Application of advanced metabolomics methods for the determination of fatty acids in seeds oils

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CONCLUSION

The main advantage of the presented method is the **identification of oil sample by using NMR spectroscopy without carry out a transesterification reaction**. Analysis of fatty acid methyl esters (FAME) often leads to erroneous results. The **main problem** in the **analysis of CLnA is their stability and correct division**. Due to the **omitting derivatisation step**, approach with **NMR spectroscopy is faster** and **less laborius**. In contrast to GC-MS**, this methodology allows to investigate the structures of CLnA isomers**.

Fig. 4 Structure of punicic acid.

Fig. 5 Structure of α-calendic acid.

WHAT'S NEW ?

Use of **nuclear magnetic resonance (NMR) spectroscopy** to **identify** and **quantify fatty acids**, especially **conjugated isomers** of **α-linolenic acid (CLNAs)** in seeds oils. Most of researches at this topic use the **gas chromatography with mass spectrometry (GC-MS)**, but this methodology doesn't allow to separate and distinguish isomers. Therefore, **approach with NMR seems to be more suitable for invesigate the vegetable oils contain CLnA isomers**.

INTRODUCTION

Conjugated fatty acids (CFA) include **positional** and **geometric isomers** of **linoleic acid** and **α-linolenic acid**. These compounds occur naturally in **high concentration** in fats of **plant** origin. Scientific reports about CFA increasingly compare biological, chemical and physical properties between CLnA isomers. The fact that individual isomers exhibit different **biological activity is particularly important in the context of their effective use as potential pharmaceuticals**. Therefore, **it is important to correct identify the conformation of isomer** occur in the sample.

