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FEATURE ARTICLE

Quo vadis, analytical chemistry?

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Abstract This paper presents an open, personal, fresh approach to the future of Analytical Chemistry in the context of the deep changes Science and Technology are anticipated to experience. Its main aim is to challenge young analytical chemists because the future of our scientific discipline is in their hands. A description of not completely accurate overall conceptions of our discipline, both past and present, to be avoided is followed by a flexible, integral definition of Analytical Chemistry and its cornerstones (viz., aims and objectives, quality trade-offs, the third basic analytical reference, the information hierarchy, social responsibility, independent research, transfer of knowledge and technology, interfaces to other scientific–technical disciplines, and well-oriented education). The framework of our discipline in the coming years can be inferred from the description of the accurate general and specific paradigms taking into account the wrong, obsolete paradigms of the past. Finally, the three possible responses of analytical chemists to the proposed changes in our discipline are discussed.

To young analytical chemists, who should play a central role in increasing appreciation of our discipline by developing cutting-edge interdisciplinary research.

This article is based on the DAC-EuCheMS Lecture held during Euroanalysis 2015.

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Introduction

The contents of this paper is the outcome of the author's personal reflection after 45 years of dedication and commitment to Analytical Chemistry, and provides the turning points it has passed over the last 50 years with almost all with which he has been concerned. The paper is by no means intended to unilaterally dictate the future of Analytical Chemistry. Rather, its contents are fully open to discussion and change for enrichment and sharing by the analytical community. Disagreement can in fact be a source of clarification, improvement, and consensus, and it is essential for our discipline to be placed in a widely accepted framework for the coming decades.

The author's intention in writing this paper is to go beyond the typical approaches based on conventional, simple trends, and on the contents of existing papers and books on the topic. Because the topic is too extensive indeed, this paper is general, basic, and philosophical rather than specific. Also, although some analytical chemists may react uncomfortably to its contents owing to the deep changes proposed, they should be willing to engage in a serious discussion about the future orientation of our discipline. This is particularly so with young analytical chemists, who are the main targets of this message; they should be encouraged with a positive, experience-based attitude to change from their seniors.

This paper contextualizes Analytical Chemistry in the realm of Chemistry and outlines the most salient wrong approaches to our discipline. These constitute the main arguments for proposing an integral definition of Analytical

Chemistry and its cornerstones with a view to establishing accurate, new general and specific paradigms for it in order to deliver a consistent message throughout.

Analytical chemistry in the context of chemistry

One crucial requirement to describe Analytical Chemistry accurately is to contextualize it in Chemistry, its mother science. As is shown in Fig. 1a, *Analysis* is an essential component (corner) of the basic triangle of *Chemistry* [1–3] in addition to *Synthesis* and *Theory*. The sides of the triangle represent desirable, fruitful relationships among the three components. In fact, the triangle would shrink to virtually a single point if the existing water-tight compartments among the basic components of Chemistry were reduced to a great extent.

If the chemical applications such as Clinical, Agricultural, Pharmaceutical Chemistry and Industrial Chemistry are considered, the triangle of Fig. 1a becomes the tetrahedron of Fig. 2b, which retains the relationships among the components of Chemistry. It should be noted that the field of action of Analytical Chemistry cannot be accurately delimited if *Analysis* is included among the *Applications* of Chemistry as some colleagues from other chemical disciplines tend to do; as can clearly be seen from Fig. 1b, the two are clearly different.

The major trend to interdisciplinary in today's and —presumably— tomorrow's Science and Technology can be expected to bring Chemistry to a prominent place in scientific and technical collaborative studies and applications; as a result, the tetrahedron of Fig. 1b can be expected to become the pentahedron of Fig. 1c. No doubt, the future of Chemistry lies at interfaces with other scientific and technical disciplines. The right and wrong roles analytical chemists can play in these interdisciplinary studies are discussed later on.

