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## Determination of the composition of linseed oil by nuclear magnetic resonance spectroscopy

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### Abstract

In this article, we determined the composition of flaxseed oil by nuclear magnetic resonance using the Bruker Avance DRX 400 spectrometer. In the obtained spectrum, peaks appear between 0.97 and 5.36 ppm. Thus, the composition of flaxseed oil is as follows: linolenic acid 18:3 - 50%, linoleic acid 18:2 - 19%, mono-unsaturated 18:1 (oleic acid) - 20% and saturated acid 18:0 - 10%.

**Keywords:** Oil linseed,  $^1\text{H}$  NMR, spectroscopy

### Introduction

Nuclear magnetic resonance spectroscopy, most commonly known as NMR spectroscopy or magnetic resonance spectroscopy (MRS), is a spectroscopic technique based on re-orientation of atomic nuclei with non-zero nuclear spins in an external magnetic field. This re-orientation occurs with absorption of electromagnetic radiation in the radio frequency region from roughly 4 to 900 MHz, which depends on the isotopic nature of the nucleus and increased proportionally to the strength of the external magnetic field <sup>[1]</sup>. Notably, the resonance frequency of each NMR-active nucleus depends on its chemical environment. As a result, NMR spectra provide information about individual functional groups present in the sample, as well as about connections between nearby nuclei in the same molecule. As the NMR spectra are unique or highly characteristic to individual compounds and functional groups, NMR spectroscopy is one of the most important methods to identify molecular structures, particularly of organic compounds.

### The principle of NMR usually involves three sequential steps

The alignment (polarization) of the magnetic nuclear spins in an applied, constant magnetic field  $B_0$ .

The perturbation of this alignment of the nuclear spins by a weak oscillating magnetic field, usually referred to as a radio-frequency (RF) pulse.

Detection and analysis of the electromagnetic waves emitted by the nuclei of the sample as a result of this perturbation.

Similarly, biochemists use NMR to identify proteins and other complex molecules. Besides identification, NMR spectroscopy provides detailed information about the structure, dynamics, reaction state, and chemical environment of molecules. The most common types of NMR are proton and carbon-13 NMR spectroscopy, but it is applicable to any kind of sample that contains nuclei possessing spin.

NMR spectra are unique, well-resolved, analytically tractable and often highly predictable for small molecules. Different functional groups are obviously distinguishable, and identical functional groups with differing neighboring substituents still give distinguishable signals. NMR has largely replaced traditional wet chemistry tests such as color reagents or typical chromatography for identification.

The most significant drawback of NMR spectroscopy is its poor sensitivity (compared to other analytical methods, such as mass spectrometry). Typically 2-50 mg, of a substance is required to record a decent quality NMR spectrum. The NMR method is non-destructive, thus the substance may be recovered. To obtain high-resolution NMR spectra, solid substances are usually dissolved to make liquid solutions, although solid-state NMR spectroscopy is also possible.

The timescale of NMR is relatively long, and thus it is not suitable for observing fast phenomena, producing only an averaged spectrum. Although large amounts of impurities do

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show on an NMR spectrum, better methods exist for detecting impurities, as NMR is inherently not very sensitive - though at higher frequencies, sensitivity is higher.

Correlation spectroscopy is a development of ordinary NMR. In two-dimensional NMR, the emission is centered around a single frequency, and correlated resonances are observed. This allows identifying the neighboring substituents of the observed functional group, allowing unambiguous identification of the resonances. There are also more complex 3D and 4D methods and a variety of methods designed to suppress or amplify particular types of resonances. In nuclear Overhauser effect (NOE) spectroscopy, the relaxation of the resonances is observed. As NOE depends on the proximity of the nuclei, quantifying the NOE for each nucleus allows for construction of a three-dimensional model of the molecule.

NMR spectrometers are relatively expensive; universities usually have them, but they are less common in private companies. Between 2000 and 2015, an NMR spectrometer cost around 500,000 - 5 million USD [3-10]. Modern NMR spectrometers have a very strong, large and expensive liquid helium-cooled superconducting magnet, because resolution directly depends on magnetic field strength. Higher magnetic field also improves the sensitivity of the NMR spectroscopy, which depends on the population difference between the two

nuclear levels, which increases exponentially with the magnetic field strength.

Less expensive machines using permanent magnets and lower resolution are also available, which still give sufficient performance for certain applications such as reaction monitoring and quick checking of samples. There are even benchtop nuclear magnetic resonance spectrometers. NMR spectra of protons ( $^1\text{H}$  nuclei) can be observed even in Earth magnetic field. Low-resolution NMR produces broader peaks which can easily overlap one another causing issues in resolving complex structures. The use of higher strength magnetic fields result in a better sensitivity and higher resolution of the peaks, and it is preferred for research purposes [5-17].

