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Supplement of

Chemotaxonomy of domesticated grasses: a pathway to understanding the origins of agriculture

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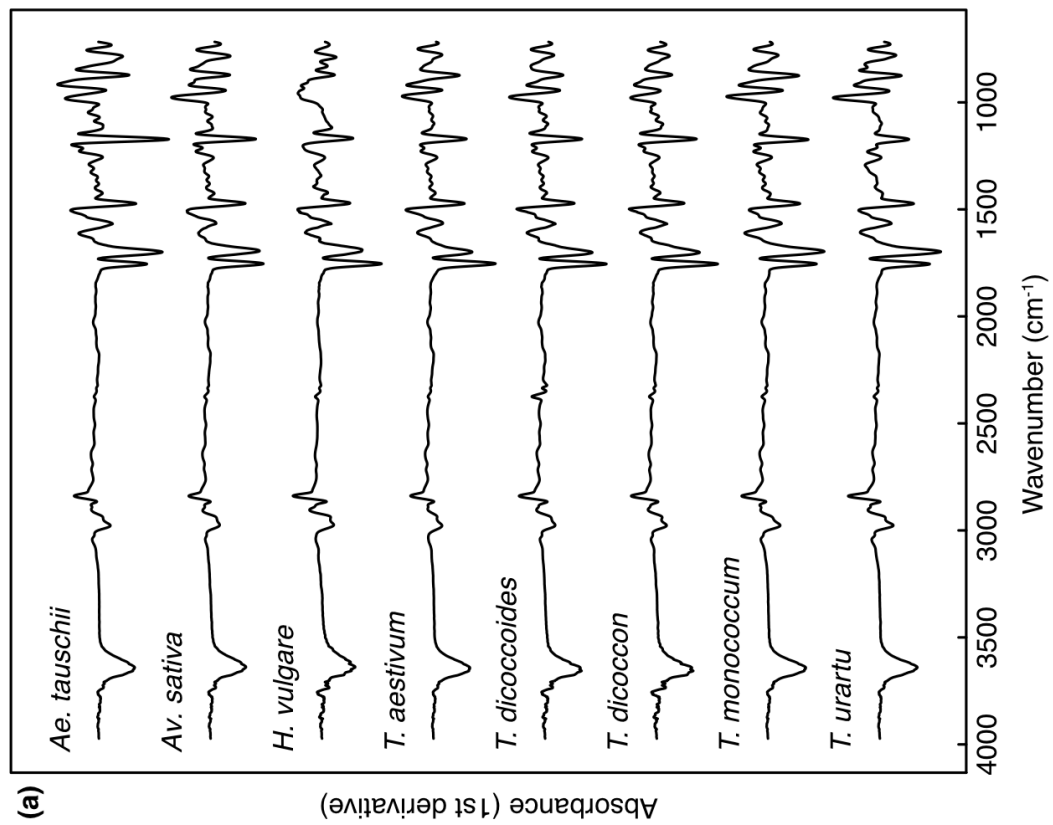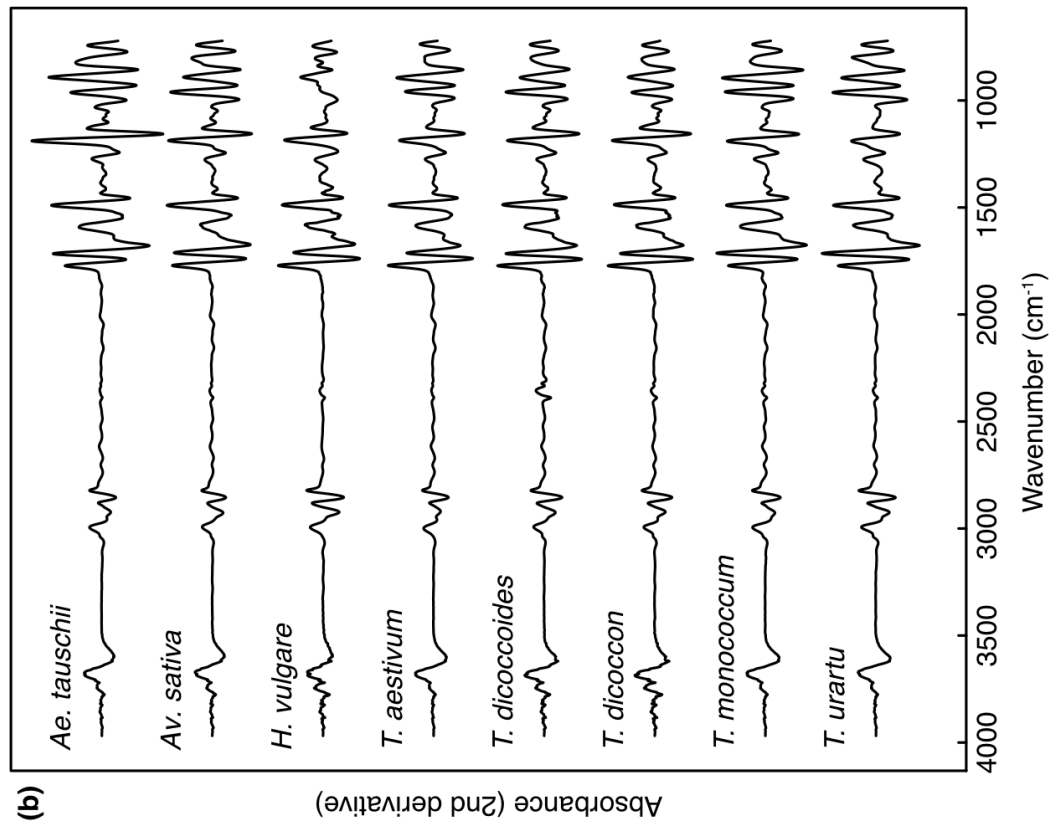*Correspondence to:* Phillip E. Jardine (jardine@uni-muenster.de)

