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Supplementary material

SUPPLEMENTARY MATERIAL TO

Discriminating cereal and pseudocereal species using binary system of GC–MS data – A pattern recognition approach

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TABLE S-I. Utilization of various GC–MS methods combined with chemometrics in authenticity confirmation of different products; PCA – principal component analysis; PLS-DA – partial least squares discriminant analysis; OPLS-DA – orthogonal projections to latent structures discriminant analysis; LDA – linear discriminant analysis; CA – cluster analysis; HCA – hierarchical cluster analysis; S-LDA – stepwise linear discriminant analysis; PCO – principal coordinate analysis

Sample	Compounds analyzed	Pattern recognition method	Reference
Vegetable oils (corn, grape seed, hazelnut, olive, peanut, sun-flower, canola, palm, soybean)	*n*-Alkane profile, fatty acids methyl esters (FAME)	PCA, PLS-DA, OPLS-DA, LDA	1,2
Almond oil cultivars	Volatile aldehydes	LDA	3
Coffee	Volatile and semivolatile compounds (pyrazine, pyridine, pyrrole, furan, ketone, aldehyde)	PCA	4
Olive oil	Various aroma compounds, FAME	LDA	2,5,6
Meat products	Volatiles (2,3-octanedione, toluene, terpenes, alkanes, alkenes, ketones)	DA	7
Fruit-flavored foods and beverages	γ-decalactone, δ-decalactone	HCA, PCA	8
Strawberry-flavored foods	Aroma active volatile components	–	9
Essential lemon oil	Various volatile compounds	–	10
Coconut oil	FAME	PCA, PLS-DA,	1,11

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	Cholesterol	OPLS-DA	
Chamomile flowers, essential oils and commercial products	Nonpolar: volatile esters/oxides Polar: phenols	PCA, PLS-DA	12
Beeswax	Hydrocarbon, alkenes and monoesters	CA, PCA, LDA	13
Wax works of art	Hydrocarbons, alcohols, ω-1-diols, fatty acids, ω-1-hydroxy acids	–	14,15
Oolong tea varieties	Volatile compounds (alkanes, alkenes, aldehydes, ketones, alcohols, esters, oxides)	HCA, PCA, S-LDA	16
Cereal flour	Fatty acids, monosaccharides, disaccharides, sugar alcohols	HCA, PCA, PCO	17–19

TABLE S-II. An overview of a number of literature data describing the analysis of fatty acids and non-saponifiable compounds in various cereal and pseudocereal species and cultivars using exclusively chromatographic methods

Species	Techniques used in fatty acid analysis	Techniques used in the non-saponifiable part (phytosterols, tocopherol and squalene) analysis
Wheat	HPLC-ELSD,[20] HPLC–MS,[20] GC-FID[20–22]	HPLC-ELSD,[20] HPLC–MS,[20,23,24] GC-FID,[20,25,26] GC–MS[25,26]
Rye	GC-FID[27]	HPLC-DAD,[25] GC-FID,[25] GC–MS[25]
Barley	GC-FID[22,27]	HPLC-DAD,[27] GC-FID,[25] GC–MS[25]
Oat	GC-FID,[22,28,29] GC–MS[29]	GC-FID,[25,28] GC–MS[25]
Triticale	GC-FID,[21] GC–ECD[30]	–
Corn	GC-FID,[25,31] GC–MS[31]	GC-FID,[31] GC–MS,[31] HPLC-DAD[27]
Spelt	GC-FID[27]	HPLC–MS,[32,33] HPLC-DAD[27]
Buckwheat	GC-FID,[27,34] HPLC–MS[35]	HPLC-DAD,[27,36] GC–MS[36]
Amaranth	GC-FID,[37] GC–MS[38]	GC-FID,[37] GC–MS[38]

Overlaid TIC chromatograms of each cultivar analyzed in this study (cultivars from Table I), separated according to the corresponding cereal/pseudocereal species, *i.e.*, botanical origin.

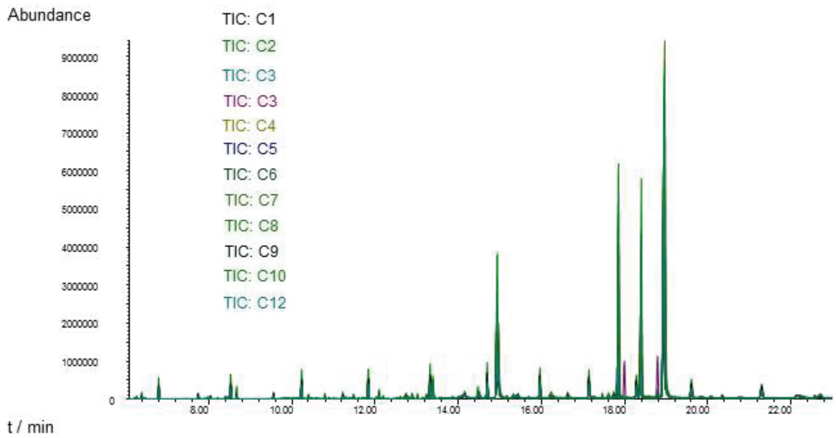

Fig. S-1. Overlain TIC chromatograms of the corn cultivars analyzed in this study.