## Materials and methods

### Nuclear Magnetic Resonance Analysis

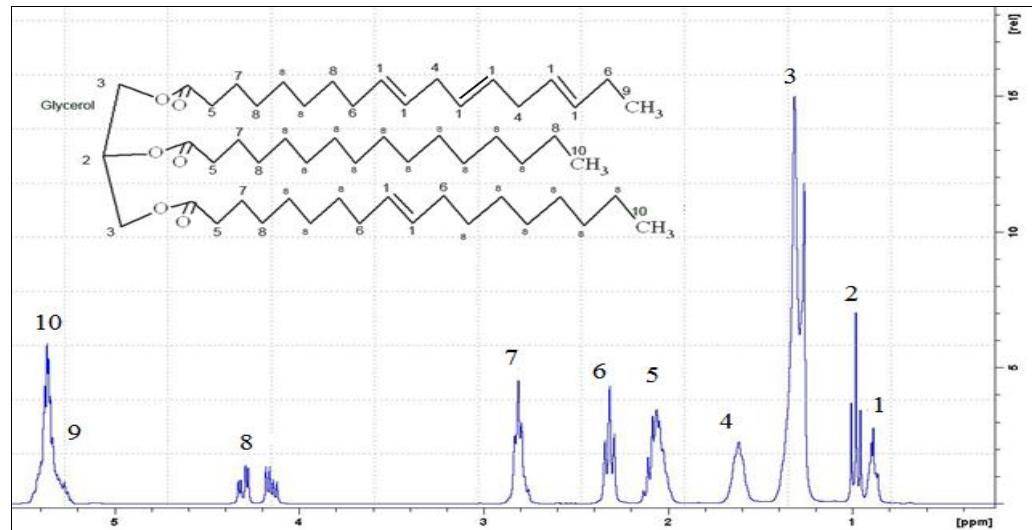
$^1\text{H}$  nuclear magnetic resonance ( $^1\text{H-NMR}$ ) spectra were recorded on a Bruker Avance DRX 400 spectrometer, operating at 9.4 Tesla, corresponding to the resonance frequency of 400.13 MHz for the  $^1\text{H}$  nucleus, equipped with a direct detection four nuclei probe head and field gradients on z axis. The chemical shifts are reported in ppm, using the TMS as internal standard.



**Fig 1:** Bruker Avance DRX 400 spectrometer

**Results and discussions:** From the recorded spectral data, the fatty acids composition of the oil linseed was calculated according to recently reported method [6]. Fig. 2 presents the

$^1\text{H-NMR}$  spectrum of linseed oil and Table 1 lists the signals and peaks assignment of the oil linseed. The fatty acid composition of oil linseed is presented in Table 2.



**Fig 2:**  $^1\text{H-NMR}$  spectrum of linseed oil

**Table 1:**  $^1\text{H-NMR}$  signals and peak assignment of linseed oil spectrum

Signal	$\delta$ (ppm)	Proton	Compound
1	0.97	-CH <sub>2</sub> =CH-CH <sub>2</sub> -CH <sub>3</sub>	linolenic acid
2	0.88	-CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>2</sub> -CH <sub>3</sub>	all acids except linolenic acid
3	1.31	-(CH <sub>2</sub> ) <sub>n</sub> -	all fatty acids
4	1.61	-CH <sub>2</sub> -CH <sub>2</sub> -COOR	all fatty acids
5	2.06	-CH <sub>2</sub> -CH=CH-	all unsaturated fatty acids
6	2.31	-CH <sub>2</sub> -COOR	all fatty acids
7	2.80	-CH=CH-CH <sub>2</sub> -CH=CH	linolenic and linoleic fatty acid
8	4.15-4.29	-CH <sub>2</sub> -O-COR	glycerol ( $\alpha$ -position)
9	5.27	-CH-O-COR	glycerol ( $\beta$ -position)
10	5.36	-CH=CH-	all unsaturated fatty acids

**Table 2:** Linseed oil fatty acid composition by  $^1\text{H-NMR}$ 

Fatty acids	Amount (%)
linolenic acid 18:3	51
linoleic acid 18:2	19
mono-unsaturated 18:1 (oleic acid)	20
saturated acid 18:0	10

## Conclusions

The composition of flaxseed oil was determined by nuclear magnetic resonance using a Bruker Avance DRX 400 spectrometer. In the obtained spectrum, peaks appear between 0.97 and 5.36 ppm. Thus, the composition of flaxseed oil is as follows: linolenic acid 18:3 - 50%, linoleic acid 18:2 - 19%, mono-unsaturated 18:1 (oleic acid) - 20% and saturated acid 18:0 - 10%.

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