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BOOK REVIEW

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Review of: *Mass Spectra of Designer Drugs 2008 CD-ROM**

REFERENCE: Roesner P. Mass spectra of designer drugs 2008. Hoboken, NJ: John Wiley & Sons, Inc., 2008, CD-ROM, ISBN 978-3-527-31899-5.

The Designer Drugs 2008 (DD2008) mass spectral library is a formidable tool for forensic drug chemists and toxicologists. Previously reviewed as Designer Drugs 2005 (DD2005; JFS, Mar. 2006, Vol. 51, No. 2), the current CD-ROM contains nearly three times as many compounds (8300) and mass spectra (9658) as the 2005 edition. Vendor-specific libraries are available on the CD-ROM for instruments from various manufacturers. This evaluation of DD2008 used the library constructed for Agilent (Hewlett-Packard) mass spectrometers. The Agilent "Data Analysis" function with "library search" was used for tentative identification of "live" samples while the "parametric retrieval" function was used for hard copies of compounds submitted by e-mail attachment as unknown mass spectra. Both functions worked very well with DD2008. Using parametric retrieval, spectral data of compounds acquired at one laboratory can be electronically transmitted as pdf, doc, or similar attachments and evaluated at another laboratory having the DD2008 database. Using this procedure, mass spectra can be identified either by mass number of the apparent molecular ion or by inputting three mass fragments and their relative intensities. However, parametric retrieval, or a similar function, may not be available for mass spectrometers from other manufacturers.

A minor shortcoming noted in the earlier review was a relatively small number of mass spectra for the tryptamine analogs. This has been remedied in the 2008 edition that now contains a substantial number of mass spectra (207) containing the tryptamine structure. A valuable feature of the previous Designer Drug (DD) versions was the large number of phenethylamine-derived substances (i.e., substituted amphetamines, butanamines, methylenedioxy analogs). The entries for this category of compounds have become even more robust, now containing over 2300 mass spectra. DD2008 also contains an impressive 257 spectra of piperazine analogs, a relatively new class of abused drugs.

Another specific area of drug identification addressed in DD2008 is that of pharmaceuticals. Often, pharmaceuticals are added to enhance or modify the effect produced by the clandestinely synthesized material. This is especially true during the tableting of illicit drugs such as 3,4-methylenedioxymethamphetamine (MDMA). Furthermore, counterfeit tablets of legitimate products that are occasionally submitted to forensic laboratories for analysis may not contain the declared active pharmaceutical ingredient (API) of the genuine product. Even in the instances where legitimate pharmaceuticals are submitted for analysis, those with unidentifiable logos or inscriptions may present a problem in identification because of lack of standards or reference materials. To aid in the identification of these compounds, DD2008 now contains 1975 mass spectra of APIs.

A further feature of this edition of Designer Drugs addresses the area of clandestine drug manufacturing operations. If a finished product is not obtained during the seizure of a clandestine laboratory, identification of precursor chemicals may be a critical factor in building a case to prosecute the clandestine chemist for intent to manufacture. DD2008 excels in this aspect of drug analysis with 446 mass spectra of DD precursors, 122 of substituted benzaldehydes, and 127 of 1-aryl-2-nitroalkenes. Two series of DD (i.e., controlled substance analogs) currently enjoying popularity are the 2,5-dimethoxy-4-substituted-phenethylamines and their alpha methyl amphetamine analogs (1) (often referred to as the "2C" and "DO" series of compounds, respectively). Synthesis of these compounds typically starts with a substituted benzaldehyde as the initial precursor. Alternatively, a number of these phenethylamines can be synthesized by reduction of the 1-aryl-2-nitroalkenes. This library has successfully identified a number of benzaldehyde and nitroalkene intermediates prepared during the in-house synthesis of the 2C and DO compounds. It was also successful in identifying some of the indoleglyoxylamides prepared as precursors to designer tryptamines.

As a practical exercise, the ability of DD2008 to identify a number of currently encountered DDs was tested with a series of compounds that were injected into the mass spectrometer. These included six compounds from the "2C" series, six from the "DO" series, one each of the bromoFLY/bromoDragonFLY series (2,3) and two tryptamine precursors. Using the library search function of the Agilent 5973 Mass Selective Detector (MSD) software, each of the compounds was successfully identified by the DD2008 library. In addition, hardcopy mass spectra of two unknowns had been submitted for identification. A parametric retrieval search based on apparent molecular weight of each compound correctly identified one drug as 1-methyl-4-benzylpiperazine and the other as 1-(3-chlorophenyl)piperazine. Agilent's format presents the mass spectrum of the "unknown" on top with the library identification appearing below it. Occasionally, the mass spectrum of the compound in question and its library identification are accompanied at the bottom of the screen by a drawing of the structure of the identified molecule. This is helpful, but only available for a limited number of molecules in the Agilent version of the library. However, it is possible to get a structural representation of the compound once its tentative identity is known by accessing http://www.chemograph.de.de/start.htm or http://designer-drugs.eu/. Right "clicking" on the name of the compound will produce the

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*Review and opinion of the reviewer do not necessarily reflect the position of the Drug Enforcement Administration.

two-dimensional drawing of the substance. Other mass spectroscopic software, such as the Thermo Scientific Excalibur™, correctly presents the library search results with the relevant structures.

The continual introduction of novel clandestinely produced drugs into the underground market contributes to the rapid obsolescence of mass spectral drug libraries. A valuable feature of the Designer Drug series of mass spectral libraries is the availability of annual upgrade supplements, thus keeping the library up to date at a fraction of the cost of buying the current issue of the software. For forensic drug chemists and toxicologists, this library excels in its ability to identify novel DDs, their precursors, and the pharmaceuticals which may accompany the drug(s) of interest.

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