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Characterisation of flaxseed cultivars based on NIR diffusion reflectance spectra of whole seeds and derived samples

Yana Troshchynska[1,2]*, Roman Bleha[2], Lenka Kumbarová[2], Marcela Sluková[2], Andrej Sinica[2], Jiří Štětina[1]

[1]Department of Dairy, Fat and Cosmetics, Faculty of Food and Biochemical Technology, University of Chemistry and Technology in Prague, Prague, Czech Republic

[2]Department of Carbohydrates and Cereals, Faculty of Food and Biochemical Technology, University of Chemistry and Technology in Prague, Prague, Czech Republic

*Corresponding author: troshchy@vscht.cz

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Abstract: Discrimination of yellow and brown flaxseed cultivars was made based on diffusion reflectance FT-NIR spectra of whole seeds. The spectra of flaxseed kernels, hulls, defatted flours, and oils were also measured for comparison. Hierarchy cluster analysis (HCA) and principal component analysis (PCA) were used for the discrimination. Multivariate analyses of FT-NIR spectra led to satisfactory discrimination of all flaxseed cultivars of this study mainly according to the nutritionally important fatty acid composition that was confirmed by comparison with the corresponding spectra of flaxseed kernel and oil. By contrast, spectral features of proteins, polysaccharides, and tannins predominated in the FT-NIR spectra of flaxseed hulls and defatted flours.

Keywords: crop seed composition; multivariate analyses; vibration spectroscopy

Flax (*Linum usitatissimum* L.) is a widely cultivated crop with many applications. It is cultivated mainly for fibre and oil production. It is possible to modify fatty acid composition in flaxseeds by breeding (Smolová *et al.* 2017). Oiliness flax varieties cultivated for seed production and nutritional purposes can be divided into three groups according to polyunsaturated fatty acid composition: (i) high linoleic, but low α-linolenic acid (Amon); (ii) low linoleic, but high α-linolenic acid (Libra, Recital); (iii) both fatty acids at comparable medium amounts (Raciol).

Reflection spectroscopy in near infrared (NIR) region (4000–10 000 cm^{-1}) is often used for qualitative and quantitative characterisation of food products and raw materials (Porep *et al.* 2015) including oils (Hourant *et al.* 2000; Sato 2014) and oilseeds (Sato *et al.* 2003; Siemens & Daun 2005). Reflectance spectroscopy in NIR and mid-infrared (MIR) regions was used for multivariate determination of linoleic and α-linolenic acids in yellow and brown flax seeds and flax seed flours (Ribeiro *et al.* 2013). However, not only the fatty acid composition is relevant for nutritional characterisation of flaxseeds, but also the contribution of proteins, polysaccharides, phenolic compounds, *etc.* There is still no reference about discrimination of flaxseed varieties by NIR spectroscopy in accordance with nutritional composition of the whole seed.

This study is devoted to discrimination of chosen flax varieties based on NIR diffusion reflectance spectra of whole seeds and derived samples.

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MATERIAL AND METHODS

Flaxseed cultivars and samples. Brown (Libra, Recital) and golden (Amon, Raciol) cultivars of flaxseed (*Linum usitatissimum*) were obtained from the local producer AGRITEC, Research, Breeding & Services, Ltd. (Czech Republic). These cultivars were grown at Rapotín locality in the Czech Republic. Specification of flax cultivars analysed in this study is represented in Table 1. Hulls were separated from kernels manually using tweezers, scalpel, and magnifying glass. For oil extraction, the whole seeds were exposed to steam for 10 min and then grounded in an electric mill. Grounded material was placed into a mortar, where an extraction of oil was made by vigorous stirring with hexane for 15 minutes. The hexane extract was filtered on a paper filtre and air dried. The obtained oil samples were placed in test tubes and stored in dark at 4°C.

Flaxseed composition. The crops were conducted according to standard methods for linseed growing. The air-dried, clean, whole and undamaged seeds and isolated kernels were used for the measurements. Total lipids in milled flaxseeds were evaluated gravimetrically using Soxhlet extraction. Fatty acid composition was determined as methyl esters (FAME) according to AOCS Official Methods Ce 1f-96 (2002) by capillary gas-liquid chromatography. Correction factors were used before conversion of peak areas into mass for accurate determination. Analysis was performed on gas chromatograph 6890N (Agilent Technologies, California, USA) with capillary column SP™ 2560 (Supelco, USA), 0.25 mm × 100 m, film thickness 0.2 µm. The conditions of analysis were as follows: hexane solution of FAME (1%) was used for the injection (1 µl), split injection (1 : 50) at 220°C; flow of carrier gas (He) 1 ml/min; analysis at 175°C for 120 min; FID detection at 250°C, flow of H_2 40 ml/min, air flow 450 ml/min and make-up gas (N_2) flow 45 ml/min. Determinations were performed minimally in triplicate. Obtained analytical data are summarised in Table 2. The represented values are typical for the corresponding flaxseed cultivars as characterised above.

