

**IDENTIFICATION OF  
ESSENTIAL OIL COMPONENTS BY  
GAS CHROMATOGRAPHY/  
MASS SPECTROMETRY, 5th Ed. (online)**

**Dr. ROBERT P. ADAMS**

**Professor**

**Biology Department  
Baylor University**

**Texensis Publishing  
Gruver, TX USA  
2017**

Neither this book nor any part may be reproduced or transmitted in any  
from by any means, electronic or mechanical, including photocopying,  
microfilming and recording, or by any information storage retrieval  
system without the permission in writing from the publisher.

5th Ed. online, 2017  
Copyright 2017 - All Rights Reserved

Texensis Publishing  
Gruver, TX UDA

ISBN 978-0-9981557-2-2

## CONTENTS

### *Preface*

vii

### ***PART A GAS CHROMATOGRAPH/MASS SPECTROSCOPY***

<b>I</b>	<b>Introduction</b>	1
<b>II.</b>	<b>Nomenclature</b>	1
<b>III.</b>	<b>Mass Spectrometry Considerations</b>	2
	A. Obtaining Quality Spectra for Identification	2
	B. The Role of Retention Times in Library Searches	3
<b>IV.</b>	<b>Operating Conditions Used for Spectra Acquisition</b>	4
<b>V.</b>	<b>Compatibility with Mass Spectrometer Data Systems</b>	5
<b>VI.</b>	<b>Explanations of Formats Used in Appendices</b>	6
<b>VII.</b>	<b>References</b>	7

### ***PART B APPENDICES***

<b>I</b>	<b>Alphabetical Listing of Compounds with Their Retention Time and Arithmetic Retention Index on DB-5</b>	9
<b>II</b>	<b>Compounds Listed in Order of Their Retention Time and Arithmetic Index on DB-5</b>	31
<b>III</b>	<b>Mass Spectra and Structures of Compounds Listed in Order of Their Retention Time/Arithmetic Index on DB-5</b>	53
<b>IV</b>	<b>Cross Index of Common Names</b>	698

