SUPPLEMENTARY DATA 3

Metabolomics quality control and principle component analysis

Tubers of the potato (*Solanum tuberosum* group Tuberosum) cultivar ‘Desiree’ and sample blanks containing only internal standards and retention standards were extracted and processed simultaneously with *L. perenne* samples, as described in the Materials and Methods section. ‘Desiree’ is run consistent in our laboratory as a rolling biological reference material. Multivariate analysis was performed on the results to check for any abnormalities, and the principal component analysis (PCA) showed that potato tuber samples and the blank segregated from the *L. perenne* dataset (Fig. S1) on the second and third principal components. The reference samples did not show significant changes throughout the sequence of injections, suggesting that the performance of the GC-MS system remained stable throughout the analysis process (Fig. S2).

FIG. S1. PCA plots generated using the data from the metabolite profiles of the ‘Cashel-P’ and ‘IRL-OP-2538’ samples as well as those from the biological standard (‘Desiree’) and blank injections. The standard and blanks are tightly grouped and segregated (e.g. PC 2 v 3) apart form each other and the *Lolium* samples, highlighting injection and machine consistency. The first principle component appears to separate root and leaf tissue and explains 36.1% of the variance. Component 2 and 3 explain 23.3 and 8.4% of the variance, respectively.

‘Desiree’, ★; Sample blanks, ★; ‘IRL-OP-2538-P’, ★; ‘Cashel-P’, ★

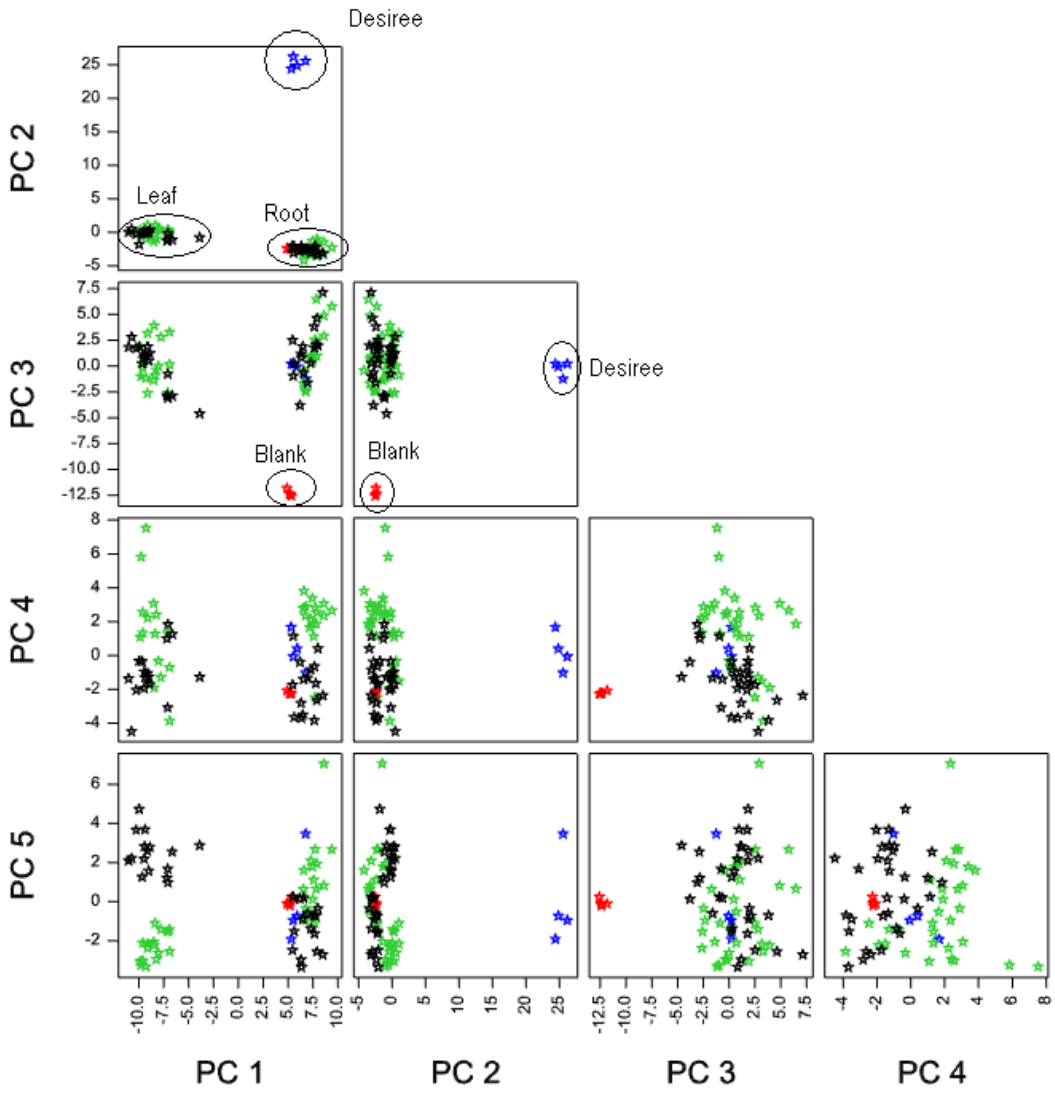

FIG. S2. PCA plots represented in Fig. S1 re-annotated according to injection sequence. Injection 1, ★; Injection 2, ★

