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Is a new approach to Analytical Chemistry possible?

Sir,

There is an impressive amount of literature about the celebration of 2011 as the International Year of Chemistry (IYC, http://www.chemistry2011.org/) which seems to converge on *six clear-cut objectives*. Two pertains to the celebration itself: the centenary of the award of the 1911 Nobel Prize in Chemistry to Marie Curie and the wish to place special emphasis on the role of women in the development of Science in general and Chemistry in particular. Two others relate to the social perception of Chemistry: to improve Chemistry's image and social appreciation by disseminating its doubtless positive contributions. The last two objectives look directly at the future: to arouse the interest of young people in Chemistry and to strengthen creativity and innovation in this science. Most of these objectives are closely related to the principles and practices of today's and tomorrow's Analytical Chemistry.

One of the cornerstones of Chemistry in addition to Synthesis and Theory is Analysis; this is the concern of Analytical Chemistry, a chemical discipline aiming at providing quality (bio)chemical information about natural and artificial objects and systems.

The two primary aims of Analytical Chemistry are to ensure a high metrological quality and to solve the analytical problems posed by the need of a variety of "clients" for accurate (bio)chemical information with a view to making correct, timely decisions. Analytical Chemistry has two major objectives, namely: (a) to obtain more, better (bio)chemical information while (b) reducing material consumption, human effort, time, costs and risks in implementing (bio)chemical measurement processes. Resolving the intrinsic contradictions between these aims and objectives is the greatest challenge of today's and tomorrow's Analytical Chemistry, one that can probably never met without adopting some "quality compromises". These aims and objectives, and their mutual relationships, constitute the framework for the proposed ten new targets in Analytical Chemistry, which are summarized below.

1. The "products" of a (bio)chemical measurement process should be related to the data–information–knowledge hierarchy, which has never been systematically used in Analytical Chemistry despite its significance. In this discipline, the data are instrument signals, the results information derived by compiling and processing the data, and the reports the materialization of knowledge by interpretation and contextualization of the results to facilitate correct, timely decisions.
2. The fact that Analytical Chemistry is an information discipline requires considering so-called "Analytical Social Responsibility" (ASR), which is a combination of Social Responsibility of Chemistry (SRC) and a peculiar way of delivering scientific and technical information. The internal (passive) and external (active) connotations of ASR materialize in the sustainable production and delivery of quality analytical information and knowledge, respectively.
3. A modern, comprehensive picture of Analytical Chemistry can only be obtained by contextualization among the large variety of written standards directly aimed at the continuous improvement of individual and collective human activities such as the guidelines on knowledge management (CAN 1494, 2004), social responsibility (ISO 25000:2010), occupational health (AS 18001:2007) and environmental management systems (ISO 14001:2004); or the standards on quality in general (ISO 9001:2008) and quality of testing and calibrating laboratories in particular (ISO 17025:2005).
4. The classical basic references for Analytical Chemistry, which are tangible (viz. Certified Reference Materials) or written standards (viz. norms, guides, official methods), should be supplemented with a third, crucial reference to (bio)chemical information needs and their contextualization.
5. A holistic approach to analytical properties emphasizing the complementary and contradictory relationships between the capital (accuracy and representativeness), basic (precision, robustness, sensitivity, and selectivity) and production-related properties (safety, expeditiousness, and cost-effectiveness) is needed. These relationships can be sometimes more useful than the individual properties towards solving analytical problems.
6. Enhancing selectivity has been the *leitmotif* of many attempts at improving Analytical Chemistry over the last few centuries. Today, this classical analytical goal has lost strength because "clients" are increasingly needing new measurands such as "total indices" rather than discriminate information about specific analytes.
7. Lowering detection limits has also been a classical focus of improvements in analytical processes and/or equipment. However, is it really necessary to be able to detect very low concentrations of substances that are completely irrelevant to the problem at hand, especially at substantial economic or even social costs?
8. The threshold limits set by legislation or clients themselves should be accompanied by their corresponding uncertainties. It makes no sense to require that results be delivered with uncertainties in accordance with ISO 17025:2005 when the reference is a datum without its uncertainty interval. The well-known

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Horwitz trumpet, which represents the dependence of precision on the concentration or amount of analyte, is probably a good reference here.

9. The philosophy behind analytical reports should switch from its present emphasis on negative connotations to a more positive approach. Such is the case with the word "uncertainty" when applied to analytical results – a legacy of Metrology in Physics which can lead non-majors in Chemistry to question the quality of a result. Replacing "uncertainty" with "confidence interval", which has the same scientific meaning, could help "market" analytical reports better.
10. There is a need to systematically consider all types of analytical results in order to ensure appropriate metrological support. Although norms and guides tend to revolve around quantitative results only, clients are increasingly requiring that their results be delivered in new forms such as binary responses, total indices, markers or method-defined parameters.

Whereas some of these goals are starting to be considered, others will probably take some time to be assimilated. A sound combination of this set is bound to allow a new, fresh approach to Analytical Chemistry to develop.

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