Table 1. Specification of flaxseed samples

Sample	Colour of seeds	Cultivar	Harvesting year	Additional information
A1	yellow	Amon	2015	low-linolenic, high-linoleic
A2			2016	
R1		Raciol	2015	medium linolenic/linoleic
R2			2016	
R3		Raciol bio	2015	
Rt	brown	Recital	2015	high-linolenic, low-linoleic
L		Libra bio	2017	

Table 2. Composition of flaxseed samples

Sample	Content (% w/w)						
	fat[a]	fatty acids[b]					
		palmitic	stearic	oleic	linoleic	linolenic
A1	41.5	7.4	2.3	18.3	68.7	3.3
A2	40.8	6.5	2.5	18.0	69.4	3.7
R1	38.6	6.9	2.3	18.2	39.3	33.4
R2	39.8	6.3	2.8	18.8	38.8	33.4
R3	39.3	6.1	2.1	18.2	44.8	28.7
Rt	41.1	5.8	2.7	20.6	16.5	54.4
L	44.7	6.3	2.0	15.7	16.2	59.8

[a]content in whole seeds; [b]composition in oils

Spectroscopic methods. Diffuse reflectance FT-NIR spectra (10 000–4000 cm^{-1}, resolution 8 cm^{-1}, 64 scans) were recorded on the FT-IR spectrometer Nicolet 6700 (ThermoFisher Scientific, USA) using CaF_2 beam splitter and smart NIR UpDRIFT holder. The samples were scanned in cuvette with glass window holding approximately 100 ml of seeds when full. During the measurement the cuvette containing seeds was rotated using special rotation device attached to the holder. The white spectralon standard was used for measuring of background. Each sample was measured five times. The spectra were converted to ASCII format and exported to Origin ver. 6.0 (Origin Lab, USA) for further processing (smoothing, baseline correction and/or normalisation) and creation of graphical outputs.

Multivariate statistics. Diffuse reflectance FT-NIR, log (1/R), spectra in ASCII format were exported to Statistica ver. 12.0 (Statsoft, USA) software for multivariate statistical evaluation. Hierarchy cluster analysis (HCA; Ward method of clustering, Euclidian distances) and principal component analysis (PCA; covariation matrix) of the FT-NIR data were made and graphical outputs, *i.e.* dendrograms of similarity and component score graphs, were created using Statistica ver. 12.0 and Origin ver. 6.0.

RESULTS AND DISCUSSION

FT-NIR spectra of whole seeds. Average normalized diffuse reflectance FT-NIR spectra of whole seeds

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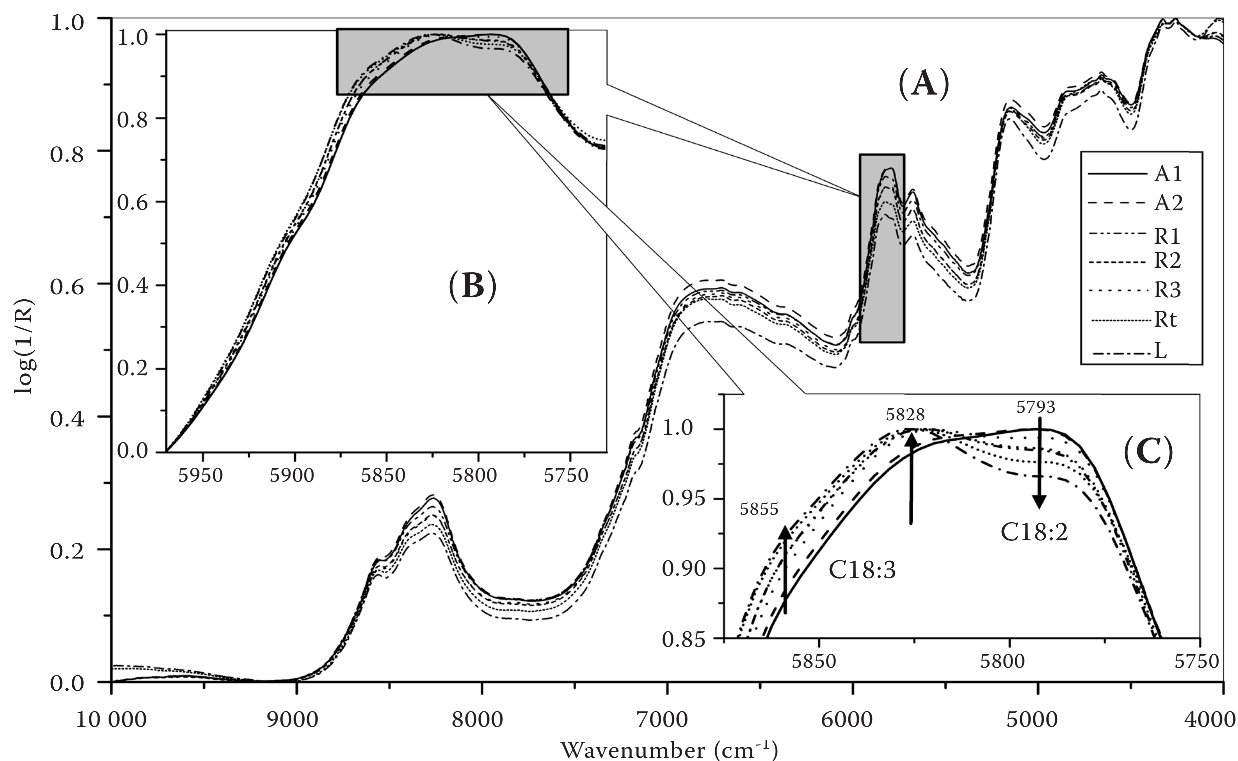