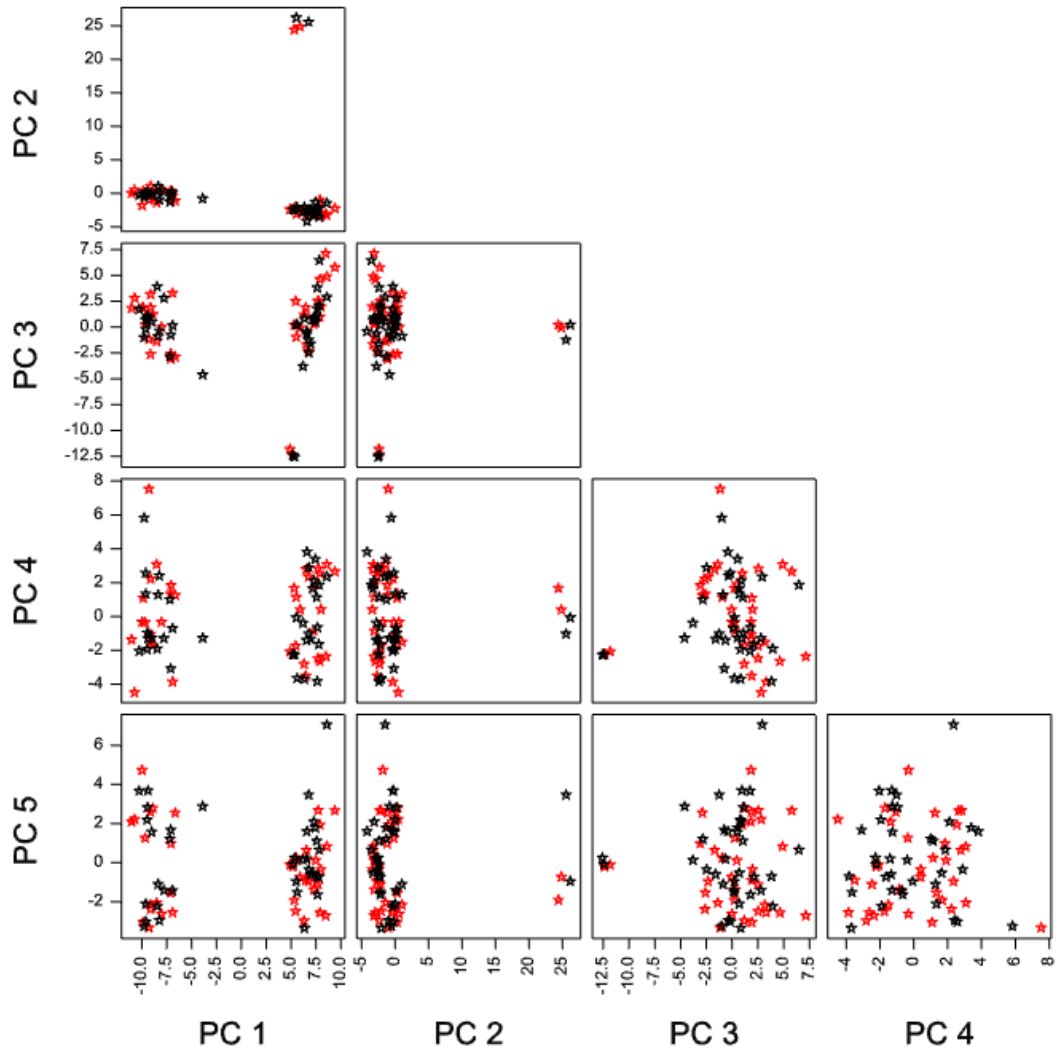

FIG. S3.PCA plot representing the first (PC 1) and second (PC 2) components of the metabolite profiles of leaf tissue samples. The second principal component appears to separate both genotypes. Components 1 and 2 explain 16.30 and 13.87%, respectively.

'Cashel-P' grown under P-limiting conditions, ★; 'Cashel-P' grown under P-sufficient conditions, ★; 'IRL-OP-2538-P' grown under P-limiting conditions, ★; 'IRL-OP-2538-P' grown under P-limiting conditions, ★

