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**Title**: ‘Beyond metabolomic imprint; towards comprehensive identification in metabolomics’ (Más allá de la huella metabolómica; hacia la identificación exhaustiva en metabolómica)

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**Summary:**

Metabolomics can be considered a discipline with standardised protocols to obtain more information about the complete set of metabolites in an organism under particular conditions. However, characterisation is not yet complete. In a typical non-targeted metabolomics study, more than 50% of the signals corresponding to a molecular entity remain unidentified.

As an overall objective of the present project, we hope to increase the number of metabolites identified, thus improving specific points of the methodology. In addition, we aim to achieve a better understanding of the metabolic processes involved.

We aim to reach this objective through six specific actions:

1. Expanding GC-MS identification abilities.

Full characterisation of biological samples with authentic standards and reference materials, as well as low-energy source GC-QTOF-MS, will expand our metabolite libraries. Among these metabolites, those related to the gut microflora, which may involve a complex interaction and interrelationship between the immune system, the endocrine system and even the Central Nervous System, will form part of the previously unidentified compounds. New methodologies for sample handling and for volatile compounds, in addition to working with an alternative ionisation source, will allow us to create a more detailed and complete database of compounds.

1. Expanding CE-MS identification abilities.

The implementation of new methods for the analysis of neutral and anionic compounds, together with the source fragmentation strategy in CE-MS, will allow us to add new records to the database of identified compounds. Among the metabolites that could be identified with CE-MS, potential epi-metabolites, i.e. identified compounds that could be associated with simple metabolic processes such as methylation and acetylation, will be integrated into the biological interpretation of the processes involved in different biological processes.

1. Expansion of LC-QTOF-M identification abilities

Lipids are still under-represented in databases, and this lack of records is even greater when it comes to oxidised lipids. We plan to expand our knowledge of these compounds, through advanced analytical strategies for purification and structural elucidation, combined with work with the CEU Mass Mediator (CMM).

1. Expansion of identification capabilities by LC-QqQ-MS

 In addition, differentiation of chiral compounds by advanced analytical strategies will expand the number of processes that could be elucidated. Different strategies: the labelling agent and separation conditions will be optimised to establish the defined chiral metabolomics method to be applied at CEMBIO.

1. Development of CMM, CEU Mass Mediator <http://ceumass.eps.uspceu.es/mediator/>

We have worked hard on the CMM, and plan to continue working on this tool, adding more capabilities, such as spectral quality assessment. In addition, better ways of integrating data from different instrumental and omics platforms will be explored.

1. Applications

In the previous years, CEMBIO has been able to establish a wide network of collaborators, and the application of the metabolomics workflow already implemented to different studies: CVD, obesity, diabetes, neurodegenerative diseases, etc.