Figure 1. Average normalized FT-NIR spectra of whole seeds (**A**) and the region used for multivariate analyses (**B**) including three characteristic bands sensitive to fatty acid composition (**C**)

of seven flaxseed samples are shown in Figure 1A. In several spectral regions (for example, 10 000–9500 and 4200–4000 cm^{-1}) the spectra of whole seeds of brown cultivars differed significantly from those of yellow cultivars. Moreover, darker brown seeded cultivar Libra showed the largest spectral differences among all the samples. The assignment of NIR bands is summarised in Table 3. The positions of shoulders were obtained by the 2nd derivative algorithm. The NIR bands were assigned to combinations and overtones of the vibrations of lipids, water, proteins, tannins, and polysaccharides. It was found that the lipid bands at 4258, 4327, 5674, 5793, and 8262 cm^{-1} (Hourant *et al.* 2000) were more pronounced for the yellow seeded cultivars. By contrast, the bands or shoulders at 4659, 5153, 6007, 6811, 8559, 8774, and 9785 cm^{-1} having a contribution from tannins (Hong *et al.* 1996) were more intense for Libra and Recital. Observed differences in band intensities could be explained by the contribution of tannins in brown seeded cultivars because these compounds are responsible for brown colour of flaxseeds. The intense bands of tannins located in hulls may mask the contribution of lipids located in kernels, so lipid bands were more pronounced for yellow seeded cultivars where tannins are absent due to mutations. The difference in fat content between yellow and brown seeded cultivars (Table 1) is not so marked to be responsible for relative intensity of lipid bands observed. The contribution of lipid bands in FT-NIR spectra of whole seeds is important prerequisite for estimation of fatty acid composition. Ribeiro *et al.* (2016) used reflectance FT-NIR spectra of whole and ground seeds for determination of linoleic and linolenic acids in yellow and brown flaxseeds.

FT-NIR spectra of flaxseed kernels. Flaxseed oil is located in the kernel part inside the seed, so the FT-NIR spectra of flaxseed kernels should better detect the differences in oil composition for the cultivars of this study. In addition, the spectrum of kernel is not burdened by the contribution of phenolics and some polysaccharides present in flaxseed hulls. Indeed, it is evident that the characteristic NIR bands of oil mentioned above are much more pronounced in the spectra of kernels (Figure 2A) than in the corresponding spectra of whole flaxseeds (Figure 1A). Moreover, the regions of 1st and 2nd overtones of CH stretching (Figure 3B and C) showed significant differences in intensities of the bands sensitive to composition of unsaturated acids in flaxseed oil. The bands at 5677, 5785, and 8269 cm^{-1} having contribution of saturated residues decreased in the raw Amon-Raciol-Recital-Li-

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Table 3. NIR band assignment for flaxseeds

