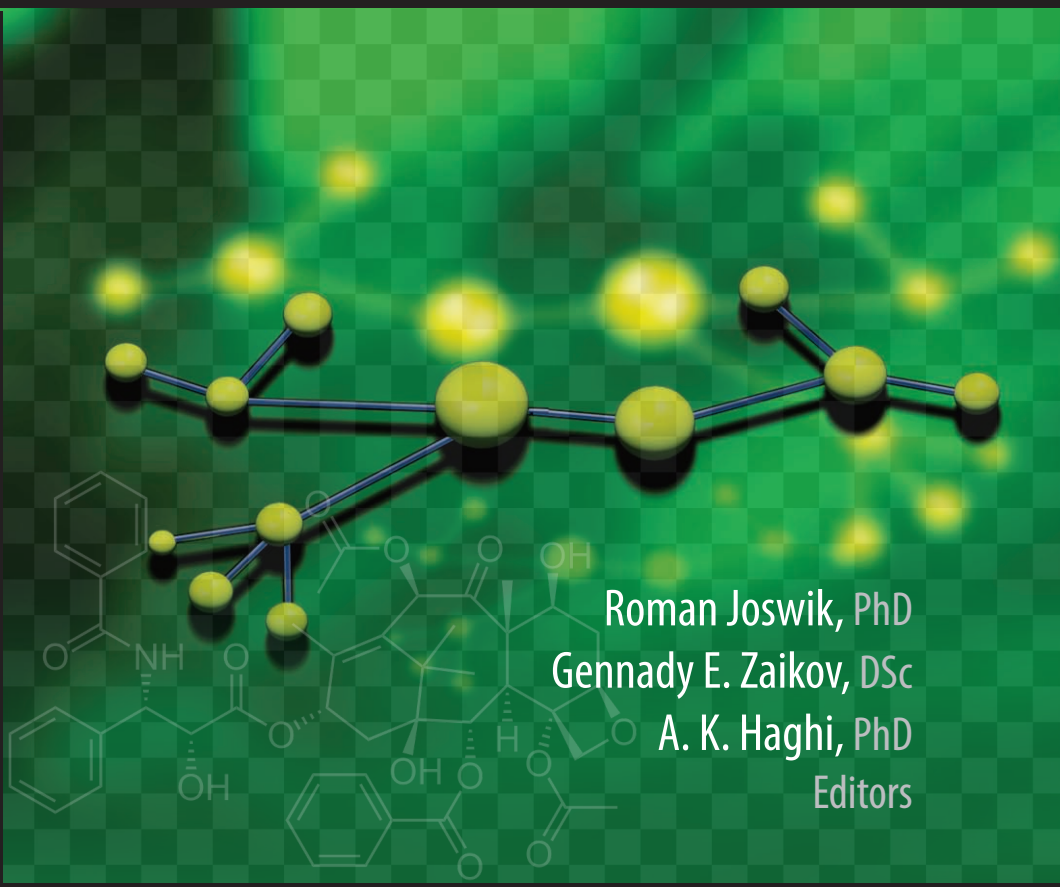
Life Chemistry Research

Biological Systems



Roman Joswik, PhD
Gennady E. Zaikov, DSc
A. K. Haghi, PhD
Editors

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LIFE CHEMISTRY RESEARCH

Biological Systems

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Edited by

Roman Joswik, PhD, Gennady E. Zaikov, DSc, and A. K. Haghi, PhD

APPLE ACADEMIC PRESS

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

Apple Academic Press, Inc
3333 Mistwell Crescent
Oakville, ON L6L 0A2
Canada

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Exclusive worldwide distribution by CRC Press an imprint of Taylor & Francis Group, an Informa business

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Version Date: 20150514

International Standard Book Number-13: 978-1-4987-0000-9 (eBook - PDF)

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ABOUT THE EDITORS

Roman Joswik, PhD

Roman Joswik, PhD, is Director of the Military Institute of Chemistry and Radiometry in Warsaw, Poland. He is a specialist in the field of physical chemistry, chemical physics, radiochemistry, organic chemistry, and applied chemistry. He has published several hundred original scientific papers as well as reviews in the field of radiochemistry and applied chemistry.

