

62. Study of chemical transformations in sunflower oil during heat treatment by NMR ^1H spectroscopy

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Introduction. Sunflower oil consists of glycerol esters and oleic and linoleic acids almost 90%. The last one is a predominance component. The purpose of the work is to study chemical transformations taking place in refined sunflower oil during long heating oil by NMR ^1H spectroscopy.

Materials and methods. Refined sunflower oil of the brand "Chumak", heat treatment of an oil sample at 230 – 240 °C. Monitoring of chemical transformations results in oil is carried out in 30, 60, 90, 120 minutes from the beginning of the experiment by NMR ^1H spectroscopy with the equipment "Varian VXR-300", as internal standard, TMS is used, a solvent CDCl_3 .

Results. The ^1H NMR spectrum of an oil sample prior to the start of the experiment shows peaks characteristic of the protons of the glycerol part. Picks of oleic and linoleic acids skeletons protons are also observed. These results are consistent with literature data regarding the fatty-acid composition of sunflower oil. The monitoring of the chemical composition of the oil sample and the comparative analysis of the integral intensities of hydrogen atoms picks in the spectra obtained show that linoleic acid moieties tend to undergo the most significant changes under heat treatment process. It is evidenced by the decrease in the area of the CH_2 signals of the bis-allylic fragment of the carbon skeleton from the beginning of the experiment to 120 minutes of heating (Table 1). The spectra show the gradual decreasing of hydrogen atoms picks that are characteristic of linoleic acid.

Table 1. Changes in the intensity of proton signals in ^1H NMR spectra from the initial value, %

The duration of the experiment	Intensities of protons signals as a percentage of the initial value, %		
	Bis-allylic- CH_2 -groups of linoleic acid at 2.77 ppm	Vinylic $-\text{CH}=\text{CH}-$ at 5.33 ppm	Allylic CH_2 groups of bond $-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_2-$ at 2.31 ppm
0 min.	100	100	100
30 min.	92	92	95
60 min.	70	80	90
90 min.	45	52	77
120 min.	36	42	76

The integral intensities of the signals of the vinylic and allylic hydrogen atoms change less as compared to bis-allylic ones.

Conclusions. During the heat treatment of sunflower oil, triglyceride molecules undergo irreversible transformations. The most sensitive fragments of triglycerides are bis-allylic groups $-\text{CH}_2-$ of linoleic acid moieties that undergo the most major transformations. The degree of irreversible transformations in oil is in direct proportion to time of heat treatment.