



## TITLE

### Analytical tools in viticulture, agri-food and forensic chemistry

## LAB & PEOPLE

- Name of the hosting lab: AGR291
- General activities of the lab:
  - Development and application of separation and spectroscopic methods of interest in wine, food and forensic chemistry
  - Automation of sample preparation and interpretation of analytical results
  - New methods for characterization and detection of food fraud
  - Advanced methods for determining food components of interest and materials used in their production and preservation
  - Use of waste and by-products from the agri-food industry
  - Evaluation of new techniques for the preparation of alcoholic beverages
  - Quality in analytical laboratories
  - Machine learning techniques in analytical sciences
- Website: agr291.uca.es
- Number of staff / PhD: 9/8
- Supervisor name and contact: María José Aliaño González ([mariajose.aliانو@gm.uca.es](mailto:mariajose.aliانو@gm.uca.es))

## TOPIC OF THE INTERNSHIP

- Scientific context of the internship (max 20 lines)

### **Characterization of raw materials, food and derivatives based on machine learning techniques**

In recent years, there have been important advances in consumer awareness of the processes carried out in the agri-food industry and the generation of by-products during these processes. In the case of industrial processes, the increase in society's knowledge about biotic and abiotic contaminants, microorganisms or adulterations and their important health consequences has led many users to become aware of the quality of the products purchased.

This line proposes the use of green chemistry techniques that have been widely and successfully used in other fields such as medicine, forensic chemistry or environmental sciences to be applied in the agri-food industry. These methods are characterized by the fact that they do not require the use of chemical solvents, do not generate waste and have minimal gas and energy

consumption. Some of the techniques combined with chemometric tools have demonstrated their great utility to be applied in the agri-food field in the detection, discrimination and quantification of adulterations in honeys, coffee and palm oil samples, proving their application in quality control in a fast, simple and reliable way.

Machine learning is a subfield of artificial intelligence that "gives computers the ability to learn without being explicitly programmed". Machine learning seeks to develop an algorithm based on the data used to create a model that can solve a problem or hypothesis. Therefore the combination of sensitive and green chemistry analytical techniques with machine learning-based techniques, will allow for analytical tools to the characterization of agri-food products and by-products helping to the detection of new functional food products, or the detection of fraud products as adulteration.

The student will be trained in a specific analytical technique to be applied in the solution of analytical problems and characterization study.

### **Keywords**

Analytical chemistry, food characterization, food frauds, wine production, fire debris analysis, machine learning.

### **Bibliography**

Our full scientific production can be found at :

<https://produccioncientifica.uca.es/grupos/8272/publicaciones>

Our most recent 20 papers are the following ones :

## **2023**

1. [The effect of ripening on the capsaicinoids composition of Jeromin pepper \(\*Capsicum annuum\* L.\) at two different stages of plant maturity](#)  
Food Chemistry, Vol. 399
2. [Sulfur dioxide-free Verdejo wines through the use of a pure stilbene extract: exploring possible synergistic effect with glutathione](#)  
Journal of the Science of Food and Agriculture, Vol. 103, Núm. 3, pp. 1152-1160
3. [Response Surface Methodology Optimization for Analytical Microwave-Assisted Extraction of Resveratrol from Functional Marmalade and Cookies Foods](#), Vol. 12, Núm. 2
4. [Optimizing an Enzymatic Extraction Method for the Flavonoids in Moringa \(\*Moringa oleifera\* Lam.\) Leaves Based on Experimental Designs Methodologies](#)  
Antioxidants, Vol. 12, Núm. 2