Wavenumber (cm^{-1})	Assignment	Compounds	Prevalence*
4023	ν(CH) + ν(CC)	polysaccharides	brown
4192sh	$\nu_{as,s}(CH_2)$ + ν(CC)	lipids	yellow
4258	$\nu_s(CH_2) + \delta(CH_2)$	lipids	yellow
4327	$\nu_{as}(CH_2) + \delta(CH_2)$	lipids	yellow
4408sh	ν(OH) + ν(CO)	polysaccharides	brown
4590sh	$\nu(=CH)_{as}$ + ν(C=C); ν(NH) + δ(NH)	lipids, proteins	yellow
4659	ν(=CH) + ν(C=C)	phenolics, lipids	brown
4725sh	ν(OH) + δ(OH)	polysaccharides	brown
4863sh	ν(NH) + δ(NH)	proteins	yellow
5048sh	$\nu(H_2O) + \delta(H_2O)$	water	yellow
5153	ν(OH) + δ(OH)	phenolics	brown
5280sh	3 × ν(C=O)	lipids	yellow
5674	2 × $\nu_s(CH_2)$	lipids	yellow
5793	2 × $\nu_{as}(CH_2)$; 2 × ν(=CH)	lipids	yellow
5828	2 × ν(=CH)	lipids	brown
5855sh	2 × ν(=CH)	lipids	brown
6007sh	2 × ν(=CH)	phenolics, lipids	brown
6352sh	ν(NH) + 2 × δ(NH)	proteins	no
6491sh	2 × ν(NH)	proteins	no
6622	2 × ν(OH)	polysaccharides	no
6707	2 × ν(OH)	polysaccharides	no
6811sh	2 × ν(OH)	phenolics	brown
6968sh	2 × $\nu_s(CH_2) + \delta(CH_2)$	lipids	yellow
7070sh	2 × $\nu_s(CH_3) + \delta_s(CH_3)$; 2 × $\nu(H_2O)$	lipids, proteins, water	no
7185sh	2 × $\nu_{as}(CH_2) + \delta(CH_2)$	lipids	yellow
7263sh	2 × $\nu_{as}(CH_3) + \delta_{as}(CH_3)$	proteins	brown
7353sh	2 × ν(CH) + δ(CH)	polysaccharides	brown
8262	3 × $\nu(CH_2)$	lipids	yellow
8412sh	3 × ν(=CH); 2 × $\nu(H_2O) + \delta(H_2O)$	lipids, water	brown
8559	3 × ν(=CH); 2 × ν(OH) + ν(C=C)	lipids, phenolics	brown
8690sh	3 × $\nu_{as}(CH_2)$	lipids	yellow
8774sh	3 × ν(=CH)	phenolics	no
9608br	3 × ν(OH)	polysaccharides	brown
9785br	3 × ν(OH)	phenolics	brown

*more pronounced NIR features for yellow or brown cultivars or no significant difference; Sato 2014; Westad *et al.* 2007; Christy *et al.* 2004; Soukupova *et al.* 2002; Hourant *et al.* 2000; Workman & Jerome1996; Hong *et al.* 1996

bra, whereas the marker bands of *cis*-unsaturation at 5832, 5870, 8412, and 8570 cm^{-1} showed the opposite changes. Other regions of the FT-NIR spectrum having contribution of fatty acid vibrations also showed similar dependences in band intensities for the mentioned cultivars, but these spectral features were not so pronounced. Therefore, comparing of the FT-NIR spectra of whole flaxseeds and kernels showed very similar trends for the studied flaxseed cultivars, and these trends can be explained by the difference in fatty acid composition of oil determined by flaxseed genotype. Removal of oil from kernel could open possibilities to estimate other biochemical compounds in kernel, mainly proteins and polysaccharides.

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FT-NIR spectra of flaxseed hulls. By contrast to the mentioned above, the FT-NIR spectra of flaxseed hulls (Figure 2D) showed significantly lower lipid bands, while the combination and overtone bands of phenolics and polysaccharides at 4015 cm^{-1} (combination of CH and CC stretching), 4717 and 5168–5172 cm^{-1} (combination of OH stretching and bending), 6820 cm^{-1} (1st overtone of OH stretching) are

