

Wiley Series on Pharmaceutical Science and Biotechnology:  
Practices, Applications, and Methods  
Mike S. Lee, Series Editor

# MASS SPECTROMETRY HANDBOOK

EDITED BY  
MIKE S. LEE

 WILEY

Copyright © 2012 by John Wiley & Sons, Inc. All rights reserved.

Published by John Wiley & Sons, Inc., Hoboken, New Jersey.  
Published simultaneously in Canada.

No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, scanning, or otherwise, except as permitted under Section 107 or 108 of the 1976 United States Copyright Act, without either the prior written permission of the Publisher, or authorization through payment of the appropriate per-copy fee to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, (978) 750-8400, fax (978) 750-4470, or on the web at [www.copyright.com](http://www.copyright.com). Requests to the Publisher for permission should be addressed to the Permissions Department, John Wiley & Sons, Inc., 111 River Street, Hoboken, NJ 07030, (201) 748-6011, fax (201) 748-6008, or online at <http://www.wiley.com/go/permissions>.

**Limit of Liability/Disclaimer of Warranty:** While the publisher and author have used their best efforts in preparing this book, they make no representations or warranties with respect to the accuracy or completeness of the contents of this book and specifically disclaim any implied warranties of merchantability or fitness for a particular purpose. No warranty may be created or extended by sales representatives or written sales materials. The advice and strategies contained herein may not be suitable for your situation. You should consult with a professional where appropriate. Neither the publisher nor author shall be liable for any loss of profit or any other commercial damages, including but not limited to special, incidental, consequential, or other damages.

For general information on our other products and services or for technical support, please contact our Customer Care Department within the United States at (800) 762-2974, outside the United States at (317) 572-3993 or fax (317) 572-4002.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic formats. For more information about Wiley products, visit our web site at [www.wiley.com](http://www.wiley.com).

***Library of Congress Cataloging-in-Publication Data:***

Mass spectrometry handbook / edited by Mike S. Lee.

p. cm.

Includes index.

ISBN 978-0-470-53673-5 (cloth)

1. Mass spectrometry—Handbooks, manuals, etc. I. Lee, Mike S., 1960–

QD96.M3M36 2012

543'.65—dc23

2011034171

Printed in the United States of America.

ISBN: 9780470536735

10 9 8 7 6 5 4 3 2 1

# CONTENTS

<b>FOREWORD</b>	<b>xi</b>
<b>PREFACE</b>	<b>xiii</b>
<b>CONTRIBUTORS</b>	<b>xvii</b>
<b>SECTION I BIOTECHNOLOGY/PROTEINS</b>	<b>1</b>
<b>1 Targeted Proteomics Using Immunoaffinity Purification</b>	<b>3</b>
<i>Karen R. Jonscher, Lei Jin, John C. Cambier, Shaikh M. Rahman, and Jacob E. Friedman</i>	
<b>2 Mass Spectrometry-Based Methods to Investigate Posttranslational Protein Modifications by Lipid Peroxidation Products</b>	<b>23</b>
<i>Navin Rauniyar and Laszlo Prokai</i>	
<b>3 Imaging Mass Spectrometry (IMS) for Biological Application</b>	<b>41</b>
<i>Yuki Sugiura, Ikuko Yao, and Mitsutoshi Setou</i>	
<b>4 Methodologies for Identifying Microorganisms and Viruses by Mass Cataloging of RNAs</b>	<b>85</b>
<i>George W. Jackson, Rafal Drabek, Mithil Soni, Roger McNichols, Richard C. Willson, and George E. Fox</i>	
<b>SECTION II PHARMACEUTICAL</b>	<b>107</b>
<b>5 Preclinical Pharmacokinetics: Industrial Perspective</b>	<b>109</b>
<i>Ayman El-Kattan and Manthena Varma</i>	
<b>6 LC-MS in Drug Metabolism and Pharmacokinetics: A Pharmaceutical Industry Perspective</b>	<b>119</b>
<i>Wenyong Jian, Wilson Shou, Richard W. Edom, Naidong Weng, and Mingshe Zhu</i>	
<b>7 Quantitative Mass Spectrometry in Support of Pharmacokinetic Studies</b>	<b>171</b>
<i>Xiaoying Xu, Wenkui Li, and Francis L.S. Tse</i>	

