

Preface

Analytical chemistry plays a very important role in most fields of science, industrial and environmental control, healthcare, and many other areas of academic, ecological, economic, and social values. Many innovations in analytics ultimately result in the discovery of new complex chemical compounds, clear and thorough understanding of living nature, improvement of quality and safety of goods, reduction in pollutant levels in the environment, and so on. Also, progress in analytical chemistry, as well as in any basic science, is certainly important as such.

In its structure, this science is the holistic unity of qualitative and quantitative analysis, which can be considered separately in the fields of research, innovation introduction, learning the discipline in universities, training and education programmes, etc. For the last two decades, a succession of scientists specialized in general analytical methodology, chemical metrology, and analytical fields where detection and identification of chemical compounds is of particular importance, perceived and expressed an opinion that modern qualitative chemical analysis had been insufficiently described in general treatises and guidances on analytics, metrology, standardization, quality assurance, and so on. Unlike analytical techniques for qualitative and quantitative determinations, well-presented in books and reviews, theoretical principles of identification and general experimental approaches to its implementation have not received comprehensive treatment in the literature. This prevents progress in the development and consistent validation of particular qualitative procedures, quality assurance of the proper analytical data, and expressing and reporting identification errors analogously to errors/uncertainties in quantitative analysis.

This book entirely devoted to chemical identification has been written especially to

- Remove “skewness” of presentation of two principal parts of chemical analytics in the literature on an analytical methodology
- Generalize approaches to identification of both various chemical compounds and samples containing these compounds
- Summarize methods of estimating trueness of identification results

- Draw the special attention of practical analysts to non-target qualitative analysis seldom or never considered in the general literature on analytical chemistry
- Spotlight issues of quality assurance and control in identification/qualitative analysis

The book is intended for anyone engaged in analytical and bioanalytical chemistry: professionals in reference, test, and control laboratories; scientists in research laboratories of universities and chemical, pharmaceutical, and biotechnology companies; graduate students of analytical chemistry, chemometrics, chromatography, spectroscopy, and quality assurance and control. In style, the book is both monograph and also laboratory guidance/manual. I hope that these two aspects complement each other.

The book begins with the consideration of basic principles of chemical identification, including main concepts and terminology (Chap. 1). Following are chapters covering analytical techniques (Chap. 2) and statistical/calculation methods (Chap. 3) required for identification purposes. Only brief information is given here, with references to comprehensive literature sources. Chapter 4 deals with different quantities and indices expressing trueness of results of qualitative analysis, detection and identification, and rates of their errors. In the book, procedures for qualitative analysis are divided into target identification by methods (Chap. 5) and unknown/non-target analysis (Chap. 7). For the latter, prior data extracted from chemical databases are very essential (Chap. 6). Identification/classification of objects such as foodstuffs, pollutions, microorganisms, materials, and so on is described in Chap. 8. Finally, issues of quality assurance and control in relation to qualitative analytical procedures are explored in Chap. 9.

Three remarks are necessary. First, because of my professional interest, low molecular compounds are covered to a greater extent than high molecular ones. Nevertheless, the latter are also of concern, in the respect that progress of analysis of high molecules, first of all in proteomics, affects the development of general analytical methodology. Second, general issues of chemical analysis are discussed only if related to identification problems. Third, qualitative procedures related to identification, such as detection, are also considered.

My view on the subject of chemical identification was formed not only by me alone but also as the result of cooperation with other persons. I would like to name them here.

Prof. Miguel Valcárcel (University of Córdoba) invited me to participate in the MEQUALAN project. Dr. Willie May (NIST) and Dr. Reenie Parris (NIST) introduced me to the analytical laboratory responsible for the development of reference methods and materials. Dr. Stephen Stein (NIST) was my supervisor in the project of building a library of tandem mass spectra. Mr. W.A. Hardcastle sent me the LGC document on qualitative analysis cited in the book. Dr. Steven Lehotay (USDA Agricultural Research Service) sent his recent articles on identification methodology. Dr. Valeri Babushok (NIST) introduced me to details of the database on retention indices. Dr. Inna Zhurkovich (Institute of Plant Protection) provided me with considerable advice about general issues of chemical analysis, and explained

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