Supplementary information

Untargeted LC-MS/MS reveals cultivar- and farming-practice associated remodeling of the oat grain foodome

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Supplementary Figure 1.

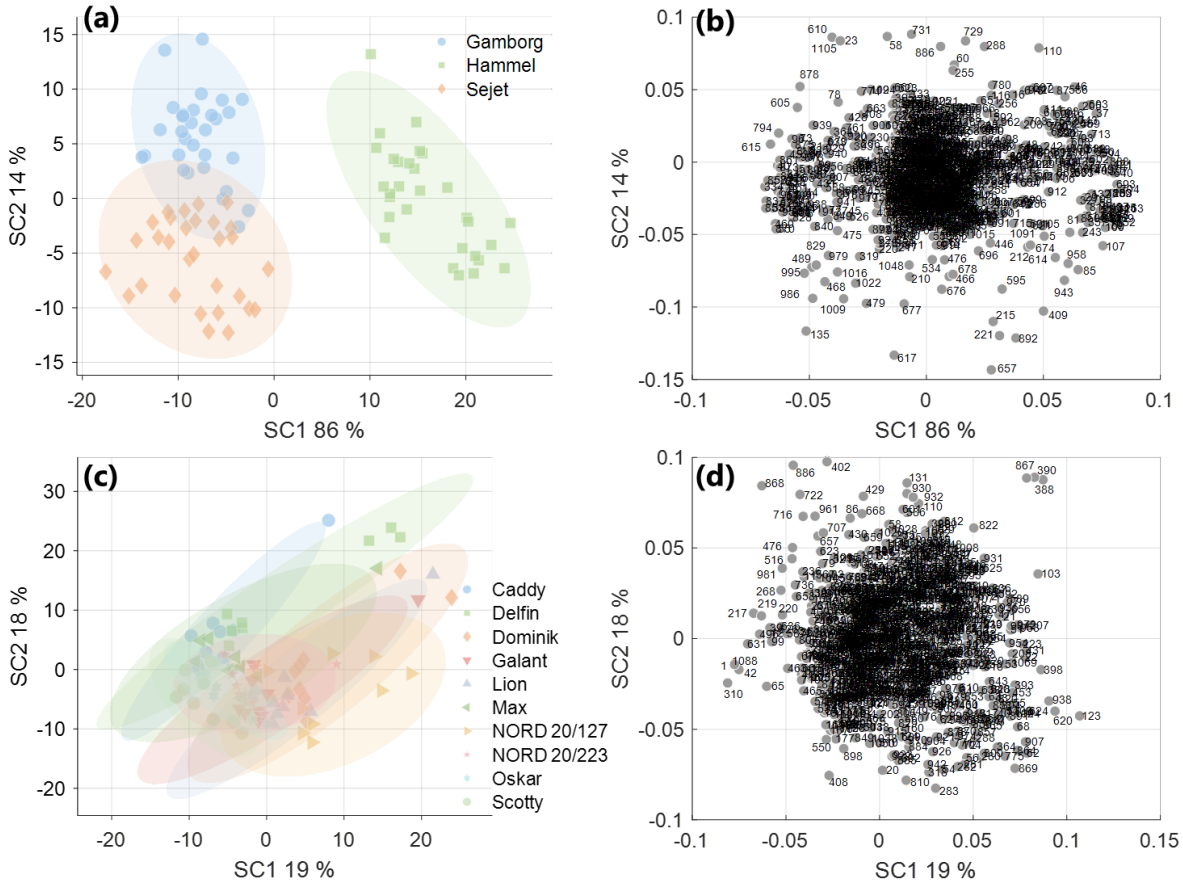
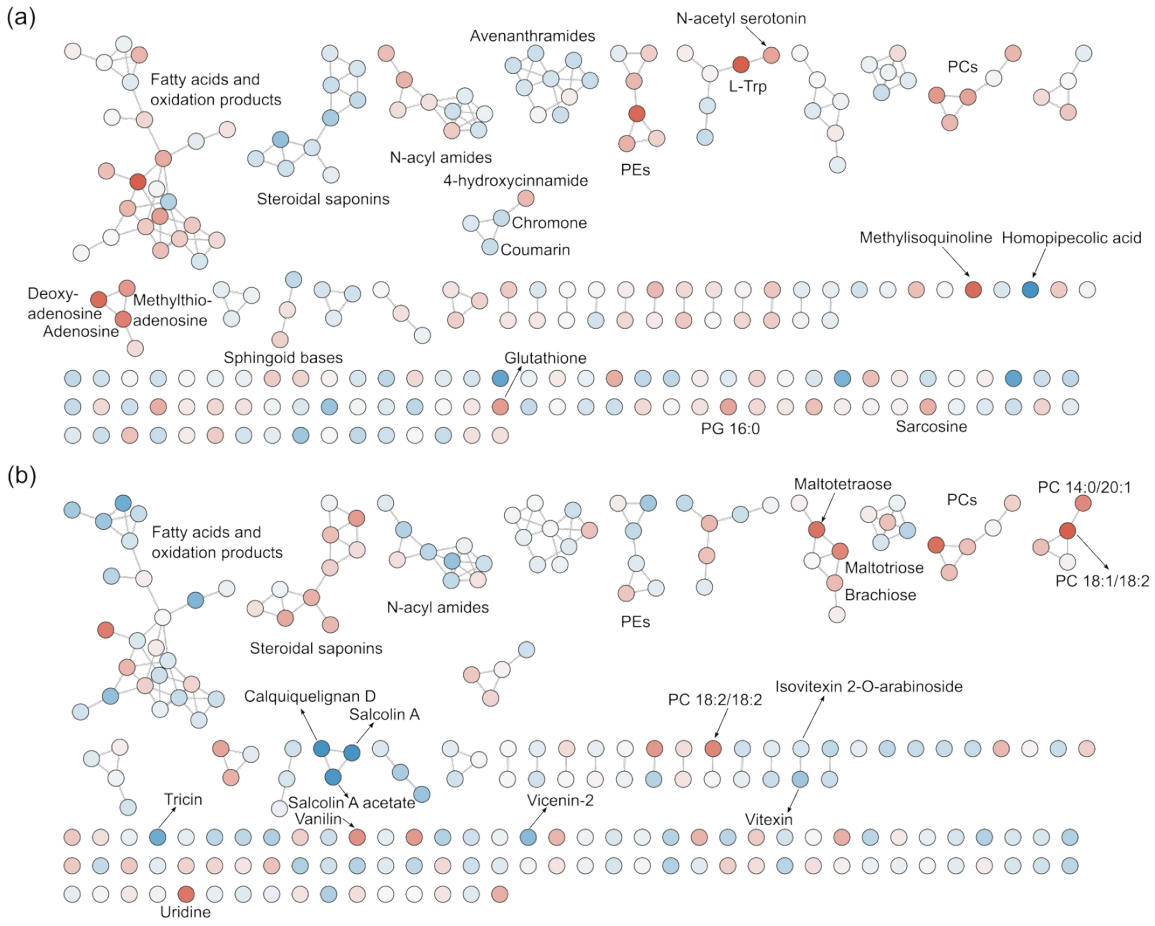


