

Supporting Information for

Kinetic profiling of metabolic specialists demonstrates stability and consistency of in vivo enzyme turnover numbers

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Table S1: Correlation between biological replicates and coverage of proteomics samples. The R^2 of protein abundance on log scale between two biological replicates is shown along with the number of unique proteins that were detected in at least one of the two replicates.

strain	R^2 between biological replicates	number of proteins detected
WT 1	0.92275	2105
WT 2	0.818324	2066
pgi 1	0.862347	2076
pgi 2	0.928284	2158
pgi 3	0.85155	2161
pgi 4	0.904126	2117
pgi 5	0.912196	2164
pgi 6	0.919021	2017
pgi 7	0.883619	2033
pgi 8	0.884893	2045
ptsHlcr 1	0.920072	2132
ptsHlcr 2	0.908835	2138
ptsHlcr 3	0.92805	2129
ptsHlcr 4	0.897441	2159
sdhCB 1	0.923292	1934
sdhCB 2	0.920167	2033
sdhCB 3	0.849117	1981
tpiA 1	0.921315	2147

tpiA 2	0.923444	2003
tpiA 3	0.913019	1818
tpiA 4	0.927285	1991

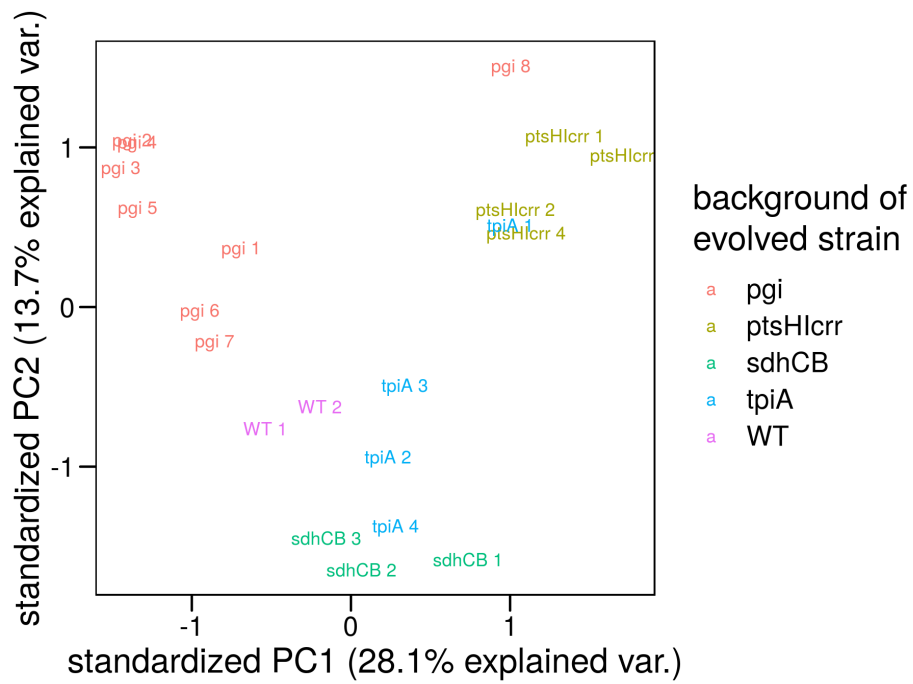


Figure S1: PCA biplot of protein abundances. Protein abundances were log-transformed, centered, and scaled. Only proteins that were detected in all samples were used for this analysis (n = 829).