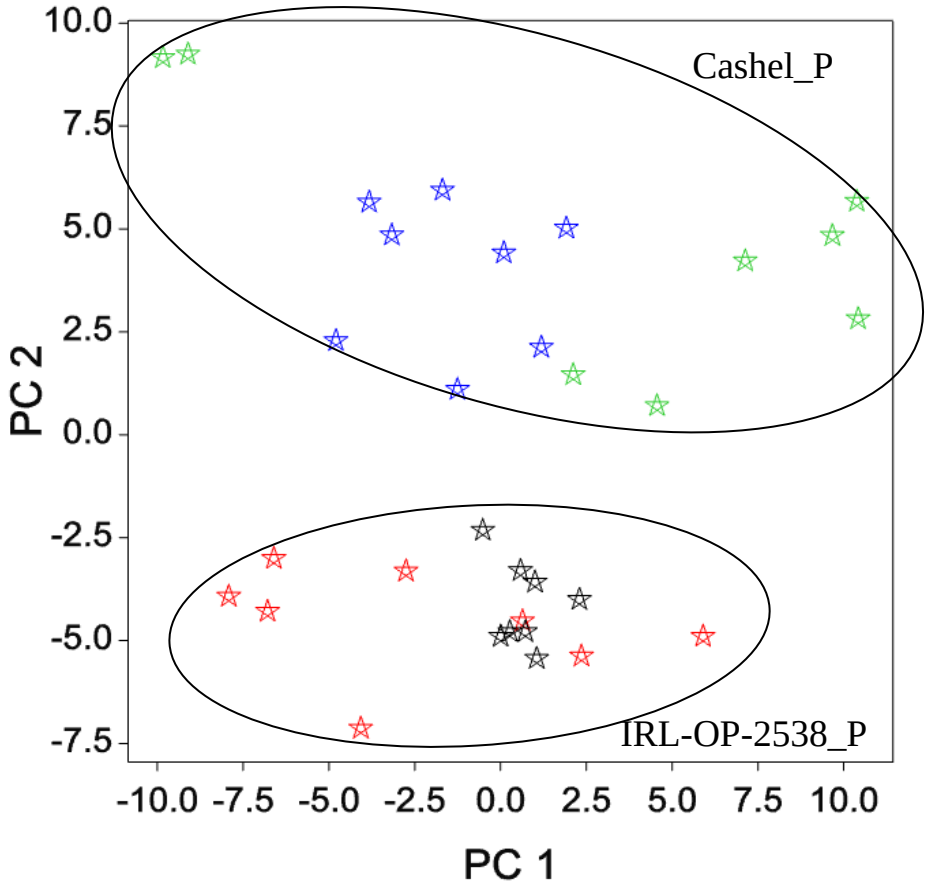

FIG. S4. PCA plot representing the second (PC 2) and third (PC 3) components of the metabolite profiles of root tissue samples. The second and third components explain 10.99 and 9.70% of the total variation in the metabolite profiles, respectively.

'Cashel-P' grown under P-limiting conditions, ★; 'Cashel-P' grown under P-sufficient conditions, ★; 'IRL-OP-2538-P' grown under P-limiting conditions, ★; 'IRL-OP-2538-P' grown under P-limiting conditions, ★