**Supplementary Table S2.** Absolute metabolite concentrations (nmol $g^{-1}$ CDW) in *E.coli* BL21 extracted using different ratios of extraction solvents for quantification using the zic-HILIC MS/MS method. The table indicates average values from technical replicates (n=3), standard deviation (SD), and relative standard deviation (RSD,%) for each metabolite. No peak was observed for 1-mNAM. Outliers were removed using Dixon's Q tests with a 95% confidence level [31]

| Extraction Solvent | | NAM | NCA | NR | FAD | NADH | ADPR | $NAD^+$ | NMN | NAMN | NADPH | $NADP^+$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ACN: MeOH: $H_2O$, 15 mM $NH_4OAc$ pH 9.7 (60:20:20) | Average | 4.6 | 3.4 | 1.4 | 66.4 | 252.7 | 1.6 | 747.8 | 4.4 | 19.4 | 51.6 | 152.5 |
| | SD | 1.3 | 0.3 | 0.3 | 0.7 | 18.3 | 0.2 | 41.1 | 0.3 | 2.7 | 2.9 | 24.4 |
| | RSD | 27.8 | 10.4 | 20.2 | 1.0 | 7.2 | 14.3 | 5.5 | 7.4 | 14.0 | 5.7 | 16.0 |
| ACN: MeOH: $H_2O$, 15 mM $NH_4OAc$ pH 9.7 (55:20:25) | Average | 6.1 | 7.7 | 3.0 | 74.0 | 265.3 | 1.5 | 769.7 | 2.9 | 24.5 | 62.4 | 143.9 |
| | SD | 1.8 | 1.2 | 0.1 | 5.6 | 14.5 | 0.1 | 79.6 | 0.3 | 2.3 | 3.5 | 16.2 |
| | RSD | 29.1 | 15.2 | 2.2 | 7.6 | 5.5 | 7.3 | 10.3 | 9.7 | 9.3 | 5.7 | 11.2 |