Molecular fingerprinting of a *Cannabis sativa* L. extract in medium-chain triglyceride (MCT) oil

UNIVERSITÀ DEGLI STUDI
DI MODENA E REGGIO EMILIA

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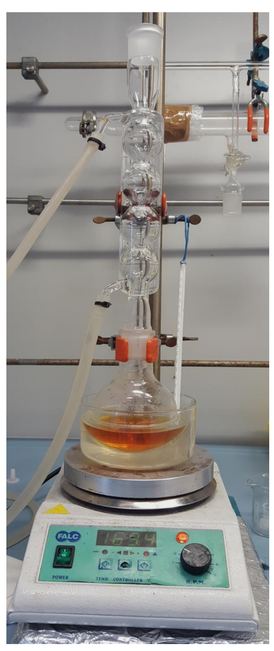


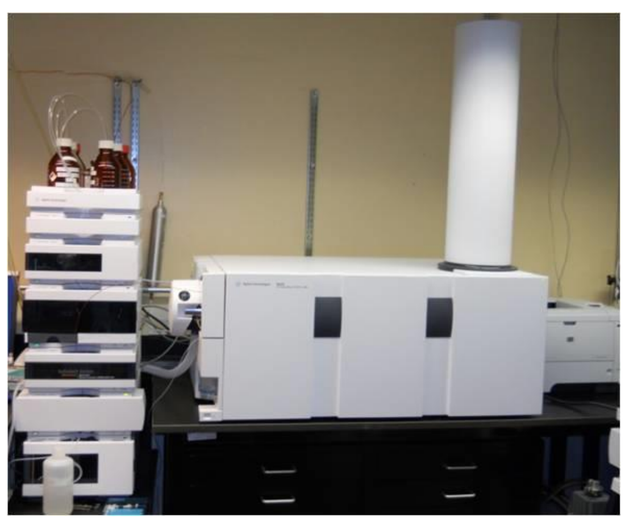
0 min

60 min

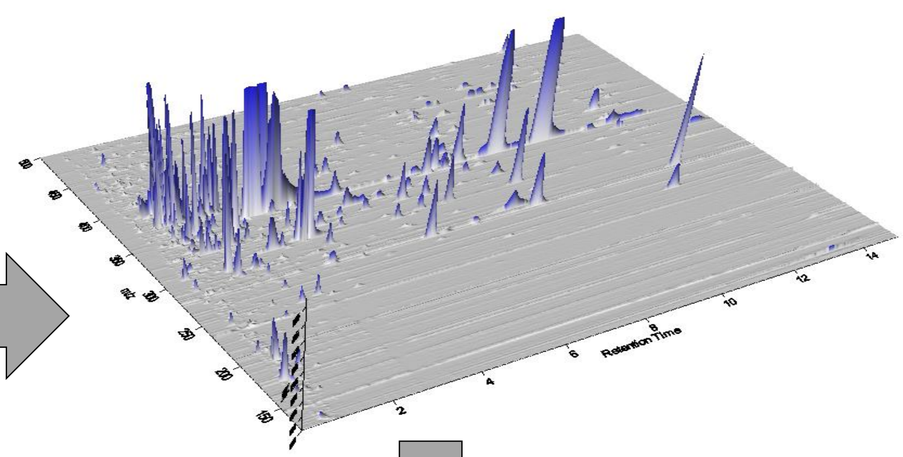
120 min

180 min

Reflux in MCT oil



Untargeted metabolomics
HPLC-ESI-QToF



Multivariate Statistical Analysis

Identified chemical structures

Arginine

Trigonelline

Choline

Proline

α-Linolenic acid

γ-Linolenic acid

Linoleic acid

Oleic acid

Cannabigerolic acid (CBGA)

Cannabidiolic acid (CBDA)

Tetrahydrocannabinolic acid (THCA)

Cannabigerol (CBG)

Cannabidiol (CBD)

Tetrahydrocannabinol (THC)

Cannabinol (CBN)

Cannabidivarin (CBDV)

Cannabidivarinic acid (CBDVA)

Cannabielsoin (CBE)

Cannabitriol (CBT)

Cannabiripsol (CBR)

