

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

| | |
|-----------------|------------|
| Yu2021_Gln_glc1 | Reference |
| Yu2021_Gln_glc2 | Suboptimal |
| Yu2021_Gln_N30 | |
| Yu2021_Phe_std | Reference |
| Yu2021_Phe_N30 | Suboptimal |
| Yu2021_Ile_std | Reference |
| Yu2021_Ile_N30 | Suboptimal |

Table S2 – Experimental proteomics measurements used for *Escherichia coli*

| Condition | Usage by PARROT | Reference |
|----------------------|-----------------|------------------------|
| GLYC_BATCH_mu=0.47_S | Reference | Schmidt et al. (2016) |
| 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 | | |
| XYL_BATCH_mu=0.55_S | | |
| GLC_CHEM_mu=0.12_S | Reference | Valgepea et al. (2013) |
| 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 | | Peebo et al. (2015) |
| GLC_CHEM_mu=0.31_V | Suboptimal | |
| GLC_CHEM_mu=0.40_V | | |
| GLC_CHEM_mu=0.49_V | | |
| GLC_CHEM_mu=0.21_P | Reference | Peebo et al. (2015) |
| GLC_CHEM_mu=0.22_P | | |
| GLC_CHEM_mu=0.26_P | Suboptimal | |
| 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

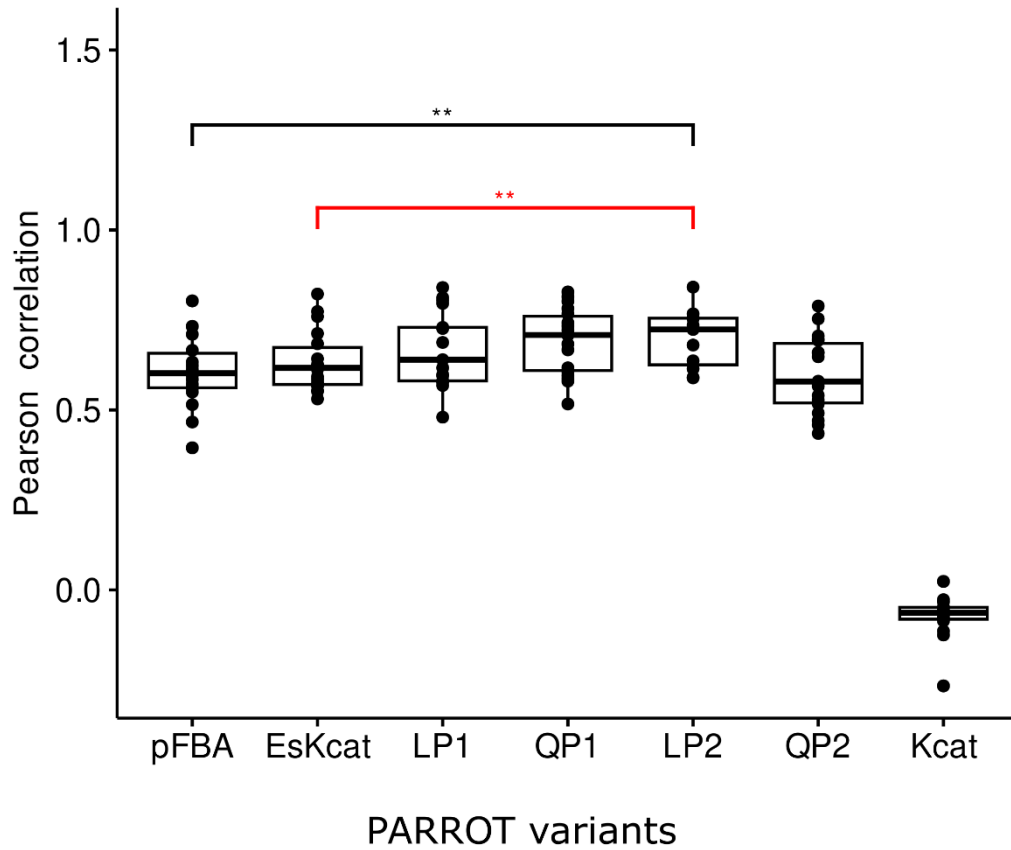


Fig. S1. Pearson correlation calculated between predicted enzyme distribution and the baseline obtained from minimizing the second norm of the experimental enzyme usage distribution, in *S. cerevisiae*. All values were log10-transformed prior to comparisons. A pairwise Wilcoxon rank sum assesses the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