## Preface

This is the fifth edition on mass spectra and retention times of common components in plant essential oils. It differs from the previous in edition that this is the first online edition. All of the compounds have been analyzed on an HP5970 MSD mass spectrometer using HP Chemstation software. I hope it will be a useful as a tool for the identification of compounds in this format. In addition, the library (including retention times) is available for the most common mass spectrometer/ computer systems. Changes in technology allow us to make this available now. For instance, when I began research on essential oils in 1966, a major portion of my thesis work involved the identification of components in Juniperus by IR spectra. Of course that involved cold trapping compounds as they eluted from the TC detector on GC. With current mass spectrometers, we can now accomplish in a couple of hours the analysis that took months or years. This book is an outgrowth of the previous books (*Identification of Essential Oils by Ion Trap Mass Spectroscopy*, Academic Press, 1989; *Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy*, Allured Publishing, 1995), but its roots reach back to 1976 when I took a sabbatical study with Ernst von Rudloff and Lawrence Hogge at the National Research Council of Canada. Our collaborative efforts yielded numerous mass spectra on their quadrupole mass spectrometer. Later, as I visited with colleagues in chemical ecology, I began to appreciate the library that I had assembled. So this book is an outgrowth of much collaboration, starting with Ernst von Rudloff and now reaching around the world. I owe a special debt of thanks to colleagues who unselfishly sent samples of oils, mass spectra, marked chromatograms, and even purified compounds. These colleagues include: E. A. Aboutabl, Egypt; Aldrich Chemical Co., USA; J. Altarjos, Spain; Applied Science Co., USA; A. Badoc, France; A; J. Barroso, Portugal; K. H.C. Baser, Turkey; A. F. Barrero, Spain; J. Berlin, Germany; H. Bussenius, Haiti; J. J. Brophy, Australia; E.-J. Brunke, Symrise GmbH & Co. (formerly Dragoco), Germany; J. L. R. Canavate, Spain; R. M. Carman, Australia; J. Casanova, France; F. M. Chaudary, Pakistan; T. S. Chamblee, Coca Cola Co., USA; A. Chaintreau, Nestec, Switzerland; J. C. Chalchat, France; M. Chien, Givaudan, USA; G. Collin, Canada; D. Clark, New Zealand; L. Cool, USA; A. Cornat, France; A. A. Craveiro, Brazil; W. Cretney, Canada; R. Croteau, USA; Jian-Qin Cu, China; C. Demetzos, Greece; H. De Pooter, Belgium; M. Deyrup, USA; V. Dev, USA; R. P. Doss, USA; V. Dragar, Australia; G. Dugo, Italy; L. Doimo, Australia; F. S. El-Ferally, Saudi Arabia; G. Elzen, USA; W. W. Epstein, USA; N. Fisher, Germany; R. Estell, USA; Z. Fleisher, Crompton & Knowles, USA; C. Franz, France; R. P. Garry, France; S. Geribaldi, France; K. Gollnick, Germany; J. Hafizoglu, Turkey; K. J. Harkiss, England; C. Harvala, Greece; S. Hasegawa, Japan; A. R. Hayman, New Zealand; E. Hethelyi, Hungary; H. G. Hills, USA; J. Hendrickson, USA; L. Hogge, Canada; G. Honda, Japan; M. Ito, Japan; P. Joseph-Nathan, Mexico; D. Joulain, France; A. J. Kahn, USA; W. A. Konig, Germany; S. Kral, IFF, USA; J. Langenheim, USA; D. Lamparsky, Givaudan, Switzerland; A. Lara, Spain; B. M. Lawrence, USA; N. G. Lewis, USA; M. Maffei, Italy; M. L. Maheshwari, India; C. S. Mathela, India; C. A. McDaniel, USA; B.Y. Meklati, Algeria; A. Michet, France; C. Menut, France; L. N. Mishra, India; D. McMahon, Union Carbide Corp., USA; K. Moriai, Japan; M. G. Moshonas, USA; R. D. H. Murray, Scotland; S. Nagahama, Japan; K. R. Neisess, USA; I. Nykanen, Finland; J. Oda, Japan; T. H. Ohaski, Japan; S. Park, USA; F. Perineau, France; W. Phillips, USA; G. Prestwich, USA; R. A. Raguso, USA; P. Raharivelomanana, France; P. Richomme, France; B. Rodriguez, Spain; V. Roussis, Greece; A. San Feliciano, Spain; J. J. C. Scheffer, Netherlands; R. Scheffrahn, USA; G. Schmaus, Symrise GmbH & Co. (formerly Dragoco), Germany; N. Sellier, France; D. Senalik, USA; S. Shatar, Mongolia; H. Shiota, Japan; E. Silva, Mexico; I. Southwell, Australia; E. Stahl-Biskup, Germany; R. Stipanovic, USA; A. B. Svendsen, Netherlands; A. Tara, Italy; A. Tenaglia, France; R. S. Thakur, India; R. K. Thappa, India; A. F. Thomas, Firmenich, Switzerland; M. Toyoota, Japan; R. R. Trenkle, IFF, USA; A. O. Tucker, USA; A. Ulubelen, Turkey; T. A. van Beek, Netherlands; A. Velasco-Negueruela, Spain; J. P. Vidal, France; O. Vostrowsky, Germany; G. J. Wagner, USA; P. Waterman, U.K.; R. Weavers, New Zealand; H. Weyerstahl, Germany; P. Weyerstahl, Germany; P. T. White, USA; M. Whitten, USA; H. J. Woerdenbag, Netherlands; K. C. Wong, Malaysia; Xu Ji-Qing, China; Xiaobing Yu, China; P. Yates, Canada; Y. Yuesa, Japan; T. A. Zanoni, USA; M. G. B. Zoghbi, Brazil; J. A. Zygaldo, Argentina; and J. H. Zwaving, Netherlands.

Special thanks Maarten Posthumus who faithfully sent me typo and structural errors from previous editions and printings. His keen eyes and cooperative spirit have been important in producing this book.

Thanks to Tonya Yanke, Lou Garrett, Madeline Reed and Ryan Perez for assistance with word processing and drawing structures. Also thanks to several young students who helped: Carlos Borunda, Blake Fitzgerald and Ryan Remick.

Finally, I would like to thank my wife, Janice, for her patience and encouragement.