<b>8</b>	<b>Determination of Pharmacokinetic Parameters by HPLC-MS/MS and UPLC-MS/MS</b>	<b>191</b>
	<i>Margrét Thorsteinsdóttir, Baldur Bragi Sigurðsson, and Gísli Bragason</i>	
<b>9</b>	<b>Methods for Screening Enantioselective Interactions in the Solution Phase Using ESI-MS</b>	<b>209</b>
	<i>Kevin A. Schug</i>	
<b>10</b>	<b>Hydrogen/Deuterium Exchange Mass Spectrometry (HDX MS) in the Studies of Architecture, Dynamics, and Interactions of Biopharmaceutical Products</b>	<b>227</b>
	<i>Igor A. Kaltashov, Cedric E. Bobst, and Rinat R. Abzalimov</i>	
<b>11</b>	<b>TOF-SIMS Applications to Bioimaging and Biomolecule Evaluation Methods</b>	<b>243</b>
	<i>Satoka Aoyagi</i>	
<b>12</b>	<b>Accelerator Mass Spectrometry in Pharmaceutical Development</b>	<b>259</b>
	<i>Benjamin J. Stewart, Graham Bench, Bruce A. Buchholz, Kurt W. Haack, Michael A. Malfatti, Ted J. Ognibene, and Kenneth W. Turteltaub</i>	
<b>SECTION III CLINICAL ANALYSIS</b>		<b>271</b>
<b>13</b>	<b>Mass Spectrometry in Clinical Analysis: Screening for Inborn Errors in Metabolism</b>	<b>273</b>
	<i>Donald H. Chace</i>	
<b>14</b>	<b>Mass Spectrometry for Steroid Analysis</b>	<b>297</b>
	<i>William J. Griffiths, Michael Ogundare, Anna Meljon, and Yuqin Wang</i>	
<b>SECTION IV FORENSICS</b>		<b>339</b>
<b>15</b>	<b>Forensic Applications of Isotope Ratio Mass Spectrometry</b>	<b>341</b>
	<i>Sarah J. Benson</i>	
<b>16</b>	<b>Analysis of Triacetone Triperoxide Explosive by Mass Spectrometry</b>	<b>373</b>
	<i>Michael E. Sigman and C. Douglas Clark</i>	
<b>SECTION V SPACE EXPLORATION</b>		<b>389</b>
<b>17</b>	<b>Mass Spectrometry in Solar System Exploration</b>	<b>391</b>
	<i>Paul V. Johnson, Luther W. Beegle, and Isik Kanik</i>	
<b>18</b>	<b>Application of GC × GC–TOFMS to the Characterization of Extraterrestrial Organic Matter</b>	<b>407</b>
	<i>Jonathan S. Watson</i>	
<b>SECTION VI HOMELAND SECURITY</b>		<b>417</b>
<b>19</b>	<b>Methods of Mass Spectrometry in Homeland Security Applications</b>	<b>419</b>
	<i>Ünige A. Laskay, Erin J. Kaleta, and Vicki H. Wysocki</i>	

