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НАУКОВИЙ КОМІТЕТ

ЧЛЕНИ КОМІТЕТУ

СЕКРЕТАР

1. THE STUDY OF THE FATTY ACIDS COMPOSITION OF DOMESTIC BRANDS OF SUNFLOWER OIL BY NMR 1H SPECTROSCOPY

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97% of sunflower oil triglycerides are represented by esters of oleic (Omega-9) and linoleic (Omega-6) acids. The technological and nutritional value of sunflower oil is determined by the ratio of these components. Sunflower oil with a high content of oleic acid (Omega-9) and a sufficiently low content of polyunsaturated lenoleic acid (Omega-6) is characterized by a lower nutritional value but greater chemical stability at high temperatures and in the presence of oxidizing agents [1]. Therefore, that type of oil, especially refined, is more suitable for high temperature processing of food and can be stored longer saving its properties. The purpose of this work was to study the TAG composition of sunflower oil samples by ^{1}H-NMR spectroscopy. This method based on estimation and comparison the proton integral intensities of allyl and diallyl CH_2 groups with intensity of glycerol protons in ^{1}H-NMR spectra that allows determining the amounts of each of these unsaturated fatty acids.

Samples of sunflower oil of commercial brands "Chumak", "Oleyna", "Maslinka" and "Shchedriy Dar" purchased in the local supermarkets, NMR ^{1}H spectroscopy, deuterated chloroform.

Vinylic hydrogens (H_v), allylic hydrogens (H_a) and bisallylic hydrogens (H_b) have own characteristic chemical shifts, and could be used to detect the unsaturated moieties of oleic and linoleic acids (see Figure 1).

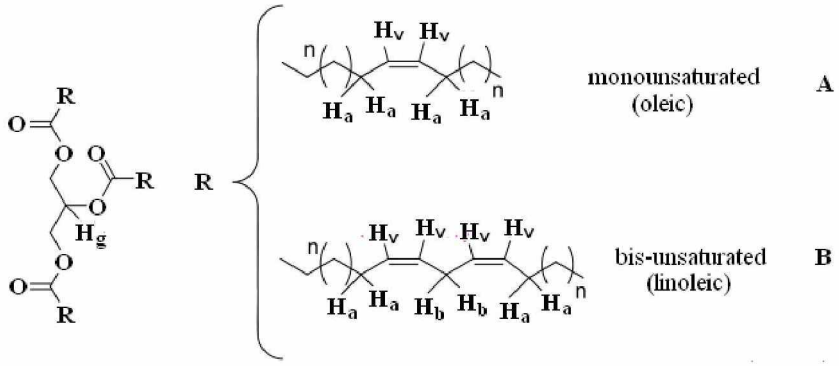

Figure 1. The general structure of triglyceride of sunflower oil

Integral intensities of these hydrogens can be compared with intensity of the tertiary hydrogen in the glycerin moiety (H_g). That allows making a conclusion about fatty acids composition of the oil samples.

The oil samples were solved in deuterated chloroform. The spectra of prepared solutions were recorded on a Varian VXR-300 spectrometr (300 MHz). Despite the fact that the data obtained do not allow the exact integration of the tertiary hydrogen of the Hg of the glycerol moiety, it is possible to determine the quantitive ratio of oleic and linoleic esters based on the

comparison of integral intensities of typical signals. The proton resonances of the TAG acyl chains were assigned according to the literature data [2, 3] and are shown in Table 1.

Table 1. Chemical shifts of protons in NMR spectra

Signal	Functional group	Chemical shift (ppm)	
		Oleic ester	Linoleic ester
1	$-CH_3$	0.96 – 0.82 (dd)	0.96 – 0.82 (dd)
2	$-CH_2-$	1.43 – 1.16 (m)	1.43 – 1.16 (m)
3	$-CH_2-C-CO_2$	1.70 – 1.51 (m)	1.70 – 1.51 (m)
4	$-CH_2-CO_2-$	2.11 – 1.91 (m)	2.11 – 1.91 (m)
5	$-C-CH_2-C=C-$	3.38 – 2.21 (m)	3.38 – 2.21 (m)
6	$-C=C-CH_2-C=C-$	-	2.83 – 2.73 (t)
7	$-C-CH_2-O-CO-C$	4.21 – 4.08 (dd)	4.21 – 4.08 (dd)
8	$-C-CH_2-O-CO-C$	4.36 – 4.22 (dd)	4.36 – 4.22 (dd)
9	$-CH(-C-O-CO-C-)_2$ $+C-HC=CH-C$	5.43 – 5.13 (m)	5.43 – 5.13 (m)

Signal multiplicity: s, single; d, doublet; t, triplet; m, multiplet

Data on the contents of oleic (Omega-9) and linoleic (Omega-6) acids in sunflower oil of domestic brands and, for comparison, data on fatty acids composition of olive oil and high-oleic oil* obtained as a result of analysis of their spectra, are represented in Table 2.

Table 2. The contents of fatty acids in the samples of sunflower oil

Number	Name	Oleic/linoleic acid ratio	Percentage, %	
			Oleic acid	Linoleic acid
1	«Chumak»	1:2	32.06	63.64
2	«Maslinka»	5:7	40.05	55.65
3	«Shchedriy Dar»	5:7	40.05	55.65
4	«Oleyna»	1:1	48.03	47.67
5	Olive oil	9:1	86.19	9.51
6	High-oleic oil *	200:1	95.23	0.47

* The oil sample from sunflower seeds provided by Institute of Oilseeds of the National Academy of Agrarian Sciences of Ukraine

Among the sunflower oil samples of domestic brands, the highest content of oleic acid and the lowest content of linoleic acid were found in oil «Oleyna». Therefore, this oil among all samples studied is the most suitable for high-temperature processing of food products.

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