



¹³C NMR STUDY OF THE OILS OBTAINED FROM BERIBA FRUIT AND FISH

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The investigation of the chemical structure of the oils obtained by fruits comparing with fish oil can be a contribution to the improvement of their applications. The study of the chemical composition of beriba oil (*Duguetia lanceolata* St. Hil) and fish oil (salmon) was carried out focusing solution nuclear magnetic resonance (NMR). The based purpose of this work was to compare the chemical positional distribution of the fatty acids present in the natural oils obtained from vegetal and animal source.

The ¹³C and ¹H NMR solution spectra were recorded on a VARIAN MERCURY 300 spectrometer, operating at 300 MHz for ¹H and 75.4 MHz for ¹³C. The samples concentration for ¹³C analyses was about 20% of oil in 3.5 ml of CDCl₃ using a 10mm NMR tube at 26°C. The quantitative ¹³C NMR spectrum was acquired using 16K data point, spectral width 220 ppm, acquisition time 1.6 s, relaxation delay 6 s, pulse width 90° and 7500 scans. The high resolution carbonyl spectrum was recorded with a 32K data point, spectral width 10 ppm, acquisition time 21 s, relaxation delay 5 s and a 90° pulse. For the ¹H NMR spectrum the sample concentration was about 2% of oil in 0.7 ml of CDCl₃ using a 5mm NMR tube at 26°C. The ¹H NMR spectrum was acquired using 16K data point, spectral width 12 ppm, acquisition time 3.3 s, relaxation delay 1 s, pulse width 45° and 256 scans.

The ¹³C NMR spectra of both type of oils were acquired and the results showed that they are mainly constituted by triacylglycerol and some free fatty acids. The fatty acids detected for the triacylglycerol are those based on the of C₁₆-C₁₈. Saturated alkane, mainly are palmitic and stearic. Alkenes (C₁₈), constituted by monounsaturated and diunsaturated, mostly oleic and linoleic, respectively. The ¹³C chemical shift values found for the beriba oil are listed in Table 1. The analysis of the carbonyl region of the beriba oil showed that the saturated chains are in low proportion and the oleic/linoleic ratio is approximately 1:1, which was also confirmed by examination of the olefinic region. ¹³C NMR seems to represent the only direct instrumental method by which the positional distribution of fatty acids on glycerol can be specifically identified. According to Sacchi¹ works, in beriba oil considering the oleic/linoleic ratio, the saturated chain of the palmitic (P) component is normally located in the position 3, as a consequence the triacylglycerol chains distribution is OOP, 1,2-dioleoyl –3-palmitoylglycerol.

The ¹³C chemical shift values detected for the fish oil are listed in Table 2. From the analysis of fish oil, obtained by ¹³C spectra, the oleic/linoleic ratio is approximately the same as it was found for the beriba oil.

Comparing the oils extracted from different natural source it is interesting that they present the same positional distribution of the fatty acids on glycerol chains.

Table 1 - The ^{13}C chemical shift values found for the beriba oil

δ (ppm)	type of carbon	Type of compounds
173.3 – 172.5	C=O	triacylglycerols
130.0	CH=CH	oleic
129.8-129.4	CH=CH	oleyl
127.7-127.7	CH=CH	linoleyl
68.9	CH-OH	triacylglycerols
62.1	CH₂-OH	triacylglycerols
34.0-33.8	CH₂	all acyl chains
31	CH₂	saturated chains
31.3-28.7	CH₂	all acyl chains
27.0	CH₂	oleyl/linoleyl
25.9	CH₂	oleyl/linoleyl
24.7-22.40	CH₂	all acyl chains
17.1-13.8	CH₃	all acyl chains

Table 2 - The ^{13}C chemical shift values found for the fish oil

δ (ppm)	Type of carbon	Type of compounds
177.1 – 177.2	C=O	triacylglycerols
171.1-172.5	C=O	triacylglycerols
131.5	CH=CH	oleic
129.6	CH=CH	oleyl
128.2-127.0	CH=CH	linoleyl
69.0-70.8	CH-OH	triacylglycerols
57.5-62.6	CH₂-OH	triacylglycerols
33.8-32.0	CH₂	all acyl chains
31.4-	CH₂	saturated chains
31.4-29.2	CH₂	all acyl chains
26.9-27.2	CH₂	oleyl/linoleyl
25.2	CH₂	oleyl/linoleyl
24.8-22.0	CH₂	all acyl chains
20.5-13.6	CH₃	all acyl chains

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