1.)

(a)

Table of pathway metabolites and abbreviations. Rows of this table match the metabolites of the respective rows below

|  |  |  |
| --- | --- | --- |
| Metabolite | Abbreviation | Formula |
| Aspartate | Asp | C4H7NO4 |
| Argininosuccinate | Arg-s | C10H18N4O6 |
| Fumarate | Fum | C4H4O4 |
| Arginine | Arg | C6H14N4O2 |
| Urea | Urea | CH4N2O |
| Ornithine | Orn | C5H12N2O2 |
| Carbamoyl Phosphate | Carb-P | CH4NO5P |
| Citrulline | Cit | C6H13N3O3 |
| AMP | AMP | C10H14N5O7P |
| ATP | ATP | C10H16N5O13P3 |
| Phosphate | P | H3PO4 |
| Diphosphate | PP | H4P2O7 |
| Water | Water | H2O |
| Ammonia | Amm | NH3 |

where reactions m1-5 are sources and sinks for the metabolites AMP, ATP, Phosphate, Diphosphate, and water, respectively

(b)

Metabolites on each column correspond to the respective row of the table. Rows correspond to elements C, H, N, O, and P, respectively.

Multiplying A and S yields a matrix with rows that sum to 0, which indicates the elements are balanced.

(c)

This stoichiometric matrix was used to solve a linear programming FBA problem to determine optimal flux to the Urea sink (b4 set as -1 in objective function).

To provide an upper bound to each flux, the enzyme concentration was multiplied by the kcat and a further correction factor with metabolite concentrations and saturation constants found in BRENDA. The Julia code wrapper Flux.jl using the GPLK linear programming algorithm was used to solve the FBA problem and gave a maximum rate of urea production of ~0.838