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Emerging Trends in Gas Chromatography and Mass Spectrometry Instrumentation for Analytical & Bioanalytical Techniques

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Description

Innovations in Gas Chromatography (GC) and Mass Spectrometry (MS) instrumentation from a variety of scientists working in the public and private sectors of research and development have driven this traditional two-dimensional hyphenated technology, and/or recently three- and four-dimensional hyphenated technologies in the case of a second GC and/or a MS equivalent being added, to become one the dominate platforms for use in a wide assortment of analytical and bioanalytical techniques. The analysis of drugs, metabolites, pesticides, chemical warfare agents, food ingredients, medications, fuels, and etcetera [1-3] and/or in the main category of volatile and semi-volatile organic compound analysis in fields such as forensic, toxicology, environment, defense, food and beverage, pharmaceutical, petrochemical, and etcetera [4-6] are all now considered to be growing in size and in scope in the use of GC-MS instrumentation. The advancement in GC-MS instrumentation was initially and still is driven by the need for a more comprehensive analytical and bioanalytical technique that can accurately and precisely discriminate targeted and untargeted analytes from higher complexity sample mixtures in a sensitive and selective way. To that end, this review, like the preceding review on LC-MS [7], will briefly attempt to focus on the most current emerging trends in GC-MS instrumentation and their respective contributions to the field of analytical and bioanalytical techniques.

A couple of distinctions, often found in use with LC-MS, can be applied in the use and discussion of GC-MS in the forms of qualitative and quantitative analysis of higher complexity sample mixtures. With qualitative GC-MS and GCxGC-MS often taking the form of discovery types of assays employing GC coupled to mass spectrometers that can include for example quadrupole-ion trap and time-of-flight mass spectrometers (i.e. QITMS, TOFMS respectively), or GCxGC coupled to TOFMS [8-10]. Whereas with quantitative GC-MS and GCxGC-MS often taking the form of directed types of assays that can employ GC coupled to a variety of mass spectrometers that utilize high resolution magnetic sector, single quadrupole, and triple quadrupole mass spectrometers (i.e. HRMS, QMS, QqQMS), or GCxGC coupled to QqQMS [11-13]. These two types of distinctions in use in instrumentation (i.e. qualitative and quantitative) have now started to become more integrated with the emergence of a new class of GC-MS instrumentation that has the ability to a degree to do both routine qualitative as well as routine quantitative analysis of targeted and untargeted analytes of higher complexity sample mixtures. This new class of GC-MS instrumentation, for example, typically takes the form of a GC or GCxGC separation system that is interfaced to two or more mass spectrometers that are placed in series to form a hybrid mass spectrometer such as a three-dimensional GC-QMS/TOFMS or a four-dimensional GCxGC-QMS/TOFMS system [14-17].

Before a continuation of our discussions of new class of GC-MS instrumentation a moment should be taking to briefly review the trend of the combination of serially stacking two standalone one-dimensional GC systems together to form a two-dimensional GCxGC system of separation. Here a pair of GC columns typically located in two separate oven compartments that are generally employing nonpolar and polar packed stationary phases are connected in series via a modulator that repeatedly traps and focuses the eluent from the first column before injecting it into the second column. This results in a two-dimensional chromatogram with retention times along both the x- and y-axis. Why do this and what advantages does this bring to the scientist, is common set of questions that come to mine. In addressing these two questions specifically let's take a look at what GCxGC facilitates in the form of compounds with similar boiling points that could not be separated with baseline resolution with single GC can now be separated based upon their differences in polarity. This in turn now allows for the analysis of higher complexity samples that were previously difficult to separate. Additionally, GCxGC allows for the recognition of patterns that can be correlated to groupings of compound structural classes such as alkanes, alkenes, alkynes, and etcetera. Overall the main advantages of GCxGC can often be summarized with an increased sensitivity, enhanced selectivity, increased number of compounds resolved with baseline resolution per unit of time, and as mention above, the formation of visualized organized patterns of compounds with the same functional class groups [18-22].

