$ WV5-1) ²	$(P_{ave}$ WV5-2) ²	$(P_{ave}$ WV5-3) ²	P_{ave} WV6-1	P_{ave} WV6-2	P_{ave} WV6-3	$(P_{ave}$ WV6-1) ²	$(P_{ave}$ WV6-2) ²	$(P_{ave}$ WV6-3) ²	P_{ave} WV7-1	P_{ave} WV7-2	P_{ave} WV7-3	$(P_{ave}$ WV7-1) ²	$(P_{ave}$ WV7-2) ²	$(P_{ave}$ WV7-3) ²
25	0.84	10.44	33.56	0.75	109.01	1126.01	0.56	0.98	0.99	0.99	0.97	0.97	0.99	143.07	137.67	3.34	20467.79	18951.84	11.18	8.02	1.56	0.96	64.28	2.44	0.93	0.99	11.68	1.21	0.99	136.45	1.47	0.00	5.96	1.05	1.00E-006	35.52	1.09
25	49.36	-15.80	7.82	0.72	249.55	61.20	0.52	1.02	1.03	1.04	1.03	1.06	1.07	142.46	137.45	3.31	20295.82	18892.31	10.98	7.92	1.72	1.04	62.79	2.95	1.07	1.01	11.19	1.18	1.02	125.29	1.40	-0.03	5.96	1.04	0.00	35.55	1.09
25	28.58	-9.69	11.13	0.72	93.80	123.88	0.52	1.02	1.03	1.04	1.04	1.06	1.08	141.89	136.94	3.30	20132.26	18752.29	10.88	8.12	1.42	0.99	65.96	2.01	0.99	1.01	11.25	1.21	1.03	126.55	1.46	-0.02	5.94	1.06	0.00	35.29	1.13
25	28.58	-25.82	-2.95	0.71	666.52	8.68	0.50	0.99	1.00	0.99	0.97	1.00	0.98	144.43	138.74	3.41	20860.80	19248.18	11.63	7.86	1.81	1.04	61.72	3.26	1.08	0.97	11.60	1.19	0.93	134.59	1.42	0.01	6.08	1.10	6.40E-005	36.93	1.22
25	28.58	-14.64	7.29	0.72	214.45	53.17	0.52	1.02	1.03	1.04	1.04	1.07	1.08	141.39	135.89	3.27	19991.67	18465.66	10.66	7.98	1.63	1.02	63.70	2.66	1.04	1.03	11.17	1.19	1.05	124.80	1.41	-0.03	5.94	1.05	0.00	35.32	1.11
25	24.27	-10.11	8.62	0.72	102.27	74.27	0.52	1.02	1.03	1.04	1.04	1.06	1.08	138.63	134.05	3.15	19218.69	17969.08	9.95	8.12	1.42	1.00	65.93	2.01	1.01	1.01	11.12	1.16	1.02	123.71	1.33	-0.01	5.98	1.06	0.00	35.79	1.12
25	52.85	-8.11	10.02	0.72	65.76	100.46	0.52	1.00	1.01	1.01	1.00	1.02	1.03	138.11	133.47	3.14	19075.73	17814.16	9.83	7.99	1.53	1.00	63.88	2.34	1.00	0.98	11.43	1.10	0.95	130.62	1.20	0.01	6.04	1.06	3.60E-005	36.47	1.12
25	52.85	-12.91	7.83	0.72	166.75	61.25	0.52	1.03	1.04	1.05	1.06	1.08	1.11	138.53	134.52	3.16	19191.12	18096.73	9.97	8.01	1.57	1.03	64.18	2.47	1.05	1.01	11.02	1.14	1.03	121.39	1.29	-1.39E-017	6.06	1.07	1.93E-034	36.77	1.14
25	52.85	-10.64	9.26	0.72	113.17	85.67	0.52	1.01	1.02	1.02	1.01	1.03	1.04	140.57	135.74	3.22	19760.88	18423.99	10.39	7.94	1.67	1.02	63.07	2.78	1.04	0.97	11.67	1.12	0.94	136.24	1.26	0.00	6.05	1.06	4.00E-006	36.58	1.12
