# Quantitative Applications of Mass Spectrometry

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*To our past, present and future students who stimulate our interest in the research and who, hopefully, have learnt or will learn something from our efforts*

# Contents

# Preface

This book has been born from the long-term collaboration (and friendship!) existing between two research groups operating in the Padova area. The first has operated for more than 30 years in the field of analytical chemistry, the second for nearly the same amount of time in organic mass spectrometry. The exchange of specific knowledge and experiences between the two groups has been very fruitful, in particular in the development phase of quantitative analyses by mass spectrometry. Both operative and theoretical aspects have been the objects of many discussions and this was fundamental to clarify those doubts that have arisen for those working in the research and analytical fields.

In the last two decades mass spectrometry has shown a phenomenal growth and nowadays it is an essential tool in environmental and biomedical fields. The problem that can arise from this wide expansion is that mass spectrometry is often mainly considered as a 'magic box' in which on one side a sample is introduced and on the other side the analytical data come out. The software (and the marketing!) has removed all the doubts and critical analysis of the data.

With this book we wish to present some very basic information to the scientists and technicians working in the field of quantitative organic mass spectrometry.

Our efforts have been devoted to authoring a book that is easy to read for researchers who are not necessarily physicists or chemists, but mainly for those who, for the first time, face all the problems arising from the development and use of a quantitative procedure. The last chapter presents a description of the theoretical aspects related to calibration and data analysis and is devoted to those who wish to learn more about these aspects.

The picture we have chosen for the cover is a Dolomite peak. Leaving aside the banal shape similarity with a chromatographic peak, this choice was made because the mountain is a good teacher of life: if you want to reach the top of the peak directly you must exert a lot of energy or, alternatively, you must study its structure and choose the right way to reach the summit with less effort. In other words each

mountain climbed requires both a general strategy and many tactical choices to be performed along the way. Thus, the same approach must be used in the development of a quantitative analysis by mass spectrometry: be sure of each step you are doing, otherwise the peak will remain out of reach!

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# Introduction

Nowadays, mass spectrometry (MS) is one of the most frequently employed techniques in performing quantitative analysis. Its specificity, selectivity and typical limit of detection are more than enough to deal with most analytical problems.

This is the result of significant effort, either from the scientists working in the field or from the manufacturing industry, devoted to the development of new ionization methods, expanding the application fields of the technique, and new analysers capable of increasing the specificity mainly by collisional experiments (MS/MS or ''tandem mass spectrometry'') or by high mass accuracy measurements.

Thus, the MS panorama is made up of many instrumental configurations, each of which have specific positive and negative aspects and different cost/benefit ratios.

Of course, these mass spectrometric approaches are usually employed when linked to suitable chromatographic (C) systems. The synergism obtained allows C-MS to be used worldwide and is of considerable interest to researchers involved in basic chemistry, environmental and food controls, biochemistry, biology and medicine.

It is to be expected that this diffusion will grow in the future, due to the relevance of the information that quantitative MS can provide, in particular in the field of public health. For this reason, some basic information on the phenomena which form the basis of different instrumental approaches, the general strategy to be employed for the development of a quantitative analysis, the role of the specificity in this context and some theoretical aspects on calibration and data analysis, are of interest and this book aims to cover, as simply as possible, all these aspects.