Gennady E. Zaikov, DSc

Gennady E. Zaikov, DSc, is Head of the Polymer Division at the N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, Russia, and Professor at Moscow State Academy of Fine Chemical Technology, Russia, as well as Professor at Kazan National Research Technological University, Kazan, Russia. He is also a prolific author, researcher, and lecturer. He has received several awards for his work, including the Russian Federation Scholarship for Outstanding Scientists. He has been a member of many professional organizations and on the editorial boards of many international science journals.

A. K. Haghi, PhD

A. K. Haghi, PhD, holds a BSc in urban and environmental engineering from University of North Carolina (USA); a MSc in mechanical engineering from North Carolina A&T State University (USA); a DEA in applied mechanics, acoustics and materials from the Université de Technologie de Compiègne (France); and a PhD in engineering sciences from the Université de Franche-Comté (France). He is the author and editor of 165 books as well as 1,000 published papers in various journals and conference proceedings. Dr. Haghi has received several grants, consulted for a number of major corporations, and is a frequent speaker to national and international audiences. Since 1983, he served as a professor at several universities. He is currently Editor-in-Chief of the *International Journal of Chemoinformatics and Chemical Engineering and Polymers Research Journal* and on the editorial boards of many international journals. He is a member of the Canadian Research and Development Center of Sciences and Cultures (CRDCSC), Montreal, Quebec, Canada.

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LIST OF CONTRIBUTORS

O. M. Alekseeva
Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, ul. Kosygina, 4, Moscow, 119334; E-mail: olgavek@yandex.ru

A. I. Bastrakov
A.N. Severtsov Institute of Ecology and Evolution, RAS, 33 Leninskij prosp., Moscow, 119071, Russia.

O. S. Berdyugina
FGBU "I.I. Mechnikov Research Institute for Vaccines and Sera" RAMS., Moscow 105064 Maliy Kazenniy per. 5a. E-mail labpitsred@yandex.ru

A. I. Beresnev
Institute of Microbiology, National Academy of Sciences, 220141, Minsk, Belarus.

Sanjay Kumar Bharti
School of Pharmaceutical Sciences, Guru Ghasidas Vishwavidyalaya (A Central University), Bilaspur, Chattisgarh, India

L. P. Blinkova
FGBU "I. I. Mechnikov Research Institute for Vaccines and Sera" RAMS. Moscow 105064 Maliy Kazenniy per. 5a. e-mail labpitsred@yandex.ru.

S. B. Bokieva
N. N. Semenov Institute of Chemical Physics, RAS, Moscow, Russia

A. A. Brilliant
GBUZSO Institute of Medical Cell Technologies, 620036 Yekaterinburg.

E. B. Burlakova
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia

M. S. Chirikova
Institute of Microbiology, National Academy of Sciences, Belarus, 220141, Minsk, Belarus, E-mail: margarita.chirikova@mail.ru.

O. V. Dmitrieva
FGBU "I. I. Mechnikov Research Institute for Vaccines and Sera" RAMS., Moscow 105064 Maliy Kazenniy per. 5a. e-mail labpitsred@yandex.ru.

Sergey Gaydamaka
Moscow State University, Chemistry Faculty, Department of Chemical Enzymology. 119991, Moscow, Russia.

N. Yu. Gerasimov
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia

M. D. Goldfein
Saratov State University named after N.G. Chernyshevsky, Russia, goldfeinmd@mail.ru

A. N. Goloshchapov
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia

N. A. Grebenkina
Higher Chemical College, RAS, Moscow, Russia

K. Z. Gumargalieva
N. N. Semenov Institute of Chemical Physics, RAS, Moscow, Russia

A. N. Inozemtsev
M. V. Lomonosov MSU, Biological Faculty, Leninskie Gory, 119991, Moscow, Russia

V. V. Kasparov
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia

Yu. A. Kim
Institute of Cell Biophysics, Russian Academy of Sciences, Pushchino, Moscow, Russia

M. A. Klyuchnikova
A. N. Severtzov Institute of Ecology and Evolution, 33 Leninski prospect, Moscow, 119071, Russia; e-mail: veravoznessenskaya@gmail.com

Sergei S. Kolesov
The Institute of Organic Chemistry of the Ufa Scientific Centre the Russian Academy of Science, Russia, Republic of Bashkortostan, Ufa, 450054, October Prospect 71.