25	52.85	-6.03	14.37	0.73	36.39	206.50	0.53	1.01	1.02	1.03	1.03	1.04	1.06	140.22	135.50	3.22	19660.75	18360.71	10.36	7.95	1.62	1.01	63.17	2.62	1.02	0.98	11.33	1.15	0.97	128.27	1.33	-0.02	5.94	1.05	0.00	35.24	1.09
25	48.54	-3.21	16.31	0.73	10.30	265.95	0.53	0.99	1.00	1.00	0.99	1.01	1.01	135.68	130.95	3.02	18410.12	17148.37	9.15	8.03	1.52	0.99	64.49	2.32	0.97	1.06	10.79	1.21	1.13	116.47	1.47	-0.01	5.98	1.04	0.00	35.79	1.07
25	6.98	0.15	19.61	0.73	0.02	384.36	0.54	1.02	1.03	1.04	1.05	1.05	1.09	139.44	135.03	3.19	19443.65	18232.10	10.18	8.01	1.55	1.00	64.11	2.40	1.01	0.97	11.31	1.14	0.94	128.02	1.29	-0.04	5.90	1.03	0.00	34.77	1.07
25	0	-20.70	2.99	0.72	428.53	8.91	0.51	1.04	1.05	1.06	1.08	1.10	1.13	140.37	136.18	3.23	19704.66	18544.39	10.46	7.91	1.80	1.07	62.57	3.23	1.14	1.01	10.96	1.16	1.02	120.06	1.35	-0.01	6.07	1.07	0.00	36.80	1.14
25	20.78	-12.19	12.68	0.73	148.67	160.81	0.53	1.02	1.03	1.04	1.04	1.05	1.07	146.57	140.73	3.48	21483.56	19804.43	12.13	8.03	1.57	1.01	64.50	2.48	1.03	0.98	11.42	1.18	0.97	130.52	1.39	-0.03	5.99	1.06	0.00	35.82	1.12
25	4.31	-5.24	16.95	0.73	27.43	287.30	0.53	1.02	1.03	1.04	1.04	1.06	1.07	140.23	135.40	3.23	19665.01	18333.08	10.45	8.05	1.52	1.00	64.83	2.31	0.99	1.01	11.25	1.18	1.01	126.55	1.40	-0.04	5.91	1.04	0.00	34.91	1.08
50	0.84	10.44	33.56	0.75	109.01	1126.01	0.56	0.98	0.99	0.99	0.97	0.97	0.99	143.07	137.67	3.34	20467.79	18951.84	11.18	8.02	1.56	0.96	64.28	2.44	0.93	0.99	11.68	1.21	0.99	136.45	1.47	0.00	5.96	1.05	1.00E-006	35.52	1.09
50	49.38	-15.80	7.82	0.72	249.55	61.20	0.52	1.02	1.03	1.04	1.03	1.06	1.07	142.46	137.45	3.31	20295.82	18892.31	10.98	7.92	1.72	1.04	62.79	2.95	1.07	1.01	11.19	1.18	1.02	125.29	1.40	-0.03	5.96	1.04	0.00	35.55	1.09
50	28.60	-9.69	11.13	0.72	93.80	123.88	0.52	1.02	1.03	1.04	1.04	1.06	1.08	141.89	136.94	3.30	20132.26	18752.29	10.88	8.12	1.42	0.99	65.96	2.01	0.99	1.01	11.25	1.21	1.03	126.55	1.46	-0.02	5.94	1.06	0.00	35.29	1.13
50	28.60	-25.82	-2.95	0.71	666.52	8.68	0.50	0.99	1.00	0.99	0.97	1.00	0.98	144.43	138.74	3.41	20860.80	19248.18	11.63	7.86	1.81	1.04	61.72	3.26	1.08	0.97	11.60	1.19	0.93	134.59	1.42	0.01	6.08	1.10	6.40E-005	36.93	1.22