Figure S1: First derivative (a) and second derivative (b) spectra, showing the mean spectrum for each species.
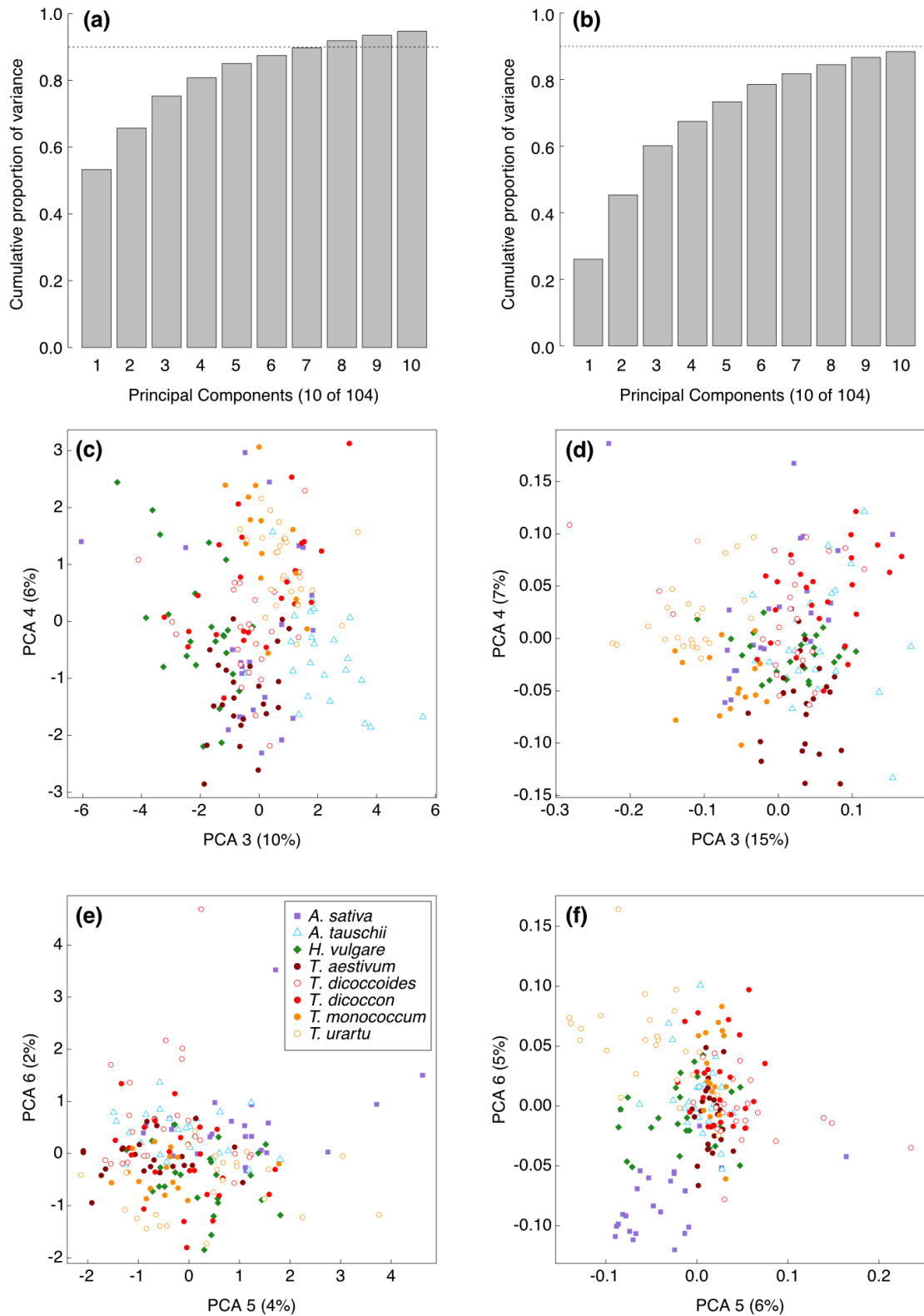
Figure S2: Further PCA information for (a, c, e) unprocessed FTIR spectra, and (b, d, f) FTIR spectra processed with Savitzky-Golay smoothing and first derivatives. (a and b) cumulative proportion of variance explained by PCA axes, with horizontal dashed line showing 90% explained variance. (c and d) PCA axes 3 and 4, (e and f) PCA axes 5 and 6.