Ethoxy-cannabitriolvarin (CBTVE)

10-Ethoxy-9-hydroxy-Δ6a-THC

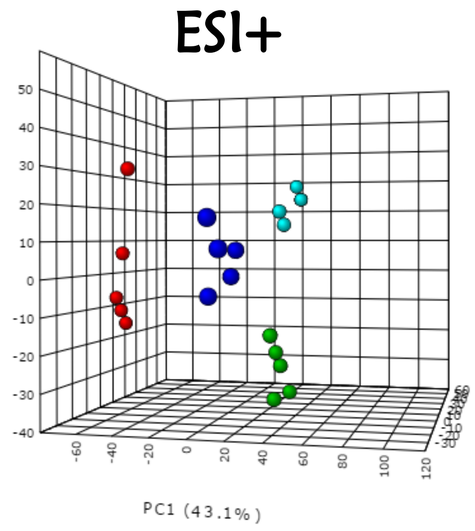
Cannabistilbene I

Canniprene

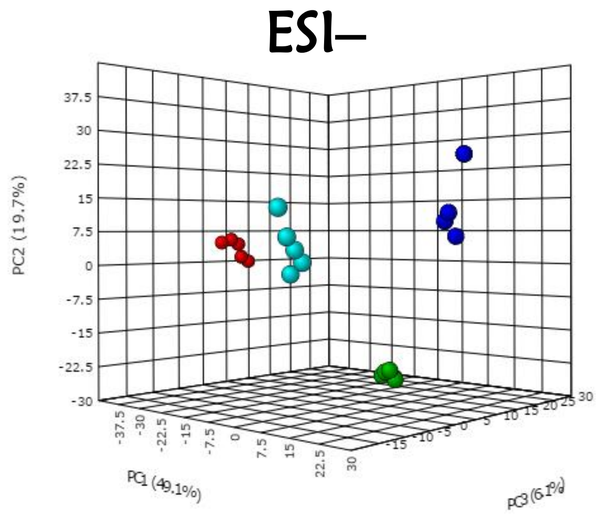
Cannaflavin A

Cannaflavin B

ESI+



ESI–



The complete characterization of the chemical composition of cannabis extracts represents a substantive challenge. In this context, an ***untargeted metabolomic approach*** and a multi-group comparison of the different extracts revealed significant variations of the extracted metabolites concentrations. The data obtained suggested that the extraction procedure dramatically affects the chemical composition of the cannabis medicinal extracts. When dealing with medicinal cannabis, which is intended for patients, it is important to know exactly the chemical content and the amount of each constituent of the final extract. A deeper investigation is required to identify the hundreds, if not thousands, of molecules comprised in the cannabis phytocomplex. Our ongoing studies are devoted to the identification of a greater number of interesting and pharmacologically active molecules. The results obtained suggested that, notwithstanding the use of a **standardized starting plant material**, there is the urgent need to develop and **standardize an extraction protocol** in order to produce every time a known amount of cannabinoids and other bioactive molecules

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Keywords: cannabis, medium-chain triglyceride oil, molecular fingerprinting, liquid chromatography, high-resolution mass spectrometry.

Cannabis sativa L. is a powerful medicinal plant and its use has recently increased for the treatment of several pathologies [1-4]. Moreover, cannabis products, spanning from cosmetics to food, have recently regained much attention due to their high pharmacological and nutritional potential [5]. The chemical composition of *Cannabis sativa* L. extracts has already been explored in several studies, but they were mainly focused on phenotype and cultivar distinction [6]. In this study, a high performance liquid chromatography coupled to tandem high-resolution mass spectrometry (HPLC-HRMS/MS) method has been employed for the evaluation of the chemical composition of a cannabis extract in medium-chain triglyceride (MCT) oil. HPLC-HRMS/MS data were processed and analysed with a single-job by XCMS Online web platform (https://xcmsonline.scripps.edu) and the most abundant metabolites were identified using authentic standards or METLIN online database (https://metlin.scripps.edu).