50	28.60	-14.64	7.29	0.72	214.45	53.17	0.52	1.02	1.03	1.04	1.04	1.07	1.08	141.39	135.89	3.27	19991.67	18465.66	10.66	7.98	1.63	1.02	63.70	2.66	1.04	1.03	11.17	1.19	1.05	124.80	1.41	-0.03	5.94	1.05	0.00	35.32	1.11
50	24.28	-10.11	8.62	0.72	102.27	74.27	0.52	1.02	1.03	1.04	1.04	1.06	1.08	138.63	134.05	3.15	19218.69	17969.08	9.95	8.12	1.42	1.00	65.93	2.01	1.01	1.01	11.12	1.16	1.02	123.71	1.33	-0.01	5.98	1.06	0.00	35.79	1.12
50	52.88	-8.11	10.02	0.72	65.76	100.46	0.52	1.00	1.01	1.01	1.00	1.02	1.03	138.11	133.47	3.14	19075.73	17814.16	9.83	7.99	1.53	1.00	63.88	2.34	1.00	0.98	11.43	1.10	0.95	130.62	1.20	0.01	6.04	1.06	3.60E-005	36.47	1.12
50	52.88	-12.91	7.83	0.72	166.75	61.25	0.52	1.03	1.04	1.05	1.06	1.08	1.11	138.53	134.52	3.16	19191.12	18096.73	9.97	8.01	1.57	1.03	64.18	2.47	1.05	1.01	11.02	1.14	1.03	121.39	1.29	-1.39E-017	6.06	1.07	1.93E-034	36.77	1.14
50	52.88	-10.64	9.26	0.72	113.17	85.67	0.52	1.01	1.02	1.02	1.01	1.03	1.04	140.57	135.74	3.22	19760.88	18423.99	10.39	7.94	1.67	1.02	63.07	2.78	1.04	0.97	11.67	1.12	0.94	136.24	1.26	0.00	6.05	1.06	4.00E-006	36.58	1.12
50	52.88	-6.03	14.37	0.73	36.39	206.50	0.53	1.01	1.02	1.03	1.03	1.04	1.06	140.22	135.50	3.22	19660.75	18360.71	10.36	7.95	1.62	1.01	63.17	2.62	1.02	0.98	11.33	1.15	0.97	128.27	1.33	-0.02	5.94	1.05	0.00	35.24	1.09
50	48.56	-3.21	16.31	0.73	10.30	265.95	0.53	0.99	1.00	1.00	0.99	1.01	1.01	135.68	130.95	3.02	18410.12	17148.37	9.15	8.03	1.52	0.99	64.49	2.32	0.97	1.06	10.79	1.21	1.13	116.47	1.47	-0.01	5.98	1.04	0.00	35.79	1.07
50	6.98	0.15	19.61	0.73	0.02	384.36	0.54	1.02	1.03	1.04	1.05	1.05	1.09	139.44	135.03	3.19	19443.65																				

External glucose, mM	metabolic flux, mmol min ⁻¹	P_{ave} WV1-1	P_{ave} WV1-2	P_{ave} WV1-3	$(P_{ave}$ WV1-1) ^{∧2}	$(P_{ave}$ WV1-2) ^{∧2}	$(P_{ave}$ WV1-1-3) ^{∧2}	P_{ave} WV2-1	P_{ave} WV2-2	P_{ave} WV2-3	$(P_{ave}$ WV2-1) ^{∧2}	$(P_{ave}$ WV2-2) ^{∧2}	$(P_{ave}$ WV2-3) ^{∧2}	P_{ave} WV3-1	P_{ave} WV3-2	P_{ave} WV3-3	$(P_{ave}$ WV3-1) ^{∧2}	$(P_{ave}$ WV3-2) ^{∧2}	$(P_{ave}$ WV3-3) ^{∧2}	P_{ave} WV5-1	P_{ave} WV5-2	P_{ave} WV5-3	$(P_{ave}$ WV5-1) ^{∧2}	$(P_{ave}$ WV5-2) ^{∧2}	$(P_{ave}$ WV5-3) ^{∧2}	P_{ave} WV6-1	P_{ave} WV6-2	P_{ave} WV6-3	$(P_{ave}$ WV6-1) ^{∧2}	$(P_{ave}$ WV6-2) ^{∧2}	$(P_{ave}$ WV6-3) ^{∧2}	P_{ave} WV7-1	P_{ave} WV7-2	P_{ave} WV7-3	$(P_{ave}$ WV7-1) ^{∧2}	$(P_{ave}$ WV7-2) ^{∧2}	$(P_{ave}$ WV7-3) ^{∧2}
