

PROPOSAL OF DOCTORAL PROJECT 2022-2025

New analytical developments for metabolomics and annotation of dyeing plant extracts: Applications in a cultural heritage context

Context of the proposal

As part of a collaboration between the UMR "Mediterranean Institute of marine and terrestrial Biodiversity and Ecology (IMBE)", IRPNC team (<https://www.imbe.fr/ingenierie-de-la-restauration-des.html>) and the UMR "Safety and Quality of Plant Products (SQPOV)", MicroNut team (<https://www6.paca.inrae.fr/sqpov/Equipes-Personnes/MicroNut>), as well as the 3A analytical platform of Avignon University, we are looking for a candidate wishing to carry out a doctoral thesis linking metabolomics, chemistry of natural products and archaeometry.

This PhD thesis is **submitted to the competition** on a doctoral contract funded by the Implanteus Graduate School (<https://implanteus.univ-avignon.fr/>) and is part of the final selection (<https://univ-avignon.fr/recherche/le-doctorat/je-souhaite-preparer-un-doctorat-27687.kjsp>) counting only 2 subjects. The defense for the competition will take place at Avignon University on June 2, 2022.

The success of the competition would make it possible to initiate this doctoral contract, which would then begin between September and December 2022 for a period of 3 years.

Description of the project

This doctoral project will aim to:

- 1) establish a complete metabolomic workflow by LC-HRMS involving the implementation of an annotation step using molecular networks and apply it to a wide range of dyeing plants representative of the chemical diversity of coloring molecules (e.g., flavonoids, anthocyanins, anthraquinones, indigoids...). This workflow will be developed in close collaboration with the 3A platform. The IMBE-IRPNC laboratory already holds many reference samples related to natural dyes (plant extracts, chemical standards). A collaboration will also be implemented with the "Jardin des plantes tinctoriales de Lauris (Vaucluse, France)", which has more than 250 different species of dyeing plants and the association "Couleur Garance", which aims to promote plant dyes and their applications.
- 2) develop a methodology to anticipate the behavior of natural coloring substances by *in silico* metabolization and apply it to the experimental study of the stability of extracts and molecules of selected dyes. To this end, different degradation mechanisms (as a function of pH and temperature) and interactions (e.g., with phenolic copigments, metal ions) will be considered and compared to the ancient applications of these dye extracts.
- 3) the search for characteristic dye chemomarkers in the field of cultural heritage, as the identification of natural dyes contained in historical samples could make it possible to decipher ancestral dyeing recipes. In addition, such studies are necessary for the documentation of artworks and can be decisive for the development of effective and appropriate conservation strategies. Various samples (textiles, votive objects...) will be selected from the regional, national and international collaborations of the IMBE-IRPNC team.

Competences expected

We look for a talented student with a completed MSc. Degree in (bio)chemistry. The PhD student has a demonstrated track record of excellence in analytical (bio)chemistry and has extensive practical and theoretical experience in at least two of the following three areas:

- liquid chromatography and high-resolution mass spectrometry,
- structural characterization of natural products,
- metabolomics, data analysis and chemometrics.

The PhD student will acquire in-depth knowledge in the field of natural plant dyes (plant physiology, chemistry, dyeing processes) and in cultural heritage chemistry. He/she will learn to answer scientific questions using a variety of approaches and methods.

The PhD student will have to develop ability to work in team, rigor, enthusiasm, organization, together with strong oral and written communication skills.

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