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Book Reviews: Technical Books Section

...AN ESSENTIAL BOOK FOR FORENSIC TOXICOLOGISTS ...Forensic toxicologists would benefit from this book most... This book shall remain a ready reference tool for me...

Quantitation and Mass Spectrometric Data of Drugs and Isotopically Labeled Analogs, 1st Edition, by Ray H. Liu, Sheng-Meng Wang and Dennis V. Canfield. Hardcover, 11" x 8.6" x 1.3".
CRC Press LLC, 6000 Broken Sound Parkway NW, Suite 300, Boca Raton, FL 33487-2742. , . Publication Date August 05, 2009. 510 pages, ISBN-10: 1420094971; ISBN-13: 9781420094978 (alk. paper). Price: $189.95.

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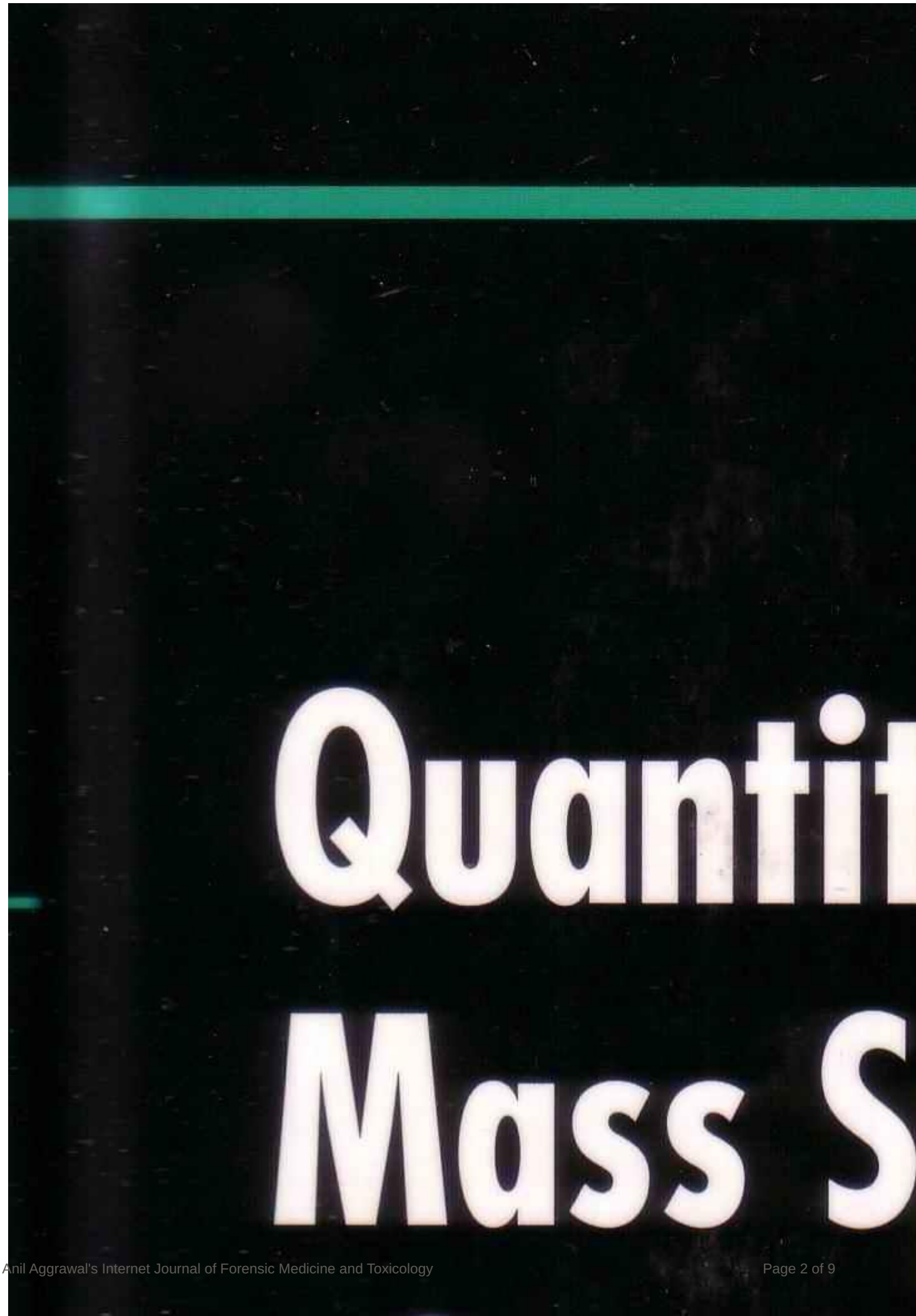
Quantit
Mass S

