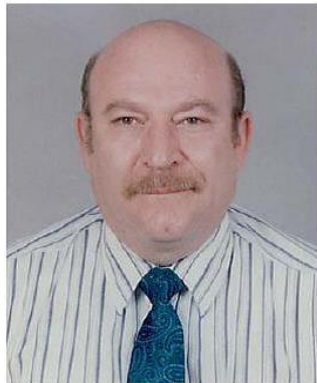


# **Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences**



Edited by  
**Andrei A. Bunaciu, Hassan Y. Aboul-Enein  
and Vu Dang Hoang**

**ANDREI A. BUNACIU   HASSAN Y. ABOUL-ENEIN   VU DANG HOANG**



## **Vibrational spectroscopy**

Applications in Biomedical, Pharmaceutical and Food sciences



# Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences

---

Andrei A. Bunaciu  
Hassan Y. Aboul-Enen  
Vu Dang Hoang



Elsevier  
Radarweg 29, PO Box 211, 1000 AE Amsterdam, Netherlands  
The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, United Kingdom  
50 Hampshire Street, 5th Floor, Cambridge, MA 02139, United States

© 2020 Elsevier Inc. All rights reserved.

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system, without permission in writing from the publisher. Details on how to seek permission, further information about the Publisher's permissions policies and our arrangements with organizations such as the Copyright Clearance Center and the Copyright Licensing Agency, can be found at our website: [www.elsevier.com/permissions](http://www.elsevier.com/permissions).

This book and the individual contributions contained in it are protected under copyright by the Publisher (other than as may be noted herein).

#### Notices

Knowledge and best practice in this field are constantly changing. As new research and experience broaden our understanding, changes in research methods, professional practices, or medical treatment may become necessary.

Practitioners and researchers must always rely on their own experience and knowledge in evaluating and using any information, methods, compounds, or experiments described herein. In using such information or methods they should be mindful of their own safety and the safety of others, including parties for whom they have a professional responsibility.

To the fullest extent of the law, neither the Publisher nor the authors, contributors, or editors, assume any liability for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions, or ideas contained in the material herein.

#### Library of Congress Cataloging-in-Publication Data

A catalog record for this book is available from the Library of Congress

#### British Library Cataloguing-in-Publication Data

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

ISBN: 978-0-12-818827-9

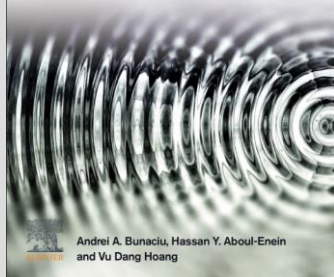
For information on all Elsevier publications  
visit our website at <https://www.elsevier.com/books-and-journals>

*Publisher:* Susan Deans  
*Acquisitions Editor:* Kathryn Eryilmaz  
*Editorial Project Manager:* Lena Sparks  
*Production Project Manager:* Debasish Ghosh  
*Designer:* Greg Harris

Typeset by SPi Global, India



Vibrational Spectroscopy  
Applications in Biomedical,  
Pharmaceutical and  
Food Sciences



Andrei A. Bunaciu, Hassan Y. Aboul-Enein  
and Vu Dang Hoang

# Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences

- **Andrei A. Bunaciu**, AAB-IR Research Laboratory, Bucharest, Romania;
  - **Hassan Y. Aboul-Enein**, Professor Emeritus, Pharmaceutical and Medicinal Chemistry Department, National Research Center, Cairo, Egypt
- and
- **Vu Dang Hoang**, Associate Professor, Department of Analytical Chemistry and Toxicology, Hanoi University of Pharmacy, Hanoi, Vietnam

**ISBN:** 978-0-12-818827-9  
**PUB DATE:** May 01, 2020  
**LIST PRICE:** £115.00 / \$150.00 /  
€131.00

**DISCOUNT:** Reference

**FORMAT:** Paperback

**TRIM:** 6w x 9h

**PAGES:** c. 240

**AUDIENCE:** Primary: Researchers and scientists in analytical chemistry, quality control and assurance, and clinical chemistry involved the application of vibrational spectroscopy in pharmaceutical or biomedical analysis, clinical research and development, bioinorganic chemistry, forensic science, and food science. Secondary: Graduate students, and faculty members, and scholars studying vibrational spectroscopy in physics and chemistry

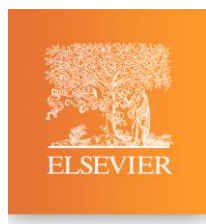
**Synthesizes the latest research on the wide variety of vibrational spectroscopy applications across several disciplines**

## KEY FEATURES

- Presents a critical discussion of many of the applications of vibrational spectroscopy
- Covers details of the analytical methodologies used in pharmaceutical and biomedical applications
- Discusses the latest developments in pharmaceutical and biomedical analysis of both small and large molecules

## DESCRIPTION

*Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences* synthesizes the latest research on the applications of vibrational spectroscopy in biomedical, pharmaceutical and food analysis. Suitable for graduate-level students as well as experienced researchers in academia and industry, this book is organized into five distinct sections. The first deals with the fundamentals of vibrational spectroscopy, with the second presenting the most important sampling methodology used for infrared and Raman spectroscopy in various fields of interest. Since spectroscopy is the study of the interaction of electromagnetic radiation with matter, this section deals with the characteristics, properties and absorption of electromagnetic radiation. Final sections describe the analytical studies performed all over the world in biomedical, pharmaceutical and in the food sciences.



