**Project proposal**

*Objective*

The proposed Project aims at developing untargeted and multiplatform analytical approaches in two main research contexts: food and environment. The link between the two is sustainability. In food research salient aspects are on one hand supporting local high-quality food production to reduce environmental impact and promote economy also in disadvantages areas, such as mountain and on the other one, to recover as much as possible agrifood production waste. As for environment, a very critical issue is nowadays preserving water resource, monitoring and preventing contamination as well as enhancing its reuse, according to the circular economy principles, highlighted in Agenda 2030. To guarantee a safety reuse of reclaimed wastewater, it is of utmost importance to implement control systems of inorganic and emerging contaminants presence, since these chemicals may be dangerous for the environment and human health. These fields share the need for reliable analytical techniques capable, given the complexity of the matrices to be studied, to provide a full characterization of the investigated systems. Thus, I would like to adopt a holistic approach, beyond the traditional chemical analysis and characterization, which focuses mainly on single classes of constituents. Consequently, the preferred analytical techniques will be those furnishing one hand a complete compositional profile, such as chromatography mass spectrometry, NMR and on the other hand, a quick to acquire but unique fingerprint, such as fast non-destructive spectroscopy. The preferred approach is untargeted analysis of the responses which does not require a priori knowledge of the analytes to be sought. Here comes into play chemometrics which is fundamental to unravel the distinctive compositional traits from these complex responses or to speed up the resolution and putative identification process in hyphenated chromatographic techniques.

*Possible methods*

*Experimental*

For developing untargeted and multiplatform analytical approaches in a sustainable context, it is important to adopt a systematic study based on representative samples (in terms of number, sampling sites and seasonality) and different analysis techniques coupled to multivariate data analysis. Sampling plays a crucial role influencing the results reliability and models robustness. In this respect, I would like to explore the capability of an innovative sampling approach, Polar Organic Chemical Integrative Samplers (POCIS), for the monitoring of emerging contaminants (industrial and agricultural additives, personal care products and pharmaceuticals). This sampling approach meets some of the principles recently proposed for green sample preparation, including the reduction of energy consumption and solvents use. To learn about this sampling typology, I would like to spend at least one month at Prof. Magi research group, University of Genoa, that have a consolidated experience in the use of these devices in many applications. Furthermore, since profiling/fingerprinting volatile organic compounds (VOCs) combined with multivariate statistical methods also offers a large potential in food and environmental sustainability, I would like to deepen some aspects regarding volatilomics approach. Isolation of volatile compounds from the food and environmental matrices is a challenging task and, thanks to the expertise acquired during my master thesis, I would like to test a Solid Phase Micro-Extraction (SPME)-Arrow based methodology, which is a new green chemistry extraction technology, to define a fingerprint of the complex investigated matrices.

*Data analysis*

The multivariate approach could furnish proper tools to approach the theme. Starting from the planning of data collection, optimization of the analytical preparative and instrumental methodologies, data pre-processing, through the elaboration, to conclude with an effective graphical representation of the results and effective way to share the modelling results with the end-users. In this respect, I would like to learn and exploit the more recent areas such as Data Fusion and recent multiblock methods, in addition to automatic

resolution and putative identification tools based on multiway, as Paradise, and multivariate curve resolution methods, as MCR-ROI.

*Expected outcomes*

At the end of the research project the idea is to have proper guidelines and practitioners' toolboxes to find the best way to approach data fusion of untargeted data from multiplatform analytical techniques. With respect to the specific research themes to be afforded they could be: (i) developing authenticity models to assess mountain product authenticity and quality models for bakery products; (ii) accomplish a feasibility study for the re-use of waste from food production chains, such as pasta, bread or sauces (in collaboration with Barilla company) and (iii) monitoring of emerging chemicals in waste water and proposing possible re-use in hydroponic cultures (in collaboration with Hera and DSV research groups).