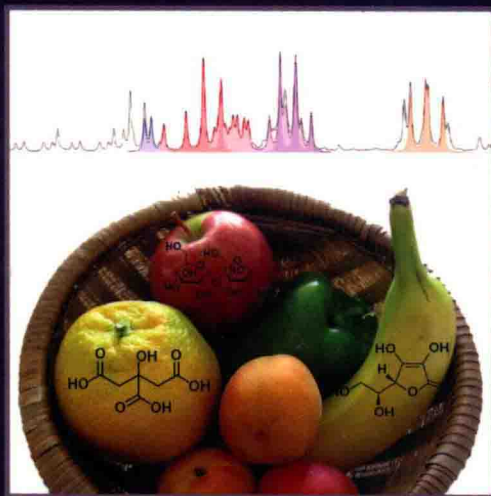


WOODHEAD PUBLISHING SERIES IN FOOD SCIENCE, TECHNOLOGY AND NUTRITION



Metabolomics in food and nutrition

Edited by Bart C. Weimer and Carolyn Slupsky

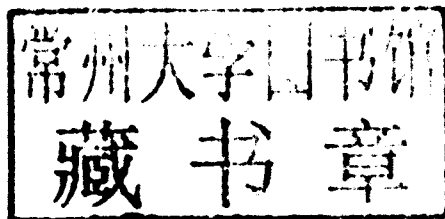
WP
WOODHEAD
PUBLISHING

Woodhead Publishing Series in Food Science, Technology and Nutrition:
Number 251

Metabolomics in food and nutrition

Edited by

Bart C. Weimer and Carolyn Slupsky



WP

WOODHEAD
PUBLISHING



Oxford Cambridge Philadelphia New Delhi

Published by Woodhead Publishing Limited,
80 High Street, Sawston, Cambridge CB22 3HJ, UK
www.woodheadpublishing.com
www.woodheadpublishingonline.com

Woodhead Publishing, 1518 Walnut Street, Suite 1100, Philadelphia, PA 19102-3406, USA

Woodhead Publishing India Private Limited, 303, Vardaan House, 7/28 Ansari Road, Daryaganj,
New Delhi – 110002, India
www.woodheadpublishingindia.com

First published 2013, Woodhead Publishing Limited

© Woodhead Publishing Limited, 2013. The publisher has made every effort to ensure that permission for copyright material has been obtained by authors wishing to use such material. The authors and the publisher will be glad to hear from any copyright holder it has not been possible to contact.

The authors have asserted their moral rights.

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission, and sources are indicated. Reasonable efforts have been made to publish reliable data and information, but the authors and the publishers cannot assume responsibility for the validity of all materials. Neither the authors nor the publishers, nor anyone else associated with this publication, shall be liable for any loss, damage or liability directly or indirectly caused or alleged to be caused by this book.

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

The consent of Woodhead Publishing Limited does not extend to copying for general distribution, for promotion, for creating new works, or for resale. Specific permission must be obtained in writing from Woodhead Publishing Limited for such copying.

Trademark notice: Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation, without intent to infringe.

British Library Cataloguing in Publication Data

A catalogue record for this book is available from the British Library.

Library of Congress Control Number: 2013944629

ISBN 978-1-84569-512-5 (print)

ISBN 978-0-85709-881-8 (online)

ISSN 2042-8049 Woodhead Publishing Series in Food Science, Technology and Nutrition (print)

ISSN 2042-8057 Woodhead Publishing Series in Food Science, Technology and Nutrition (online)

The publisher's policy is to use permanent paper from mills that operate a sustainable forestry policy, and which has been manufactured from pulp which is processed using acid-free and elemental chlorine-free practices. Furthermore, the publisher ensures that the text paper and cover board used have met acceptable environmental accreditation standards.

Typeset by RefineCatch Ltd, Bungay, Suffolk

Printed by Lightning Source

Metabolomics in food and nutrition

Related titles:

Diet, immunity and inflammation
(ISBN 978-0-85709-037-9)

Designing functional foods: Measuring and controlling food structure breakdown and nutrient absorption
(ISBN 978-1-84569-432-6)

Food for the ageing population
(ISBN 978-1-84569-193-6)

Details of these books and a complete list of titles from Woodhead Publishing can be obtained by:

- visiting our web site at www.woodheadpublishing.com
- contacting Customer Services (e-mail: sales@woodheadpublishing.com; fax: +44 (0) 1223 832819; tel.: +44 (0) 1223 499140 ext. 130; address: Woodhead Publishing Limited, 80, High Street, Sawston, Cambridge CB22 3HJ, UK)
- in North America, contacting our US office (e-mail: usmarketing@woodheadpublishing.com; tel.: (215) 928 9112; address: Woodhead Publishing, 1518 Walnut Street, Suite 1100, Philadelphia, PA 19102-3406, USA)

If you would like e-versions of our content, please visit our online platform: www.woodheadpublishingonline.com. Please recommend it to your librarian so that everyone in your institution can benefit from the wealth of content on the site.

