

Figure S1. PCA scores plots of $1D^1H$ -NMR data, indicating clustering of Tora and Resolution leaf and stem samples. Indication within the coloured clusters is highlighted to show clustering of the three technical replicates. **(a)** PC1 vs PC2 of leaf data only, coloured by genotype and harvest position; **(b)** PC1 vs PC2 of stem data only, coloured by genotype and harvest position. Harvest position: B:bottom; M:middle; T:top.