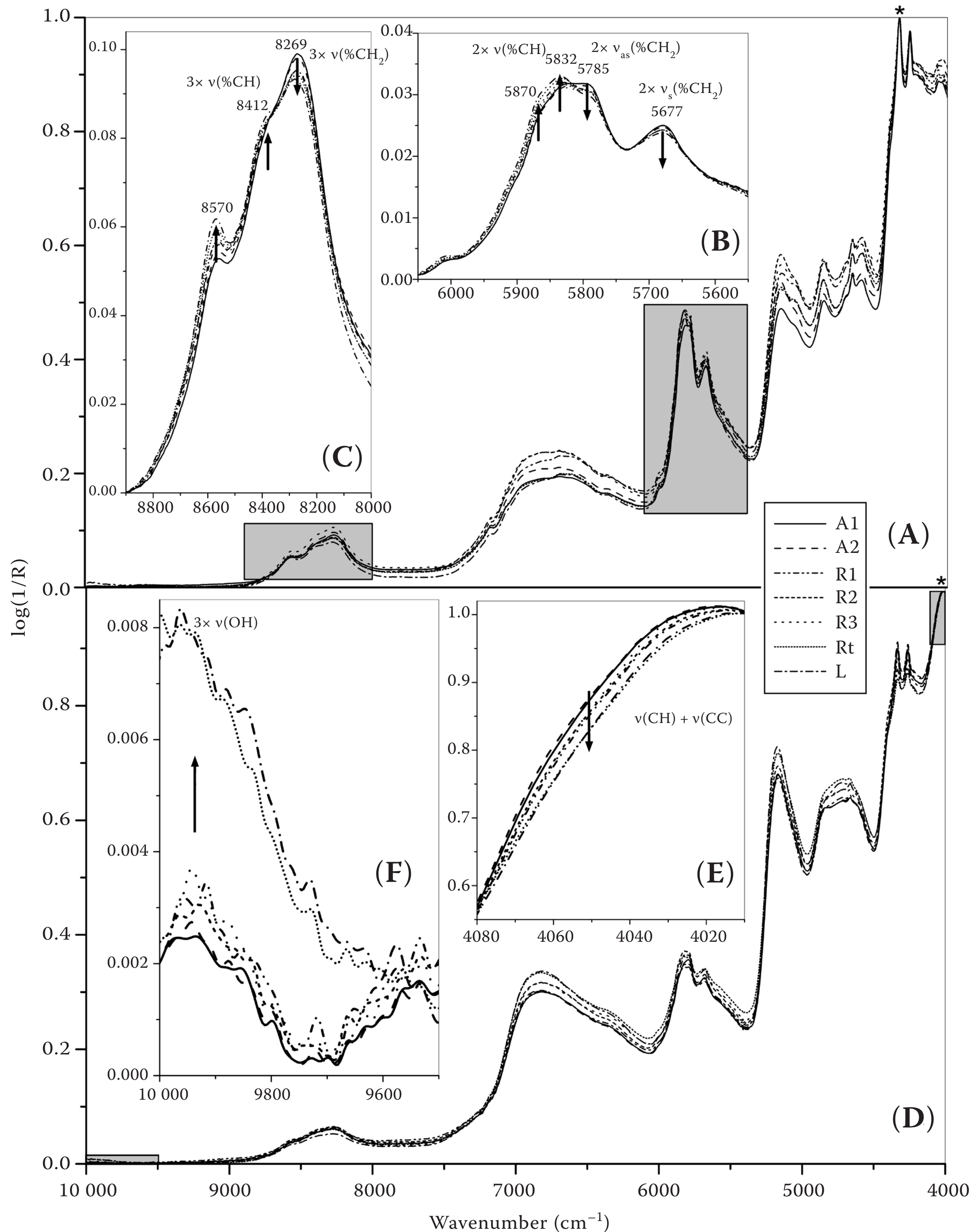

Figure 2. Average normalized FT-NIR spectra of flaxseed kernels (**A–C**) and hulls (**D–F**): four small panels (**B**, **C**, **E**, and **F**) demonstrated the cut out regions in details

