Mass Spectral and GC Data of Drugs, Poisons, Pesticides, Pollutants and Their Metabolites, Volume 1: Methods and Tables; Volume 2: Mass Spectra, 3rd Revised and Enlarged Edition

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This book provides mass spectral and gas chromatography data for large number of drugs, poisons, pesticides, pollutants and their metabolites, artifacts, degradation products, and endogenous biomolecules. The fact that all the mass spectra and GC retention indices given in the book have been generated at the laboratory of the authors Hans H. Maurer, Karl Pfleger, and Armin A. Weber gives high credentials to this book. It is really amazing that the authors could collect data from so many pure substances and also from real biological samples. The methods adopted for generating these data have been published by H. H. Maurer, and 97 references of the quoted 141 references belong to his group. This book is divided into Volume 1 and Volume 2; Volume 1 deals with methods used for generating the data and Volume 2 contains 7840 mass spectra.

The Preface given by H. H. Maurer clearly explains the changes brought into the enlarged 3rd edition. The enlarged version is quite acceptable. Volume 1 is divided into eight chapters. The Introduction chapter outlines the contents of all the chapters in this volume. Chapter 2, the Experimental section, gives details about various sample preparation procedures. This includes different extraction procedures suitable for biological samples such as urine, plasma, and gastric liquid. All the recommended derivatization procedures are nicely described. This section will find high utility by researchers and diagnostic laboratory personnel because all the necessary methods for the practical use are available in one section of the book. This section also gives a brief description of the GC-MS instruments used for generating the data, operating conditions, and quality assurance procedure followed. The method for determining the retention indices of studied compounds is explained.

Section 2.5 dealing with systematic toxicological analysis (STA) of several classes of drugs and their metabolites by GC-MS is highly commendable. This section gives screening procedures for 200 drugs in blood plasma and for the basic and neutral drugs in urine after acid hydrolysis, STA procedures for acidic drugs and their metabolites, and general screening procedure for zwitterionic compounds. The three tables detailing the characteristic ions (*m/z* values) to be monitored for different classes of drugs will be extremely useful for setting up the instrument for quick analysis.

Correlations between structure and fragmentation are discussed in section 3, which gives a brief description of the principles of electron ionization and discusses the correlation between fundamental structures, or side chains, and fragment ions. Formation of common artifacts during extraction, acid hydrolysis, and GC analysis is discussed with suitable examples in section 4. Section 5 gives a table of atomic masses used for calculation of molecular weight and section 6 contains a table giving the meanings for all the abbreviations used in Volumes 1 and 2 with reference to the relevant sections. Section 7 contains 141 references related to the data generated in the book. Section 8 is a very valuable section of the book because it contains all the necessary data such as retention indices, characteristic ions, and their signal intensities in the respective mass spectra, page references to the mass spectra in Volume 2, and the corresponding entry numbers. This table also contains an additional column describing the conditions in which a particular compound is detected. Thus, this section not only is useful for rapid identification of drugs, poisons, pesticides, pollutants and their metabolites, but also provides strong justification for this book. Section 9 contains a table of compounds in order of categories such as that of drugs, pesticides, pollutants, solvents, and so forth.

Volume 2 starts with the explanatory notes on the layout of the mass spectra given, explained on the mass spectra and also in the text. The meaning of abbreviations used is again given in section 2. Section 3 contains the compound index in alphabetical order with respective page numbers in Volume 2. This section is followed by the presentation of 7840 mass spectra arranged in ascending order of molecular weight of the compounds.

Overall, Volumes 1 and 2 will prove to be valuable references for clinical toxicology, forensic, and pharmacology laboratories; moreover, the 3rd edition has been published in a pleasing format with suitable font size and does not cause strain to the eyes. In addition to the mass spectra, the availability of retention indices data increases the value of the book. This book is also a source of many research problems for undergraduate students (e.g., identifying the correct structures of

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many unknown isomers, artifacts, and endogenous biomolecules).

The electronic form of the book, the possible linking of the mass spectral data with AMDIS (Automated Mass Spectral Deconvolution and Identification System) and use of the data with different GC-MS instruments will make this book even more valuable and well worth its price. The graphical representation of mass spectra is generally good.

There are certain concerns that can be considered by the authors during the next edition or while making a supplementary volume. These suggestions do not in any way diminish the quality of the data available in this book. A general comment is that IUPAC nomenclature should also be used for all the known compounds. The mass spectra of some of the compounds are already available in NIST or WILEY libraries. A reference to the latest version of these libraries would be useful and allow comparisons to those data for additional confirmation. This is important because, in some places, I do find discrepancies. One such example is for 3-β-etiocholonone, CAS No. 571-31-3 (NIST 2002; MS #13,943). The mass spectra given in the book and in the library are different. Another case of some concern is where the same structures are given with different RI and mass spectra. For example, o-toluidine AC and Prilocaine-M (deacetyl-)-AC are given the same structures. There are many such cases, and correcting these should be seriously addressed in future editions or supplements. It may be that one of the structures is uncertain, but the problem is the second structure is graphically depicted differently, causing some confusion among users. Data for many diastereomeric compounds also fall in this category because the structures of diastereomeric compounds are not depicted correctly. Care may be taken to use correct templates so that chemists do not question this. Use of correct templates is also essential for all the structures. Appropriate bond lengths and bond angles are not followed in many structures.

In some cases the molecular ions are either absent or least noticeable. In such cases, I am sure the authors must have used chemical ionization to support the molecular weight. This may be mentioned in the text at a suitable place. Molecular ions are depicted invariably as M^+ and it is recommended that they be depicted as $M^{+\cdot}$ in future editions.

Presentation of mass spectra in alphabetical order has its own merits. One will be able to compare the mass spectra of a compound with all its metabolites, artifacts, degradation products, and so forth in one page or on adjoining pages. Electronic versions will have the option for this kind of usage.

The number of mistakes that went unnoticed during editing and proofreading is minimal for this kind of voluminous work. The authors and the publisher have done a good job of maintaining the standard and they are to be complimented for their good work.

I strongly recommend these two volumes for libraries and for all the GC-MS users carrying out environmental, toxicological, clinical, and pharmacological studies.