100	52.88	-12.91	7.83	0.72	166.75	61.25	0.52	1.03	1.04	1.05	1.06	1.08	1.11	138.53	134.52	3.16	19191.12	18096.73	9.97	8.01	1.57	1.03	64.18	2.47	1.05	1.01	11.02	1.14	1.03	121.39	1.29	-1.39E-017	6.06	1.07	1.93E-034	36.77	1.14
100	52.88	-10.64	9.26	0.72	113.17	85.67	0.52	1.01	1.02	1.02	1.01	1.03	1.04	140.57	135.74	3.22	19760.88	18423.99	10.39	7.94	1.67	1.02	63.07	2.78	1.04	0.97	11.67	1.12	0.94	136.24	1.26	0.00	6.05	1.06	4.00E-006	36.58	1.12
100	52.88	-6.03	14.37	0.73	36.39	206.50	0.53	1.01	1.02	1.03	1.03	1.04	1.06	140.22	135.50	3.22	19660.75	18360.71	10.36	7.95	1.62	1.01	63.17	2.62	1.02	0.98	11.33	1.15	0.97	128.27	1.33	-0.02	5.94	1.05	0.00	35.24	1.09
100	48.56	-3.21	16.31	0.73	10.30	265.95	0.53	0.99	1.00	1.00	0.99	1.01	1.01	135.68	130.95	3.02	18410.12	17148.37	9.15	8.03	1.52	0.99	64.49	2.32	0.97	1.06	10.79	1.21	1.13	116.47	1.47	-0.01	5.98	1.04	0.00	35.79	1.07
100	6.98	0.15	19.61	0.73	0.02	384.36	0.54	1.02	1.03	1.04	1.05	1.05	1.09	139.44	135.03	3.19	19443.65	18232.10	10.18	8.01	1.55	1.00	64.11	2.40	1.01	0.97	11.31	1.14	0.94	128.02	1.29	-0.04	5.90	1.03	0.00	34.77	1.07
100	-5.68E-014	-20.70	2.99	0.72	428.53	8.91	0.51	1.04	1.05	1.06	1.08	1.10	1.13	140.37	136.18	3.23	19704.66	18544.39	10.46	7.91	1.80	1.07	62.57	3.23	1.14	1.01	10.96	1.16	1.02	120.06	1.35	-0.01	6.07	1.07	0.00	36.80	1.14
100	20.79	-12.19	12.68	0.73	148.67	160.81	0.53	1.02	1.03	1.04	1.04	1.05	1.07	146.57	140.73	3.48	21483.56	19804.43	12.13	8.03	1.57	1.01	64.50	2.48	1.03	0.98	11.42	1.18	0.97	130.52	1.39	-0.03	5.99	1.06	0.00	35.82	1.12
100	4.32	-5.24	16.95	0.73	27.43	287.30	0.53	1.02	1.03	1.04	1.04	1.06	1.07	140.23	135.40	3.23	19665.01	18333.08	10.45	8.05	1.52	1.00	64.83	2.31	0.99	1.01	11.25	1.18	1.01	126.55	1.40	-0.04	5.91	1.04	0.00	34.91	1.08

^a estimated by the Hynne's kinetic model as described in Material and Methods;

^b in accordance with 10 VARIMAX-derived scales (Georgiev, 2009 [18]) which represent generalized numerical scores for physical-chemical and structural features of amino acids.