Now in focus, when paring for example a hybrid MS system (i.e. QMS/TOFMS) as mentioned previously above, with that of a GC and/or a GCxGC system, the serial stacking of two typically independent MS instruments provides in this case a uniquely integrated qualitative and quantitative analysis workflow for the analysis of targeted and untargeted analytes of higher complexity sample mixtures of volatile and semi-volatile organic compounds into a single platform. Here the frontend of this MS system employs a QMS that is employing an Electron Ionization (EI) and/or a Chemical Ionization (CI) source that enables precursor ion scan regimes along with nominal mass EI spectral library searches over a mass range of 20-1050 Da. The middle of this MS system employs a linear hexapole Collision Induced Dissociation (CID) cell that enables precursor to product ion transitions to aid in, for example, structural elucidation for most components in higher complexity sample mixtures. With the backend of this MS system employing a TOFMS that enables precursor ion scan, product ion scan, and Multiple Reaction Monitoring (MRM) scan regimes that typically delivers acquisition speeds of 1 to 50 spectra

per second, a dynamic range of 10^3 to 10^5, a level of sample peak resolution of 13,000 to 15,000 FWHM, a level of mass accuracy of 2 to 5 ppm, and a mass range of 20-1700 Da with 15-3000 Da extended. It should be noted that since the TOFMS continuously acquires all masses for a given mass range simultaneously the MRM scan regime mimics QqQMS instruments by using accurate mass extracted ion mass and/or masses from the product ion scan. These TOFMS attributes, with emphasis being on accurate mass identification determinations of both precursor and product ions, allows for the effective analysis of higher complexity sample mixtures thereby enabling the construction and utilization of exact mass libraries of compounds (i.e. drugs, pesticides, metabolites, and etcetera). To that end, when the combination of the QMS with that of a TOFMS takes place to form a hybrid QMS/TOFMS instrument scientists are able to utilize a rapid, sensitive, selective, higher-resolution, accurate mass hybrid style of MS that is able to help facilitate, for example, the deconvolution of coeluting GC chromatographic peaks during routine qualitative and quantitative analysis assays even if only a single GC system is used [14,15,19,23].

As scientists build upon these innovative progressions of GC-MS instrumentation that has the unique ability to a degree to do both routine qualitative and routine quantitative analysis of targeted and untargeted analytes of higher complexity sample mixtures of volatile and semi-volatile organic compounds for analytical & bioanalytical techniques we feel optimistic that this new emergent class of GC-MS instrumentation employing hybrid QMS/TOFMS technology will begin to phase out some of the traditional classes of standalone GC-MS instrumentation that are currently found in many present day laboratories. It should be noted, as was the case with that of LC-MS employing hybrid QMS/TOFMS technology, that the ability to combine routine qualitative and quantitative analysis into one instrument is not just the savings in cost of the replacement of two standalone instruments with that of one, but rather an increase in the amount of information obtained by the scientist from a single analysis. This has become especially important and advantageous to scientists working with and/or screening higher complexity samples wishing to re-investigate rich data sets of virtually unlimited numbers of compounds that were previously assayed but not analyzed for all targeted and/or untargeted component compounds of interest at that time. In comparison, conventional screening methods of higher complexity samples that employ for example standard non-hybrid QqQMS technology are limited to a narrow number of targeted compounds analyzed only and do not allow for a retrospective analysis of previously collected untargeted data. Overall, this emerging trend in GC-MS instrumentation employing hybrid QMS/TOFMS technology may just be the shift scientists have been waiting for in the main category of volatile and semi-volatile organic compound analysis in the offering of three- and/or four-dimensional, temporally resolved, information in a single GC-MS instrument for analytical & bioanalytical techniques. Lastly, as we conclude this review scientists have taken yet another innovative step forward in the research and development of an integrated five-dimensional hyphenated technology in the form of adding liquid chromatography separations to GC-MS in the form of an LC-GCxGC-QqQMS system [24]. Here, as highlighted by the authors, depending upon the analytical & bioanalytical techniques required for a given assay a number of instrumental configurations may be employed.

Conflict of Interest

The views expressed in this manuscript are those of the author(s) and do not reflect the official policy or position of the Department of Army, Department of Defense, or the U.S. Government.

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