We are always happy to receive suggestions for new books from potential editors. To enquire about contributing to our Food Science, Technology and Nutrition series, please send your name, contact address and details of the topic/s you are interested in to nell.holden@woodheadpublishing.com. We look forward to hearing from you.

The team responsible for publishing this book:

Commissioning Editor: Nell Holden
Publications Coordinator: Emily Cole
Project Editor: Kate Hardcastle
Editorial and Production Manager: Mary Campbell
Production Editor: Mandy Kingsmill
Project Manager: Annette Wiseman
Copyeditor: Sue Clements
Proofreader: Dave Cummings
Cover Designer: Terry Callanan

Contributor contact details

(* = main contact)

Editors

B. C. Weimer
University of California, Davis
School of Veterinary Medicine
One Shields Avenue
Davis, CA 95616, USA

E-mail: bcweimer@ucdavis.edu

C. M. Slupsky
University of California, Davis
Department of Nutrition and
Department of Food Science and
Technology
One Shields Avenue
Davis, CA 95616, USA

E-mail: cslupsky@ucdavis.edu

Chapter 1

C. J. Wachsmuth, P. J. Oefner and
K. Dettmer*
Institute of Functional Genomics
University of Regensburg
Josef-Engert-Str. 9
93053 Regensburg, Germany

E-mail: katja.dettmer@klinik.uni-regensburg.de

Chapter 2

J. Sotelo and C. M. Slupsky*
University of California, Davis
Department of Nutrition and
Department of Food Science and
Technology
One Shields Avenue
Davis, CA 95616, USA

E-mail: jssotelo@ucdavis.edu;
cslupsky@ucdavis.edu

Chapter 3

J. R. Stevens
Department of Mathematics and
Statistics
Utah State University
3900 Old Main Hill
Logan, UT 84322-3900, USA

E-mail: john.r.stevens@usu.edu

Chapter 4

P. D. Karp
SRI International
333 Ravenswood Ave, AE206
Menlo Park, CA 94025, USA

E-mail: pkarp@ai.sri.com

Chapter 5

P. D. Whitfield* and M. K. Doherty
Lipidomics Research Facility
Department of Diabetes and
Cardiovascular Science
University of the Highlands and
Islands
Centre for Health Science
Old Perth Road
Inverness IV2 3JH, Scotland, UK

E-mail: phil.whitfield@uhi.ac.uk;
mary.doherty@uhi.ac.uk

Chapter 6

S. Moco, A. Ross, F.-P. J. Martin,
S. Collino, J.-P. Godin, S. Rezzi and
S. Kochhar*
BioAnalytical Science
Nestlé Research Center
Vers-chez-les-Blanc, PO Box 44
1000 Lausanne 26, Switzerland

E-mail: sunil.kochhar@rdls.nestle.
com

Chapter 7

L. R. Ruhaak and C. B. Lebrilla*
University of California, Davis
Department of Chemistry
One Shields Avenue
Davis, CA 95616, USA

E-mail: cblebrilla@ucdavis.edu

Chapter 8

T. Frank and K.-H. Engel*
Technische Universität München
Lehrstuhl für Allgemeine
Lebensmitteltechnologie
Maximus-von-Imhof-Forum 2
D-85350 Freising-Weihenstephan
Germany

E-mail: k.h.engel@wzw.tum.de

Chapter 9

D. Stewart*
Environmental & Biochemical
Sciences Group
The James Hutton Institute
Invergowrie
Dundee DD2 5DA, Scotland, UK

and

School of Life Sciences
Heriot-Watt University
Edinburgh EH14 1AS, Scotland, UK

E-mail: derek.stewart@hutton.ac.uk

L. V. T. Shepherd
Environmental & Biochemical
Sciences Group
The James Hutton Institute
Invergowrie
Dundee DD2 5DA, Scotland, UK

Chapter 10

E. Chin and C. M. Slupsky*
University of California, Davis
Department of Nutrition and
Department of Food Science and
Technology
One Shields Avenue
Davis, CA 95616, USA