Not completely correct overall approaches

One must admit that overall, Analytical Chemistry is not optimally perceived, mainly because of long-lasting prejudices. Thus, Analytical Chemistry is often viewed as a second-class discipline of Chemistry despite the undeniable need for reliable (bio)chemical information in making grounded, timely decisions in many fields of action, such as environmental sustainability, healthcare, nutrition, agriculture, hygiene, transport, sports, dressing, culture, home, or building. Whether by ignorance or by interest, the information-related component of Chemistry is frequently missed. For example, the definitions of Chemistry in such highly reputable English dictionaries as the OED [4] and Webster's [5] fail to mention this essential component. Also, a recent editorial article about the present and future of Chemistry

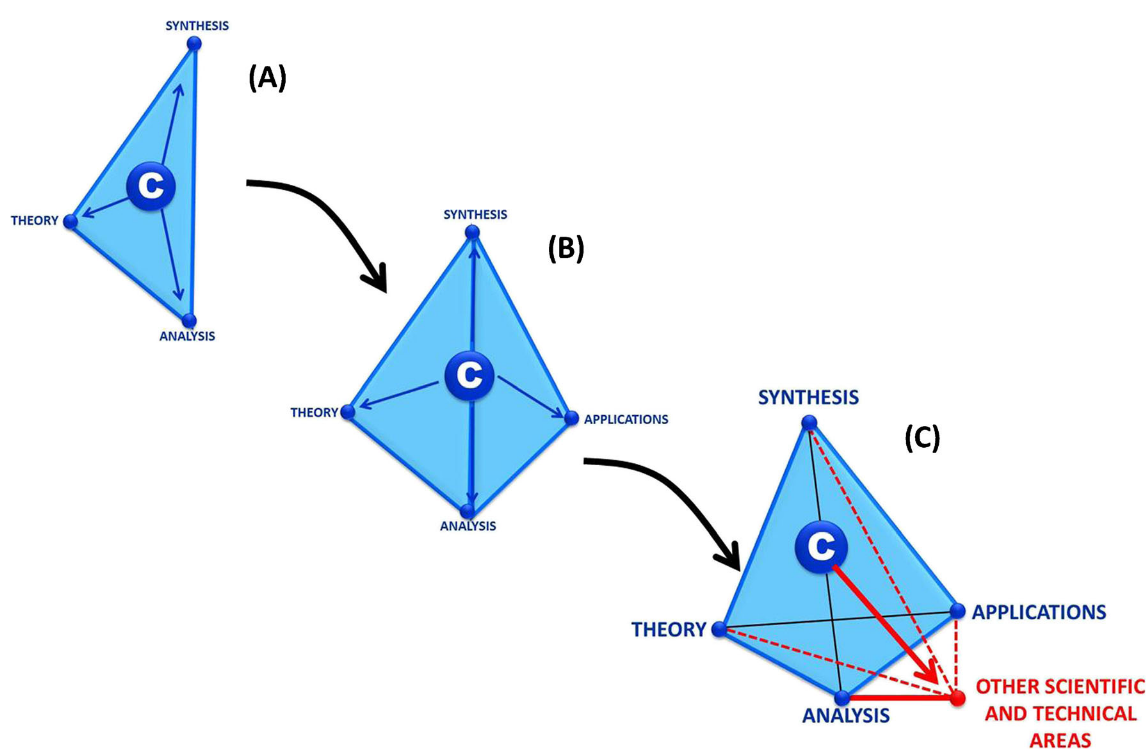


Fig. 1 Evolution of Chemistry from the basic triangle (**a**) through a tetrahedron to a pentahedron. The component "Analysis" is substantial in all

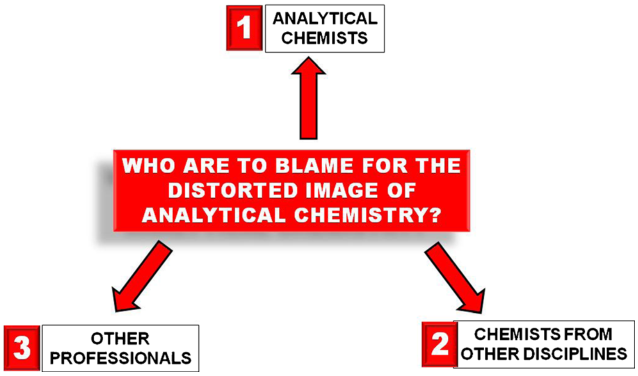


Fig. 2 Who is to blame for the distorted image of Analytical Chemistry?

published in *Science* placed little emphasis on the importance of (bio)chemical information [6], and the editors of *Analytical Chemistry* recently defined the scope of our discipline without explicitly providing for its information-related component [7].

As can be seen from Fig. 2, the responsibility for the distorted, occasionally poor image of Analytical Chemistry is to be shared by three types of individuals. First, there are analytical chemists themselves (Fig. 2.1), many of whom have implicitly accepted other chemists' downgrading of the importance of Analytical Chemistry, possibly because of an underlying inferiority complex. These colleagues have done little to improve the image of our discipline. As shown below, wrong approaches to quality analytical research and education have also contributed to distorting the view of our discipline.