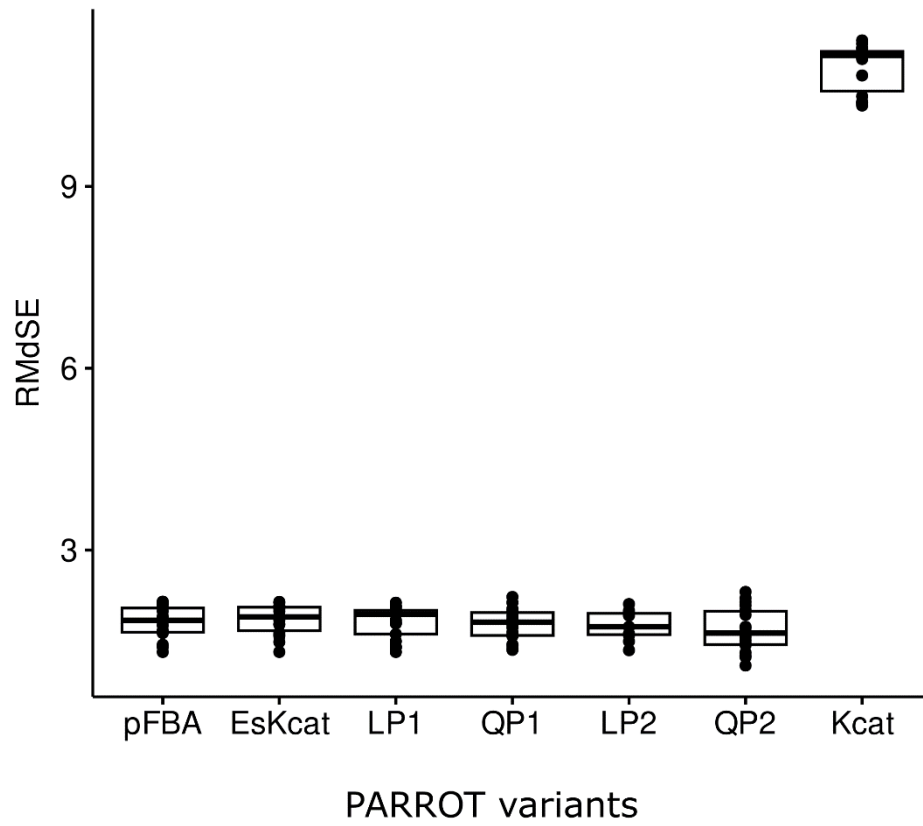


Fig. S2. Assessment of model performance based on the root median squared error (RMdSE).
The minimization of the second norm of the experimental enzyme usage distribution in *S. cerevisiae* was used. All values were log10-transformed prior to comparisons.

