

Supplementary appendix

PARROT: Prediction of enzyme abundances using protein-constrained metabolic models

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Supplementary tables

Table S1 – Experimental proteomics measurements used for yeast

Condition	Usage by PARROT	Reference
Lahtvee2017_REF	Reference	
Lahtvee2017_EtOH20		
Lahtvee2017_EtOH40		
Lahtvee2017_EtOH60	Suboptimal	Lahtvee et al. (2017)
Lahtvee2017_Osmo02		
Lahtvee2017_Osmo04		
Lahtvee2017_Osmo06		
Yu2020_Clim	Reference	
Yu2020_CN30		Yu et al. (2020)
Yu2020_CN50	Suboptimal	
Yu2020_CN115		
Yu2021_std_010	Reference	
Yu2021_N30_005		
Yu2021_N30_010		
Yu2021_N30_013	Suboptimal	Yu et al. (2021)
Yu2021_N30_018		
Yu2021_N30_030		
Yu2021_N30_035		

Yu2021_Gln_glc1	Reference
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Yu2021_Gln_glc2	Suboptimal
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Yu2021_Gln_N30	
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Yu2021_Phe_std	Reference
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Yu2021_Phe_N30	Suboptimal
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Yu2021_Ile_std	Reference
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Yu2021_Ile_N30	Suboptimal
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Table S2 – Experimental proteomics measurements used for *Escherichia coli*

Condition	Usage by PARROT	Reference
GLYC_BATCH_mu=0.47_S	Reference	
ACE_BATCH_mu=0.3_S		
GAM_BATCH_mu=0.46_S		
GLC_BATCH_mu=0.58_S	Suboptimal	
MAN_BATCH_mu=0.47_S		
PYR_BATCH_mu=0.4_S		Schmidt et al. (2016)
XYL_BATCH_mu=0.55_S		
GLC_CHEM_mu=0.12_S	Reference	
GLC_CHEM_mu=0.20_S		
GLC_CHEM_mu=0.35_S	Suboptimal	
GLC_CHEM_mu=0.50_S		
GLC_CHEM_mu=0.11_V	Reference	
GLC_CHEM_mu=0.21_V		
GLC_CHEM_mu=0.31_V	Suboptimal	Valgepea et al. (2013)
GLC_CHEM_mu=0.40_V		
GLC_CHEM_mu=0.49_V		
GLC_CHEM_mu=0.21_P	Reference	
GLC_CHEM_mu=0.22_P		
GLC_CHEM_mu=0.26_P	Suboptimal	Peebo et al. (2015)
GLC_CHEM_mu=0.31_P		