The second group of individuals to be blamed for the poor image of Analytical Chemistry are chemists from other chemical disciplines (Fig. 2.2), most of whom think ours is not a key contributor to Chemistry. In the second half of the XX century, some powerful instrumental techniques were wrongly associated with other chemical disciplines (e.g., X-ray Spectroscopy with Inorganic Chemistry, Mass Spectrometry with Organic Chemistry) owing to the type of chemical information they provided; as a result, the field of action of Analytical Chemistry was markedly shrunk. In addition, the majority of chemists have acquired a wrong picture of Analytical Chemistry from the very beginning because they were misguidedly educated in our discipline.

The third group of individuals who fail to give proper credit to Analytical Chemistry (Fig. 2.3) consists of other professionals who tend to minimize the importance of analytical expertise simply because instruments and analysers provide data in some form and such data can apparently be acquired and interpreted by technicians. Such individuals are unaware of the need to assure that the analytical information is factual, and also of the significance of R&D&I in Analytical Chemistry to solving information-related (analytical) problems. The principal role of analytical chemists is to produce not mere data, but rather quality (bio)chemical information and knowledge; an analytical chemist is not a —high-level— technician.

Integral definition

A comprehensive definition of Analytical Chemistry should place it properly in the context of Chemistry and consider the wrong overall approaches described above. Over-simplistically, Analytical Chemistry can be defined as the discipline in charge of the third component of Chemistry (Fig. 1a) or that of producing (bio)chemical information by implementing (bio)chemical measurements—and hence belonging in the field of Metrology.

More comprehensively, Analytical Chemistry can be defined as the chemical metrological discipline that develops (R&D), optimizes, and uses tools and measurement processes in order to strengthen its capabilities to extract information—particularly to obtain quality (bio)chemical information about objects and systems of natural/artificial nature in order to fulfil specific needs or requirements with a view to facilitating grounded, timely decisions in scientific, technological, economic, and social areas.

The distinct feature making Analytical Chemistry an independent, first-class discipline of Chemistry is *(bio)chemical information*, which should be the polar star of analytical chemists. Analytical information is thus equivalent to (bio)chemical information.

Judging by the growing demand for (bio)chemical information, Analytical Chemistry possesses undeniable importance. Its basic and transversal vocation has materialized in a strong impact on a wide variety of fields that require reliable chemical and biochemical information to make grounded, timely decisions of high social and economic significance (see Fig. 3).

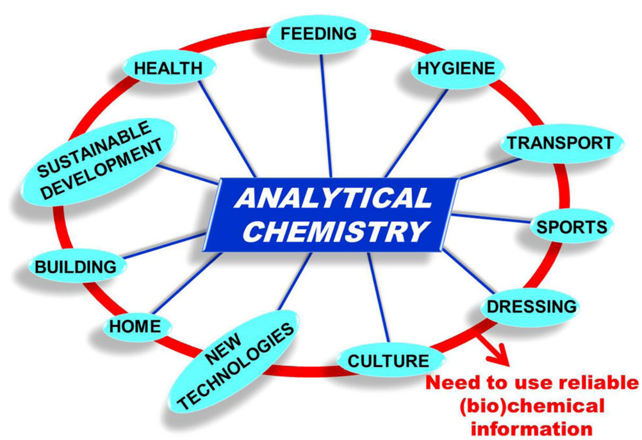


Fig. 3 Analytical Chemistry has an undeniable impact on a wide variety of fields

Pillars of the definition

The previous definition of Analytical Chemistry should rely on the firm, solid supports of Fig. 4. All rest on social responsibility, which is another pillar.

The *main aims* of Analytical Chemistry are to achieve high metrological quality (high accuracy, low uncertainty) and to solve information-related (analytical) problems. Its *overall objectives* are of the *magnifying* [viz., providing more, better (bio)chemical information] and *reducing* type (viz., expending less materials and time with as little human resources and low risks as possible). The two aims (Metrology and problem solving), and the two overall objectives (magnifying and reducing) are contradictory. Thus, one crucial aspect of Analytical Chemistry is to establish *quality trade-offs* among them to solve each analytical problem [8] in order to ensure consistency between required and delivered analytical information [9].

Analytical Chemistry has two types of classical *basic references*, namely: tangible references and written standards. Clearly, these references do not suffice to support a modern, accurate view of our discipline, and a third basic reference [viz., the (bio)chemical information needed to make decisions] is required. Integral analytical quality is a combination of metrological quality, which is related to the two classical standards, and practical quality, which is related to the new basic reference.