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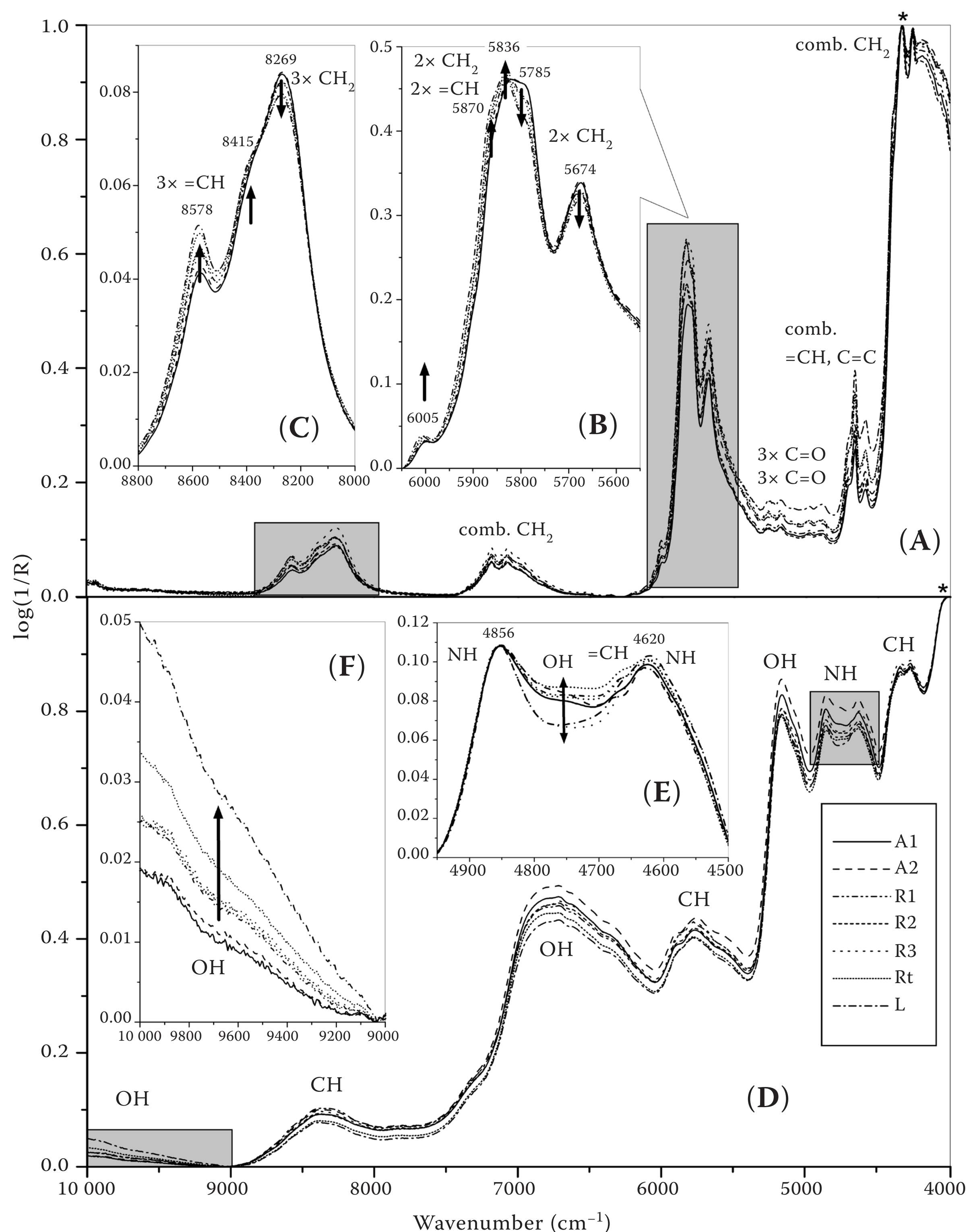

Figure 3. Average normalized FT-NIR spectra of flaxseed oils (**A-C**) and defatted flowers (**D-F**): four small panels (**B**, **C**, **E**, and **F**) demonstrated the cut out regions in details

more pronounced. Moreover, the end regions of the spectra, *i.e.* those at 9500–10 000 cm^{-1} (2nd overtone of OH stretching in tannins) and 4010–4080 cm^{-1} (combination of OH and CC stretching in polysaccharides), well illustrate the differences between cultivars of this study (Figure 2E and F). In contrast to kernels,

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FT-NIR spectra of flaxseed hulls can be used for discrimination of flax cultivars based on the contributions of tannins and polysaccharides.

FT-NIR spectra of flaxseed oils. FT-NIR spectra of flaxseed oils isolated from whole seed samples are represented in Figure 3A. There are six spectral regions corresponding to specific vibrations of fats (Hourant *et al.* 2000; Westad *et al.* 2007): (1) 4000–4500 cm^{-1}, CH combinations; (2) 4500–4830 cm^{-1}, CH and C=C combinations; (3) 4830–5320 cm^{-1}, 3rd overtones of C=O and C=C; (4) 5320–6350 cm^{-1}, 1st overtones of CH; (5) 6350–7300 cm^{-1}, CH combinations; (6) 7300–9000 cm^{-1}, 2nd overtones of CH. All these regions were examined on their sensitivity to fatty acid composition of flaxseed oils. It was found that, like in the cases of whole seeds (Figure 1C) and kernels (Figure 2B and C) described above, the regions of 1st and 2nd overtones of CH stretching vibrations showed pronounced differences in the intensities of several bands (Figure 3B and C). For the other regions, the differences were less pronounced or slight. The contribution of flaxseed oil including fatty acid composition (Siemens & Daun 2005) should play the key role in distinguishing flax cultivars by the FT-NIR spectra of whole seeds, flour or kernels like it has been reported for other crops (Sato *et al.* 2002, 2003).

FT-NIR spectra of defatted flaxseed flours. FT-NIR spectra of defatted flaxseed flours isolated from whole seed samples are represented in Figure 3D. By contrast to the spectra of flaxseed hulls and kernels, no pronounced lipid bands were found in this case due to removal of fats during oil extraction. Two marked bands at 4620 and 4956 cm^{-1} (Figure 3E) were assigned to NH combination vibrations in proteins (Workman & Jerome 1996). The region between these protein bands showed high variability in band intensity but without any correlation with flaxseed cultivars. The weak bands in this region have contributions of OH and CH combination vibrations in polysaccharides and phenolic compounds (Hong *et al.* 1996; Soukupova *et al.* 2002). Like in the case of flaxseed hulls, the high wavenumber region of the spectra at 9000–10 000 cm^{-1} having contribution of 2nd overtone of OH stretching in tannins showed evident intensity increase in the raw Amon-Raciol-Recital-Libra according to the seed colour (Figure 3F). Therefore, the distinguishing of flaxseed cultivars by the NIR spectra of defatted flour or hulls could be based on the differences in composition, but in these cases the key compounds could be proteins, polysaccharides and polyphenols. Composition of proteins or polysaccharides in defatted flours could be sensitive to flax cultivar and thus be used as biochemical markers of specificity.

