ISOBC Newsletter

August 2021

Volume 16, Number 2

Iran Society of Biophysical Chemistry

ISOBC NEWSLETTER 2021

Volume 16, Number 2

News

Prediction of proteins structure using artificial intelligence

Understanding the structure of proteins is essential to enhance medical science, but so far only a small part of them have been identified. Understanding protein folding mechanism helps explain its function, which can help to improve fundamental research on designing new medicines and treatments. Experimental techniques to determine protein structures are time consuming and expensive.

Last year researchers at Deep Mind Labs, a subsidiary of Google, for the first time announced with the help of an artificial intelligence program called Alphafold, they had been able to accurately determine shape of proteins which is one of the biggest challenges in biology. According to the researchers, this development could significantly accelerate biological research over the long term, revealing new possibilities in disease understanding and drug discovery.

According to the Company CEO and co-founder Demis Hassabis, they can fold an average protein in a matter of minutes, most cases seconds.

In an article has published by Nature entitled highly accurate protein structure prediction for the human proteome, particularly for tasks where high accuracy is advantageous like molecular replacement or the characterization of binding sites. Also different metrics developed by building on the AlphaFold model is introduced, and use them to interpret the dataset, identifying strong multi-domain predictions and disordered regions.

Currently, DeepMind protein predictions are used for medical research, including the study of the function of SARS-CoV-2, the virus that causes COVID-19.

References

Tunyasuvunakool, Kathryn, et al. "Highly accurate protein structure prediction for the human proteome." *Nature* (2021): 1-9.

https://www.theverge.com

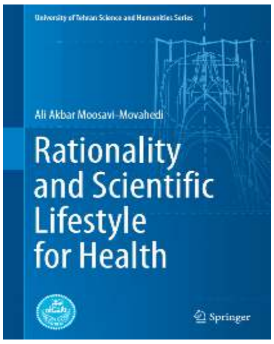
Prepared by:

Elnaz Hosseini, PhD student

Institute of Biochemistry and Biophysics

University of Tehran

New books



Book: Rationality and Scientific Lifestyle for Health

Edited by: Ali A. Moosavi-Movahedi

Publisher: Springer

Language: English

ISBN 978-3-030-74326-0

Published date: 2021

Technologies strongly influence lifestyle behaviors; therefore, knowledge, rationality, and behavior are more important in healthy living. Today, many artificial technologies are abnormal and create pollutants that produce stress (unbalanced free radicals) for humans and creature. Molecular stress generates a variety of unbalanced free radicals from which many diseases originate, like cancer and diabetes. Our scientific evidence shows that diabetes type 2 is not just a disease of sugar but also a stress disease. Stress avoidance is one of the most important criteria of a healthy lifestyle, and one of the highest wealth in the world today is tranquility. In this book, an attempt has been made to link science with reason and lifestyle so that the anomalies of technology branching out from science are under the control of rationality.

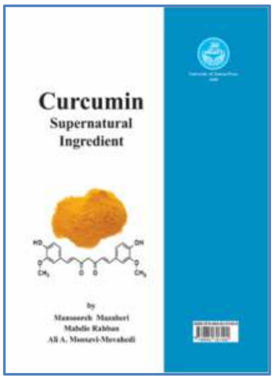
This book is written for the health and well-being of people to lead everyone to true prosperity. The best and healthiest for human beings is to have a balance between life and nature. Therefore, this book introduces useful nutritious, functional foods, nutraceuticals, antioxidants, and how natural molecules which are from the generosity of nature, can be the best medicine for human beings. Besides, it expresses a healthier lifestyle by considering the psycho-emotional dimension of wellness, and finally states that good sleep is the principle of health and happiness for human beings and how it removes stress and how unbalanced free radicals in good sleep are expelled from their bodies.

In this book, the scientific and research achievements of the authors and other worldwide researchers have been written and for this purpose, the following chapters are written:

Chapter one: Philosophy Virtue of Nature, Mankind and Natural Health

Chapter two: Bioinspiration and Biomimicry in Lifestyle

Chapter three: Nature's Generosity in Protecting Human Health
Chapter four: Biodiversity and Drug Discovery Approach to Natural Medicine
Chapter five: Nutraceuticals and Superfoods
Chapter six: Spices as Traditional Remedies: Scientifically Proven Benefits
Chapter seven: Halal Products and Healthy Lifestyle
Chapter eight: Lifestyle in the Regulation of Diabetic Disorders
Chapter nine: Healthier Lifestyle by Considering Psychoemotional Dimension of Wellness
Chapter ten: Good Sleep as an Important Pillar for a Healthy Life



Book: Curcumin: Supernatural Ingredient (The active ingredient of turmeric)

Authors: M. Mazaheri, M. Rahban and Ali A. Moosavi-Movahedi

Publisher: University of Tehran Press, 1nd edition 2021

Language: Persian

ISBN: 978-964-03-0145-6

Turmeric is one of the most popular medicinal herbs with a long history of administration. Curcumin (diferuloylmethane; 1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione) is a primary active compound of turmeric, which is a hydrophobic polyphenol yellow pigment obtained from the dried rhizomes. Curcumin exhibits therapeutic activity attributed mainly to its chemical structure and unique physical, chemical, and biological properties. Curcumin contains two functional phenolic groups, and 7-carbon dienone spacer with a linear diarylheptanoid structure. The o-methoxyphenol group and methylenic hydrogen of curcumin are responsible for the antioxidant activity. Curcumin interacts with proteins through non-covalent and covalent bonding.