Consistency between Analytical Chemistry and the *data–information–knowledge hierarchy* is also very important here [10]. Raw data are typically signals from instruments that are compiled and processed to obtain information: the results of an analytical process. Processing and interpreting such information provides *knowledge* in the form of (bio)chemical reports, which constitute the foundations for correct decisions. However, in times of crisis, knowledge is not enough—according to Einstein, imagination is also required to break the traditional frontiers of knowledge and create new paradigms. Such is the case with the analysis of the nanoworld. The current crisis arose because of the exponential growth of information demands in this area, which could not be met owing to a lack of experience and effective tools. No doubt, analytical chemists should work hand-in-hand with other professionals to create new paradigms in order to successfully face the new challenges.

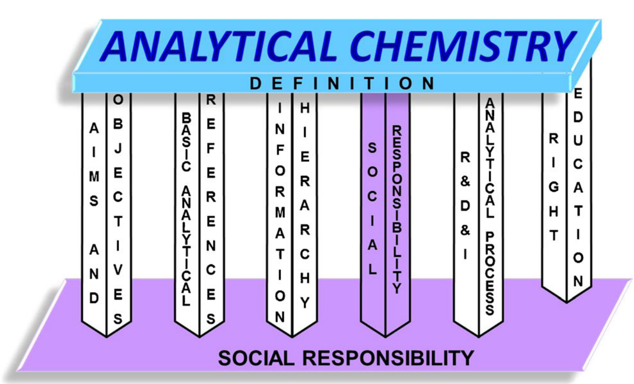


Fig. 4 Pillars of the definition of Analytical Chemistry

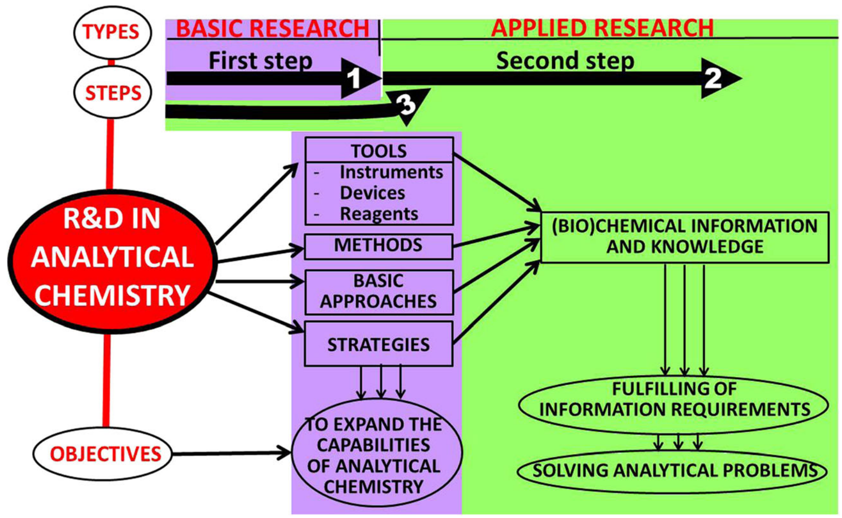
Interfaces to other areas and disciplines are essential with a view to approaching Analytical Chemistry in a modern, correct way. Analytical Chemistry should establish fruitful internal relationships with other chemical disciplines (viz., Physical, Organic, Inorganic, and Applied Chemistry, Chemical Engineering) and external relationships with other branches of Science and Technology (e.g., Physics, Biology, Mathematics, Engineering) to accomplish its aims and objectives. Also, obtaining an integral view of Analytical Chemistry entails considering the two-way relationships (interfaces) [11] with the six types of written standards for

- knowledge management (CEN-CWA 14924:2004);
- social responsibility (ISO 26000:2010);
- management of occupational health and safety (OHSAS 18001/2);
- environmental management systems (ISO 14001:2004);
- quality management systems (ISO 9001:2008); and hence
- requirements of competence of testing and calibration laboratories (ISO 17025:2004).

Analytical Chemistry can only become an independent discipline by ensuring *efficient analytical R&D*. Figure 5 depicts the main types, steps, and objectives of analytical research and development. The first step (Fig. 5.1) corresponds to basic research, which is primarily intended to expand the capabilities of Analytical Chemistry by developing a great variety of analytical tools (e.g., instruments, analysers, devices, reagents), methods, approaches, and strategies (e.g., vanguard–rearguard strategies [12]). The second step (Fig. 5.2) involves using existing analytical capabilities to produce (bio)chemical information and knowledge from objects and systems in order to meet the information requirements of a variety of "clients" with a view to solving analytical problems. This may require developing research from scratch (Fig. 5.3) if the existing repository of tools and methods does not allow a particular information problem to be reliably addressed.