A. L. Kovarskij
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia.

A. A. Kozlova
A. N. Severtsov Institute of Ecology and Evolution, RAS, 33 Leninskij prosp., Moscow, 119071, Russia.

L. Z. Kravtsova
The "NTC BIO", LLC, 309292, Russia, Belgorod Region, Shebekino town, e-mail: ntcbio@mail.ru

E. I. Kulish
Bashkir State University, Russia, Republic of Bashkortostan, Ufa, 450074, ul. Zaki Validi.

S. V. Kvach
Institute of Microbiology, National Academy of Sciences, 220141, Minsk, Belarus.

C. A. Liman
the "Agroakademia", LLC, 309290 Russia, Belgorod region, Shebekino town, A., e-mail: agroakademia@mail.ru

Murygina Lomonosov
Moscow State University, Chemistry Faculty, Department of Chemical Enzymology. 119991, Moscow, Leninsky gory 1/11

Debarshi Kar Mahapatra
School of Pharmaceutical Sciences, Guru Ghasidas Vishwavidyalaya (A Central University), Bilaspur, Chattisgarh, India

T. V. Malanina
A.N.Severtzov Institute of Ecology & Evolution, 33 Leninski prospect, Moscow, 119071, Russia, email: veravoznessenskaya@gmail.com.

E. I. Martirosova
Emanuel Institute of Biochemical Physics, RAS, 119334, Moscow, Russia. Email: ms_martins@mail.ru

O. V. Nevrova
Emanuel Institute of Biochemical Physics RAS, 119334, Moscow, Russia

I. R. Oviya
Department of Bioinformatics, Bharathiar University, Coimbatore, India.

Yu. D. Pakhomov
FGBU "I.I. Mechnikov Research Institute for Vaccines and Sera" RAMS., Moscow 105064 Maliy Kazenniy per. 5a. e-mail labpitsred@yandex.ru.

D. S. Pavlov
A.N. Severtsov Institute of Ecology and Evolution, Russian Academy of Sciences, 119071 Russia, Moscow.

I. G. Plashchina
Emanuel Institute of Biochemical Physics, RAS, 119334, Moscow, Russia.

V. V. Podmasteryev
N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, 119334, Moscow, Russia

S. V. Ponomarev
the "Bioaquapark" Innovation Centre– The Scientific Centre of the Aqua-Culture at the ASTU, 414025, Astrakhan, e-mail: kafavb@yandex.ru

V. G. Pravdin
The "NTC BIO", LLC, 309292, Russia, Belgorod region, Shebekino town, e-mail: ntcbio@mail.ru

S. D. Razumovsky
N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Mascow, Russia.

E. I. Rodionova
A. A. Kharkevich Institute for Information Transmission, 19 B. Karetny, Moscow, 127994, Russia.

E. G. Rozantsev
Saratov State University named after N.G. Chernyshevsky, Russia.

A. S. Samsonova
Institute of Microbiology, National Academy of Sciences, Belarus, 220141, Minsk, Belarus

R. Sathishkumar
Dept. of Biotechnology, Salem Sowdeswari College, Salem, India.

I. P. Savchenkova
All Russian State Research Institute of Experimental Veterinary Medicine of Ya.R. Kovalenko, 109428, Russia, Moscow, E–mail: s-ip@mail.ru

S. V. Sazonov
GBUZSO Institute of Medical Cell Technologies, 620036 Yekaterinburg.

T. P. Shakun
Institute of Microbiology, National Academy of Sciences, Belarus, 220141, Minsk, Belarus, E-mail: margarita.chirikova@mail.ru.

