BOOK REVIEW

Quantitation and Mass Spectrometric Data for Drugs and Isotopically Labeled Analogs

Ray H. Liu, Sheng-Meng Wang, and
Dennis V. Canfield, Editors
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This book represents years of work by the authors compiling the mass spectra of the many drug forms and derivatives, their metabolites, and their isotopically labeled variants. The first author is Ray H. Liu, a lawyer and a Ph.D. chemist who is currently professor in Fooyin University (Taiwan). He was formerly on the faculty at the University of Alabama at Birmingham. Dr. Sheng-Meng Wang is professor of forensic science of the in the Department of Forensic Sciences of Central Police University (Taiwan). Dr. Dennis V. Canfield earned his Ph.D. in forensic chemistry and is currently at the Bioaeronautical Sciences Research Lab at the Federal Aviation Administration's Civil Aerospace Medical Institute. As these authors point out in the Preface, drug analysis is now quite advanced and is expected to be $\pm 20\%$ accurate at the ng/mL level. This kind of accuracy requires the use of internal standards. The purpose of the book is to present their EI mass spectra and guide analysts in their use. These spectra are obviously of high utility for those who work in the area of drug analysis.

Part I of the book is a short section comprised of two chapters that describes quantitation approaches using internal standards. It discusses the optimal choice of an internal standard for drug quantitation while minimizing cross contributions of internal standard and analyte. This section contains detailed descriptions of the approach and the use of the data.

Part II of the book makes up the majority and contains the mass spectra of commonly abused drugs and their isotopically labeled analogs in various derivatized forms. The EI mass spectra were obtained by GC-MS; they are organized in various figures and located in an appendix. Appendix One is comprised of seven figures. Figure I contains the mass spectra of stimulants; Figure II, Opioids; Figure III, Hallucinogens; Figure IV, Depressants/Hypnotics; Figure V, Antianxiety Agents;

Figure VI, Antidepressants, and Figure VII, Others. This section constitutes a major portion of the book, from page 33 to 371. Each page contains bar graphs of six mass spectra.

In Figure I are 523 mass spectra of 21 stimulants. For example, the first entry (Figure 1-1) is devoted to amphetamine. Contained in this large figure are mass spectra of amphetamine, amphetamine- d_5 , d_6 , d_8 , d_{10} , d_{11} . These spectra are followed by the mass spectra of the acetyl derivative of amphetamine: d_0 , d_5 (two isotopomers), d_6 , d_8 , d_{10} , d_{11} . Next is the trichloroacetyl derivative, followed by the pentafluoropropionyl derivative, etc. Figure I-2 contains the mass spectra of methamphetamine and its deuterated analogs, Figure I-3 contains the mass spectra of ephedrine and ephedrine- d_3 . With the exception of a few mass spectra of caffeine labeled with ^{13}C , all the labeled compounds contain d .

Figure II is a compilation of the mass spectra of 21 opioids, starting with heroin, d_0 , d_3 , d_9 , followed by spectra of 6-acetylmorphine, morphine, hydromorphone, etc. (total of 454 mass spectra). For the vast majority, the label is d . This organization is repeated for five more figures for the substances summarized above.

Part III of the book presents data showing drugs and their isotopically labeled analogs that show some cross contribution. The purpose is to understand and correct for the contribution of an ion from the labeled material (usually an internal standard) to the unlabeled (the analyte). These data were experimentally acquired in a variety of ways by selected ion monitoring. One of a number of approaches is illustrated in the Introductory section. Imagine that a certain ion in the mass spectrum of a compound has an ion intensity (peak area) of 10,000 whereas the isotopically labeled analog has an intensity of 300 for the same m/z ion. The cross contribution of the labeled material to the unlabeled is 3%. The authors admit there is some error in the determination because the data come from two separate injections of presumably the same quantities of labeled and unlabeled material. In a later table, the cross contribution data are assessed for accuracy so that an analyst can select the most appropriate pair of ions for a given analyte and its internal standard. This portion of the book extends from page 377 to 492. The book ends with an index.

The book is of obvious utility to those analysts who work in drug analysis and to those who are confronted occasionally with a drug-analysis problem. The strategies outlined in this work are important to anyone who is conducting trace analysis by chromatography coupled with mass spectrometry. The fragmentation outcomes of labeled materials may also have some use for scientists interested in mass spectral fragmentation mechanisms. It would be even more useful if these spectra were available in electronic format.