Automation of mass spectrometric detection of analytes and related workflows: A review

Decibel P. Elpa,b, Gurpur Rakesh D. Prabhu,a,b, Shu-Pao Wua,*, Kheng Soo Tayc, Pawel L. Urbanb,d,*

a Department of Applied Chemistry, National Chiao Tung University, 1001 University Rd., Hsinchu, 300, Taiwan
b Department of Chemistry, National Tsing Hua University, 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan
c Department of Chemistry, Faculty of Science, University of Malaya, 50603 Kuala Lumpur, Malaysia
d Frontier Research Center on Fundamental and Applied Sciences of Matters, National Tsing Hua University, 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan

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ABSTRACT

The developments in mass spectrometry (MS) in the past few decades reveal the power and versatility of this technology. MS methods are utilized in routine analyses as well as research activities involving a broad range of analytes (elements and molecules) and countless matrices. However, manual MS analysis is gradually becoming a thing of the past. In this article, the available MS automation strategies are critically evaluated. Automation of analytical workflows culminating with MS detection encompasses involvement of automated operations in any of the steps related to sample handling/treatment before MS detection, sample introduction, MS data acquisition, and MS data processing. Automated MS workflows help to overcome the intrinsic limitations of MS methodology regarding reproducibility, throughput, and the expertise required to operate MS instruments. Such workflows often comprise automated off-line and on-line steps such as sampling, extraction, derivatization, and separation. The most common instrumental tools include autosamplers, multi-axis robots, flow injection systems, and lab-on-a-chip. Prototyping customized automated MS systems is a way to introduce non-standard automated features to MS workflows. The review highlights the enabling role of automated MS procedures in various sectors of academic research and industry. Examples include applications of automated MS workflows in bioscience, environmental studies, and exploration of the outer space.

1. Introduction

Mass spectrometry (MS) is an analytical technique with colorful past and bright future. Since the discovery of electron by Thomson [1], and construction of the early prototypes of mass spectrometers by Aston [2], there has been enormous progress in the theory, instrumentation, and applications of MS [3–5]. Nowadays, mass spectrometrists capitalize on the technique’s virtues, and implement it in discovery-oriented research as well as routine analyses in the areas of clinical, food, environmental chemistry, and beyond. The important features of MS include high sensitivity that enables detection of molecules at low concentrations or in confined samples [5], high resolution that enables identification of molecules by matching their m/z or comparing fragmentation patterns [7,8], quantitative capabilities that allow one to report on the concentrations of analytes in real samples [9], and high speed of analysis that permits monitoring fast processes or increases analytical throughput [5].

Automation plays a central role in modern analytical laboratories [10–22]. The proliferation of automated analytical systems has been sustained due to the developments in microcomputer technology. In many cases, automated MS systems are simple expansions of generic automated systems, which integrate a mass spectrometer instead of an optical detector. MS augments the automated analytical methods by ensuring high selectivity. Certainly, the automated MS systems are characterized with higher throughputs than those obtained with manual sample introduction systems. Automation allows analysts to perform multiple and remote sample processing operations for MS detection of analytes. The automated MS systems have an enabling potential in various science disciplines. This review provides an evaluation of the main achievements in automation of MS detection of analytes and various related workflows. First, we define the concepts related to automation in MS workflows. Second, we discuss different steps of analytical workflows involving MS, where...

* Corresponding author. Department of Chemistry, National Tsing Hua University, 101, Section 2, Kuang-Fu Rd., Hsinchu, 30013, Taiwan.
** Corresponding author. Department of Applied Chemistry, National Chiao Tung University, 1001 University Rd., Hsinchu, 300, Taiwan.
E-mail addresses: spwu@mail.nctu.edu.tw (S.-P. Wu), urban@mx.nthu.edu.tw (P.L. Urban).

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