Systematic *transfer of knowledge and technology* is a pending goal of Analytical Chemistry. In fact, the need remains to bridge the gap between analytical research "products," which can be tangible or intangible (see Fig. 6), and their use in practice [13]. As shown in Fig. 6, Analytical R&D centers currently transfer analytical tools, such as new instruments, reagents, or extraction devices, to the producers of analytical tools; there is two-way communication between the two parties. Also,

Fig. 5 Dual approach to R&D in Analytical Chemistry

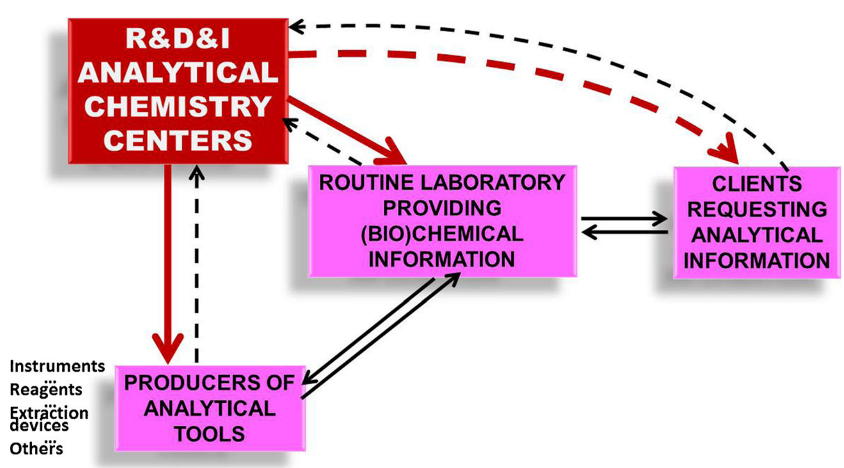


some centers are directly engaged in two-way communication with routine laboratories producing (bio)chemical information and receiving tools from producers in exchange. In some cases, research centers relate directly to clients requiring unusual analytical information.

Social Responsibility is an urgent goal in Science and Technology [14]. *Social Responsibility of Analytical Chemistry* [15] is also extremely important because it provides support for its definition and other cornerstones (see Fig. 4). Social Responsibility in our discipline can be defined as "the impact on society at large, and on health, industry, agrifood, environment, etc., in particular, of the (bio)chemical information and knowledge derived from the analysis of objects and systems." Analytical Social Responsibility rests on two essential pillars as regards (bio)chemical information and knowledge, namely: (*a*) reliable, sustainable production of both —an internal connotation—; and (*b*) consistency with reality (i.e., raising no false expectations and no false alarms)—and external connotation. Directly transferring analytical data and information to society may result in their misinterpretation. On the other hand, transferring (bio)chemical information and knowledge through reports is acceptable as long as the reports provide contextualized information and thus allow grounded decisions to be made and hypotheses or mechanisms to be formulated in basic studies. Analytical Social Responsibility should definitely be introduced as a topic in modern approaches to the teaching of Analytical Chemistry [16].

As in other scientific and technical disciplines and activities, a *different, modern orientation of the teaching of Analytical Chemistry* is essential (see Fig. 4). The image of Analytical Chemistry acquired by graduate students depends strongly of the way they are first exposed to it. Analytical Chemistry should not be associated almost exclusively with concepts such as "calculations," "ionic equilibria," "titrations," "gravimetry," or "instrumental techniques"—a gross strategic error. In fact, these concepts constitute the starting contents of most Analytical Chemistry textbooks—even some

Fig. 6 Transfer of analytical knowledge and technology from analytical research laboratories to various recipients. For details, see text



recently published books that continue to ignore the actual foundations of our discipline. One of the fist chapters in a textbook by Laitinen and Harris [17] is devoted to those standards that are essential for a measurement-based (metrological) discipline. The first atypical textbook departing from the traditional way of teaching Analytical Chemistry was published by the author in the early XXI century [1]. The switch is clearly reflected in the changes from the first (1998) to the second edition (2004) [2] of the textbook "Analytical Chemistry," the first few chapters of which are concerned with its place in Chemical Science, foundations, aims and objectives, tangible and intangible standards, peculiarities, etc. In my opinion, this approach should be better reflected in the Analytical Chemistry Euro-curriculum [18, 19].