<b>20</b>	<b>Homeland Security</b>	<b>441</b>
	<i>Christina L. Crawford and Herbert H. Hill, Jr.</i>	
<b>21</b>	<b>Mass Spectrometry in Homeland Security</b>	<b>477</b>
	<i>Yasuaki Takada</i>	
<b>22</b>	<b>Measurements of Surface Contaminants and Sorbed Organics Using an Ion Trap Secondary Ion Mass Spectrometer</b>	<b>491</b>
	<i>Gary S. Groenewold, Anthony D. Appelhans, Garold L. Gresham, and John E. Olson</i>	
<b>23</b>	<b>Determination of Actinides: Determination of Low-Concentration Urine Uranium 235/238 Isotope Ratios</b>	<b>509</b>
	<i>R. Steven Pappas</i>	
	<b>SECTION VII FOOD ANALYSIS</b>	<b>529</b>
<b>24</b>	<b>Mass Spectrometry in Agriculture, Food, and Flavors: Selected Applications</b>	<b>531</b>
	<i>Maciej Stobiecki, Piotr Kachlicki, and Henryk Jeleń</i>	
<b>25</b>	<b>Top-Down Proteomic Identification of Protein Biomarkers of Food-Borne Pathogens Using MALDI-TOF-TOF-MS/MS</b>	<b>559</b>
	<i>Clifton K. Fagerquist and Omar Sultan</i>	
	<b>SECTION VIII ENVIRONMENTAL</b>	<b>575</b>
<b>26</b>	<b>Determination of Dithiocarbamate Fungicides in Food by Hydrophilic Interaction Liquid Chromatography/Mass Spectrometry</b>	<b>577</b>
	<i>Wolfgang Schwack</i>	
<b>27</b>	<b>Disinfectant and By-Product Analysis in Water Treatment by Membrane Introduction Mass Spectrometry</b>	<b>593</b>
	<i>Chongzheng Na and Terese M. Olson</i>	
<b>28</b>	<b>Proton Transfer Reaction Mass Spectrometry (PTR-MS)</b>	<b>605</b>
	<i>Yujie Wang, Chengyin Shen, Jianquan Li, Haihe Jiang, and Yannan Chu</i>	
<b>29</b>	<b>Determination of Chlorinated Compounds in Dialysis Water and in Biological Fluids/Matrices</b>	<b>631</b>
	<i>Diana Poli</i>	
	<b>SECTION IX GEOLOGICAL</b>	<b>645</b>
<b>30</b>	<b>Mass Spectrometry Techniques for Analysis of Oil and Gas Trapped in Fluid Inclusions</b>	<b>647</b>
	<i>Simon C. George, Herbert Volk, and Adriana Dutkiewicz</i>	
<b>31</b>	<b>LA-MC-ICP-MS Applied to U-Pb Zircon Geochronology</b>	<b>675</b>
	<i>Alain Cocherie and Michèle Robert</i>	
<b>32</b>	<b>Hydrocarbon Processing</b>	<b>707</b>
	<i>Maoqi Feng, Thomas Andrews, and Eloy Flores III</i>	