One of the crucial components of forensic drug testing is the detection of drugs and their metabolites in biological tissues and fluids. Sometimes, these drugs may be in very low quantities. Thus a crucial requirement is to be able to detect drugs at very low concentrations. Currently the analysis of drugs and their metabolites in biological media are expected to routinely achieve ± 20% accuracy in the ng/mL concentration level. Thus the availability and the selection of quality ion-pairs designating the analytes and their isotopically labeled analogs (ILAs) are important considerations in achieving the accuracy of quantitation results. Assisting scientists with this process, Quantitation and Mass Spectrometric Data of Drugs and Isotopically Labeled Analogs provides an extremely valuable reference for labs involved in the analysis of therapeutic and abused drugs.

View this book on Amazon

The book comprises of three parts. Part One illustrates approaches, mechanisms, and challenges pertaining to the use of isotopic analogs as internal standards for drug quantitation. Part two – the most extensive part - is a systematic compilation of full-scan mass spectra of drugs and their analogs, as parent compounds and as derivatives resulting from various chemical derivatization approaches, commonly encountered in today's labs. Based on the mass spectra data presented in the second section, Part Three provides corresponding tables of ion-pairs which can potentially be adapted to designate the drugs and their isotopic analogs in the analytical processes. Relative quality of these ion-pairs (cross-contribution to the intensity of these ions by their isotopic analogs) is included in these tables.

...Forensic toxicologists would benefit from this book most. Other professionals that would benefit from this book are clinical toxicologists and clinical sports toxicologists – the professionals who perform drug testing in sporting people. With more than 1500 full-scan mass spectra and quick access data tables, this text represents mass spectra of the many chemical derivatization forms of drugs, their metabolites, and their isotopically labeled counterparts...

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Excerpts from the book:

This book is a significant addition to the literature on forensic toxicology. So that our readers can get some idea about what the book contains, the editors at the journal office decided to run some excerpts from this book. This is how the authors start chapter 2, entitled "**Isotopically Labeled Analog of the Analyte as Internal Standard for Drug Quantitation - Chemical Derivatization and Data Collection and Evaluation**"....

INTRODUCTION

With *internal standard method* as the preferred calibration approach and an isotopically labeled analog (ILA) of the analyte as the internal standard (IS) of choice, the cross-contribution (CC)

phenomenon - contribution of IS to the intensities of the ions designating the analyte, and vice versa - is undoubtedly the most significant interference factor in a quantitative determination protocol. Successful quantitation of a drug in biological matrices relies on the availability of ion-pairs that are free of (or with minimal) CC for designating the analyte and the IS.

An ideal complementary ILA of the analyte serving as the IS, that can produce ion-pairs with the desirable characteristics, maybe synthesized with full understanding of the analyte's ion fragmentation pathways and skillful positioning of the labeling isotopic atoms in the analyte's molecular framework. Desirable ion-pairs may also become available when the analyte/IS pair, possessing active functional groups, are derivatized with an appropriate derivatization group.

Sections included in this chapter illustrate the generation and selection of favorable ion-pairs using various derivatization groups and ILAs. Also illustrated are methods used to evaluate the quality of the ion-pairs of interest. *Full-scan mass spectra* of the analytes (and their ILAs) studied, in various derivatization forms, are compiled in **Part Two** (**Appendix One**, pp 31-371), while the *CCdata* evaluated for potentially favorable ion pairs are shown in **Part Three** (**Appendix Two**, pp 373-492) of this book. Information included in Parts Two and Three should be of valuable reference to those who are interested in the analysis of drugs in various forms.

I. CHEMICAL DERIVATIZATION

Chemical derivatization was traditionally incorporated into the sample preparation process to convert the analyte to a form that is more *compatible to the chromatographic environment. Creating or optimizing separation* and *enhancing detection and structural elucidation efficiency* have later become the reasons for practicing chemical derivatization prior to the instrumental measurement step. The primary objective of chemical derivatization discussed in this chapter is the generation of favorable ion-pairs for designating the analyte and the ILA serving as the IS. Specifically, it is hoped that the chemically derivatized analyte and IS would produce ion-pairs that are free of (or with minimal) CCs between the intensities of ions designating the analyte and the IS.