E-mail: elichin@ucdavis.edu;
cslupsky@ucdavis.edu

Woodhead Publishing Series in Food Science, Technology and Nutrition

- 1 **Chilled foods: A comprehensive guide** Edited by C. Dennis and M. Stringer
- 2 **Yoghurt: Science and technology** A. Y. Tamime and R. K. Robinson
- 3 **Food processing technology: Principles and practice** P. J. Fellows
- 4 **Bender's dictionary of nutrition and food technology Sixth edition** D. A. Bender
- 5 **Determination of veterinary residues in food** Edited by N. T. Crosby
- 6 **Food contaminants: Sources and surveillance** Edited by C. Creaser and R. Purchase
- 7 **Nitrates and nitrites in food and water** Edited by M. J. Hill
- 8 **Pesticide chemistry and bioscience: The food-environment challenge** Edited by G. T. Brooks and T. Roberts
- 9 **Pesticides: Developments, impacts and controls** Edited by G. A. Best and A. D. Ruthven
- 10 **Dietary fibre: Chemical and biological aspects** Edited by D. A. T. Southgate, K. W. Waldron, I. T. Johnson and G. R. Fenwick
- 11 **Vitamins and minerals in health and nutrition** M. Tolonen
- 12 **Technology of biscuits, crackers and cookies Second edition** D. Manley
- 13 **Instrumentation and sensors for the food industry** Edited by E. Kress-Rogers
- 14 **Food and cancer prevention: Chemical and biological aspects** Edited by K. W. Waldron, I. T. Johnson and G. R. Fenwick
- 15 **Food colloids: Proteins, lipids and polysaccharides** Edited by E. Dickinson and B. Bergenstahl
- 16 **Food emulsions and foams** Edited by E. Dickinson
- 17 **Maillard reactions in chemistry, food and health** Edited by T. P. Labuza, V. Monnier, J. Baynes and J. O'Brien
- 18 **The Maillard reaction in foods and medicine** Edited by J. O'Brien, H. E. Nursten, M. J. Crabbe and J. M. Ames
- 19 **Encapsulation and controlled release** Edited by D. R. Karsa and R. A. Stephenson
- 20 **Flavours and fragrances** Edited by A. D. Swift
- 21 **Feta and related cheeses** Edited by A. Y. Tamime and R. K. Robinson
- 22 **Biochemistry of milk products** Edited by A. T. Andrews and J. R. Varley
- 23 **Physical properties of foods and food processing systems** M. J. Lewis
- 24 **Food irradiation: A reference guide** V. M. Wilkinson and G. Gould

- 25 **Kent's technology of cereals: An introduction for students of food science and agriculture** Fourth edition *N. L. Kent and A. D. Evers*
- 26 **Biosensors for food analysis** Edited by *A. O. Scott*
- 27 **Separation processes in the food and biotechnology industries: Principles and applications** Edited by *A. S. Grandison and M. J. Lewis*
- 28 **Handbook of indices of food quality and authenticity** *R. S. Singhal, P. K. Kulkarni and D. V. Rege*
- 29 **Principles and practices for the safe processing of foods** *D. A. Shapton and N. F. Shapton*
- 30 **Biscuit, cookie and cracker manufacturing manuals Volume 1: Ingredients** *D. Manley*
- 31 **Biscuit, cookie and cracker manufacturing manuals Volume 2: Biscuit doughs** *D. Manley*
- 32 **Biscuit, cookie and cracker manufacturing manuals Volume 3: Biscuit dough piece forming** *D. Manley*
- 33 **Biscuit, cookie and cracker manufacturing manuals Volume 4: Baking and cooling of biscuits** *D. Manley*
- 34 **Biscuit, cookie and cracker manufacturing manuals Volume 5: Secondary processing in biscuit manufacturing** *D. Manley*
- 35 **Biscuit, cookie and cracker manufacturing manuals Volume 6: Biscuit packaging and storage** *D. Manley*
- 36 **Practical dehydration** Second edition *M. Greensmith*
- 37 **Lawrie's meat science** Sixth edition *R. A. Lawrie*
- 38 **Yoghurt: Science and technology** Second edition *A. Y. Tamime and R. K. Robinson*
- 39 **New ingredients in food processing: Biochemistry and agriculture** *G. Linden and D. Lorient*
- 40 **Benders' dictionary of nutrition and food technology** Seventh edition *D. A. Bender and A. E. Bender*
- 41 **Technology of biscuits, crackers and cookies** Third edition *D. Manley*
- 42 **Food processing technology: Principles and practice** Second edition *P. J. Fellows*
- 43 **Managing frozen foods** Edited by *C. J. Kennedy*
- 44 **Handbook of hydrocolloids** Edited by *G. O. Phillips and P. A. Williams*
- 45 **Food labelling** Edited by *J. R. Blanchfield*
- 46 **Cereal biotechnology** Edited by *P. C. Morris and J. H. Bryce*
- 47 **Food intolerance and the food industry** Edited by *T. Dean*
- 48 **The stability and shelf-life of food** Edited by *D. Kilcast and P. Subramaniam*
- 49 **Functional foods: Concept to product** Edited by *G. R. Gibson and C. M. Williams*
- 50 **Chilled foods: A comprehensive guide** Second edition Edited by *M. Stringer and C. Dennis*
- 51 **HACCP in the meat industry** Edited by *M. Brown*
- 52 **Biscuit, cracker and cookie recipes for the food industry** *D. Manley*
- 53 **Cereals processing technology** Edited by *G. Owens*
- 54 **Baking problems solved** *S. P. Cauvain and L. S. Young*
- 55 **Thermal technologies in food processing** Edited by *P. Richardson*
- 56 **Frying: Improving quality** Edited by *J. B. Rossell*
- 57 **Food chemical safety Volume 1: Contaminants** Edited by *D. Watson*
- 58 **Making the most of HACCP: Learning from others' experience** Edited by *T. Mayes and S. Mortimore*

