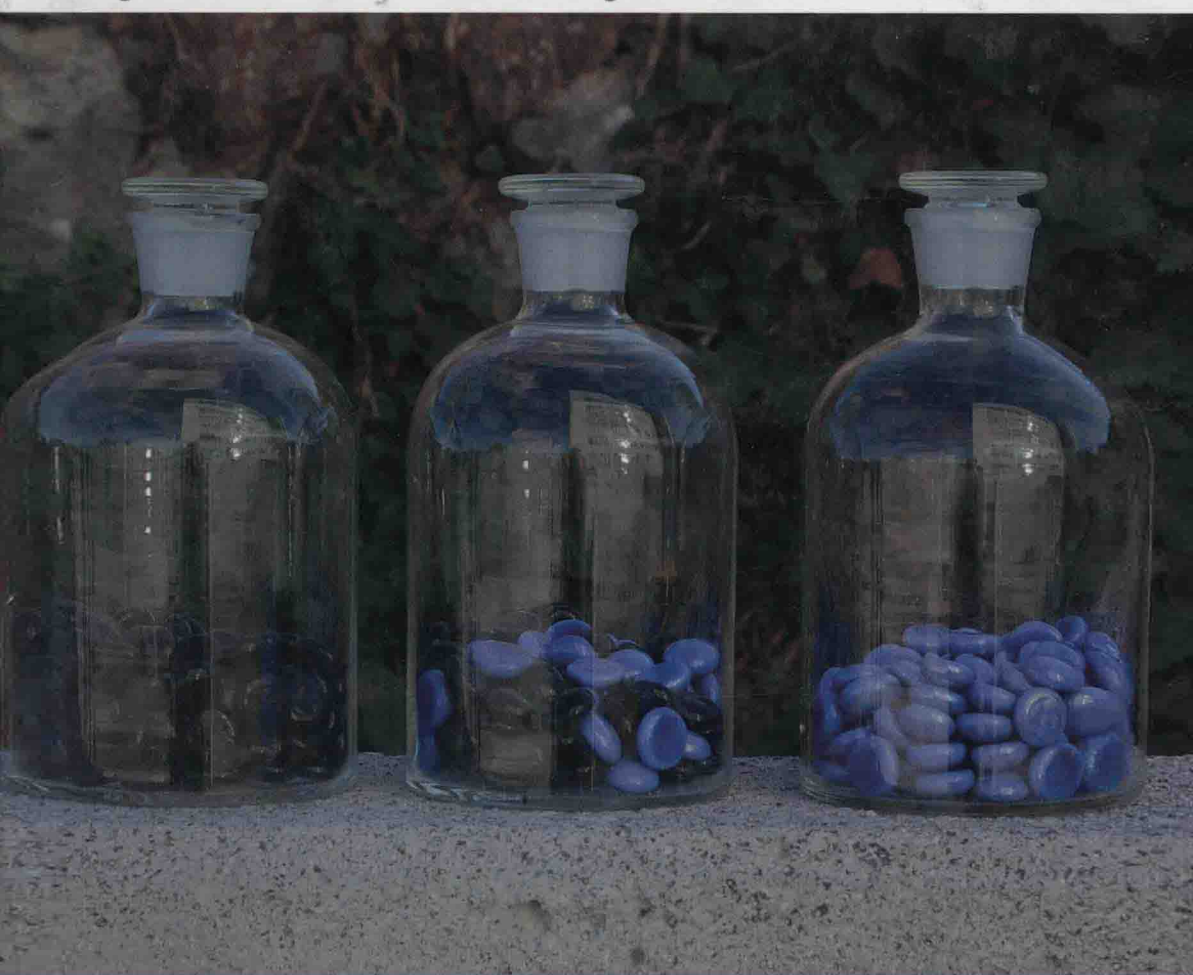
Isotope Dilution Mass Spectrometry

J. Ignacio García Alonso and Pablo Rodríguez-González



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Preface

The aim of this book is provide a comprehensive account of the developments in the field of Isotope Dilution Mass Spectrometry (IDMS) from a tutorial point of view. The book focuses on the routine implementation of IDMS and it is intended primarily for postgraduate students and laboratory personnel. However, given the large range of applications of IDMS and the clear fragmentation between the field of "organic" and "inorganic" analysts, this book may offer a global view for advanced researchers working in any of these fascinating topics.