Discrimination of flax cultivars based on NIR data. The region of 5730–5970 cm^{-1} (Figure 1B) in FT-NIR spectra of whole seeds was used for discrimination of flax cultivars using multivariate statistical methods (HCA and PCA). This region corresponds mainly to 1st overtones of CH stretching modes in unsaturated fatty acids having C=C bonds in *cis* configuration (Hourant *et al.* 2000; Westad *et al.* 2007). Azizian & Kramer (2005) demonstrated the differences in 2nd derivative FT-NIR spectra at this region among three model unsaturated triacylglycerols (TAG): triolein, trilinolein and trilinolenin. As the number of C=C bonds in the TAG molecule increased from 3 to 9, the peaks at 5830 and 5870 cm^{-1} became stronger, but those at 5768 and 5680 cm^{-1} weakened. Sato (2014) confirmed on the same TAGs that higher *cis*-unsaturation led to more pronounced shift of the CH stretching overtone band to higher wavenumber, *i.e.* from 5797 cm^{-1} (triolein) to 5838 cm^{-1} (trilinolein) and then to 5851 cm^{-1} (trilinolenin). According to Hourant *et al.* (2000), the bands at 5793, 5828, and 5855 cm^{-1} in the spectra of oils have the main contribution from the residues of oleic (*cis*-C18:1), linoleic (*cis*-C18:2) and linolenic (*cis*-C18:3) acids, respectively. All these acids are common in flaxseed oil. Contrary to this, the latter band was found to be sensitive to the oleic acid to linoleic acid ratio in soy flour and sesame seeds; it became stronger compared to the first band when the proportion of linoleic acid increased (Sato *et al.* 2002, 2003). The second band at 5828 cm^{-1} was used instead for the estimation of linoleic acid in husked sunflower seeds in relation to the band at ~5800 cm^{-1} having contribution from oleic acid and saturated acid chains (Sato 2014).

Therefore, the three bands mentioned above can be used for evaluation of the ratio between CC and C=C in flaxseed oil, which is contributed to the spectra of whole seeds. Partially, the relationship between these bands should indicate the differences in relative amounts of the corresponding unsaturated fatty acids. Indeed, the FT-NIR spectra of cultivar Amon having a low amount of linolenic acid (~3.5%) and a high amount of linoleic acid (~69%) showed a maximum at 5793 cm^{-1} (Figure 1B and C). In the raw Amon-Raciol-Recital-Libra this band subsequently decreased with increasing the ratio between linolenic and linoleic acids. There is also the growth of a new band at 5828 cm^{-1} and a shoulder near 5855 cm^{-1}. Finally, the spectra of cultivar Libra (58.5% of linolenic acid, 15.3% of linoleic acid) have a significant maximum at 5828 cm^{-1} and

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less pronounced shoulder near 5793 cm^{-1}. Therefore, the ratio between intensities of these two bands determines the difference in relative amounts of the major polyunsaturated fatty acids in flaxseed oil. In comparison with other spectroscopic methods, NIR spectroscopy has an advantage that it is able to check fatty acid composition in whole seeds. This feature, together with seed colour, is a key difference between flaxseed cultivars. Moreover, fatty acid composition has nutritional importance because regular flaxseed oil having high ~50% of linolenic acid is not suitable for food purposes because of undesirable odour and taste reversion due to auto-oxidation of this fatty acid (Ralph 1992). Despite characteristic NIR bands of other whole seed constituents are not so pronounced like lipid bands, it is possible to use FT-NIR spectra of seed fractions (kernel, hull, oil or defatted flour) to reach discrimination of flaxseed cultivars based on the contribution of proteins, polysaccharides or phenolic compounds.