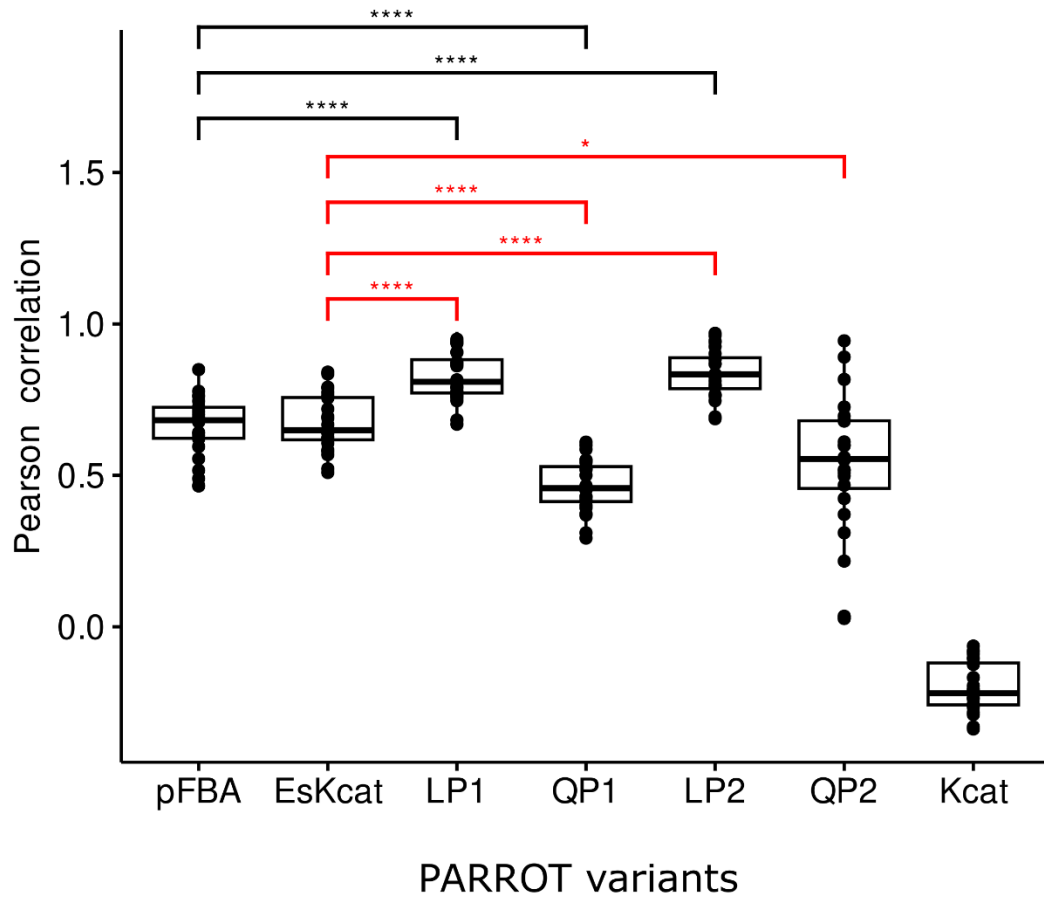


Fig. S3. Pearson correlation calculated between predicted enzyme distribution and the baseline obtained from minimizing the second norm of the experimental enzyme usage distribution, in *E. coli*. All values were log10-transformed prior to comparisons. A pairwise Wilcoxon rank sum assesses the statistical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

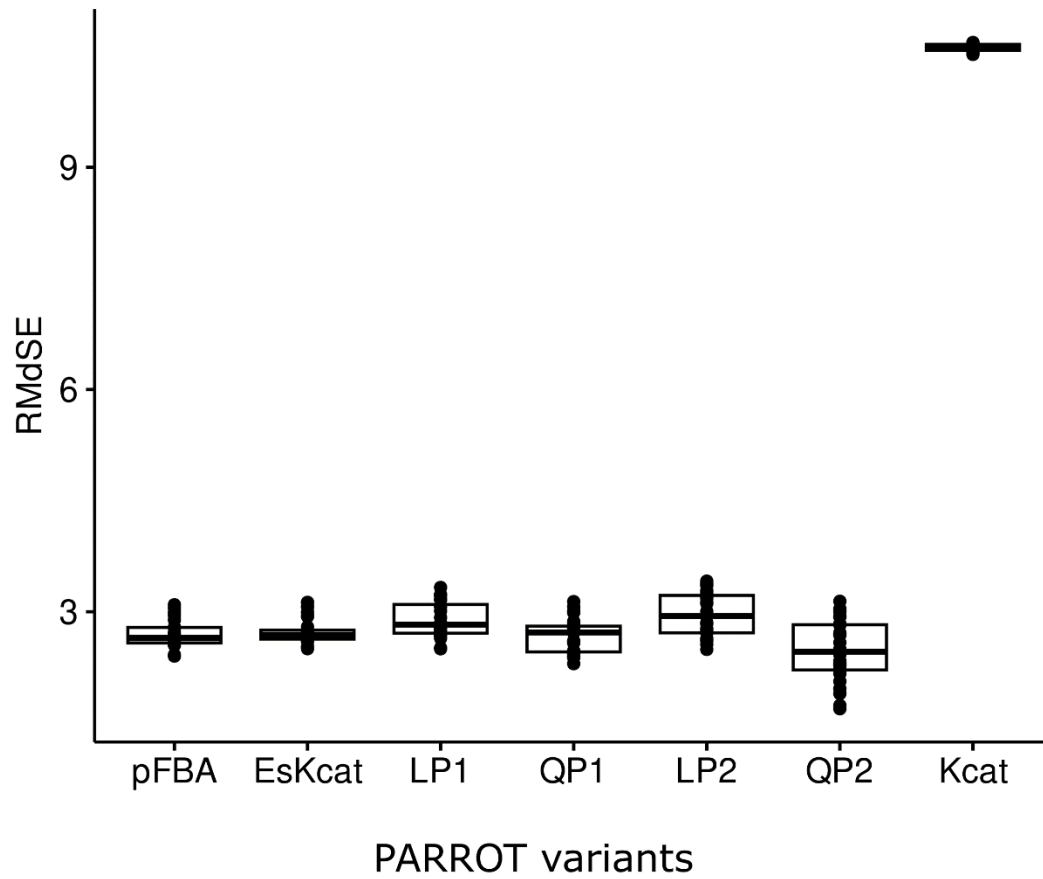


Fig. S4. Assessment of model performance based on the root median squared error (RMdSE).

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.