GLC_CHEM_mu=0.36_P

GLC_CHEM_mu=0.41_P

GLC_CHEM_mu=0.46_P

GLC_CHEM_mu=0.51_P

Supplementary figures

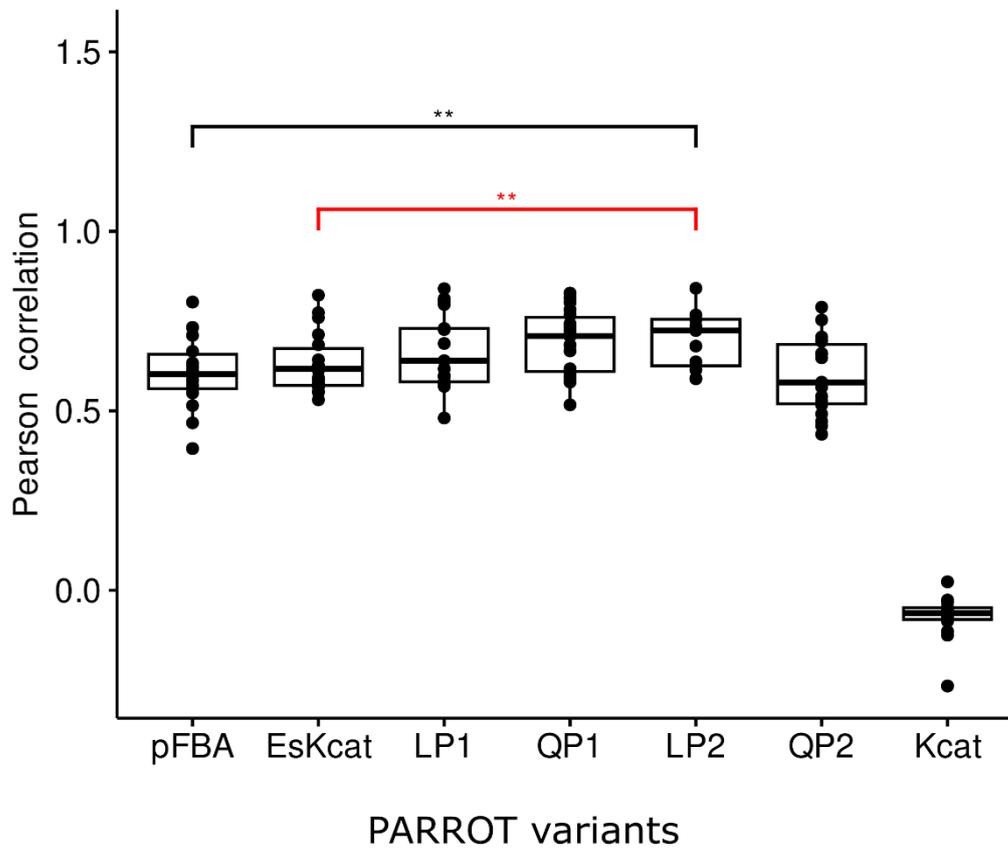


Fig. S1. Pearson correlation calculated between predicted enzyme distribution and the baseline obtained from minimizing the second norm of the experimental enzyme usage distribution, in *S. cerevisiae*. All values were log₁₀-transformed prior to comparisons. A pairwise Wilcoxon rank sum assesses the statistical significance: ** p-value < 0.0009. Black significance bar indicates comparisons to pFBA. Red significance bar indicates comparisons to EsKcat.