- 59 **Food process modelling** Edited by L. M. M. Tijskens, M. L. A. T. M. Hertog and B. M. Nicolai
- 60 **EU food law: A practical guide** Edited by K. Goodburn
- 61 **Extrusion cooking: Technologies and applications** Edited by R. Guy
- 62 **Auditing in the food industry: From safety and quality to environmental and other audits** Edited by M. Dillon and C. Griffith
- 63 **Handbook of herbs and spices Volume 1** Edited by K. V. Peter
- 64 **Food product development: Maximising success** M. Earle, R. Earle and A. Anderson
- 65 **Instrumentation and sensors for the food industry Second edition** Edited by E. Kress-Rogers and C. J. B. Brimelow
- 66 **Food chemical safety Volume 2: Additives** Edited by D. Watson
- 67 **Fruit and vegetable biotechnology** Edited by V. Valpuesta
- 68 **Foodborne pathogens: Hazards, risk analysis and control** Edited by C. de W. Blackburn and P. J. McClure
- 69 **Meat refrigeration** S. J. James and C. James
- 70 **Lockhart and Wiseman's crop husbandry Eighth edition** H. J. S. Finch, A. M. Samuel and G. P. F. Lane
- 71 **Safety and quality issues in fish processing** Edited by H. A. Bremner
- 72 **Minimal processing technologies in the food industries** Edited by T. Ohlsson and N. Bengtsson
- 73 **Fruit and vegetable processing: Improving quality** Edited by W. Jongen
- 74 **The nutrition handbook for food processors** Edited by C. J. K. Henry and C. Chapman
- 75 **Colour in food: Improving quality** Edited by D. MacDougall
- 76 **Meat processing: Improving quality** Edited by J. P. Kerry, J. F. Kerry and D. A. Ledward
- 77 **Microbiological risk assessment in food processing** Edited by M. Brown and M. Stringer
- 78 **Performance functional foods** Edited by D. Watson
- 79 **Functional dairy products Volume 1** Edited by T. Mattila-Sandholm and M. Saarela
- 80 **Taints and off-flavours in foods** Edited by B. Baigrie
- 81 **Yeasts in food** Edited by T. Boekhout and V. Robert
- 82 **Phytochemical functional foods** Edited by I. T. Johnson and G. Williamson
- 83 **Novel food packaging techniques** Edited by R. Ahvenainen
- 84 **Detecting pathogens in food** Edited by T. A. McMeekin
- 85 **Natural antimicrobials for the minimal processing of foods** Edited by S. Roller
- 86 **Texture in food Volume 1: Semi-solid foods** Edited by B. M. McKenna
- 87 **Dairy processing: Improving quality** Edited by G. Smit
- 88 **Hygiene in food processing: Principles and practice** Edited by H. L. M. Lelieveld, M. A. Mostert, B. White and J. Holah
- 89 **Rapid and on-line instrumentation for food quality assurance** Edited by I. Tothill
- 90 **Sausage manufacture: Principles and practice** E. Essien
- 91 **Environmentally-friendly food processing** Edited by B. Mattsson and U. Sonesson
- 92 **Bread making: Improving quality** Edited by S. P. Cauvain
- 93 **Food preservation techniques** Edited by P. Zeuthen and L. Bøgh-Sørensen
- 94 **Food authenticity and traceability** Edited by M. Lees
- 95 **Analytical methods for food additives** R. Wood, L. Foster, A. Damant and P. Key

