

# Metabolites identification in non-targeted metabolomics approches multi-analytical mass spectrometry platform view

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### Introduction

Non-targeted metabolomics approaches include various steps, among these, structural elucidation of metabolites of interest still remains important bottleneck [1]. To facilitate metabolite identification, an in house-LC-HRMS database containing information about chromatographic retention time, accurate mass and fragmentation pattern, using ACD/Labs software, has been developed [2]. In addition, an automatic Excel® macro to help filtering and allowing a fast and direct annotation of compounds in the XCMS table has been elaborated. Nevertheless, these criteria are not always sufficient for unequivocal identification being the use of other analytical and complementary techniques necessary. As a result, a multi-analytical platform based on both LC-HRMS using the complementarities of reversed phase and HILIC separations, and GC-MS has been developed for a comprehensive metabolome and lipidome characterization, coupled to an in-house reference database [3].

### Metabolites identification & automatic annotation



#### Conclusion

Correct assignment of chemical identities to signals generated by MS based metabolomic approaches is a pre-requisite for any scientific outcome. Therefore, raw data have to be correctly processed through properly developed scripts and identification of revealed markers must become high-throughput. Indeed, the development of an experimental spectral database greatly facilitates metabolite identification based on retention time, accurate mass and fragmentation pattern. However, this spectral database will be continuously completed to increase the number of metabolites. On the other hand, the use of a

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