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Editorial

Modern qualitative analysis 2015

This Special Issue of ***TrAC*** presents the state of the art in chemical and biochemical qualitative analysis. Modern qualitative analysis is the multidisciplinary R&D field covering both identification and structure elucidation of individual chemical compounds and characterization, identification and classification of analyzed samples of, for example, specimens, materials, products, foodstuffs, pollutions, microorganisms, and cells.

At the beginning of the twenty-first century, several research projects were devoted to general principles and features of qualitative chemical analysis. The projects appeared for two reasons. First was evident progress in analytical instrumentation, chemical metrology and methodology, and statistics of chemical analysis. Second was that the general principles of qualitative analysis and general experimental approaches to its implementation had not previously received comprehensive treatment in the literature.

The results and the conclusions of those projects were generalized in a series of reviews covered by the Special Issue of ***TrAC*** on Modern Qualitative Analysis, edited by M. Valcárcel and S. Cárdenas, issued 10 years ago, which remains readable and citable. Nevertheless, in the past decade, there have been large developments in chemical analysis demanding both updated reviews on traditional subjects of qualitative analysis and the appearance of publications to summarize the frontiers of research.

Advances in qualitative analysis are expressed in reviews in this updated Special Issue. Many reviews (Milman; Vaniya and Fiehn; Lehotay, Sapozhnikova, and Mol; and, Szabó and Janáky) are devoted or related to mass spectrometry. Among different analytical techniques, there are nuclear magnetic resonance (Elyashberg), chromatography (Babushok), and miniaturized analytical systems (Rios and Zougagh). The special reviews in chemometrics (Szymanska, Gerretzen, Engel, Geurts, Blanchet, and Buydens) and drug analysis (Görög) also express the particular progress in several analytical techniques.

All reviews of this Special Issue are multi-faceted. General approaches to performing procedures of qualitative analysis are considered in two works (Milman, and Szymanska). Criteria for chemical identification or qualitative determination and related terminology are covered (Milman, Lehotay, and Szymanska). Analysis in metabolomics (Vaniya, Szymanska), proteomics (Szabó), food (Lehotay, and Rios), drugs (Görög), and clinical diagnostics (Rios) are presented. Validation of qualitative methods is discussed (Lehotay, Szymanska, and Elyashberg). Some aspects of chemoinformatics and bioinformatics (Babushok, Elyashberg, Vaniya, Milman, Szabó, and Szymanska) are captured.

We hope that the readers of ***TrAC*** will find this collection of reviews useful. We would like to thank all authors and reviewers for their cooperation, as well as the Publisher in making possible this Special Issue. We also thank Professor M. Valcárcel for supporting the idea of preparing this Special Issue of ***TrAC***.

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