

Identification of Essential Oil Components by Gas Chromatography / Mass Spectroscopy

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Allured Publishing Corporation

Carol Stream, IL, 60188, USA

1995, \$95 Book, \$395 Book & Disk, 469 pp.

ISBN 0-931710-42-1

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Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy is a collection of electron ionization mass spectra acquired on a Finnigan ITD-800 quadrupole ion trap mass spectrometer along with DB-5 retention time data. The data are presented as bar-graph spectra and are also available in electronic format for a variety of different gas chromatography/mass spectrometry (GC/MS) data system library search routines. The printed format has spectra of 1211 compounds, and the electronic format has 1252 spectra.

Although not reflected in the title, the author clearly states in the Preface that this is the second edition of a previous publication entitled *Identification of Essential Oils by Ion Trap Mass Spectrometry* (Academic, San Diego, CA, 1989; ISBN: 0-12-044230-2). The primary differences are the availability of an electronic format from the publisher, more than twice as many compounds (the first edition contained 502 spectra), and the arrangement of the spectra by retention time, rather than in alphabetical order, in an attempt to make the book more useful in the identification of these compounds as they are found in analytical samples.

The book is divided into two parts: 1) "Ion Trap Mass Spectrometry" with five sections, and 2) "Appendices," which includes the database arranged by various sorts of orders. The "Ion Trap Mass Spectrometry" section is almost verbatim a repeat of the text in the section of the same title in the previous edition. In an attempt to explain some spectral anomalies, the author presents information about ion trap mass spectrometry that is not consistent with what is known today. For the most part, the spectra in this collection do not differ substantially from those that could be obtained on a beam-type instrument. The explanations of ion trap mass spectrometry are the only real weak points of the book, and readers should be cautioned not to rely on them in understanding ion trap mass spectrometry or the spectral anomalies that may be observed when these types of instruments are used to generate electron ionization mass spectra. In addition, these explanations do not take into account changes that have occurred in currently available instrumenta-

tion, nor the increased understanding of how they should be operated.

The "Appendices" consist of an alphabetical listing of compounds (mostly common names) with their retention times and Kovat's index on a DB-5 capillary GC column. This is followed by a listing of the compounds arranged in increasing retention time order. Following the presentation of the bar-graph spectra is a cross index of common names. This listing only gives references to other names used in the database with no referenced page numbers or retention times. In order to find the spectrum of a compound whose synonym appears in this index, the listing name must be found in the alphabetical index in order to retrieve the retention time, which is necessary to locate the spectrum. This seems to be a little awkward.

The bar-graph spectra are nicely presented three per page along with structures of compounds with indications of stereochemistry where appropriate. In addition to the name, DB-5 retention time, and Kovat's index, the compound's Chemical Abstracts Service (CAS) registry number, empirical formula, formula weight (nominal mass), library entry number for the electronic format, and a list of synonyms are provided.

One of the things that sets this collection of mass spectra apart from others that have been published is that the gas chromatographic and mass spectrometric conditions under which the data were acquired is meticulously documented. The format of the spectral presentations is carefully annotated in the "Ion Trap Mass Spectrometry" section.

The collection of compounds of interest to the essential oil chemist that have been amassed for this work is outstanding; however, by the author's own admission, "Unfortunately, several compounds are not in the [database] because we could not obtain authentic reference compounds." Just as unfortunately, a list of these compounds is not included in the book.

The electronic format of the data does not contain the same level of annotation that is available in the printed format. The "name" field includes the compound name and the DB-5 retention time. The only other information contained in the electronic format is the empirical formula and the molecular weight (nominal mass) of the compound. The electronic library was assembled using the ITD-800 data system software, which does not allow for the inclusion of additional information such as structures, CAS registry numbers, and synonyms. It is not stated whether the spectra in the printed format were taken from a display of the electronic library spectrum or from the data file before adding the spectrum to the library. The significance of this information has to do with the INCOS algorithm for building a mass spectral library in the ITD-800 software. This algorithm performs a condensation on the spectrum to be entered into the library so that no

more than 50 peaks are in any spectrum. While this has little effect on the ability to identify a compound by matching its spectrum with the corresponding spectrum in the library, it can cause some visual confusion. Of course, if the spectrum has fewer than 50 peaks before its addition to the library, it will have the same number of peaks when added to the library. Since all the different instrument manufacturers' electronic formats of this database were produced by converting the ITD-800 library, any spectral condensation will be carried over to these formats.

Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy is a valuable collection of mass spectra for anyone working with essential oils. It should be available in any laboratory, both as the printed and electronic formats, using GC/MS for the analysis of these types of compounds. This is the first time that a publication of this type has essentially made full spectra available in electronic format as well as the printed format. Both the author and publisher should be congratulated on this publication.