M. Sharanya
Department of Bioinformatics, Bharathiar University, Coimbatore, India.

Angela S. Shurshina
Bashkir State University, Russia, Republic of Bashkortostan, Ufa, 450074.

V. S. Sibirtsev
GiproRjibFlot (Research and design institute on development and exploitation of a fish fleet), lab. Technical microbiology; Instrumentalnaja ul. 8, 197022 Russia, e-mail: vs1969r@mail.ru; site: http:\\www.vs1969r.narod.ru\publen.htm

Anamika Singh
Maitreyi Collage, University of Delhi, India. E-mail: 10rsingh@gmail.com

Rajeev Singh
Division of Reproductive and Child Health, Indian Council of Medical Research, New Delhi

G. G. Sivets
Institute of Bioorganic Chemistry, National Academy of Sciences, 220141, Minsk, Belarus

N. N. Skorlupkina
FGBU "I. I. Mechnikov Research Institute for Vaccines and Sera" RAMS., Moscow 105064 Maliy Kazenniy per. 5a. e-mail labpitsred@yandex.ru tel.: +7 495 916-11-52, fax: +7 495 917-54-60.

N. A. Ushakova
A. N. Severtsov Institute of Ecology and Evolution, Russian Academy of Sciences, 33 Leninskij prosp., Moscow, 119071 Russia, fax (8495) 954-55-34, e-mail naushakova@gmail.com

P. Valentina
Moscow State University, Chemistry Faculty, Department of Chemical Enzymology, 119991, Moscow, Russia.

A. E. Voznesenskaya
A. A. Kharkevich Institute for Information Transmission, 127994, Moscow, Russia

V. V. Voznessenskaya
A. N. Severtzov Institute of Ecology & Evolution, 33 Leninski prospect, Moscow, 119071, Russia, Email: veravoznessenskaya@gmail.com.

Bataeva Yulia
Federal State Budget Educational Institution of Higher Professional Education, Astrakhan State University. E-mail: aveatab@mail.ru

A. A. Zagorinsky
A. N. Severtsov Institute of Ecology and Evolution, RAS, 33 Leninskij prosp., Moscow, 119071, Russia.

G. E. Zaikov
N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow 119334, Russia, Chembio@sky.chph.ras.ru

Y. M. Zasadkevich
GBUZSO Institute of Medical Cell Technologies, 620036 Yekaterinburg, Russia.

A. I. Zinchenko
Institute of Microbiology, National Academy of Sciences, 220141, Minsk, Belarus.

LIST OF ABBREVIATIONS

AD	Alzheimer's disease
AFO	ankle foot orthotics
AHB	alkylhydroxybenzenes
AMS	amikacin sulfate
AMS	antibiotics - amikacin
BSA	bovine serum albumin
CBC	cyano-bacterial communities
CBT	cognitive behavioral therapy
ChTA	chitosan acetate
CMC	critical micelle concentration
CTD	common technical document
EMEA	evaluation of medicinal products
EPR	electron paramagnetic resonance
ETP	electron transport particles
FFA	free fatty acids
FSR	fragmented sarcoplasmic reticulum
HAS	human serum albumin
INNs	international non-proprietary names
LMWC	low molecular weight chitosans
LT	longitudinal tubules
MFC	minimal fungicidal concentration
MFD	minimum fungicidal dilution
MIC	minimal inhibitory concentration
MID	minimum inhibitory dilution
NMR	nuclear magnetic resonance
PD	Parkinson's disease
PRCA	pure red cell aplasia
PRET	progressive resisted exercise training
RyR	ryanodine receptor
SIRS	system inflammatory response syndrome
SR	sarcoplasmic reticulum
TC	terminal cysternaes
TCM	traditional chinese medicine
TGA	therapeutic goods administration
UPSIT	University of Pennsylvania Smell Identification Test

LIST OF SYMBOLS

m_∞	relative amount of water in equilibrium swelling film sample
k	constant connected with parameters of interaction polymer
n	indicator characterizing the mechanism
c_0	surface concentration
τ	constant of proportionality
τ_c	rotational diffusion correlation time
V	volume of the radical
η	dynamic viscosity of the medium
K	Boltzmann constant
T	absolute temperature
n	number of cracks
l	length of a crack
h	depth
D	optical density
α	solubility coefficient

PREFACE

This book, with contributions from many world leaders in the field, is equally appropriate for graduate or research courses in biochemistry. The book has been extensively class-tested and includes tutorials in biology and biochemistry to aid students of varying backgrounds. This exciting new book will be a must-read for years to come for all students and researchers interested in the field of biological chemistry.