Figure 7 provides a schematic view of the proposed changes in the teaching of Analytical Chemistry. Obvious teaching innovations (Fig. 7.1) include the use of new (information) technologies (see, for example, [20]); however, the most salient innovations relate to the principles of our discipline (Fig. 7.2). The first main change should be a switch to a bottom-up approach (viz., from common, characteristic principles to the description of classical and instrumental techniques and analytical processes) [1, 21], avoiding topics that are not directly related to Analytical Chemistry and can be replaced with others, such as metrology in chemistry, quality, solving (bio)chemical information problems, and social responsibility, among others. This can help to improve the first impression students acquire about Analytical Chemistry. Other proposed changes include a holistic approach to teaching analytical properties based on their contradictory and complementary relationships [22, 23], as well as a hierarchical approach [24] to the most salient key words in Analytical Chemistry in order to avoid the obsolete traditional definitions (see, for example [1]).

Almost obsolete paradigms

The answer to the question "Is a new approach to Analytical Chemistry possible?" [25] is obviously "yes." Wrong overall approaches to Analytical Chemistry have left a number of now obsolete paradigms that should be removed or replaced, namely:

1. *Analytical Chemistry starts at the laboratory door and ends at the printer or plotter.* This assertion ignores the fact that external tasks and systematic relationships of analytical chemists are essential. Such is the case with the planning and monitoring of sampling or with two-way relationships with those requesting (bio)chemical information, among others.
2. *Analytical Chemistry is a discipline using instruments to develop methods and ends with data acquisition*. This is wrong because analytical chemists are meant to generate (bio)chemical information and knowledge by developing and applying analytical processes (R&D, Fig. 5).
3. *Only tangible and written standards are relevant to Analytical Chemistry.* In fact, the (bio)chemical information required constitutes the third basic analytical standard—which, however, is frequently ignored.

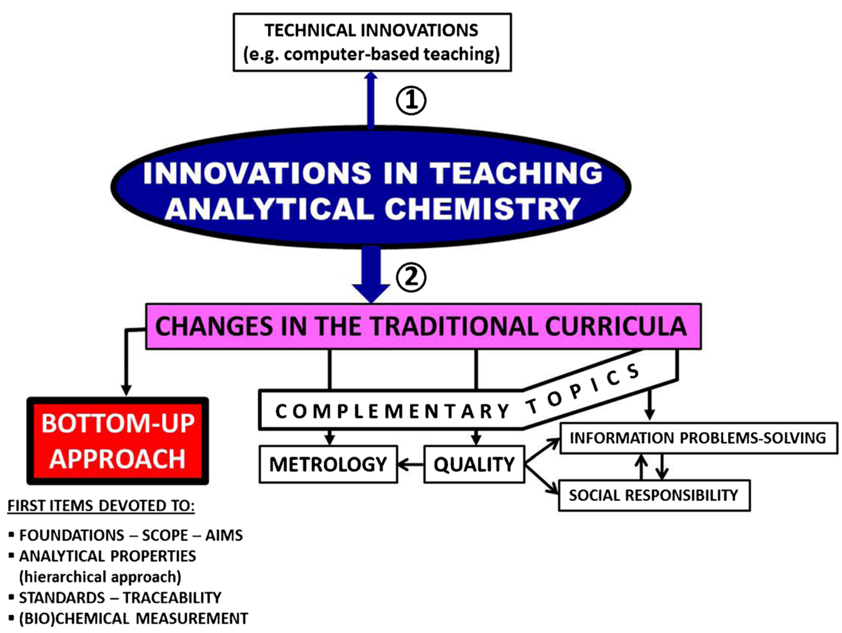


Fig. 7 New ways of teaching Analytical Chemistry departing from the typical technical approach (1) and involving the teaching sequence and complementary topics to be dealt with (2) in addition to classical and instrumental analysis