<b>33 Hydrocarbon Processing: MALDI-MS of Polydisperse Hydrocarbon Samples</b>	<b>725</b>
<i>Alan A. Herod</i>	
<b>34 Renewable Energy: Mass Spectrometry in Biofuel Research</b>	<b>749</b>
<i>Ingvar Eide and Kolbjørn Zahlse</i>	
<b>SECTION X ARCHAEOLOGY</b>	<b>763</b>
<b>35 Mass Spectrometry in Archaeology</b>	<b>765</b>
<i>Robert Hedges and James McCullagh</i>	
<b>36 Archaeometric Data from Mass Spectrometric Analysis of Organic Materials: Proteins, Lipids, Terpenoid Resins, Lignocellulosic Polymers, and Dyestuff</b>	<b>797</b>
<i>Maria Perla Colombini, Francesca Modugno, and Erika Ribechini</i>	
<b>37 Laser Ablation ICP-MS in Archaeology</b>	<b>829</b>
<i>Hector Neff</i>	
<b>38 Spatially Resolved MS in the Study of Art and Archaeological Objects</b>	<b>845</b>
<i>Giuseppe Spoto</i>	
<b>39 Laser Ablation–Inductively Coupled Plasma Mass Spectrometry for the Investigation of Archaeological Samples</b>	<b>859</b>
<i>Martín Resano, Esperanza García-Ruiz, and Frank Vanhaecke</i>	
<b>SECTION XI SURFACE ANALYSIS</b>	<b>885</b>
<b>40 Mass Spectrometry in Semiconductor Research</b>	<b>887</b>
<i>Stefan Flege and Wolfgang Ensinger</i>	
<b>41 Analysis of Thin and Thick Films</b>	<b>943</b>
<i>Philippe Le Coustumer, Patrick Chapon, Agnès Tempez, Yuriy Popov, George Thompson, Igor Molchan, Nicolas Trigoulet, Peter Skeldon, Antonino Licciardello, Nunzio Tuccitto, Ivan Delfanti, Katrin Fuhrer, Marc Gonin, James Whitby, Markus Hohl, Christian Tanner, Nerea Bordel Garcia, Lara Lobo Revilla, Jorge Pisonero, Rosario Pereiro, Cristina Gonzalez Gago, Alfredo Sanz Medel, Mihai Ganciu Petcu, Ani Surmeian, Constantin Diplasu, Andreea Groza, Norbert Jakobowski, Roland Dorka, Stela Canulescu, Johann Michler, Philippe Belenguer, Thomas Nelis, Abdellatif Zahri, Philippe Guillot, Laurent Thérèse, Arnaud Littner, Richard Vaux, Julien Malherbe, Frédéric Huneau, Fred Stevie, and Hugues François-Saint-Cyr</i>	
<b>42 SIMS for Organic Film Analysis</b>	<b>961</b>
<i>Taoufiq Mouhib and Arnaud Delcorte</i>	
<b>43 Ceramics: Contribution of Secondary Ion Mass Spectrometry (SIMS) to the Study of Crystal Chemistry of Mica Minerals</b>	<b>1017</b>
<i>Luisa Ottolini, Emanuela Schingaro, and Fernando Scordari</i>	
<b>SECTION XII POLYMERS</b>	<b>1061</b>
<b>44 ETV-ICPMS for Analysis of Polymers</b>	<b>1063</b>
<i>Maite Aramendia Marzo, Martín Resano, and Frank Vanhaecke</i>	

<b>45 Polymers</b>	<b>1079</b>
<i>Maurizio S. Montaudou and Salvatore Battiato</i>	
<b>46 Mass Spectroscopy in Polymer Research</b>	<b>1107</b>
<i>Jale Hacaloglu and Talat Yalcin</i>	
<b>47 Laser Mass Spectrometry Applied to the Analysis of Polymers</b>	<b>1135</b>
<i>Jérôme Bour and David Ruch</i>	
<b>SECTION XIII ANALYTICAL TECHNIQUES</b>	<b>1143</b>
<b>48 Measuring Thermodynamic Properties of Metals and Alloys</b>	<b>1145</b>
<i>Evan H. Copland and Nathan S. Jacobson</i>	
<b>49 High-Performance Thin-Layer Chromatography–Mass Spectrometry for Analysis of Small Molecules</b>	<b>1181</b>
<i>Gertrud E. Morlock</i>	
<b>50 Laser Ionization Mass Spectrometry of Inorganic Ions</b>	<b>1207</b>
<i>Julius Pavlov and Athula B. Attygalle</i>	
<b>51 Mass Spectrometry in the SSITKA Studies</b>	<b>1229</b>
<i>L.G. Pinaeva, E.M. Sadovskaya, A.P. Suknev, V.B. Goncharov, and B.S. Bal'zhinimaev</i>	
<b>52 Proton Transfer Reaction Mass Spectrometry: Applications in the Life Sciences</b>	<b>1257</b>
<i>Elena Crespo, Marco M.L. Steeghs, Simona M. Cristescu, and Frans J.M. Harren</i>	
<b>INDEX</b>	<b>1283</b>