Development of innovative analytical methods based on the omics sciences for the characterization of structurally related classes of compounds in complex matrices

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Abstract

In the latest years, the development of high-resolution mass spectrometry (HRMS) instrumentation has smoothed the path in many undisclosed directions in the field of omics sciences. HRMS, in fact, has allowed projecting untargeted approaches, in which previous knowledge on the analytes is not required, leading to the discovery of unexpected or still unknown compounds of interest. In the development of untargeted strategies in the field of omics sciences, there are several troubles to face: wide dynamic range intervals, uneven method performances for structurally diverse classes of compounds, the need for data processing software programs for raw data management, and the need for spectral libraries and manual validation for compound identification[1]. In this context, strategies aimed at structurally related classes of compounds, with homogeneous physicochemical properties, provide several advantages and higher performances. Sample pretreatment is of crucial importance when dealing with complex matrices, for removing interferences and concentrating analytes present in trace amounts. Data acquisition is the core of any analytical method, and HRMS techniques offer a wide range of different approaches, i.e., direct infusion, flow injection, LC-MS, full-scan acquisition, data-dependent acquisition, and data-independent acquisition[2]. Finally, data processing and compound identification have become critical as soon as untargeted HRMS approaches have been spreading. The large raw dataset obtained by HRMS analysis, in fact, cannot be handled without the use of specific software programs which extract the m/z, group the adducts, align the peaks, predict the elemental compositions, and remove compounds present in the background. Extracted data are not only highly dependent on the instrumental conditions but also on the algorithms and parameters of the chosen data processing workflow. Moreover, online MS databases are needed for associating extracted features to existing compounds. Whenever a deep and detailed characterization of structurally related classes of compounds is needed, default data processing workflows and generic MS databases are not sufficient. In the course of the seminar, several analytical approaches intervening in the sample pretreatment step, data acquisition step, and data processing step are discussed. In particular, several case studies will be reported for highlighting different crucial aspects, i.e., short-chain peptides[3,4], phytocannabinoids[5], and phosphocholine-containing lipids.

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