- 96 **Handbook of herbs and spices Volume 2** Edited by *K. V. Peter*
- 97 **Texture in food Volume 2: Solid foods** Edited by *D. Kilcast*
- 98 **Proteins in food processing** Edited by *R. Yada*
- 99 **Detecting foreign bodies in food** Edited by *M. Edwards*
- 100 **Understanding and measuring the shelf-life of food** Edited by *R. Steele*
- 101 **Poultry meat processing and quality** Edited by *G. Mead*
- 102 **Functional foods, ageing and degenerative disease** Edited by *C. Remacle and B. Reusens*
- 103 **Mycotoxins in food: Detection and control** Edited by *N. Magan and M. Olsen*
- 104 **Improving the thermal processing of foods** Edited by *P. Richardson*
- 105 **Pesticide, veterinary and other residues in food** Edited by *D. Watson*
- 106 **Starch in food: Structure, functions and applications**
Edited by *A.-C. Eliasson*
- 107 **Functional foods, cardiovascular disease and diabetes** Edited by *A. Arnoldi*
- 108 **Brewing: Science and practice** *D. E. Briggs, P. A. Brookes, R. Stevens and C. A. Boulton*
- 109 **Using cereal science and technology for the benefit of consumers: Proceedings of the 12th International ICC Cereal and Bread Congress, 24 – 26th May, 2004, Harrogate, UK** Edited by *S. P. Cauvain, L. S. Young and S. Salmon*
- 110 **Improving the safety of fresh meat** Edited by *J. Sofos*
- 111 **Understanding pathogen behaviour: Virulence, stress response and resistance**
Edited by *M. Griffiths*
- 112 **The microwave processing of foods** Edited by *H. Schubert and M. Regier*
- 113 **Food safety control in the poultry industry** Edited by *G. Mead*
- 114 **Improving the safety of fresh fruit and vegetables** Edited by *W. Jongen*
- 115 **Food, diet and obesity** Edited by *D. Mela*
- 116 **Handbook of hygiene control in the food industry** Edited by *H. L. M. Lelieveld, M. A. Mostert and J. Holah*
- 117 **Detecting allergens in food** Edited by *S. Koppelman and S. Hefle*
- 118 **Improving the fat content of foods** Edited by *C. Williams and J. Buttriss*
- 119 **Improving traceability in food processing and distribution** Edited by *I. Smith and A. Furness*
- 120 **Flavour in food** Edited by *A. Voilley and P. Etievant*
- 121 **The Chorleywood bread process** *S. P. Cauvain and L. S. Young*
- 122 **Food spoilage microorganisms** Edited by *C. de W. Blackburn*
- 123 **Emerging foodborne pathogens** Edited by *Y. Motarjemi and M. Adams*
- 124 **Benders' dictionary of nutrition and food technology Eighth edition**
D. A. Bender
- 125 **Optimising sweet taste in foods** Edited by *W. J. Spillane*
- 126 **Brewing: New technologies** Edited by *C. Bamforth*
- 127 **Handbook of herbs and spices Volume 3** Edited by *K. V. Peter*
- 128 **Lawrie's meat science Seventh edition** *R. A. Lawrie in collaboration with D. A. Ledward*
- 129 **Modifying lipids for use in food** Edited by *F. Gunstone*
- 130 **Meat products handbook: Practical science and technology** *G. Feiner*
- 131 **Food consumption and disease risk: Consumer–pathogen interactions** Edited by *M. Potter*
- 132 **Acrylamide and other hazardous compounds in heat-treated foods** Edited by *K. Skog and J. Alexander*

- 133 **Managing allergens in food** Edited by C. Mills, H. Wichers and K. Hoffman-Sommergruber
- 134 **Microbiological analysis of red meat, poultry and eggs** Edited by G. Mead
- 135 **Maximising the value of marine by-products** Edited by F. Shahidi
- 136 **Chemical migration and food contact materials** Edited by K. Barnes, R. Sinclair and D. Watson
- 137 **Understanding consumers of food products** Edited by L. Frewer and H. van Trijp
- 138 **Reducing salt in foods: Practical strategies** Edited by D. Kilcast and F. Angus
- 139 **Modelling microorganisms in food** Edited by S. Brul, S. Van Gerwen and M. Zwietering
- 140 **Tamime and Robinson's Yoghurt: Science and technology Third edition**
A. Y. Tamime and R. K. Robinson
- 141 **Handbook of waste management and co-product recovery in food processing Volume 1** Edited by K. W. Waldron
- 142 **Improving the flavour of cheese** Edited by B. Weimer
- 143 **Novel food ingredients for weight control** Edited by C. J. K. Henry
- 144 **Consumer-led food product development** Edited by H. MacFie
- 145 **Functional dairy products Volume 2** Edited by M. Saarela
- 146 **Modifying flavour in food** Edited by A. J. Taylor and J. Hort
- 147 **Cheese problems solved** Edited by P. L. H. McSweeney
- 148 **Handbook of organic food safety and quality** Edited by J. Cooper, C. Leifert and U. Niggli
- 149 **Understanding and controlling the microstructure of complex foods** Edited by D. J. McClements
- 150 **Novel enzyme technology for food applications** Edited by R. Rastall
- 151 **Food preservation by pulsed electric fields: From research to application** Edited by H. L. M. Lelieveld and S. W. H. de Haan
- 152 **Technology of functional cereal products** Edited by B. R. Hamaker
- 153 **Case studies in food product development** Edited by M. Earle and R. Earle
- 154 **Delivery and controlled release of bioactives in foods and nutraceuticals** Edited by N. Gardi
- 155 **Fruit and vegetable flavour: Recent advances and future prospects** Edited by B. Brückner and S. G. Wyllie
- 156 **Food fortification and supplementation: Technological, safety and regulatory aspects** Edited by P. Berry Ottaway
- 157 **Improving the health-promoting properties of fruit and vegetable products** Edited by F. A. Tomás-Barberán and M. I. Gil
- 158 **Improving seafood products for the consumer** Edited by T. Borresen
- 159 **In-pack processed foods: Improving quality** Edited by P. Richardson
- 160 **Handbook of water and energy management in food processing** Edited by J. Klemeš, R. Smith and J.-K. Kim
- 161 **Environmentally compatible food packaging** Edited by E. Chiellini
- 162 **Improving farmed fish quality and safety** Edited by Ø. Lie
- 163 **Carbohydrate-active enzymes** Edited by K.-H. Park
- 164 **Chilled foods: A comprehensive guide Third edition** Edited by M. Brown
- 165 **Food for the ageing population** Edited by M. M. Raats, C. P. G. M. de Groot and W. A Van Staveren
- 166 **Improving the sensory and nutritional quality of fresh meat** Edited by J. P. Kerry and D. A. Ledward