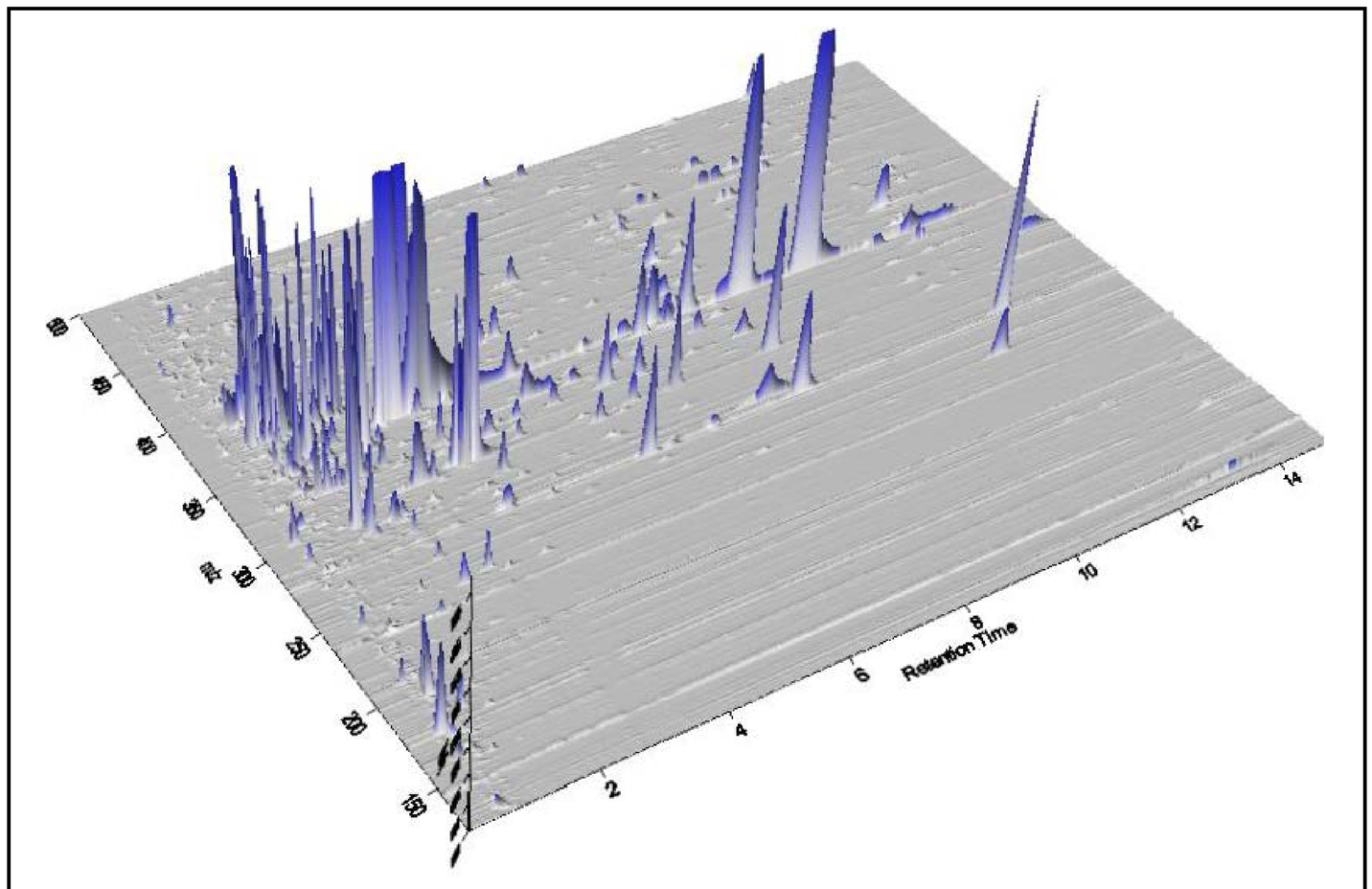

Figure 1. HPLC-HRMS 3D Total Ion Chromatogram of MCT oil extract in positive ionization mode indicates the chemical complexity. The retention time (min) is represented on the *x* axis, the peak intensity (ion counts) on the *y* axis and the m/z values on

[1] Borgelt L.M. *et al.*, *Pharmacotherapy: The Journal of Human Pharmacology and Drug Therapy* **2013**, *33* (2), 195-209.
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