

NMR Study of Cumbaru Oil to Apply as Mechanical Engineering Lubricant

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Abstract

According to the great importance that seed oils has in relation to human health, cumbaru seed oil (DIPTERYX ALATA VOGEL) had its chemical structure and positional distribution of glycerol chains investigated by solution ^1H and ^{13}C NMR, as well as the natural degradation has been evaluated. The NMR techniques applied to the study of this oil showed that it is mainly constituted by oleic and linoleic glycerols with low content of saturated glycerols such as palmitic. Another important point was that this oil did not degraded or oxidated by itself or by light action quickly, it was stored at normal laboratory conditions during two years, and it was analyzed after that time and both ^1H and ^{13}C solution NMR spectra presented the same signals since this oil was extracted from the seed.

Keywords: Cumbaru oil; ^{13}C NMR; Chemical characterization

Introduction

Seeds are a great source of fiber, lignans, protein, fat, vitamins, minerals and oils. An extensive range of seed oil has high quality for nutritional uses, focusing on bulk nutritional oils. Seeds are also one of the best sources for the essential fatty acid alpha linolenic acid. Alpha linolenic acid is so important for bodybuilders because it “enhances insulin sensitivity within muscle cells.” This omega-3 fatty acid also has many other beneficial effects. Fruit seed from which oil is extracted, such as cumbaru have high oil content (30-40%). When the whole seeds are eaten, it is suspected that the oil portion is very slowly released and metabolized, preserving and enhancing both stable energy levels and favorable blood fat chemistry. The oils in oily seeds are an excellent energy source and the seed oil is also a rich source of linolenic acid [1-3].

Seed oils derived from tropical fruit can have a high commercial value, because of diversity uses such as pharmacological, cosmetics and food industries, which depends of its chemical composition. The content of linoleic and/or linolenic acids may promote aggregate values to those oils. According to the composition of seed oils they can be used in a wide variety of applications, from analgesic to digestive. The cumbaru fruit comes from Fabaceae family, its seed presents a high nutritional value with ~26% of proteins and can be eating crude or toasted [4,5]. The chemical components and properties of this fruit have a great importance in Brazil, especially in Mato Grosso State. Because of this different researcher have been developed and several studies to improve its production and application are in progress. The nutritional properties of the virgin oil have a good quality and it is frequently used for the people as tobacco aromatizing and also as anti-rheumatic [6]. According to those people speculations, the objective of this work is to study the chemical composition of cumbaru seed oil. For that reason, we have chosen nuclear magnetic resonance (NMR) employing ^1H and ^{13}C nuclei, as they are one of the best probes to generate response on this type of information [5-11]. Another purpose for choose NMR is based on the fact that no previous sample treatment like separation, esterification and other need to be done.

Experimental

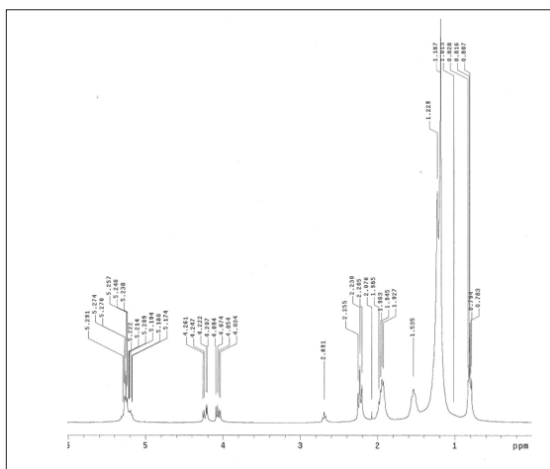
NMR Spectroscopy

Cumbaru seed oil was extracted with acetone; this oil is yellow and has a sweet smell. The analyzes of ^{13}C NMR solution were recorded on VARIAN MERCURY 300 spectrometer, operating at 300MHz for ^1H and 75.4MHz for ^{13}C . The samples concentration for ^{13}C analyses

was about 20% of oil in 3.5ml of chloroform-d using a 10mm NMR tube at temperature of 26C, in the broadband proton decoupling mode. The quantitative ^{13}C NMR spectrum was acquired using 16K data point, spectral width 220ppm, acquisition time 1.8s, relaxation delay 6s, pulse width 90, no NOE effect and 25000 scans. High-resolution carbonyl spectrum was recorded with a 32K data point, spectral width 10ppm, acquisition time 21s, relaxation delay 5s and a 90 pulse [3]. For the ^1H NMR spectrum the sample concentration was about 2% of oil in 0.7ml of CDCl_3 using a 5mm NMR tube at 26C. The ^1H NMR spectrum was acquired using 16K data point, spectral width 12ppm, acquisition time 3.3s, relaxation delay 1s, pulse width 45 and 256 scans.

Result and Discussion

The assignments of partial ^1H spectrum of the cumbaru seed oil acquired after solvent extraction of the cumbaru fruit seed are listed in Table 1. From the assignments it can be seen that the oil is mainly constituted by triacylglycerols, with long aliphatic chains (Table 1). The same NMR study was carried out after it has been stored for six months, one year and two years. The results of both hydrogen and ^{13}C assignments were the same as it was done immediately the oil has been extracted from the seed. No difference on chemical shift assignments for the proton spectra after two years stored at room temperature was found, indicating that the sample did not change by itself along this time. The ^1H NMR spectrum of the cumbaru oil showed oxidation stability and don't have demonstrated the presence of minor components (Figure 1) (Table 2).



which is a carbon that probably presents a branch (Figure 3). This signal was also observed in the Figure 2 showing that the oil did not show any evidence of degradation or un-stability due to oxidation process. From the ^{13}C high-resolution carbonyl spectrum the positional distribution of the glycerols along the chains was determined. The relation of the integration area of the carbonyls located at 172.8ppm represents the substitution in sn-1,3 position and the carbonyls located at 172.4ppm shows the substitution in sn-2 position.

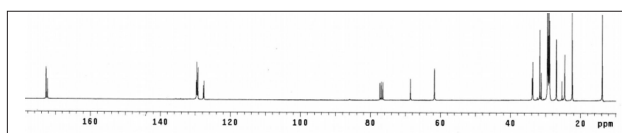


Figure 2: ^{13}C NMR spectrum of cumbaru seed oil after it has been extracted from the seed.

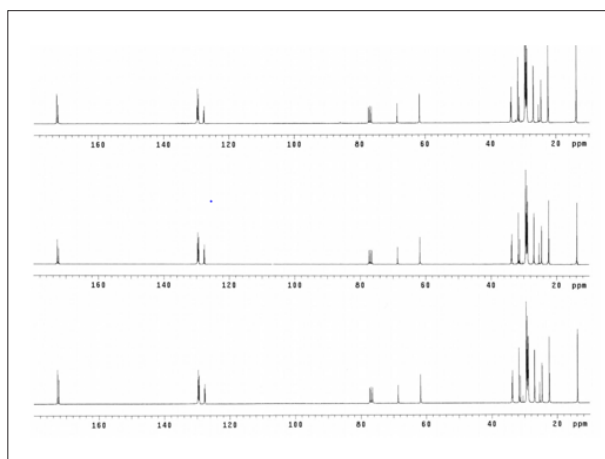


Figure 3: Comparison of ^{13}C NMR spectrum of the cumbaru oil:

1. After six month
2. Two years and
3. Immediately extracted.

Conclusion

According to the main purpose of this work, the NMR techniques were applied to the oil and the data obtained showed the main chemical compounds and the positional distribution on triacylglycerol chains. The most important conclusion was that this oil did not degraded by itself or by lights during the time studied, which is very good, for example, food and lubricant applications.

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