This volume also contains experiments related to the content of biological chemistry courses as well as basic/preparatory chemistry courses. These research studies give students an opportunity to go beyond the lectures and words in the textbook to experience the scientific process from which conclusions and theories are drawn.

This book:

- Focuses on fundamental and relevant connections between chemistry and life.
- Elegantly portrays the complementary nature of chemistry and biology. By describing biological processes in detailed chemical terms, the authors have provided a resource that provides an unparalleled look into the fascinating and emerging field of chemical biology.
- Satisfies a major need in chemistry curricula, bridging the gap between introductory organic chemistry and biochemistry/biology.
- Delivers need-to-know information in a succinct style for today's students.

PART I

BIOLOGICAL MEDICINE

CHAPTER 1

A STEP TOWARD PERSONALIZED MEDICINE

I. R. OVIYA

Department of Bioinformatics, Bharathiar University, Coimbatore - 641 046, India

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1.1 INTRODUCTION

The age-old practice of traditional medicine is gaining momentum today. The traditional and alternative medicinal practices like Ayurveda, Siddha, Unani, Kampo, traditional Chinese medicine, etc., have promising therapeutic values. They constitute the group of evidence-based medicine. Though not scientifically proven then, but the practical knowledge of our forefathers have unbelievably exceeded today's scientific practice when the whole foundation was based upon personalized medicinal concept or "Prakriti" which is also mentioned in our ancient text as follows [3], [2]:

> *"Every individual is different from another*
>
> *and hence should be considered as a different entity.*
>
> *As many variations are there in the Universe, all are seen in Human being"*.

With the advancement in biological science, the root cause of all human diseases is mapped to the genomic and phenotypic variations which are important to understand for personalized medicine concept. Prakriti-based medicine is based on three doshas, namely, vata, pitta, and kapha explaining the different conditions of the body.

1.2 WHAT IS ALTERNATIVE MEDICINE?

Alternative medicine which includes Ayurveda, Siddha, Unani, Kampo, traditional Chinese medicine, to name a few, is a substitute for present conventional medicine, namely Allopathy. They are practiced with traditional knowledge for healing in different parts of the world. The ancestral medicinal knowledge documented by various scholars of their era is now being used to gain knowledge for alternative medicinal practice.

1.2.1 PROS AND CONS

1. Alternative medicines are based on evidence-based practice since ancient times. Thus, it has a strong foundation for sustaining its practice.
2. They are believed to possess lesser side effects.
3. Alternative medicine is based on personalized medicine concept. Hence, drug selection and dosage quantity is based on the prakriti or tridosha of a person under treatment.
4. Alternative medicines are believed to cure some of the most menacing disease of present era which the present conventional medicine is unable to cure.

5. Presently there is no standardization of herbal medicine which compromises on the purity of the medicine.
6. Still various practices of the tribal communities are undisclosed. Hence, very little is known of different traditional remedies practiced today.
7. Scientific research is still lagging in understanding the mechanism of action of the herbal formulations and its synergistic activity in the biological system.

1.3 WHAT IS BIOINFORMATICS?

Bioinformatics is an interdisciplinary area for analyzing the biological systems with a computational approach. The area of bioinformatics has diversified into many sister areas of research namely, genomics, proteomics, metabolomics, systems biology, pharmacogenomics, etc. More recently few new areas seem to emerge like ayugenomics [2], reverse pharmacogenomics [1], and pathogenomics [11]. Few areas are briefly described here:

1.3.1 GENOMICS

Genomics is the study of sequence, structure, and function of genome. The completion of the human genome project held high hopes of the scientists in undeciphering the genetic puzzle in humans in medical perspective. Breakthrough in establishing basis of individual differences with VNTRs, SNPs, EST, and other genomic elements gave hope toward a personalized medication approach. However, the science of human body is too complex to understand and apply these concepts to the whole.