AIM

Aim of this work was to develop approach for identification CLnA isomers using two seeds oils: **pot marigold oil** and **pomegranate oil.**
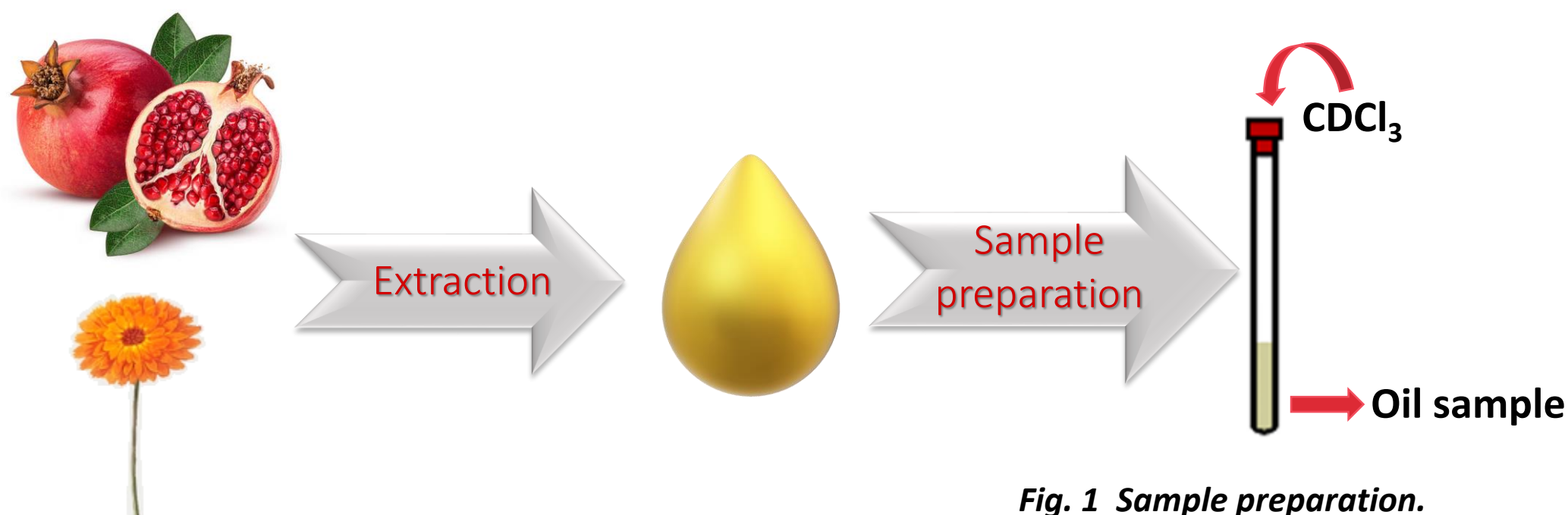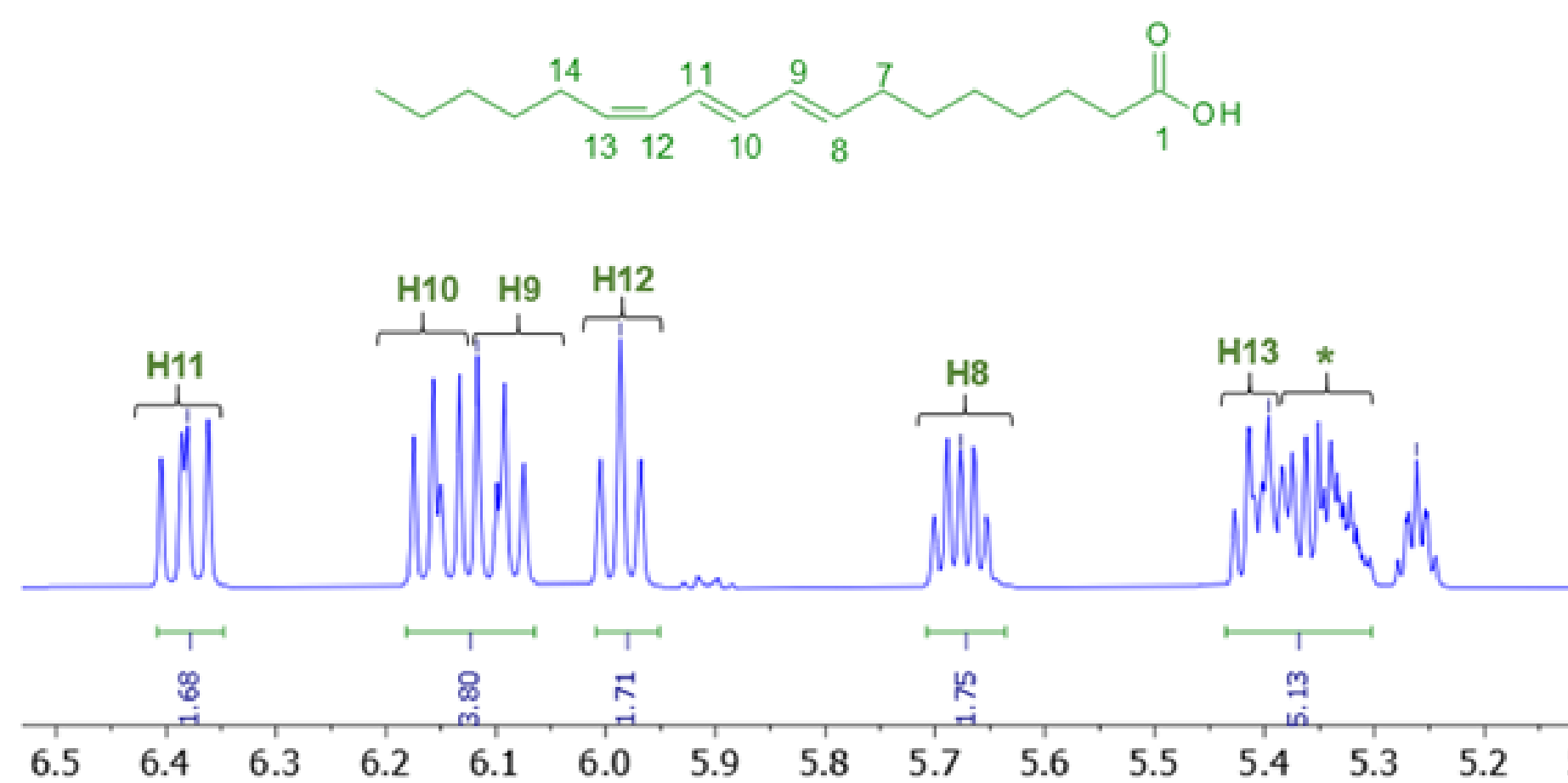
Fig. 1 Sample preparation.

MATERIALS & METHODS

- **Soxhlet extraction**

The seeds were grounded and extracted by **n-hexane** in Soxhlet apparatus **under inert atmosphere**. Then solvent was evaporated and obtained oil was stored at 4°C before analysis.

- **Sample preparation**

To 5mm NMR tube contain **10 µl of oil sample, introduced the 550 µl of deuterated chloroform and mixed**. The Spectrometer Bruker ULTRASHIELD™ PLUS AV2 was applied for analysis of the sample.

Fig. 2 ^{1}H NMR spectrum of the pot marigold seeds oil – CLnA isomers range.