Resulting graphical outputs from HCA and PCA of NIR spectra (5730–5970 cm^{-1}) are represented in Figure 4. The dendrogram of similarity illustrate clustering of seeded cultivars according to the fatty acid composition. Three main clusters corresponded to cultivars Amon (high-linoleic/low-linolenic), Raciol (medium linoleic and linolenic) and Libra plus Recital (low-linoleic/high-linolenic); then brown seeded Libra and Recital formed own clusters (Figure 4A). The component score graph for NIR data PC1 versus PC3 illustrates discrimination of individual cultivars according to fatty acid composition (Figure 4B): PC1 separated three main groups mentioned above, *i.e.* Amon (positive PC1), Raciol (PC1 around zero) and two brown cultivars (negative PC1), while PC3 additionally separated Raciol having similar amounts of two polyunsaturated fatty acids (positive PC3) from the other cultivars having extremely different amounts of these fatty acids (negative PC3). Moreover, PC3 also separated smaller clusters according to cultivar, harvesting year or conditions, *i.e.* the pair Libra/Recital as well as individual samples of Amon and Raciol. Therefore, multivariate analyses of FT-NIR spectra at specific spectral region sensitive to fatty acid composition led to successful discrimination of whole seeds according to phenotypic differences including cultivar and harvesting year.

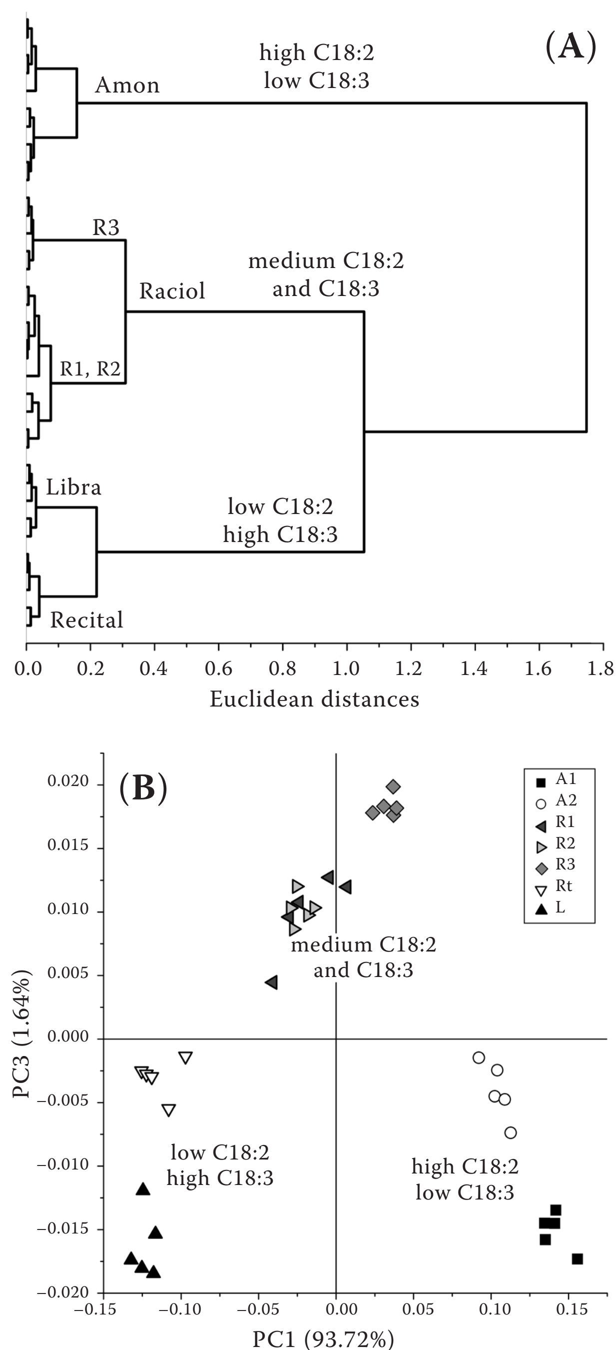

Figure 4. Dendrogram of similarity (**A**) and component score graph PC1 versus PC3 (**B**) for FT-NIR spectra of whole seeds

CONCLUSIONS

Obtained results confirmed that FT-NIR spectroscopy can be used as effective tool in characterisation of flaxseed composition. FT-NIR spectra of whole seeds were successfully used for discrimination of several flaxseed cultivars according mainly to unsaturated fatty acid compositions. The NIR spectra processing by HCA and PCA demonstrated well separation of the clusters corresponding to individual cultivars. FT-NIR spectra of seed fractions (kernel, hull, oil or defatted flour) were used for more detailed analysis of

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the chemical composition of flaxseeds. These results contribute to characterisation of crop cultivars and estimation of their quality that is important for food processing. Moreover, fractionation of flaxseed used in this work permits to evaluate the major constituents in the specific parts or extracts, *i.e.* fatty acids in seed oil, proteins in defatted kernel, polysaccharides or tannins in hull. Use of FT-NIR spectroscopy for quantitative estimation of the main flaxseed constituents like fats, proteins, and polysaccharides could be the subjects of future investigations.

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