2023 Master internship at University of Cádiz

TITLE

FORENSIC CHEMISTRY

Research group- AGR 291-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: Marta Ferreiro González (marta.ferreiro@uca.es) / +34657961915

TOPIC OF THE INTERNSHIP

- Scientific context of the internship (max 20 lines)

We offer internship positions related to the following research line: **Forensic Chemistry.**

This research line includes the development of fast and green analytical methods for the charaterization of samples of forensic interest. The student will be trained in a specific spectroscopic technique (NIRS, FT-IR or electronoic noses) in combination with machine learning and chemometric tools for the characterization of samples of forensic interests such as fire debris, adulterated foodstuff, oil spills, combustion residues, human scent ...

The student will collaborate in the following tasks:

- Preparation of samples of interest in Forensic Chemistry. This includes: simulation of samples of fire debris, fuel adulteration, food adulteration or other types of samples that need to be created and cannot be acquired.
- Development and optimization of analytical methods for the identification of samples of interest.
- Development of fingerprints through the application of chemometric techniques or machine learning) of the different samples for the rapid and automated identification of suspicious samples.
- Interpretation of the results.

Keywords

Analytical Chemistry; Forensic Chemsitry ;Food Frauds, Fire debris analysis ; Food adulteration ; Spectroscopic Techniques ; Electronic nose ; Machine Learning ; Chemometrics ; Green Chemistry.

Bibliography

My full scientific production can be found at :
https://produccioncientifica.uca.es/investigadores/112519/publicaciones

My ***20 most recent JCR articles related to the proposal*** are as follows:

1. Application of Direct Thermal Desorption–Gas Chromatography–Mass Spectrometry for Determination of Volatile and Semi-Volatile Organosulfur Compounds in Onions: A Novel Analytical Approach. (2023) Pharmaceuticals, 16 (5), art. no. 715, .DOI: 10.3390/ph16050715.
2. Machine learning approaches over ion mobility spectra for the discrimination of ignitable liquids residues from interfering substrates.(2022) Talanta Open, 6, art. no. 100125, DOI: 10.1016/j.talo.2022.100125
3. Optimization through a Box–Behnken Experimental Design of the Microwave-Assisted Extraction of the Psychoactive Compounds in Hallucinogenic Fungi (Psylocibe cubensis).(2022) Journal of Fungi, 8 (6), art. no. 598. DOI: 10.3390/jof8060598
4. Rapid Detection and Quantification of Adulterants in Fruit Juices Using Machine Learning Tools and Spectroscopy Data. (2022) Sensors, 22 (10), art. no. 3852, . DOI: 10.3390/s22103852
5. Detection of Adulterations in Fruit Juices Using Machine Learning Methods over FT-IR Spectroscopic Data. (2022) Agronomy, 12 (3), art. no. 683.DOI: 10.3390/agronomy12030683
6. Assessment of Volatile Compound Transference through Firefighter Turnout Gear (2022) International Journal of Environmental Research and Public Health, 19 (6), art. no. 3663. DOI: 10.3390/ijerph19063663
7. Comparison of different processing approaches by SVM and RF on HS-MS eNose and NIR Spectrometry data for the discrimination of gasoline samples. (2022) Microchemical Journal, 172, art. no. 106893, DOI: 10.1016/j.microc.2021.106893

8. A methodology based on ft-ir data combined with random forest model to generate spectralprints for the characterization of high-quality vinegars. (2021) Foods, 10 (6), art. no. 1411, . DOI: 10.3390/foods10061411
9. A novel method based on headspace-ion mobility spectrometry for the detection and discrimination of different petroleum derived products in seawater. (2021) Sensors, 21 (6), art. no. 2151, pp. 1-16. DOI: 10.3390/s21062151
10. Discrimination of ignitable liquid residues in burned petroleum-derived substrates by using HS-MS eNose and chemometrics. (2021) Sensors (Switzerland), 21 (3), art. no. 801, pp. 1-12. DOI: 10.3390/s21030801
11. Characterization of biodegraded ignitable liquids by headspace-ion mobility spectrometry. (2020) Sensors (Switzerland), 20 (21), art. no. 6005, pp. 1-11. DOI: 10.3390/s20216005
12. Development of a methodology based on headspace-gas chromatography-ion mobility spectrometry for the rapid detection and determination of patin fish oil adulterated with palm oil. (2020) Arabian Journal of Chemistry, 13 (10), pp. 7524-7532. DOI: 10.1016/j.arabjc.2020.08.026
13. Novel method based on ion mobility spectroscopy for the quantification of adulterants in honeys. (2020) Food Control, 114, art. no. 107236 . DOI: 10.1016/j.foodcont.2020.107236
14. Characterization of Arabica and Robusta coffees by ion mobility sum spectrum. (2020) Sensors (Switzerland), 20 (11), art. no. 3123 . DOI: 10.3390/s20113123
15. A screening method based on Visible-NIR spectroscopy for the identification and quantification of different adulterants in high-quality honey. (2019) Talanta, 203, pp. 235-241. DOI: 10.1016/j.talanta.2019.05.067
16. Novel method based on ion mobility spectrometry sum spectrum for the characterization of ignitable liquids in fire debris. (2019) Talanta, 199, pp. 189-194. DOI: 10.1016/j.talanta.2019.02.063
17. A screening method based on headspace-ion mobility spectrometry to identify adulterated honey. (2019) Sensors (Switzerland), 19 (7), art. no. 1621, . DOI: 10.3390/s19071621
18. FT-IR, Vis spectroscopy, color and multivariate analysis for the control of ageing processes in distinctive Spanish wines. (2019) Food Chemistry, 277, pp. 6-11. DOI: 10.1016/j.foodchem.2018.10.087
19. Escape ClassRoom: Can You Solve a Crime Using the Analytical Process?. (2019) Journal of Chemical Education, 96 (2), pp. 267-273. DOI: 10.1021/acs.jchemed.8b00601
20. Interpreting the near infrared region of explosives. (2018) Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 204, pp. 81-87. DOI: 10.1016/j.saa.2018.06.002

- 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´s degree

- Field(s) of study: chemistry, food, forensics or environmental studies

- Scientific skills : basic experience in labs

- Language skills required : English

THE INTERNSHIP ASSIGNMENT:

Desired duration of the internship (in months): 3-6 months

Desired Starting date of the mission: Any time between September 2023 to March 2024 to be finished by July 2024

Indicative weekly schedule: *35h / week*

Remuneration *? no*

Erasmus grant ? no

This internship will receive finacial support from Erasmus+

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, marta.ferreiro@uca.es before November 2023