A. Production of Most Favorable Ion-Pairs for Drug Quantitation

Approaches that may potentially help generate favorable ion-pairs for a specific analyte/ILA IS system include:

a. Positioning the isotopic atoms at the most desirable positions in the molecular framework; .

b. Experimenting various chemical derivatization alternatives; and

c. Selecting an alternate ionization method, such as chemical ionization.

All three approaches have their limitations. The *number and positions of the isotopic atoms* are determined in the manufacturing process and cannot be altered by the laboratory analyst, while positioning isotopic atoms in the analyte is constrained by the availability of practical synthesis routes. *Chemical derivatization* approach is limited by existing functional groups in the analyte and reagents that are available. For practical purposes, *electron impact* and *chemical ionization* are the only ionization options. Chemical ionization procedure, typically yielding one ion for the designation of the drug and one for the IS, has been criticized for providing inferior discriminating power for definite identification under routine high throughput test environment.

In practice, the analyst can explore the best combination of ILA (serving as the IS) and derivatization options through a comprehensive evaluation process. This process includes the examination of empirical CC data of various derivatization products resulting from all combinations of available ILA and amenable derivatization alternatives.

B. Exemplar Studies

Fragmentation in the ion source of a mass spectrometer often includes [M – H_n] processes resulting in series of “cluster ions”, where n is the number of H-atom involved in the process. When this occurs, [M - ^2H_n] processes originated from a ^{2}H-analog of the analyte are likely to generate ions that may contribute to the intensities of ions designating the analyte. Thus, ^{13}C-labeled analogs may cause less interference of this nature. A very limited number of ^{13}C-labeled drug analogs are now commercially available and two of them have been thoroughly studied along with their ^{2}H -counterparts. The resulting CC data, as determined by various procedures for the secobarbital/ secobarbital-d_5 (SB/SB- d_5), secobarbital/ secobarbital - $^{13}C_4$ (SB/SB- $^{13}C_4$) systems, indeed confirmed this rationale.

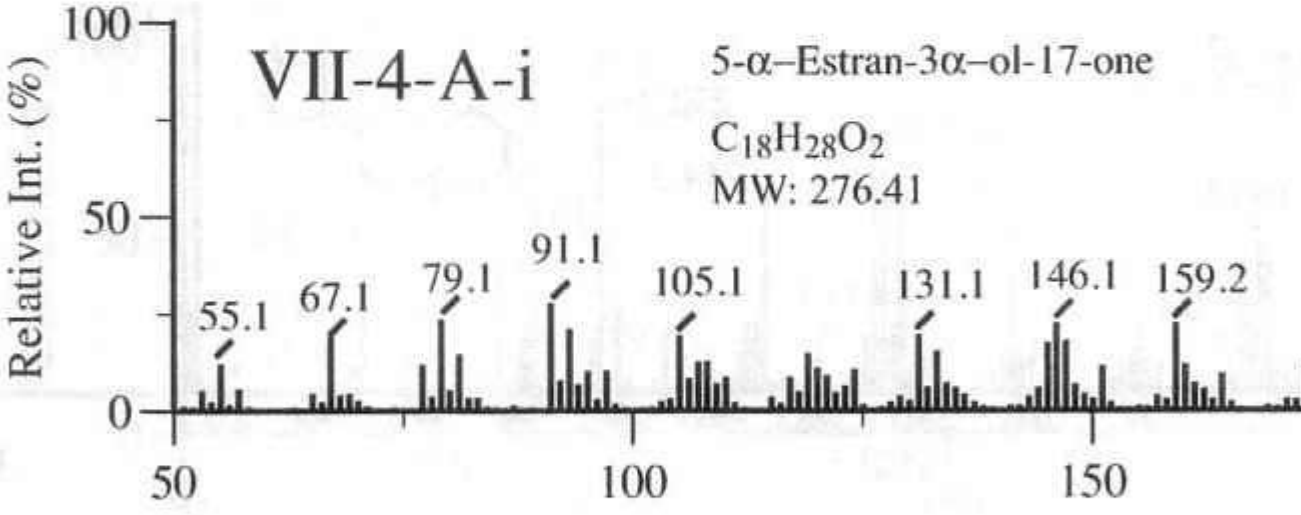
With limited availability of ^{13}C-analogs, ^{2}H -analogs are more commonly used as the ISs in routine analysis and related studies. For example, various ^{2}H -labeled analogs of amphetamine and methamphetamine, with different number of ^{2}H-atoms and positions, were evaluated for their suitability in serving as the ISs for the analysis of these two drugs. Suitability is judged primarily by the availability of three ions that are *interference free, retaining some of the drug's structural feature,* and with *relatively high mass and sufficient intensity.* Another study on this subject matter focused on evaluating the contribution (interference) of ions *m/z* 91 and 118, derived from the heptafluorobutyryl derivative of methamphetamine-d_5, -d_8, and –d_{11} to the intensities of these ions designating the analyte.