- 167 **Shellfish safety and quality** Edited by S. E. Shumway and G. E. Rodrick
- 168 **Functional and speciality beverage technology** Edited by P. Paquin
- 169 **Functional foods: Principles and technology** M. Guo
- 170 **Endocrine-disrupting chemicals in food** Edited by I. Shaw
- 171 **Meals in science and practice: Interdisciplinary research and business applications** Edited by H. L. Meiselman
- 172 **Food constituents and oral health: Current status and future prospects** Edited by M. Wilson
- 173 **Handbook of hydrocolloids** Second edition Edited by G. O. Phillips and P. A. Williams
- 174 **Food processing technology: Principles and practice** Third edition P. J. Fellows
- 175 **Science and technology of enrobed and filled chocolate, confectionery and bakery products** Edited by G. Talbot
- 176 **Foodborne pathogens: Hazards, risk analysis and control** Second edition Edited by C. de W. Blackburn and P. J. McClure
- 177 **Designing functional foods: Measuring and controlling food structure breakdown and absorption** Edited by D. J. McClements and E. A. Decker
- 178 **New technologies in aquaculture: Improving production efficiency, quality and environmental management** Edited by G. Burnell and G. Allan
- 179 **More baking problems solved** S. P. Cauvain and L. S. Young
- 180 **Soft drink and fruit juice problems solved** P. Ashurst and R. Hargitt
- 181 **Biofilms in the food and beverage industries** Edited by P. M. Fratamico, B. A. Annous and N. W. Gunther
- 182 **Dairy-derived ingredients: Food and nutraceutical uses** Edited by M. Corredig
- 183 **Handbook of waste management and co-product recovery in food processing Volume 2** Edited by K. W. Waldron
- 184 **Innovations in food labelling** Edited by J. Albert
- 185 **Delivering performance in food supply chains** Edited by C. Mena and G. Stevens
- 186 **Chemical deterioration and physical instability of food and beverages** Edited by L. H. Skibsted, J. Risbo and M. L. Andersen
- 187 **Managing wine quality Volume 1: Viticulture and wine quality** Edited by A. G. Reynolds
- 188 **Improving the safety and quality of milk Volume 1: Milk production and processing** Edited by M. Griffiths
- 189 **Improving the safety and quality of milk Volume 2: Improving quality in milk products** Edited by M. Griffiths
- 190 **Cereal grains: Assessing and managing quality** Edited by C. Wrigley and I. Batey
- 191 **Sensory analysis for food and beverage quality control: A practical guide** Edited by D. Kilcast
- 192 **Managing wine quality Volume 2: Oenology and wine quality** Edited by A. G. Reynolds
- 193 **Winemaking problems solved** Edited by C. E. Butzke
- 194 **Environmental assessment and management in the food industry** Edited by U. Sonesson, J. Berlin and F. Ziegler
- 195 **Consumer-driven innovation in food and personal care products** Edited by S. R. Jaeger and H. MacFie
- 196 **Tracing pathogens in the food chain** Edited by S. Brul, P. M. Fratamico and T. A. McMeekin

