The ultimate “analytical challenge”: what is analytical chemistry?

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Analytical chemistry is the branch of chemistry concerned with analysis. But what exactly does “analysis” mean? Until well into the nineteenth century the word “analysis” in chemistry was synonymous with decomposition [1–3]. At that time, chemical analysis was the art of decomposing substances in order to learn about the nature and proportions of their constituents [3]. The other method of learning about substances was synthesis. But analytical chemistry has changed since then. Now, with a single pass in front of an atmospheric pressure ionization mass spectrometer one can instantly detect traces of cocaine adsorbed on a banknote.

Analytical philosophy

The historical interpretation of the word “analysis” in chemistry is on par with the philosophical distinction between analysis and synthesis nowadays primarily associated with Immanuel Kant. With the advent of mass spectrometry or spectroscopy, however, it is no longer necessary to destroy the molecules to learn about their composition or structure. Hence, the traditional meaning of analysis now chiefly concerns the identification and quantification of substances, not decomposition. Yet, the goal of analytical chemists is to measure all kinds of chemical properties, not just the concentration of a substance [4]. Analytical chemists do not just provide results, but also strategies for measuring chemical properties [5].

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Analytical chemists now spend increasing amounts of time interpreting their data. Not surprisingly, McLafferty's *Interpretation of mass spectra* is among the most cited books in modern analytical chemistry [6]. Fields such as genomics and proteomics cannot be imagined without automated large-scale data analysis. Likewise, modern mass spectrometry measurements in geology are based heavily on the complicated mathematical analysis of mass bias fractionation correction. Data analysis itself now takes considerably more time than data collection in chemical analysis). Chemists have long made use of the operational definition of their subject-chemistry is simply what chemists do. In light of what analytical chemists now do, perhaps the time has come to formally define analytical chemistry from a more philosophical point of view where “analytical” judgments are supposed to unfold the contents of a concept [7]. As noted by Sir Isaac Newton, an analytical method is used to comprehend experiments and to observe phenomena [7].

With the abundance of more readily available data, the question arises as to how we can guarantee the rigor of the conclusions based on these data? For example, many of the studies of selenium metabolites in urine appear to have assigned incorrect structures and the long-held view that the $(\text{CH}_3)_3\text{Se}^+$ ion is a major human urinary metabolite appears unjustified [8]. In this vein, albeit on a much simpler level, the *Mendeleev vodka challenge* published in this issue of *ABC* is a vivid reminder of the uncritical copy-culture that surrounds us [9].

Analytical mathematics

In 1980, the International Committee for Weights and Measures realized that more attention needed to be devoted to metrology in chemistry. Just a few decades later, metrology, the science of measurement, has become an integral part of analytical chemistry, most notably with the publication of the *Guide to the expression of uncertainty in measurement* (GUM) in 1993 [10], now among the publications most referenced in this journal. The widespread use of GUM principles in analytical chemistry has clearly weakened the distinction, if any, between analytical chemistry and chemical metrology. Analytical mathematics is the representation of curves and surfaces by equations and a similar concept forms a vital part of analytical chemistry in the post-GUM-era, where all processes must be represented by a measurement model, i.e., a mathematical relation among all quantities known to be involved in a measurement. Besides the evaluation of the uncertainty budgets for measurement results, definition of the detection limit is a prominent example of analytical mathematics in chemistry.

Analytical challenges

Analytical challenges are intended to be food for thought, interesting chemical trivia or snippets of a chemical nature to be considered and analyzed. They emphasize the vital role of

information analysis in modern analytical chemistry. Identification of chemical structure from a range of types of data is a classic example, but puzzle-solving in analytical chemistry does not stop there. Many of the previous challenges were designed to bridge the gap between disciplines such as neurochemistry and probability theory [11], DNA sequencing and puzzles [12], or mass spectrometry and relativity theory [13]. Others were designed to show the beauty of structure elucidation, as for the glycoside fraxin [14], to illustrate the charm of mathematics in chemical data analysis, as in the isotopic composition of zinc [15], or to detect pitfalls in analytical methods [16]. In a way, the *Analytical challenges* are an invitation to be passionate in the quest for knowledge. In the words of Dr. Faustus, “sweet analytics, ’tis thou hast ravish’d me!” [17].

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