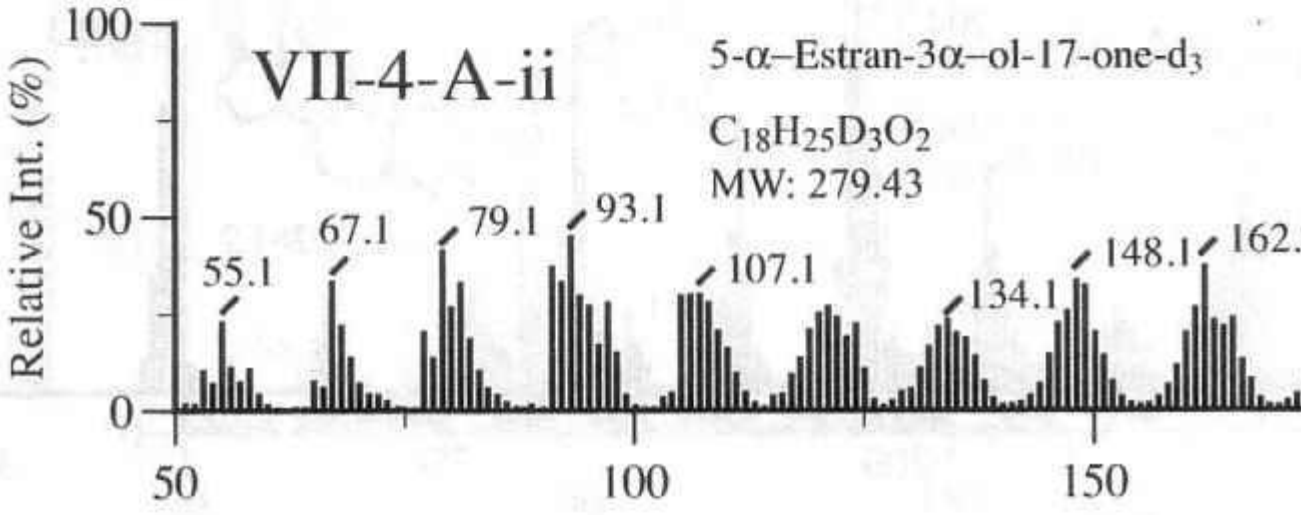
Part Two and three of the book comprises a big section of the book, and are the most valuable. Part two gives mass spectra of some commonly abused drugs and their isotopically labelled analogs in various derivatization forms. There are seven groups of mass spectra in all (referred to as figures in the book). Figure 1 gives mass spectra of stimulants, figure 2 of opioids, figure 3 of hallucinogens, figure 4 of depressants/hypnotics, figure 5 of antianxiety agents, figure 6 of antidepressants and finally figure 7 of various other drugs.

Part three describes cross-contributions of ion intensity between analytes and their isotopically labeled analogs in various derivatization forms.

The following is the mass spectra of 5-«-estran-3«-ol-17-one and its deterated analogs (page 355). Also excerpted are the mass spectra of some related compounds (pages 356 and 357). **Please click to enlarge all**.