- 197 **Case studies in novel food processing technologies: Innovations in processing, packaging, and predictive modelling** Edited by C. J. Doona, K. Kustin and F. E. Feeherry
- 198 **Freeze-drying of pharmaceutical and food products** T.-C. Hua, B.-L. Liu and H. Zhang
- 199 **Oxidation in foods and beverages and antioxidant applications Volume 1: Understanding mechanisms of oxidation and antioxidant activity** Edited by E. A. Decker, R. J. Elias and D. J. McClements
- 200 **Oxidation in foods and beverages and antioxidant applications Volume 2: Management in different industry sectors** Edited by E. A. Decker, R. J. Elias and D. J. McClements
- 201 **Protective cultures, antimicrobial metabolites and bacteriophages for food and beverage biopreservation** Edited by C. Lacroix
- 202 **Separation, extraction and concentration processes in the food, beverage and nutraceutical industries** Edited by S. S. H. Rizvi
- 203 **Determining mycotoxins and mycotoxigenic fungi in food and feed** Edited by S. De Saeger
- 204 **Developing children's food products** Edited by D. Kilcast and F. Angus
- 205 **Functional foods: Concept to product Second edition** Edited by M. Saarela
- 206 **Postharvest biology and technology of tropical and subtropical fruits Volume 1: Fundamental issues** Edited by E. M. Yahia
- 207 **Postharvest biology and technology of tropical and subtropical fruits Volume 2: Açai to citrus** Edited by E. M. Yahia
- 208 **Postharvest biology and technology of tropical and subtropical fruits Volume 3: Cocona to mango** Edited by E. M. Yahia
- 209 **Postharvest biology and technology of tropical and subtropical fruits Volume 4: Mangosteen to white sapote** Edited by E. M. Yahia
- 210 **Food and beverage stability and shelf life** Edited by D. Kilcast and P. Subramaniam
- 211 **Processed Meats: Improving safety, nutrition and quality** Edited by J. P. Kerry and J. F. Kerry
- 212 **Food chain integrity: A holistic approach to food traceability, safety, quality and authenticity** Edited by J. Hoorfar, K. Jordan, F. Butler and R. Prugger
- 213 **Improving the safety and quality of eggs and egg products Volume 1** Edited by Y. Nys, M. Bain and F. Van Immerseel
- 214 **Improving the safety and quality of eggs and egg products Volume 2** Edited by F. Van Immerseel, Y. Nys and M. Bain
- 215 **Animal feed contamination: Effects on livestock and food safety** Edited by J. Fink-Gremmels
- 216 **Hygienic design of food factories** Edited by J. Holah and H. L. M. Lelieveld
- 217 **Manley's technology of biscuits, crackers and cookies Fourth edition** Edited by D. Manley
- 218 **Nanotechnology in the food, beverage and nutraceutical industries** Edited by Q. Huang
- 219 **Rice quality: A guide to rice properties and analysis** K. R. Bhattacharya
- 220 **Advances in meat, poultry and seafood packaging** Edited by J. P. Kerry
- 221 **Reducing saturated fats in foods** Edited by G. Talbot
- 222 **Handbook of food proteins** Edited by G. O. Phillips and P. A. Williams

- 223 **Lifetime nutritional influences on cognition, behaviour and psychiatric illness**
Edited by D. Benton
- 224 **Food machinery for the production of cereal foods, snack foods and confectionery** *L.-M. Cheng*
- 225 **Alcoholic beverages: Sensory evaluation and consumer research** *Edited by J. Piggott*
- 226 **Extrusion problems solved: Food, pet food and feed** *M. N. Riaz and G. J. Rokey*
- 227 **Handbook of herbs and spices Second edition Volume 1** *Edited by K. V. Peter*
- 228 **Handbook of herbs and spices Second edition Volume 2** *Edited by K. V. Peter*
- 229 **Breadmaking: Improving quality Second edition** *Edited by S. P. Cauvain*
- 230 **Emerging food packaging technologies: Principles and practice** *Edited by K. L. Yam and D. S. Lee*
- 231 **Infectious disease in aquaculture: Prevention and control** *Edited by B. Austin*
- 232 **Diet, immunity and inflammation** *Edited by P. C. Calder and P. Yaqoob*
- 233 **Natural food additives, ingredients and flavourings** *Edited by D. Baines and R. Seal*
- 234 **Microbial decontamination in the food industry: Novel methods and applications** *Edited by A. Demirci and M.O. Ngadi*
- 235 **Chemical contaminants and residues in foods** *Edited by D. Schrenk*
- 236 **Robotics and automation in the food industry: Current and future technologies**
Edited by D. G. Caldwell
- 237 **Fibre-rich and wholegrain foods: Improving quality** *Edited by J. A. Delcour and K. Poutanen*
- 238 **Computer vision technology in the food and beverage industries** *Edited by D.-W. Sun*
- 239 **Encapsulation technologies and delivery systems for food ingredients and nutraceuticals** *Edited by N. Garti and D. J. McClements*
- 240 **Case studies in food safety and authenticity** *Edited by J. Hoorfar*
- 241 **Heat treatment for insect control: Developments and applications**
D. Hammond
- 242 **Advances in aquaculture hatchery technology** *Edited by G. Allan and G. Burnell*
- 243 **Open innovation in the food and beverage industry** *Edited by M. Garcia Martinez*
- 244 **Trends in packaging of food, beverages and other fast-moving consumer goods (FMCG)** *Edited by N. Farmer*
- 245 **New analytical approaches for verifying the origin of food** *Edited by P. Brereton*
- 246 **Microbial production of food ingredients, enzymes and nutraceuticals** *Edited by B. McNeil, D. Archer, I. Giavasis and L. Harvey*
- 247 **Persistent organic pollutants and toxic metals in foods** *Edited by M. Rose and A. Fernandes*
- 248 **Cereal grains for the food and beverage industries** *E. Arendt and E. Zannini*
- 249 **Viruses in food and water: Risks, surveillance and control** *Edited by N. Cook*
- 250 **Improving the safety and quality of nuts** *Edited by L. J. Harris*
- 251 **Metabolomics in food and nutrition** *Edited by B. C. Weimer and C. Slupsky*
- 252 **Food enrichment with omega-3 fatty acids** *Edited by C. Jacobsen, N. S. Nielsen, A. F. Horn and A.-D. M. Sørensen*
- 253 **Instrumental assessment of food sensory quality: A practical guide** *Edited by D. Kilcast*