1.3.2 PROTEOMICS

Proteomics is the study of structure and function of proteins. In recent times, there has been a boom in structure elucidation of various proteins and its mode of action. These structures give us better understanding of the protein behavior with different molecules. The identification of the active site and the active residues are the main components into probing the possible drug-target interaction.

1.3.3 TRANSCRIPTOMICS

Transcriptomics is the study of expression level of different proteins in a given cell population. It is also referred as expression profiling and is based on microarray technology. This technology is used to study the differences in the expres-

sion of different genetic elements in more than one condition such as normal vs. disease conditions.

1.3.4 METABOLOMICS

The study of various intermediate metabolites in cellular processes and decoding the chemical fingerprints is known as metabolomics.

1.3.5 SYSTEMS BIOLOGY

Systems biology focuses on integrating the data from genomics, proteomics, transcriptomics, and metabolomics. It focuses on computational model building using the data involving metabolic networks or cell signaling networks. Network building is an integral part of systems biology.

1.3.6 PHARMACOGENOMICS

Pharmacogenomics aims toward personalized medicine approach. It involves technology combining genomics, proteomics, metabolomics, etc., to analyze the individual's genetic makeup affecting his drug response.

This integrative field is still in its infancy with respect to understanding of complexity of the biological entities. However, the advances made in the sister areas can't be ignored.

1.4 BIOINFORMATICS AND ALTERNATIVE MEDICINE—THE PRESENT SCENARIO

The promises of the computational models for studying the biological systems is not new but the advent of the technology post the completion of the human genome project has been huge. High throughput sequencing data, microarray, and expression data compiled systematically in a database is a boon for the modern biologist for extracting the experimental knowledge and its application henceforth. The present-day approaches in alternative medicine are mainly focuses on QSAR studies, molecular modeling, docking, dynamic, and other validation studies. These studies are mainly focused on the application of the developed strategies. The prospects of bioinformatics is not only limited to the usage of available data and softwares but to develop more robust network models to comply with the dynamicity of the biological systems. Human system is complex as well as variable. The earliest scientific approach was restricted to understand the human complexicity. Recent studies have to be extended to deal with the

variability in genome induced due to physiological and biological changes. The computational biology plays an integral role in bioinformatics in developing the softwares for analysis. The efficiency of the computational techniques is dependent on the mathematical models implemented using programming languages which can deal with both complexity and variability as mentioned.

1.4.1 DATABASES, TEXT MINING METHODS, OR LITERATURE-BASED STUDIES

The information on the traditional medicine is scattered and the present-day need is to gather them and present it to the researchers in a more organized manner. Various kind of information are available in different databases which minimize our searing work and allow us to effective utilize the information for further analysis. The traditional practices and usages that have been documented in different books, scriptures, and sometimes they have not been documented but have been in practice with the group or tribe for a long time. Such kind of information is highly valuable and cannot be harnessed at one place. Hence the research work comprising of field visit, collection of traditional information, and documentation in modern form (databases) is important to give other researchers a peep into the data and to carry out the further pharmacognostical or phytochemical work. Medicinal pharmacogenomics is based in the information available likewise. Similarly, along with documentation, web search needs to be more robust and specific. Text mining approaches improves not only efficiency of search but also saves time. Few databases for the reference of the reader are mentioned below:

Databases	**Information**	**References**
Supernatural	Available natural compounds	[4]
TCM-ID	Herbal ingredient, structure, function, therapeutic details	[22]
TCMGeneDIT	Association information about TCM	[5]
HIT	Herbs and their protein target information	Hao et al. (2011)
SWEETLEAD	Approved drugs, regulated chemicals, herbal isolates for CADD	[18]
INpacdb	Indian plant anticancer compounds	[20]
NAPROC-13	Indian medicinal plants	[17]

1.4.2 EXPRESSION STUDIES

Microarray analysis, spectroscopic methods, and other high throughput technology have led to the increase in the pharmacological understanding of the disease conditions. The differential gene, protein expression can help us to identify the candidate gene and thus help to identify the drug target. The expression data can be accessed by various public database like GEO, ArrayExpress, etc.