**CHEMISTRY**  
Analytical Chemistry  
[www.elsevier.com](http://www.elsevier.com)



Dr Andrei A. Bunaciu



Professor Hassan Y. Aboul-Enein



Professor Vu Dang Hoang

# Table of Contents

## 1. Introduction

### Part I. THEORETICAL ASPECTS OF VIBRATIONAL SPECTROSCOPY

2. Molecular vibration
3. Infrared absorption
4. Sampling in Infrared / Raman spectroscopy

### Part II. BIOMEDICAL ANALYSIS APPLICATIONS

5. Body fluids analysis
6. Tissues analysis
7. Biomedical analysis
8. Clinical diagnosis

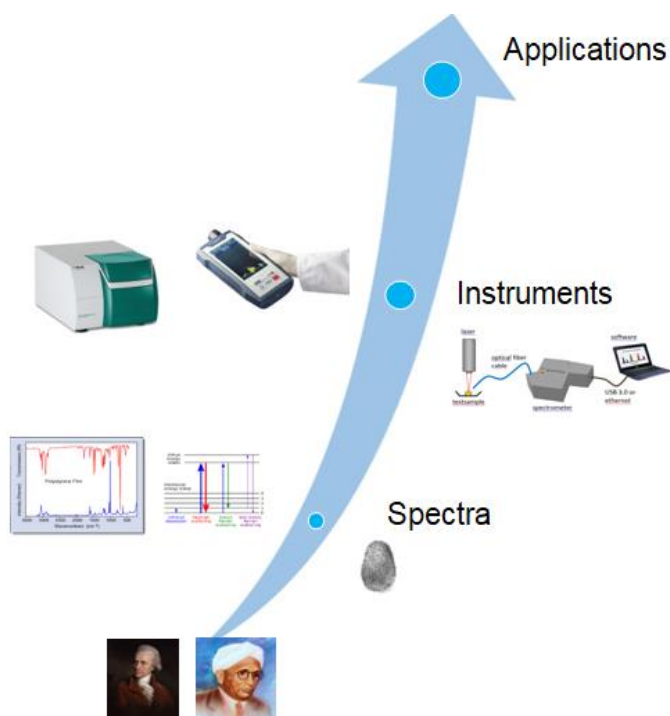
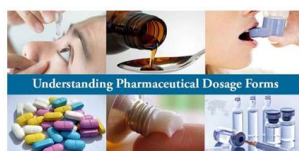
### Part III. PHARMACEUTICAL ANALYSIS APPLICATIONS

9. Drugs – chemical
10. Drugs – herbal
11. Polymorphic substances analysis

### Part IV. FOOD ANALYSIS

12. Alcohol beverages analysis
13. Milk analysis
14. Edible oil

## 15. Conclusions



# Contents

Preface	vii
<b>1. Introduction</b>	<b>1</b>
Brief history of vibrational spectroscopy	2
References	10
Further reading	11
<b>Part I</b>	
<b>Fundamental aspects of vibrational spectroscopy</b>	
<b>2. Basic theory, sampling techniques, and instrumentation</b>	<b>15</b>
Basic theory	15
Sampling techniques and instrumentation	19
References	35
<b>Part II</b>	
<b>Biomedical analysis applications</b>	
<b>3. Body fluid analysis</b>	<b>39</b>
<b>4. Tissues analysis</b>	<b>71</b>
<b>Part III</b>	
<b>Pharmaceutical analysis applications</b>	
<b>5. Chemical drug analysis</b>	<b>97</b>
Drug quantification and formulation characterization	97
Polymorphic analysis	110
Counterfeiting drug analysis	119
References	130
<b>6. Herbal drug analysis</b>	<b>137</b>

**Part IV**

**Food analysis applications**

7. Edible oil analysis	167
8. Milk analysis	189
9. Alcoholic drink analysis	205
10. Some concluding remarks	225
Appendix: Chemometric processing of spectroscopic data <i>Alessandra Biancolillo and Federico Marini</i>	227
Index	249



***Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences***

**Andrei A. Bunaciu, Ph.D.**

AAB-IR Research Laboratory, Bucharest, Romania

**Hassan Y. Aboul-Enein, Ph.D.**

Professor Emeritus, Pharmaceutical and Medicinal Chemistry Department,  
National Research Center, Cairo, Egypt

**Vu Dang Hoang, Ph.D.**

Associate Professor, Department of Analytical Chemistry and Toxicology,  
Hanoi University of Pharmacy, Hanoi, Vietnam

*Synthesizes the latest research on the wide variety of applications of vibrational spectroscopy across several disciplines*

*Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences* provides the necessary fundamentals to understand the basics of vibrational spectroscopy and synthesizes the latest research on its applications in biomedical, pharmaceutical, and food analysis.

Organized into five distinct sections, *Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences* primes readers with basic knowledge, then presents the most important sampling methodology used for infrared and Raman spectroscopy, and finally provides descriptions of analytical studies of vibrational spectroscopy applications. *Vibrational Spectroscopy Applications in Biomedical, Pharmaceutical and Food Sciences* is a valuable resource for graduate-level students as well as experienced researchers in academia and industry.

**Key Features:**

- Presents a critical discussion of many applications of vibrational spectroscopy
- Covers details of the analytical methodologies used in pharmaceutical and biomedical applications
- Discusses the latest developments in pharmaceutical and biomedical analysis of both small and large molecules

**Related Titles:**

- Larkin, *Infrared and Raman Spectroscopy*, 2e. November 2017. ISBN: 9780128041628
- Le Ru, *Principles of Surface-Enhanced Raman Spectroscopy*. March 2014. ISBN: 9780444527790
- Gupta, *Molecular and Laser Spectroscopy*. September 2017. ISBN: 9780128498835