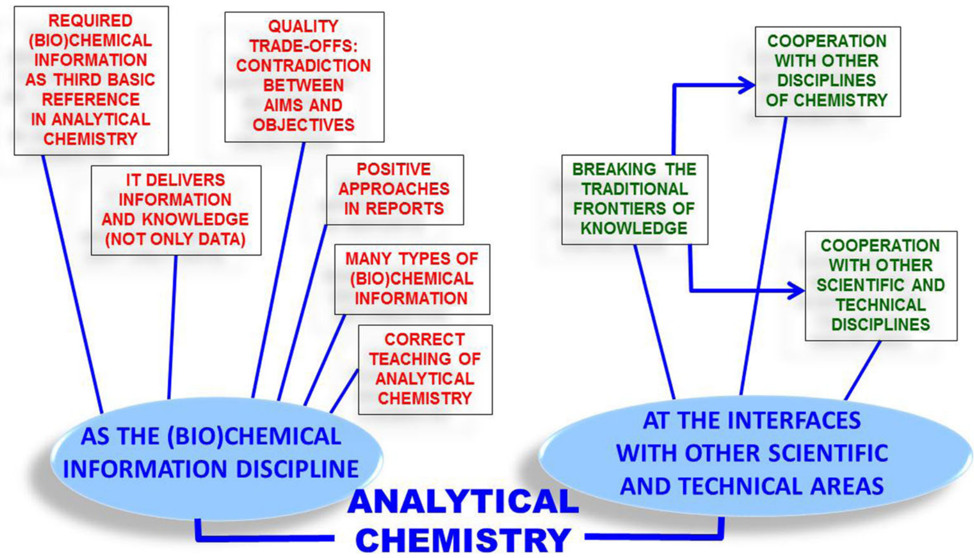


Fig. 8 Specific new paradigms based on general paradigms (1) of Analytical Chemistry as the (bio)chemical information discipline and at interfaces with other scientific and technical areas

4. *Quality-related balances between aims (metrology and problem-solving), and magnifying and reducing objectives, in Analytical Chemistry are also frequently ignored* even though they are essential in planning and validating analytical processes, and in interpreting results.
5. *Social Responsibility is irrelevant to Analytical Chemistry because it ordinarily applies to enterprises only.* This is a gross error because social responsibility principles can be as easily adapted to Analytical Chemistry [15] as they can to Science and Technology [14]. The importance of today's and tomorrow's Social Responsibility in Analytical Science can be compared with the impact of the concept "quality" two or three decades ago.
6. *A holistic view of analytical properties and their mutual relationships is a mere theoretical exercise of no practical significance.* Rather, classifying analytical properties into capital (accuracy and representativeness), basic (precision, sensitivity and selectivity), and productivity-related properties (expeditiousness, human involvement, costs-effectiveness), and establishing contradictory and complementary relationships among them is crucial with a view to planning, selecting, and interpreting the results of analytical processes.
7. *Analytical results can only be qualitative (e.g., a yes/no response) or quantitative.* In fact, new types of analytical information have emerged [10] in response to the increasing information demands. Thus, total indices [26], method-defined parameters [27], and markers [28] are currently of great practical importance, even though they lack firm metrological support.

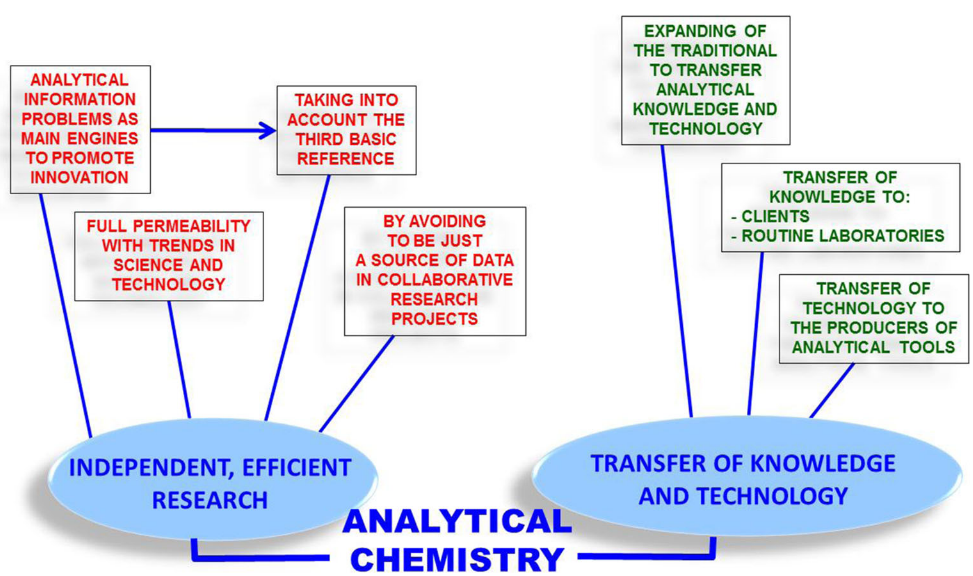


Fig. 9 Specific new paradigms based on general paradigms (2) of Analytical Chemistry (viz., efficient/independent R&D, and analytical transfer of knowledge and technology)

