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BOOK REVIEW

Terry A. Dal Cason,[1] *M.S.*

Review of: *Mass Spectra of Designer Drugs 2005*

REFERENCE: Rosner P. Mass spectra of designer drugs 2005. Hoboken, NJ: John Wiley & Sons Inc., 2005.

Although compounds that could be classified as "designer drugs" have been synthesized since the early 1980s, the last decade has seen a proliferation of these structural analogs. Keeping abreast of these new drugs is a difficult task for forensic chemists and toxicologists. *Mass Spectra of Designer Drugs 2005*, a mass spectral drug library published by John Wiley & Sons on CD-ROM, provides an additional tool to assist in the identification of a number of these compounds. The CD, as received, contained libraries for various instrumentation formats including the Agilent Chemstation (tested here), Thermo Finnigan (ICIS, INCOS, ionTrap, GCQ/TSQ/SSQ, ITS-40), Thermo Galactic, Fisons VG Masslab/LabBase, NIST/Excalibur, PE Turbomass, NetCDF, Shimadzu QP-5000, and Varian Saturn. The various library formats were located within separate directories. A brief installation manual in PDF format is also on the CD.

Prepared by Dr. Peter Rosner and his colleagues in the Regional Departments of Criminal Investigation in Germany, the library consists of 3,437 mass spectra (MS) acquired from 2,959 compounds. This number of entries is significantly larger than might be assumed from the title of the CD-ROM. The large number of "designer drug" entries results, in part, from the inclusion of commonly encountered drugs such as cocaine, heroin, morphine, caffeine, guaifenesin, etc. These drugs are typically found in the standard MS libraries such as Wiley7n.L (392,086 entries), NIST02.L (174,948 entries), or PMW-Tox3.L (6,360 entries). However, the DD2005 library consists of not only the electron impact MS of the selected compounds, but in some instances, acetyl, trifluoroacetyl, trimethylsilyl, pentafluoropropionic, or additional derivatives. The MS of drug precursors and drug "artifacts" enhanced the library and assisted in increasing the size of the "Designer Drugs 2005" database. The library also incorporated a limited number of entries of chemical ionization MS. For some drugs, such as 1-phenyl-ethylamine, more than one entry appears. Presumably, this is due to different tuning parameters used by the contributing laboratories, or to data acquisition from mass spectrometers of different manufacturers or from different models. Rosner et al. have also included a number of compounds considered to be chemical warfare agents rather than true "designer drugs." Thus the overall effect is a library with somewhat fewer individual "designer drugs" than the actual number of data entries.

DD2005.L contains an outstanding collection of ring and/or nitrogen substituted aminoacetophenones, aminopropiophenones (cathinone analogs), aminobutyrophenones, and related amino ketones up to and including the heptane side chain. A library search of several reference compounds using an Agilent 5973 MS with a standard autotune correctly identified 1-(3,4-methylenedioxyphenyl)-2-methylamino-propan-1-one (3,4-MDmethcathinone, Methylone), a compound that has recently been reported in both the Northeastern and Southwestern U.S. In addition, the *N*-ethyl and *N*,*N*-dimethyl analogs of 3,4-MDmethcathinone, as well as the *N*-ethyl, the 2-methyl-*N*-ethyl, the *N*-propyl and the *N*-isopropyl analogs of cathinone were identified in the DD2005 library. The library contains an impressive number of 2,3- and 3,4-ring and chain substituted methylenedioxyamphetamine analogs as well. It is also moderately comprehensive with respect to other phenethylamines and to drug precursors, but weaker in regard to the number of entries for ring, chain, and alkyl amine chain tryptamine analogs.

During evaluation, when DD2005 library searches did not give good "quality" matches, the mass spectral fragmentation patterns of the retrieved compounds proved to be of substantial help in elucidating a proposed identity for the "unknown" compound. For example, the DD2005 library returned an identity of *N*,*N*-diethyl-indol-3-yl-glyoxylamide having a match "quality" of 72 for an "unknown" test compound. The "unknown" was a reference standard of *N*-methyl-*N*-isopropyl-indol-3-yl-glyoxylamide. A careful comparison of the two spectra showed they were exceptionally close in structure, but not identical. Although the highest quality library match proved not to be the compound in question, the remarkable similarity of the spectra should have led an experienced analyst to suspect that the "unknown" *N*,*N*-disubstituted indole-3-glyoxylamide was likely the *N*-methyl-*N*-isopropyl or the *N*-methyl-*N*-propyl analog. Thus, even when the unknown is not in the DD2005 library, the structural similarity reflected in the fragmentation pattern of the unknown with the library "hit" may provide the analyst with a solid clue as to the identity of a new analog.

The relative instantaneous intensity of the mass fragments can change over the time interval of sample collection. Improved library matches can sometimes be achieved by reviewing a number of individual sequential acquisition time "slices" of the chromatogram, rather than either just the apex or a contiguous average of slices. Occasionally, applying background subtraction for the mass spectrum of the unknown provided better correlation ("quality") with the DD2005 library.

[1] Drug Enforcement Administration, U.S. Department of Justice, Chicago, IL 60605–1526.

The review copy of the CD also contained a library of chemical structures accessible from the file DD2005.MOL within the directory MSP. "Entry" numbers and their chemical designations accompany the mass spectral matches that result from library searches. These "entry" numbers will permit retrieval of the appropriate chemical structures, provided a chemical structure editor is resident on the hard drive. Since the library entries are assigned by number, rather than by chemical name, it was not possible to retrieve a spectrum using a name search, something that could be a potentially useful feature. Upon request, Wiley will provide a list of the library entries by name and number, thus allowing indirect name retrieval of the structural drawing. The MSP directory also included an installer package (DD2005.msp), but it could not be opened and, therefore, the program was not installed and evaluated. Use of this feature requires third party software that is not part of the DD2005 package.

The DD2005 CD will permit a structure database to be configured by the user that does allow retrieval of the chemical structure along with the mass spectrum. However, the instructions to accomplish this are found in an Agilent Technologies article "Configuring a Structure Database" not included on the CD. Wiley will provide copies of this article if requested.