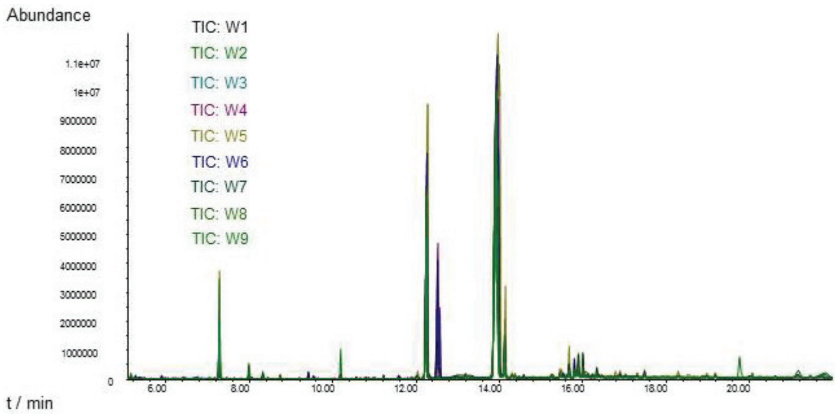

Fig. S-2. Overlain TIC chromatograms of the wheat cultivars analyzed in this study.

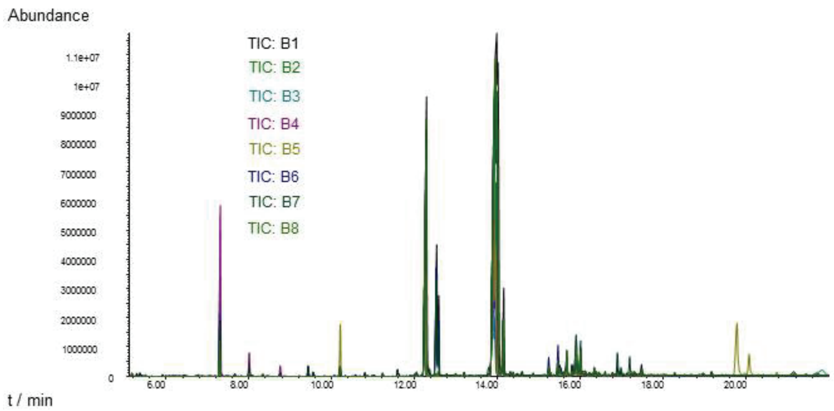

Fig. S-3. Overlain TIC chromatograms of the barley cultivars analyzed in this study.

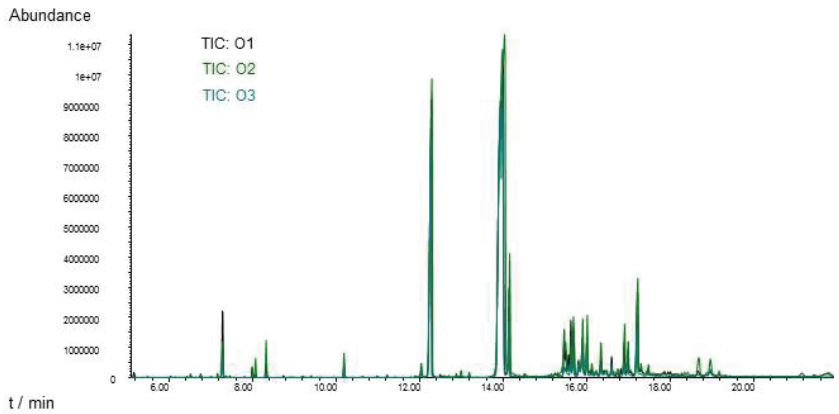

Fig. S-4. Overlain TIC chromatograms of the oat cultivars analyzed in this study.

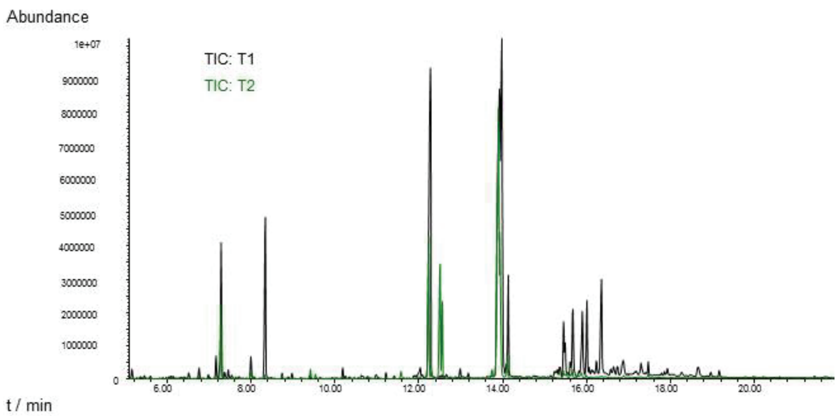

Fig. S-5. Overlain TIC chromatograms of the triticale cultivars analyzed in this study.

