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Review of: *Mass Spectra of Designer Drugs: Including Precursors, Medicinal Drugs and Chemical Warfare Agents*

REFERENCE: Rösner P, Junge T, Westphal F, Fritschi G. *Mass spectra of designer drugs: including drugs, chemical warfare agents, and precursors*. Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA, 2007, 2067 pp.

The title of this impressive two-volume set may not appeal to mainstream practitioners. However, the content of this compact, well-organized, and concise publication will be of tremendous use to clinical and forensic toxicologists as well as researchers. Over 5500 mass spectra of 4739 different compounds are presented—including designer drugs, narcotics, psychotropics and their metabolites, precursors, impurities, and byproducts (natural and synthetic). The text includes numerous designer drugs that have grown in popularity in Europe and are emerging as illicit substances in the United States. Many of these substances are not included in many of the commercial mass spectral databases that are widely used in forensic laboratories.

Mass spectra are clearly presented with non-proprietary name, systematic name, and legal category, including the appropriate schedule of the Federal Controlled Substances Act. Compound specific information includes the molecular weight, accurate weight of the molecular ion, and gas chromatographic retention indices for DB-1/OV-1 or equivalent capillary columns. Mass spectral quality indices are presented in two ways: a traditional Quality Index (QI) and a Verification Index (VI). The latter represents the number of mass spectral libraries in common use (Pfleger, NIST, and others) in which the mass spectrum corresponds with the reference mass spectrum with a spectral match of 90% or more. Only a small number of the entries have verification indices (<13%), which is an indication of the number of unique entries in this reference text.

In addition to the wealth of drug data the text also includes mass spectra for explosives and chemical warfare agents, including degradation products of many nerve agents. These agents are listed by name, military code, and number.

Of particular note is the inclusion of mass spectra for derivatized drugs and compounds of interest, making this an extremely useful text for toxicologists involved in method development, or academics involved in research. A wide variety of mass spectra are presented for some substances. Although the majority of spectra were obtained using electron impact (EI) ionization, positive chemical ionization (CI) data are also presented using methane as the reagent gas if the traditional EI mass spectrum does not yield a molecular ion. This inclusion makes the text a tremendous resource for practitioners of CI.

Drugs and compounds of interest are indexed alphabetically by name. The mass spectra themselves are normalized to the base peak and presented in order of ascending mass. This approach has some disadvantages. For example, if you are looking for mass spectra of morphine or one of its derivatives, you have the choice of 26 entries, listed throughout the text. The drug and its derivatives are not presented consecutively. This aside, the text is remarkably well organized and easy to navigate.

The inclusion of so many new illicit drugs, metabolites, precursors, and breakdown products; the complement of CI mass spectra; and the inclusion of mass spectra for chemical derivatives that are widely used in chromatographic analysis, makes this an essential complement to the electronic reference materials that are in widespread use.

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