- 254 **Food microstructures: Microscopy, measurement and modelling** Edited by *V. J. Morris and K. Groves*
- 255 **Handbook of food powders: Processes and properties** Edited by *B. R. Bhandari, N. Bansal, M. Zhang and P. Schuck*
- 256 **Functional ingredients from algae for foods and nutraceuticals** Edited by *H. Domínguez*
- 257 **Satiation, satiety and the control of food intake: Theory and practice** Edited by *J. E. Blundell and F. Bellisle*
- 258 **Hygiene in food processing: Principles and practice** Second edition Edited by *H. L. M. Lelieveld, J. Holah and D. Napper*
- 259 **Advances in microbial food safety Volume 1** Edited by *J. Sofos*
- 260 **Global safety of fresh produce: A handbook of best practice, innovative commercial solutions and case studies** Edited by *J. Hoorfar*
- 261 **Human milk biochemistry and infant formula manufacturing technology** Edited by *M. Guo*
- 262 **High throughput screening for food safety assessment: Biosensor technologies, hyperspectral imaging and practical applications** Edited by *A. K. Bhunia, M. S. Kim and C. R. Taitt*
- 263 **Foods, nutrients and food ingredients with authorised EU health claims** Edited by *M. J. Sadler*
- 264 **Handbook of food allergen detection and control** Edited by *S. Flanagan*
- 265 **Advances in fermented foods and beverages: Improving quality, technologies and health benefits** Edited by *W. Holzapfel*
- 266 **Metabolomics as a tool in nutritional research** Edited by *J.-L. Sebedio and L. Brennan*
- 267 **Dietary supplements: Safety, efficacy and quality** Edited by *K. Berginc and S. Kreft*
- 268 **Grapevine breeding programs for the wine industry: Traditional and molecular technologies** Edited by *A. G. Reynolds*
- 269 **Handbook of natural antimicrobials for food safety and quality** Edited by *M. Taylor*
- 270 **Managing and preventing obesity: Behavioural factors and dietary interventions** Edited by *T. Gill*
- 271 **Electron beam pasteurization and complementary food processing technologies** Edited by *S. Pillai and S. Shayanfar*
- 272 **Advances in food and beverage labelling: Information and regulations** Edited by *P. Berryman*
- 273 **Flavour development, analysis and perception in food and beverages** Edited by *J. K. Parker, S. Elmore and L. Methven*
- 274 **Rapid sensory profiling techniques and related methods: Applications in new product development and consumer research**, Edited by *J. Delarue, B. Lawlor and M. Rogeaux*
- 275 **Advances in microbial food safety: Volume 2** Edited by *J. Sofos*
- 276 **Handbook of antioxidants in food preservation** Edited by *F. Shahidi*
- 277 **Lockhart and Wiseman's crop husbandry including grassland: Ninth edition** *H. J. S. Finch, A. M. Samuel and G. P. F. Lane*
- 278 **Global legislation for food contact materials: Processing, storage and packaging** Edited by *J. S. Baughan*
- 279 **Colour additives for food and beverages: Development, safety and applications** Edited by *M. Scotter*

Introduction

Metabolomics has emerged as a science with the capacity to cause a major paradigm shift in the way we approach all aspects of public health, including nutrition, agriculture, and food production. Metabolomics biochemically describes the total metabolism and metabolic interactions of cells, organisms, and communities of organisms, to provide a framework on which to understand cellular and organism function in a given environment. Incorporating metabolomics into systems biology will allow a comprehensive understanding of the breadth of health and disease by linking genomics, transcriptomics, proteomics and metabolomics at the organism and/or community level. This system-level knowledge will be key to understanding the network and the communication within the metabolic network that leads to overall health or disease. Moreover, clarifying how the genome and transcriptome are ultimately related to the end products of metabolism will enable a better assessment of the impact of environment, pathogens, and genetic modification on the nutritional and sensory qualities of food. The goal of this book is to provide a working knowledge of metabolomics in health and agriculture to researchers, students, and policy makers by first outlining the technology in detail, and how the wealth of information generated is used to gain meaningful information. Secondly, this book provides several chapters on how this type of research is being used in laboratories and industries to solve important problems, and where this research will lead in the future. This book will provide an invaluable reference tool on techniques and methods in metabolomics, allowing the reader a greater understanding of this rapidly expanding field.

Progress in systems biology, and in particular metabolomics, has occurred through breakthroughs in both technology (especially equipment and techniques for mass spectrometry (MS) and nuclear magnetic resonance (NMR)) and our understanding and integration of these -omics sciences through computational methods. For MS, more sophisticated instrumentation, along with the establishment of standard chemical fragmentation libraries and advances in computer hardware and software, means that thousands of chemicals within a single sample can be measured. Similarly, for NMR, increases in magnetic field strength, the