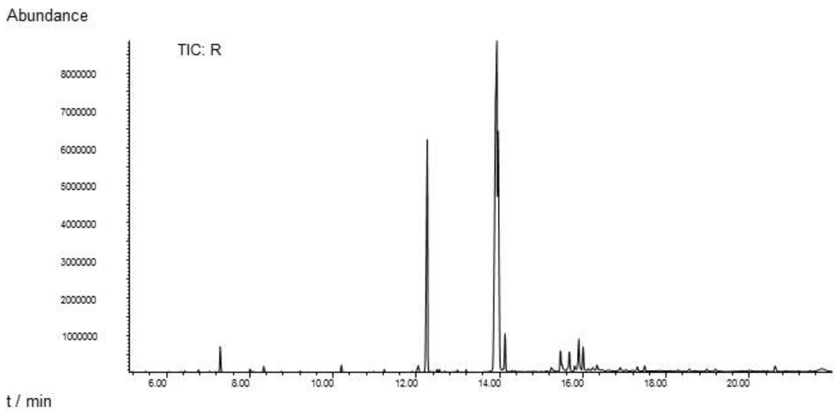

Fig. S-6. Overlain TIC chromatograms of a rye cultivar analyzed in this study.

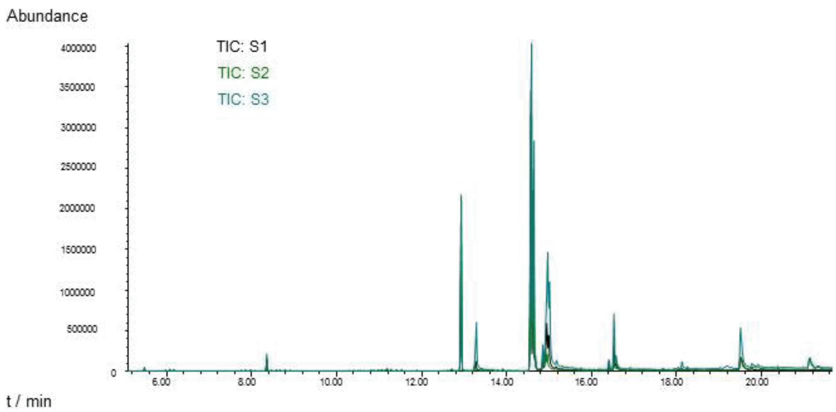

Fig. S-7. Overlain TIC chromatograms of the spelt cultivars analyzed in this study.

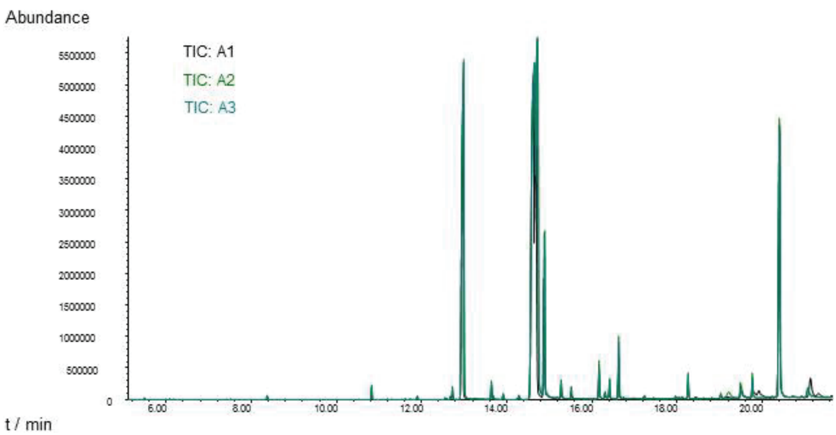

Fig. S-8. Overlaid TIC chromatograms of the amaranth cultivars analyzed in this study.

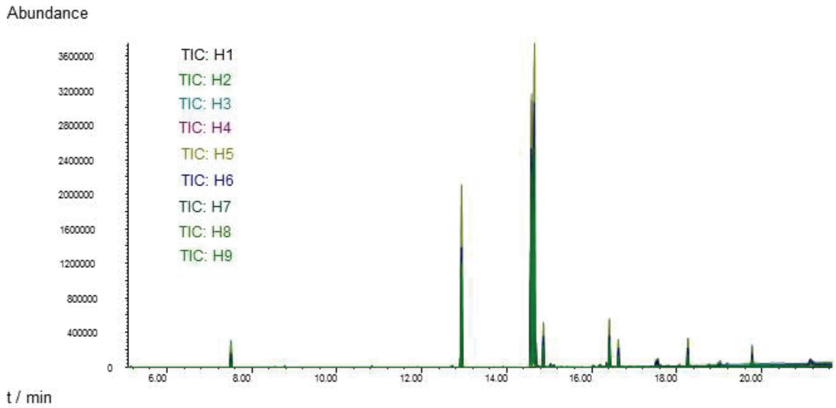

Fig. S-9. Overlain TIC chromatograms of the buckwheat cultivars analyzed in this study.

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