



**Figure S2.** PCA of the LS-means calculated from the contents of 2846 metabolites, metabolite signatures, starch and total protein measured in the panel of 29 maize hybrids grown under limiting (LN, blue circles) and optimal (HN, red squares) fertilization conditions. **(A)** Scores plot annotated with the hybrid codes. **(B)** Loadings plot in which symbols indicate the type of biochemical analyses: targeted analyses, orange triangles;  $^1\text{H}$ -NMR analyses, blue diamonds; LC-QTOF-MS analyses, grey open circles. Metabolites or identified metabolite signatures with an absolute value of loading higher than 0.015 on PC1 or PC2 are annotated. gluc = glucoside.