Figure VII-4. Mass spectra of 5-α-estran-3α-ol-17-one and i
underivatized; (B) acetyl-derivatized; (C) TMS-derivatized





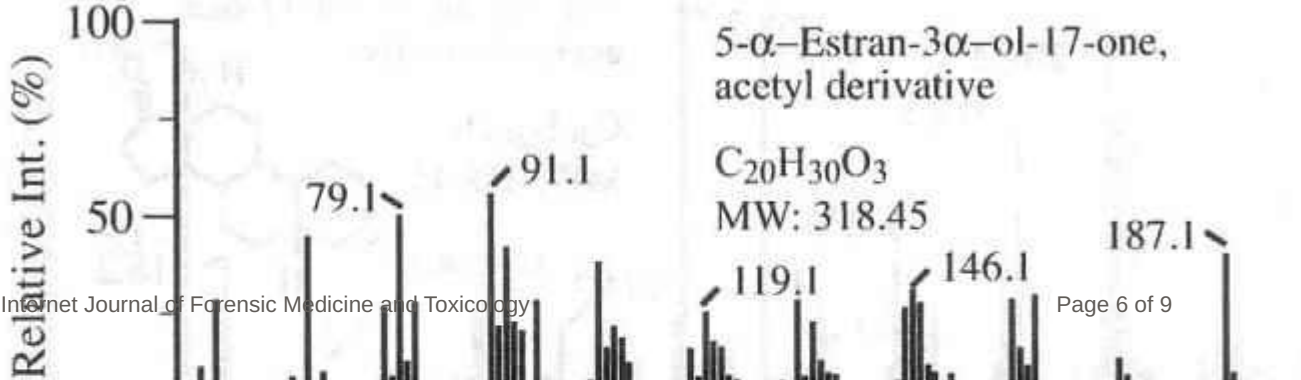
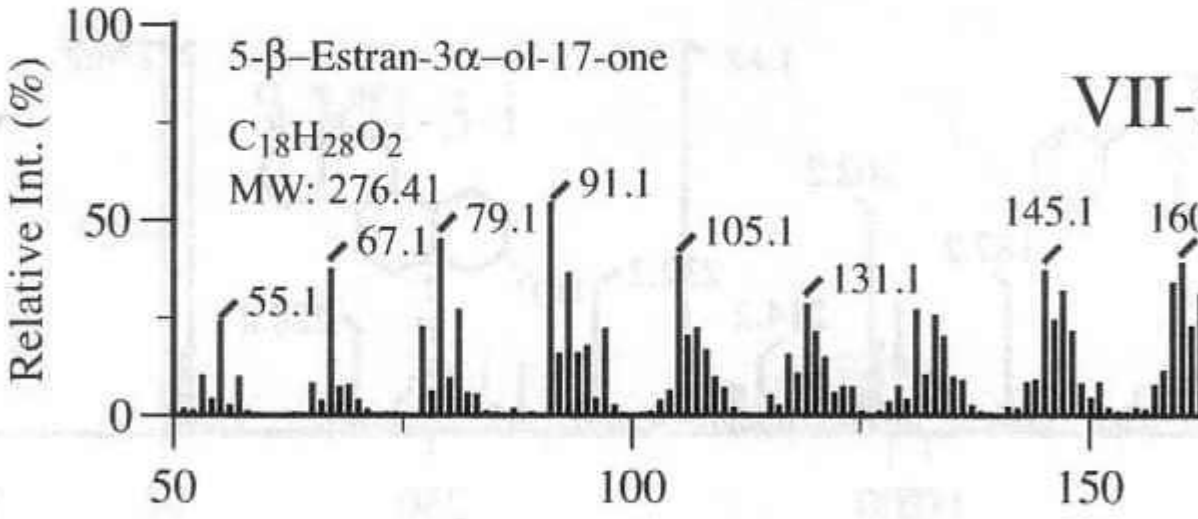
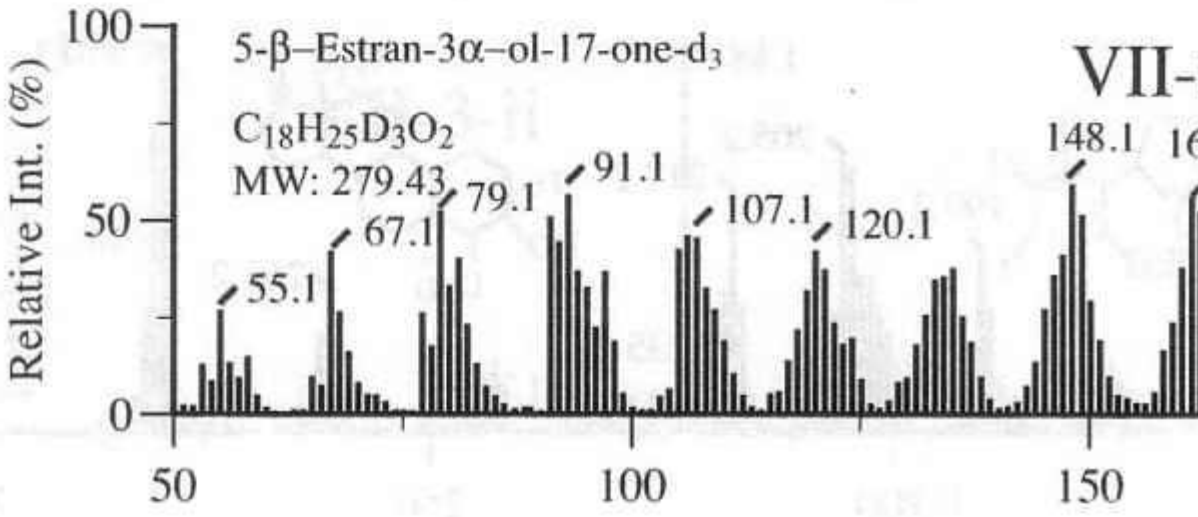