8. *The main goals of Analytical Chemistry are increasing sensitivity (viz., lowering detection and quantitation limits) and selectivity while minimizing uncertainty.* This assertion ignores recent changes in the essentials of Analytical Chemistry. For example, sensitivity should be adapted to the average concentration of the target analyte in each sample—macro components require no increased sensitivity. The classical selectivity concept contradicts the essence of overall indices, which are now widely used. Also, some degree of certainty can be sacrificed provided the results can be rapidly obtained (e.g., to make decisions on a changing object such as fresh milk). In other words: not always is the Olympic motto "Citius, Altius, Fortius" applicable in Analytical Chemistry.
9. *Analytical reports need not be easy to understand because their recipients will normally know how to interpret them*. This is definitely a wrong assumption. Also, reports should "sell themselves." For example, they should avoid negative comments that might be spuriously extrapolated to unrelated situations. Such can be the case when using uncertainty intervals rather than confidence intervals as proposed by Professor Thomas many years ago [29]. In fact, reports could be more easily understood if the limits set by national and international legislation or clients were accompanied by tolerated uncertainties.
10. *The main aims of R&D in Analytical Chemistry are to publish papers in journals of as high an impact factor as possible*, few permeability to trends in Science and Technology and low innovation to produce slight variations on a well-known topic or theme in much the same way as Ravel's bolero in musical terms, and to ignore the natural order of events by first developing a method and then trying to find applications —usually by using "easy" samples such as spiked natural water. In this way, the essentials of Analytical Chemistry are diluted or lost. Analytical R&D should clearly occur in a rather different framework (see Fig. 5).
11. *There is no need to systematically transfer analytical R&D "products."* On the contrary, transfer of analytical knowledge and technology (Fig. 6) is essential in order to obtain an accurate picture of Analytical Chemistry.

New paradigms

A positive view of today's and tomorrow's Analytical Chemistry can only be obtained by relying on a set of essential new paradigms that can be general (overall approaches) or specific (concrete approaches) in nature. Such paradigms lie at the opposite end of the pendulum where wrong overall approaches and obsolete paradigms, respectively, currently are.

The *general paradigms* relating to the overall orientation of the present and future of Analytical Chemistry are as follows: (*a*) thinking of Analytical Chemistry as the (bio)chemical information discipline; (*b*) placing it at fruitful interfaces with other scientific and technical disciplines and areas; (*c*) developing an efficient, distinct R&D system; and (*d*) systematically transferring analytical knowledge and technology—a primary goal. These are the true main supports for our discipline.

The *specific paradigms* derived from the four general paradigms are those described in this paper. Figure 8 summarizes those derived from the informative character of Analytical Chemistry and its future crucial role in interdisciplinary studies and applications. Figure 9 shows specific paradigms derived from analytical R&D, and also from the transfer of analytical knowledge and technology.

Final considerations

This paper is by no means intended to convey a catastrophist view of our discipline. Although it may be somewhat provocative, it is intended to stimulate deep changes in order to effectively support today's and tomorrow's Analytical Chemistry, make analytical chemists feel proud of their discipline, put it in the right place in the field of Chemistry, and challenge young analytical chemists—who will have its future in their hands.

Strong winds of change in Analytical Chemistry are arising from differences between zones of a high atmospheric pressure (right future view) to zones of low pressure (old-fashioned, wrong views) for the sake of equalization. We can face these winds in two different ways. One is resisting changes by clinging on to the classical, now obsolete approach; as long ago sung by The Beatles, "there will be an *answer*, let it be." A more open attitude can be adopted by looking for new ways of dealing with Analytical Chemistry; as sung by Bob Dylan, "the *answer* is blowing in the wind." The word "answer" is synonymous with "novelty" or "innovation" in both songs. Analytical chemists committed to change are likely to identify themselves with Dylan's proactive expectancy.

Finally, it should be noted that appreciation of our discipline is increasing, albeit slowly, at present. For example, in 2015, Whitesides (University of Harvard, USA) [30] recognized the importance of (bio)chemical information and stated that "*Analytical Chemistry is a more important area than it may seem.*" Also, Dyson has convincingly argued in Science [31] and other publications that "*one of the most important steps in opening new areas of science is developing new analytical techniques to make possible relevant measurements.*" Progress in this direction can be an incentive for young analytical chemists, who are bound to gain better appreciation of their innovative work.

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Compliance with ethical standards

Conflict of interest The opinions contained in this paper are of the exclusive responsibility of the author. They may not be shared by other analytical chemists, who are welcome to criticize them. After all, nobody is in possession of the whole truth about anything.

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