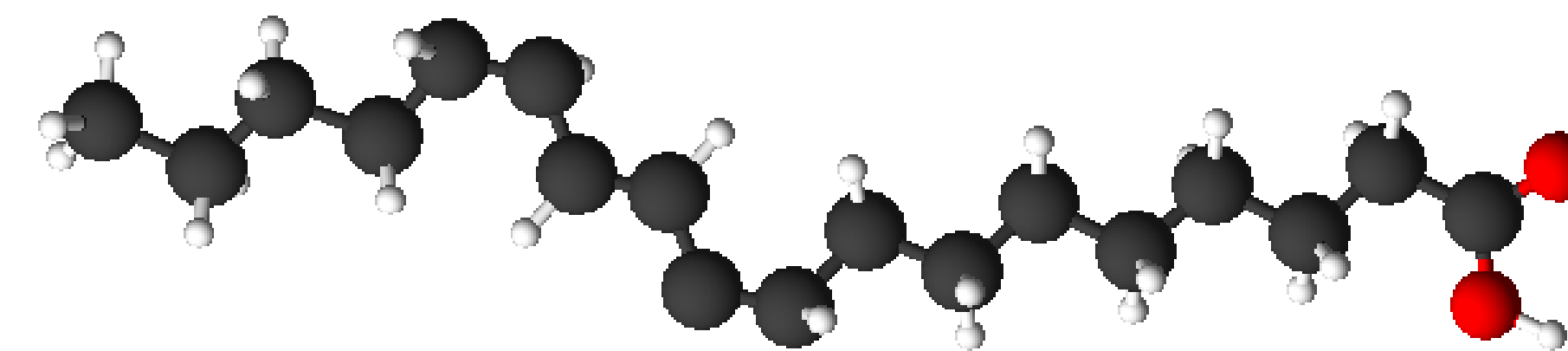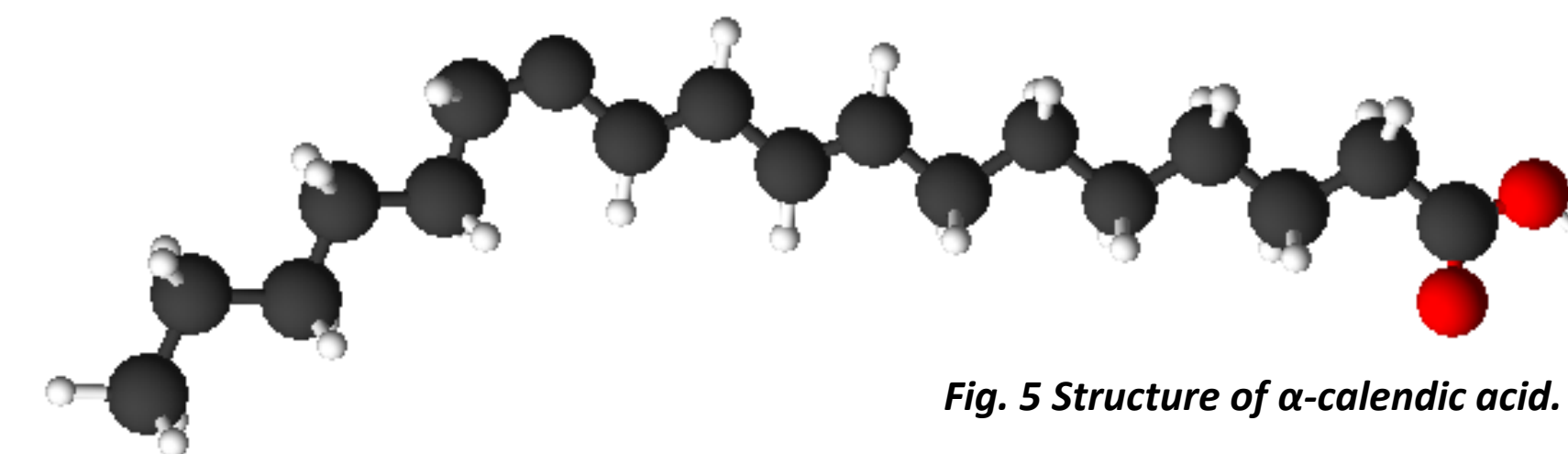*Fig. 3 ^{1}H NMR spectrum of the pomegranate seeds oil – CLnA isomers range.*

RESULTS

Fatty acids with **18 carbon atoms** are the **main group** in both investigated oils. Moreover, **CLNAs isomers are in high concentration**. It is characteristic for oils extracted from plants.

On both ^{1}**H NMR spectra analogous signals in the same chemical shifts are observed**. That's mean two oils contain the same fatty acids, for example **linoleic acid** and **oleic acid**, but **in different concentration**. In regions at range from **5,2 ppm** to **6,5 ppm signals from CLNAs isomers are observed** (**Fig. 2**, **Fig. 3**). Precise analysis of these regions allow to **determine the conformation of the present isomer**. In **pot marigold seeds oil** the main component is **α-calendic acid**, which occur in **58,67 %**. In **pomegarante seeds oil, punicic acid** is in the highest concentration – **79,5 %**.

POLSKIE TOWARZYSTWO METABOLICZNE

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