5. Optimization of a New Ultrasound-Assisted Extraction Method of Caffeic Acid from the Aerial Parts of *Coriandrum sativum* by Using Experimental Design and Ultra-Performance Liquid Chromatography  
Separations, Vol. 10, Núm. 2
6. Optimization of a Microwave-Assisted Extraction Method for the Recovery of the Anthocyanins from Jabuticaba By-Products  
Agronomy, Vol. 13, Núm. 2
7. Grapevine shoots extract as an alternative to SO<sub>2</sub> in rosé wines. A double approach: Classical measurements and <sup>1</sup>H NMR metabolomics  
Food Control, Vol. 152
8. Capsaicinoid Content in the Pericarp and Placenta of Bolilla Peppers (*Capsicum annuum* L.) throughout the Ripening of the Fruit at Two Different Stages of Plant Maturation  
Agronomy, Vol. 13, Núm. 2
9. A Rapid Method for Authentication of Macroalgae Based on Vis-NIR Spectroscopy Data Combined with Chemometrics Approach  
Water (Switzerland), Vol. 15, Núm. 1

## 2022

1. Ultrasound-Assisted Extraction of Polyphenols from Maritime Pine Residues with Deep Eutectic Solvents  
Foods, Vol. 11, Num. 23
2. Total Ion Chromatogram and Total Ion Mass Spectrum as Alternative Tools for Detection and Discrimination  
Chemosensors, Vol. 10, Num. 11
3. Ultrasound-Assisted Extraction of Betalains from *Opuntia* Fruit Pulp of Different Color Varieties  
Agronomy, Vol. 12, Num. 11
4. Optimization of an Enzyme-Assisted Extraction Method for the Anthocyanins Present in Açai (*Euterpe oleracea* Mart.)  
Agronomy, Vol. 12, Num. 11
5. Assessment of Volatile Compound Transference through Firefighter Turnout Gear  
International Journal of Environmental Research and Public Health, Vol. 19, Num. 6
6. Sulfur dioxide-free Verdejo wines through the use of a pure stilbene extract. Exploring possible synergistic effect with glutathione  
Journal of the Science of Food and Agriculture

7. **Ultrasound-Assisted Extraction of Total Phenolic Compounds and Antioxidant Activity in Mushrooms**  
Agronomy, Vol. 12, Num. 8
  8. **Machine learning approaches over ion mobility spectra for the discrimination of ignitable liquids residues from interfering substrates**  
Talanta, Vol.6
  9. **Microwave-assisted extraction of non-coloured phenolic compounds from grape cultivars**  
European Food Research and Technology
  10. **Wood Waste from Fruit Trees: Biomolecules and Their Applications in Agri-Food Industry**  
Biomolecules, Vol. 12, Num. 238
  11. **A comparison study between ultrasound–assisted and enzyme–assisted extraction of anthocyanins from blackcurrant (*Ribes nigrum* L.).**  
Food Chemistry X, Vol. 13, Num. 100192
- Tasks and duties entrusted to the student:
    1. To prepare a research proposal based on the literature provided by the supervisor (1-2 weeks)
    2. To run a training period in the lab (2-3 weeks) with the supervisor and the technicians
    3. To develop the research proposal (2-6 months)
    4. To prepare 3 reports :
      - a. Initial report including the research proposal
      - b. Intermediate report including information about the training period and the starting results from the training period
      - c. Final report including
        - i. All data obtained from the intership period
        - ii. Critical evaluation of the data, including the data analysis
        - iii. A draft of a manuscript to be evaluated by the supervisor. In case the results are excellent it will be proposed to be prepared for a scientific publication
  - Skills to be acquired or developed:
    - Experience in research duties
    - Training in specific analytical procedures
    - Training in data analysis

## **PROFILE OF THE DESIRED STUDENT**

- Minimum level of study required: Running a master degree
- Field(s) of study: chemistry, food or environmental studies
- Scientific skills : basic experience in labs
- Language skills required : English

## **THE INTERNSHIP ASSIGNMENT:**

Desired duration of the internship (in months): 5 months

Desired Starting date of the mission: *Any time between January 2024 to June 2024 to be finished by July 2024*

Indicative weekly schedule: *35h / week*

Remuneration : *No*

Internship agreement: *an internship agreement will be signed.*

*To SEA-EU students:*

*If you're interested please send your CV and letter of motivation to the scientist in charge, email : [mariajose.aliانو@gm.uca.es](mailto:mariajose.aliانو@gm.uca.es)*