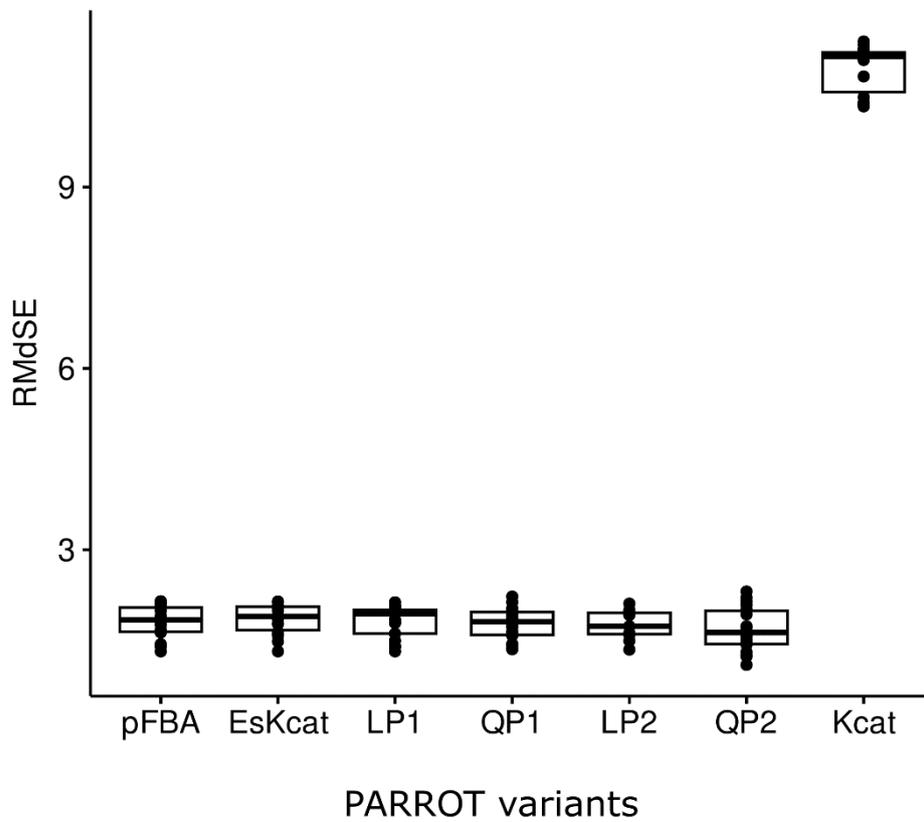


Fig. S2. Assessment of model performance based on the root median squared error (RMdSE).
The minimization of the second norm of the experimental enzyme usage distribution in *S. cerevisiae* was used. All values were log10-transformed prior to comparisons.