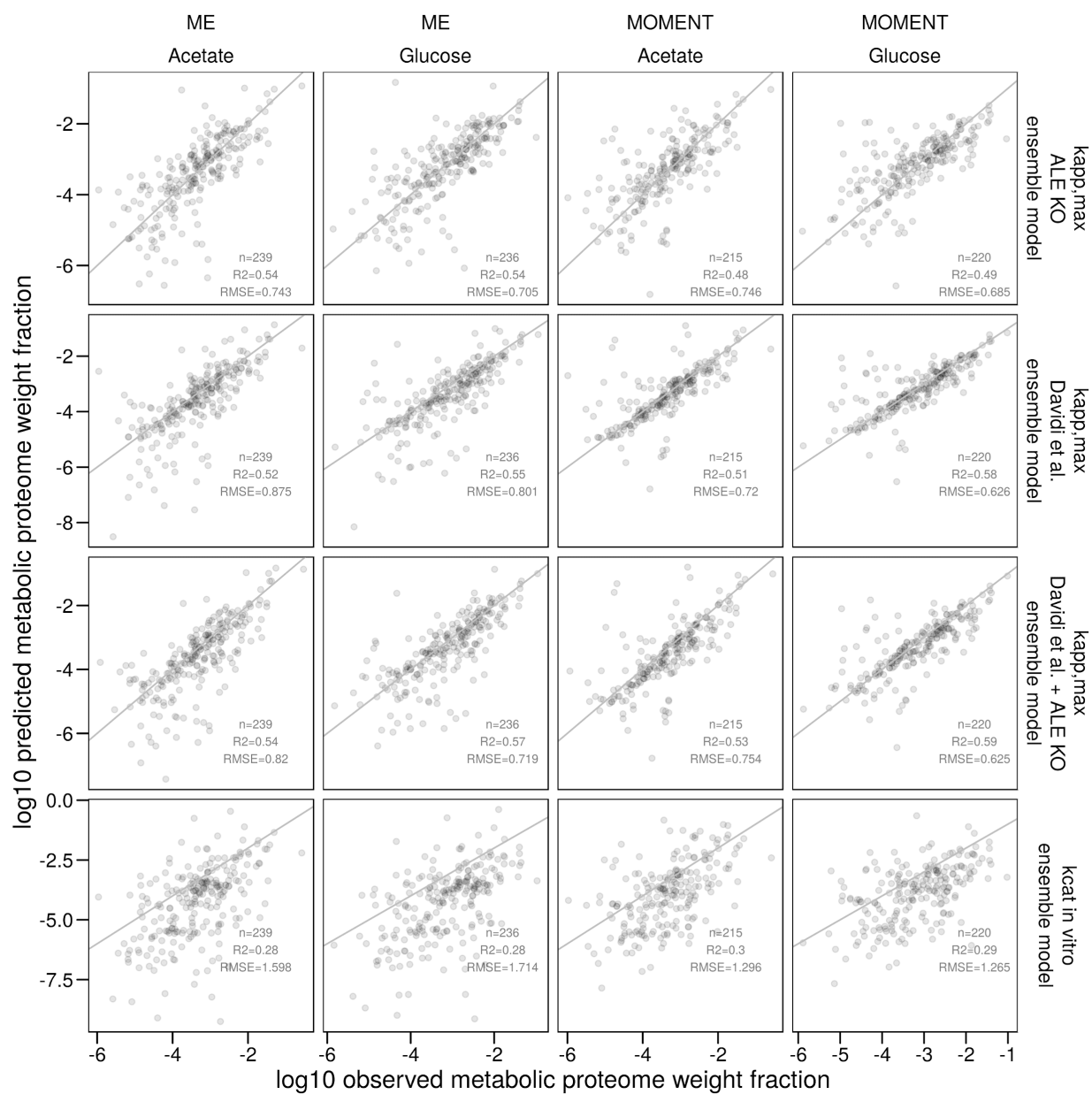


Figure S2: Direct comparison of protein abundance predictions with measured data for different k_{cat} parameterizations. Proteomics data for growth on glucoses and acetate from Schmidt et al.¹ is shown as examples.

Other Supporting Information Files

Dataset S1 (separate file). Protein abundances, MFA fluxes, and k_{app} s (S1A). Table of $k_{\text{app,max}}$ s (S1B). Table of k_{cat} in vitro and $k_{\text{app,max}}$ extrapolated with machine learning models or the median (S1C). These were used to parameterize mechanistic genome-scale models. Mutation table of the strains used in this study (S1D). Details on all data sets are given in Dataset S1.

SI References

1. Schmidt, A. *et al.* The quantitative and condition-dependent Escherichia coli proteome. *Nat. Biotechnol.* **34**, 104–110 (2016).