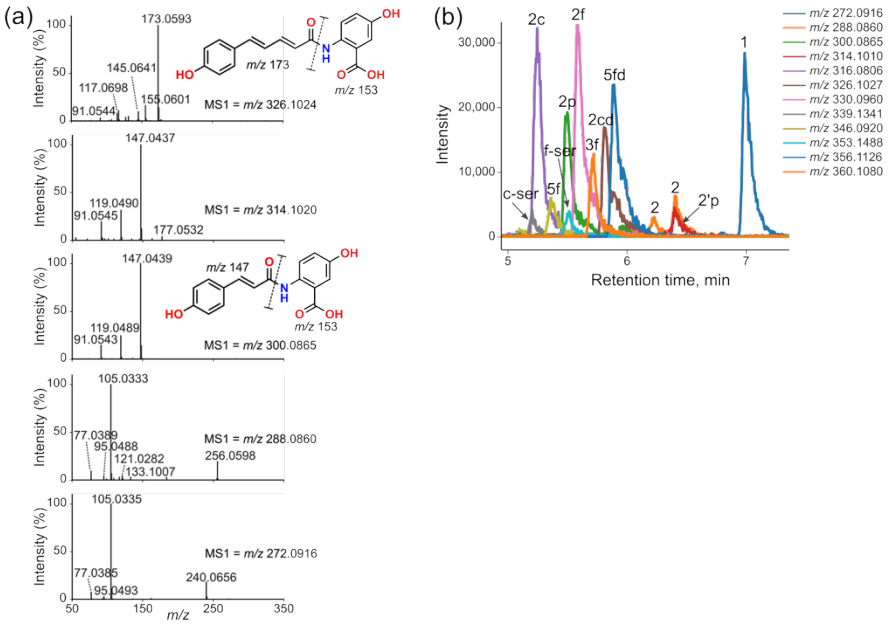
Figure S1. ANOVA–simultaneous component analysis (ASCA) performed on 1187 LC-MS/MS features and show separation of 30 oat samples originated from 10 different cultivars (Caddy, Delfin, Dominik, Galant, Lion, Max, NORD 20/127, NORD 20/223, Oskar and Scotty) grown under organic (Hammel) and conventional practices (Sejet and Gamborg).Scores (a) and loadings (b) plots show the separation of oat samples (n = 3 replicates × 30 samples) according to the farming practice (explained variance = 13.8%, p-value = 0.001) and the features contributing to this separation, respectively. Scores (c) and loadings (d) plots correspond to the cultivar effect, showing the partial separation of oat samples (n = 3 locations × 3 replicates × 10 cultivars) according to cultivar (explained variance = 13.7%, p-value = 0.001) and the features contributing this partial separation, respectively. SC1 versus SC2 scores and loadings represent the ASCA model developed on the autoscaled feature table.

Supplementary Figure 2.



ANOVA-simultaneous component analysis (ASCA) performed on 228 annotated metabolites. SC2 loadings for the location (a) and cultivar (b) effects, respectively. Loading values were normalized to a range from -1 to 1 and mapped to a color gradient which was used to encode SC1 loadings in the corresponding molecular networks. Each node in molecular network represents a metabolite and node color indicates the direction and magnitude of its SC2 loading.

Supplementary Figure 3.



Hydroxycinnamic acid amides detected in oat grains. (a) MS/MS spectra of selected compounds in hydroxycinnamic acid amides molecular network with spectral library matches and tentative structure annotation based on accurate mass and fragmentation pattern. (b) Extracted ion chromatograms of compounds in the hydroxycinnamic acid amides molecular network.