1.4.3 TRADITIONAL CHINESE MEDICINE (TCM)

The worldwide acceptance of TCM makes it a promising source of experimental studies. The concept of personalized medicine is not new and it is being practiced for thousands of years. The basis of TCM practice lies in Zheng (i.e., personalized identification and classification of the symptoms and treating it individually). Zheng describes the overall physical status of the human body based on the genotypic and phenotypic differences arising due to heredity, SNPs, environmental variations, and nutrition wherein the patients can classified into characteristic hot or cold Zheng. This has given our modern day researchers to probe into the effectiveness of TCM and its underlying mechanism. Various research papers suggest *in-silico* approach to solve the puzzle of TCM. The sequencing data, text mining resources, pharmacogenomics, microarray expression analysis, etc., all gave a reason to systematically investigate TCM further [19]. More recently systems biology and network pharmacology is the principle choice of carrying out study designs on TCM. Network pharmacology integrates the available chemical and metabolomic knowledge derived from experimental results for drug-target interaction or network studies in a computer simulated model mimicking the living systems. The mode of actions and the scientific basis behind TCM's principle is still unclear. There is a curiosity to unveil the principles behind TCM life systems. Kang et al. developed novel entropy-based models like acquired life entropy, acquired life entropy flow, and acquired life entropy production using the experimental data and has drawn comparative lines with the current TCM principles. The computational approach is also used to study molecular mechanisms like miRNA and siRNA interaction, glycolysis targeting, histone modifications, DNA methylation [7], [8], [21]. These mechanisms are particularly important to understand as they serve as the basis for the drug-target interaction studies. The present-day drugs are based on 'one drug fits all' theory which may not be a pharmacologically correct term for treating a disease. Network pharmacology is being used [13] for multicompound drug discovery. Diseases like cardiovascular disease, HIV, etc., that are being treated using TCM are being probed by computational methods into its mode of action [9].Various mathematical models have been suggested for network construction

between herbs/natural products and their targets [12], [24], [15], [14], [16], [6]. The concept of network pharmacology is explained in detail in various review articles [16, 6].

The various steps involved in bioinformatics approaches are:

1. Text mining for collection of literature.
2. Data mining of the various available resources from databases. For example, 2D and 3D structure of compounds from chemspider, pubchem, etc.
3. Understanding the problem, finding loopholes, study design
4. QSAR studies
5. Target identification, target modeling
6. Network building, interpretation, visualization, pathway-enrichment analysis
7. Genome-wide association studies
8. Evolutionary analysis
9. Docking, molecular simulation

1.5 CONCLUSION

No science can justify independently its role in a biological system. Different areas of science have to come together for sharing scientific concepts and knowledge. Bioinformatics plays an important role in understanding biological mechanism and unveiling the underlying genomic entities responsible for causing diseases. Alternative and complementary medicine is presently gaining momentum. Ethnomedicine, phytochemistry, pharmacology of the plants, and its mechanism of action are being studied by using various molecular techniques and bioinformatics tools. The need of the hour is to fasten the research by using *in-silico* methods coupled with other biological techniques to scientifically validate the usage of the herbal medicines. Also there is a need for the researchers to gain the trust of the tribal people so as to utilize their knowledge. Study designs should be more comprehensive to fill the void in the medical knowledge.

KEYWORDS

- **Alternative medicine**
- **Bioinformatics**
- **Genomics**
- **Personalized medicine**

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CHAPTER 2

TREATING FUNGAL DERMATOPHYTIC INFECTIONS

M. SHARANYA[1] and R. SATHISHKUMAR[2]

[1]Department of Bioinformatics, Bharathiar University, Coimbatore - 641 046, India

[2]Department of Biotechnology, Salem Sowdeswari College, Salem - 636 010, India

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