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Development of a compartmentalized model for insight into the structured metabolic pathway of carbon metabolism in cassava leaves

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Supplementary data 1. List of abbreviations

| KEGG | Kyoto Encyclopedia of Genes and Genomes; |
|------------|---|
| PMN | Plant Metabolic Network database; |
| ph-MeRecon | photosynthetic-Manihot esculenta metabolic pathway reconstruction |
| TCA | Tricarboxylic acid cycle |
| PPP | Pentose Phosphate Pathway |
| PSI | Photosystem I |
| PSII | Photosystem II |
| LEF | Linear electron flow |
| CEF | Cyclic electron flow |
| Cyt b6f | Cytochrome b6f complex |
| FNR | Ferredoxin-NADP+ reductase |
| PEPC | Phosphoenolpyruvate carboxylase enzyme; |
| RuBisCO | Ribulose-1,5 bisphosphate carboxylase/oxygenase enzyme |
| 2-PG | 2-Phosphoglycolate |
| G3P | Glycerate 3-phosphate |
| OAA | Oxaloacetate |
| Pi | Orthophosphate |
| PEP | Phosphoenolpyruvate |
| RuBP | Ribulose-1,5 bisphosphate |
| PQ | Plastoquinone |
| PQH2 | Plastoquinol |

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| PC | Plastocyanin |
|------|---|
| Fd | Ferredoxin |
| AMI | Amino acid metabolism |
| AMIO | Metabolism of other amino acids |
| BUT | Butanoate metabolism |
| CAL | Calvin cycle (carbon fixation) |
| CEL | Cell wall metabolism |
| COF | Cofactors and vitamin metabolism |
| FAT | Fatty acid metabolism |
| GABA | GABA shunt pathway |
| GLYC | Glycan metabolism |
| GLYO | Glyoxylate and dicarboxylate metabolism |
| NIT | Nitrogen metabolism |
| NUC | Nucleotide metabolism |
| РНО | Photosynthesis light reactions |
| PRES | Photorespiration pathway |
| PRO | Propanoate metabolism |
| RES | Respiration pathway |
| SEC | Secondary metabolism |
| STA | Starch metabolism |
| SUC | Sucrose metabolism |
| SUL | Sulfur metabolism |
| TER | Metabolism of terpenoids and polyketides. |
| | |



Fig S1. The overall workflow of ph-MeRecon pathway construction and analysis.



Fig S2. Example of gap filling process for (S)-1-Pyrroline-5-carboxylate and L-glutamate 5-semialdehyde in proline biosynthesis pathway before (A) and after (B) network refinement. The gap metabolites are marked in blue. Blue arrow shows the added gap reaction with the KEGG reaction ID (pink rectangle). The KEGG reaction IDs of reactions (black arrows) are noted in green rectangle.