Traditionally, IDMS was practised only in highly sophisticated laboratories devoted to Metrology in Chemistry, Clinical Chemistry, Geology or Nuclear Chemistry. Nowadays IDMS is slowly entering the routine analysis field. For those analysts working in routine testing laboratories there was a need for a textbook explaining all the basic concepts and their application to the different fields of IDMS. We hope that this book will cover this need and help to expand the use of IDMS in the analytical testing laboratories.

Another objective of this book is to cover the whole theory of IDMS to be useful in Master and Doctoral studies regardless of the application field. We have tried to cover all possible range of applications from elemental and speciation analysis to organic analysis and quantitative proteomics. We have also included concepts from metabolic and environmental studies where enriched stable isotopes are also employed. The mathematical aspects of IDMS are covered in detail but have been restricted to data-treatment procedures that can be performed by standard spreadsheet software.

In most cases, the examples selected to illustrate the concepts have been taken from our laboratory. The main reason for this decision is the direct access to the raw data of the experiments. In this way, we have treated these data in the best possible way to illustrate, with the help of tables and figures, the concepts at hand. If we had taken figures and

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tables directly from research publications the tutorial aspect of the book would have been compromised. However, as we are not experts in all fields of IDMS, many publications from different authors are cited in the references. For some applications we have taken numerical data from the literature and used them to build tables and figures that could better help in the discussion of the concepts.

As commented above, the field of IDMS has evolved since the 1940s into two different application fields: elemental and molecular IDMS. As a consequence, modern practitioners of "elemental" and "molecular" IDMS do not speak the same "language". If we take into account the researchers working in the field of metabolisms with enriched stable isotopes the differences are even larger. In this book we have covered all basic equations and concepts used traditionally in the different fields but propose a new integrated approach that can be employed in any IDMS application. This new approach is based on the use of isotope abundances or isotope distributions rather than isotope ratios. We think that this new approach is conceptually simple and covers all practical applications of IDMS including metabolic and environmental studies.

This book is made up of ten chapters. The first chapter is devoted to the history of IDMS and covers the basic concepts that are developed in the rest of the chapters. Chapter 2 covers the IDMS theory as applied to elemental and molecular analysis including the different calculation equations. The alternative online IDMS procedure is described in Chapter 3 together with the different application fields while the work with multiple spikes is the subject of Chapter 4. This chapter covers the applications of multiple spikes to trace element speciation and metabolism studies. Then, Chapters 5, 6, 7 and 8 cover what we could call "the sample", "the spike" and "the mixture". Chapter 5 is devoted to the isotope composition of natural abundance elements and molecules that will form the sample for most IDMS applications. A spreadsheet for the calculation of the isotope composition of natural abundance molecules is explained in this chapter. Chapter 6 focuses on the selection of the spike or tracer and on the characteristics of isotope-labelled molecules. Chapter 7 is devoted to elemental analysis by IDMS, while Chapter 8 focuses on molecular analysis. Both of the latter chapters treat the measurement of the isotope composition of elements and molecules after spiking with a suitable tracer. The different application fields of elemental and molecular IDMS are described here. However, the aim of this book is not to give a comprehensive account of all IDMS applications described in the literature. For specific application fields the reader is referred to the cited references. Finally,

Chapters 9 and 10 discuss the concepts of traceability and uncertainty propagation as applied to IDMS. These two chapters forge the final traceability chain for the implementation of IDMS in routine analysis. The certification of reference materials by IDMS is covered in chapter 9 while procedures for uncertainty propagation are described in Chapter 10.

J. Ignacio García Alonso
Pablo Rodríguez González

Author Biographies

Professor J. Ignacio García Alonso obtained his PhD in analytical chemistry from the University of Oviedo in 1985 and subsequently became a postdoctoral fellow at the University of Plymouth before returning to Oviedo in 1987. For five years he was a scientific officer of the European Commission, based in Karlsruhe and in 1995 returned to the University of Oviedo, where he is now Head of Mass Spectrometry and Full Professor of Analytical Chemistry. He is responsible for the Enriched Stable Isotopes Research Group at the University of Oviedo (www.isotopos.es).

Dr Pablo Rodríguez-González defended his PhD in 2005 at the University of Oviedo and subsequently he became a postdoctoral fellow at the CNRS in Pau (France) after three years. He has carried out his PhD and postdoc work in the field of isotope dilution analysis for elemental speciation and for the determination of organic compounds. He has written, in collaboration with Prof. Garcia Alonso several revisions on this topic. Since 2008 he has been a researcher at the University of Oviedo in the Enriched Stable Isotopes Research Group.

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