Figure VII-5. Mass spectra of 5-β-estran-3α-ol-17-one
underivatized; (B) acetyl-derivatized; (C) TMS-derivati





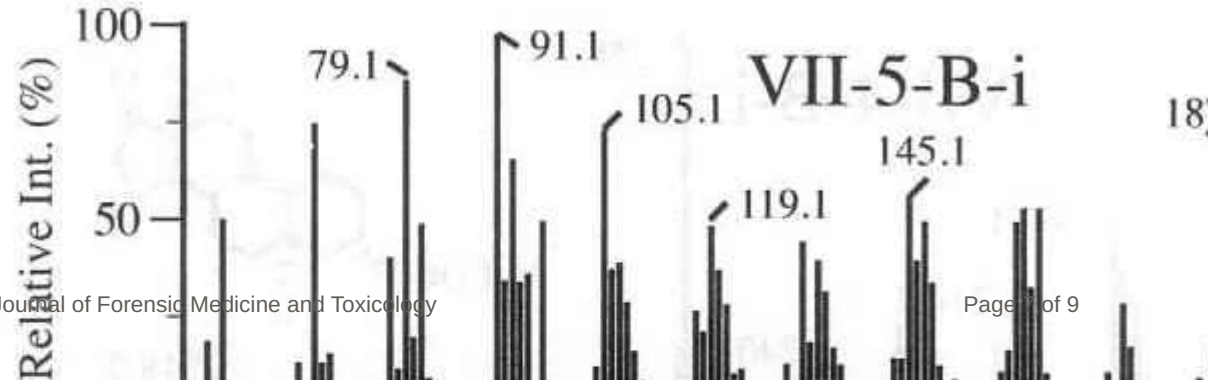
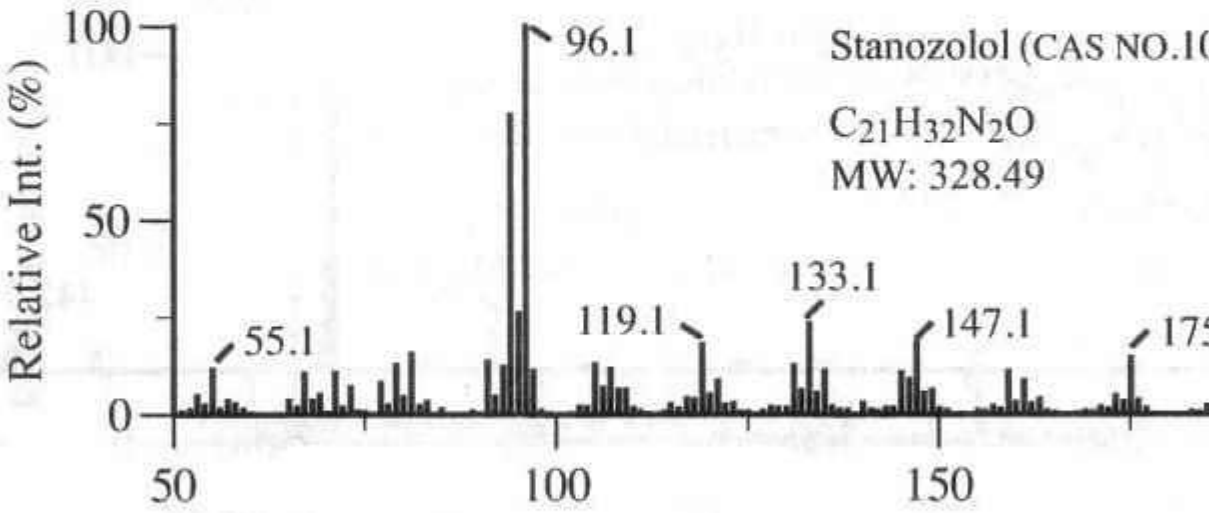
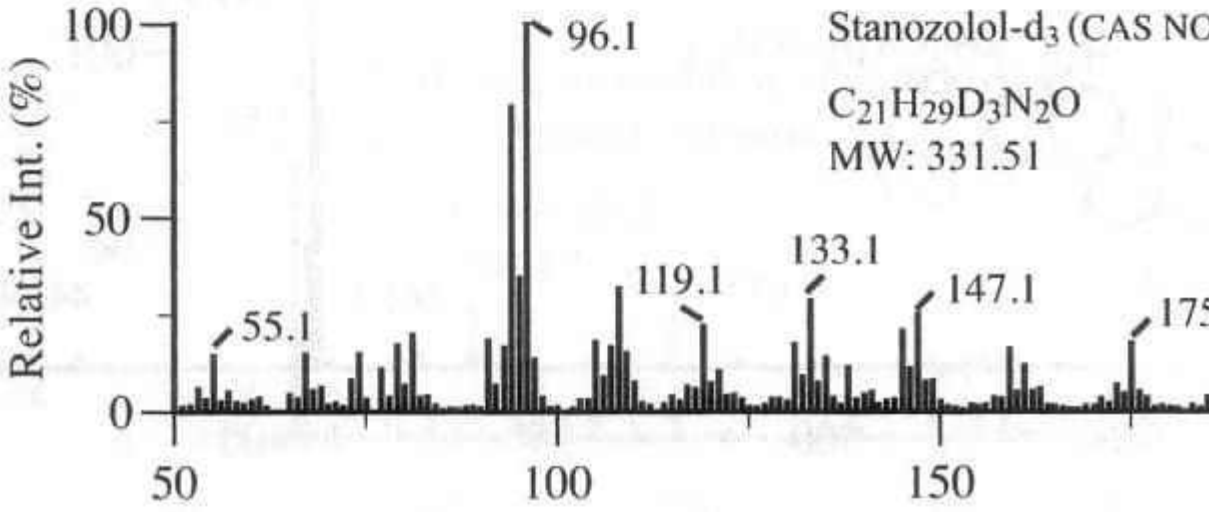
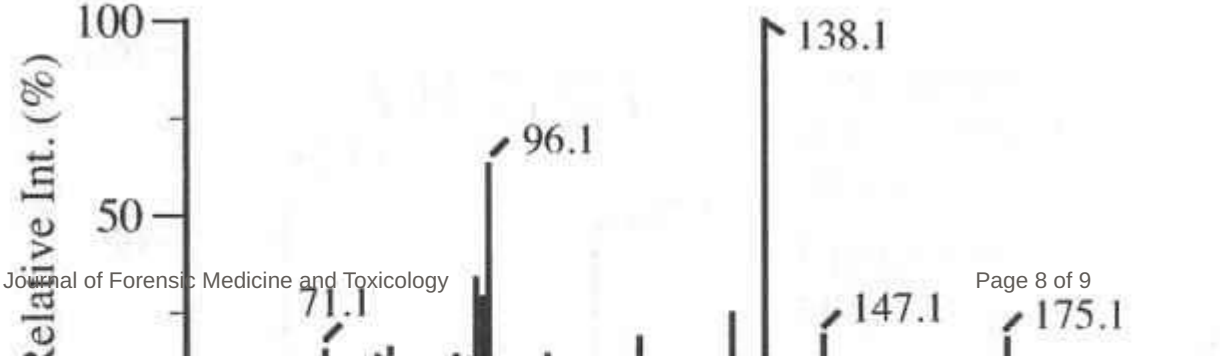


Figure VII-6. Mass spectra of stanozolol and its deutera
derivatized; (C) $[TMS]_2$-derivatized. (D) *t*-BDMS-deriva







The book gives mass spectra of several other drugs of importance. A great resource for forensic toxicologists indeed....

View this book on Amazon

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Editor's recommendation. This book is recommended by the editor.