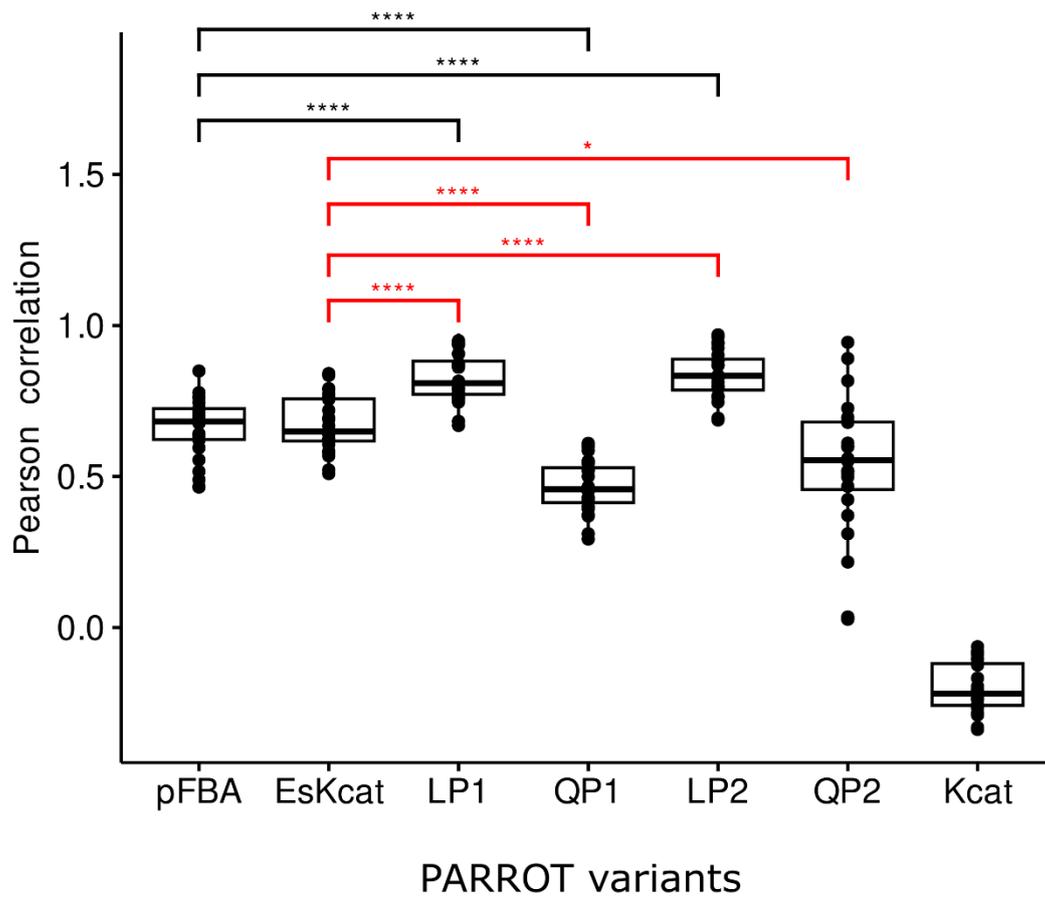


Fig. S3. Pearson correlation calculated between predicted enzyme distribution and the baseline obtained from minimizing the second norm of the experimental enzyme usage distribution, in *E. coli*. All values were log₁₀-transformed prior to comparisons. A pairwise Wilcoxon rank sum assesses the statistical significance: **** p-value < 0.000005, * p-value < 0.03. Black significance bar indicates comparisons to pFBA. Red significance bar indicates comparisons to EsKcat.

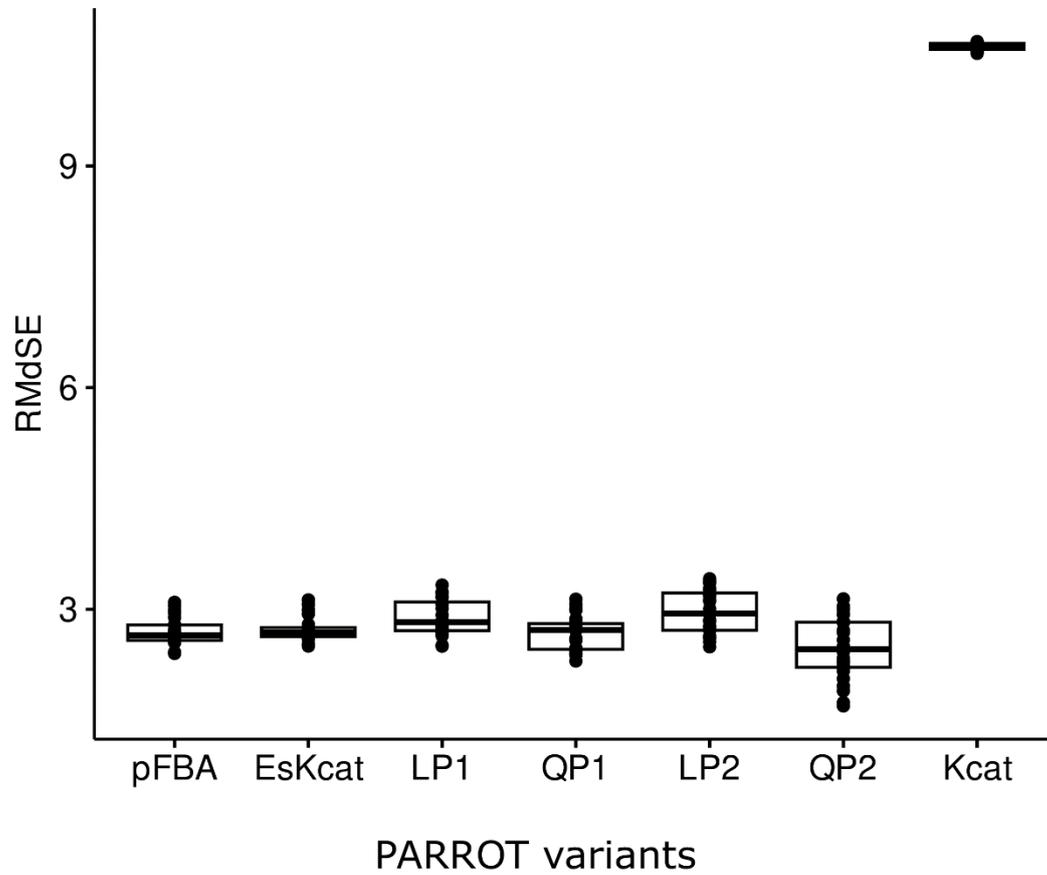


Fig. S4. Assessment of model performance based on the root median squared error (RMdSE).

The minimization of the second norm of the experimental enzyme usage distribution in *E. coli* was used. All values were log10-transformed prior to comparisons.