Our extensive research and studies show that curcumin has a wide appreciated range of beneficial properties, including anti-inflammatory, anti-diabetic, anti-oxidant, anti-microbial, anti-arthritic, anti-carcinogenic activity, and wound healing effects. Curcumin could modify multiple cell signaling pathways and downregulates cell survival gene expression profile by its effects on multiple cellular targets. Curcumin exhibits antioxidant activity by donating hydrogen and scavenging free radicals. Curcumin also inhibits the production of pro-inflammatory monocyte/macrophage-derived cytokines [interleukin- 8 (IL-8), monocyte inflammatory protein-1 (MIP-1), monocyte chemotactic protein-1 (MCP-1), interleukin-1b (IL-1b), and tumor necrosis factor-α (TNF-α). Curcumin is able to improve energy homeostasis through its direct and indirect antioxidant effects by eliminating ROS. As a result, curcumin is a non-toxic natural product, and due to its broad range of beneficial activities, could be utilized as a therapeutic agent in various diseases that we mentioned in this book.

The scientific and research achievements of the authors and other worldwide researchers have been presented, and more than 490 scientific references have been studied. However, the scientific contents of this book are simplified to be accessible for everybody; therefore, the book is linked to a healthy lifestyle by offering the methods of turmeric usage in ordinary meals.

In this book, the properties and biological studies of turmeric and curcumin are reviewed, and for this purpose, the following chapters are written:

Chapter One: Overview of the Amazing Properties of Curcumin
Chapter Two: Curcumin and Sugar Disease
Chapter Three: Curcumin and its Anti-Cancer Properties
Chapter Four: Curcumin and the Impact of Alzheimer's Improvement
Chapter Five: Curcumin and its Impact on Improving Other Diseases
Chapter Six: Limitation of Curcumin for using
Chapter Seven: Methods of using Curcumin and Turmeric

Introduction of two specialist approach to Raman spectroscopy

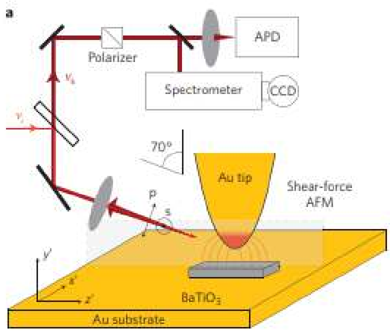
Tip-enhanced Raman spectroscopy (TERS)

Surface and interfaces play key roles in heterogeneous catalysis, electrochemistry and photo(electro)chemistry. Tip-enhanced Raman spectroscopy (TERS) combines plasmon-enhanced Raman spectroscopy with scanning probe microscopy to simultaneously provide a chemical fingerprint with which specific molecules can be identified and morphological information for the sample at the nanometer spatial resolution. It is an ideal tool for achieving an in-depth understanding of the surface and interfacial processes, so that the relationship between structure and chemical performance can be established.

TERS is a unique spectroscopic technique that possesses single-molecule sensitivity and high spatial resolution. Both of these properties are due to 1) extremely high confinement of an electromagnetic field at the apex of the scanning probe and 2) precise positioning of the scanning probe at the surface of the analyzed specimen.

The earliest reports of tip enhanced Raman spectroscopy typically used a Raman microscope coupled with an atomic force microscope. Tip-enhanced Raman spectroscopy coupled with a scanning tunneling microscope (STM-TERS) has also become a reliable technique, since it utilizes the gap mode plasmon between the metallic probe and the metallic substrate.

The technique is ideal for probing samples in aqueous medium. Also, it doesn't require the use of labels, so it can be employed to study chemical composition and molecular dynamics in biological samples, such as protein, lipid and cell membranes and nucleic acids, peptides and pathogens, directly.



Schematic of the experimental TERS setup for backscattering Raman imaging of nanocrystals based on phonon Raman selection rules [3]

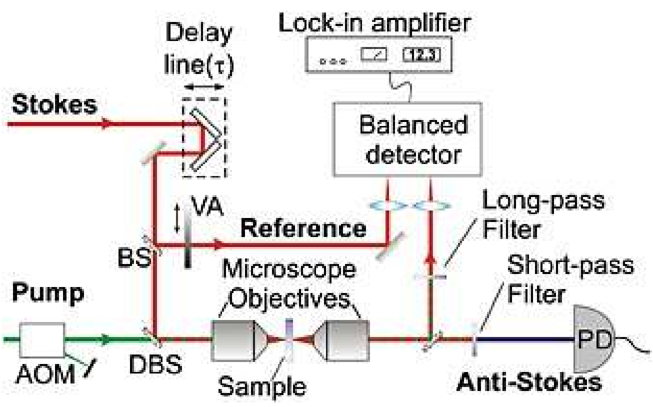
Coherent Anti-Stokes Scattering (CARS)

Coherent anti-Stokes Raman Scattering (as well as Stimulated Raman Scattering) create high imaging contrast without labeling. The technology involves two laser beams. The pump laser beam and a Stokes laser beam interact, producing an anti-Stokes signal. CARS is sensitive to the vibrational modes of samples and visualizes the vibrational contrast of molecules. The samples, even living objects, remain almost unaffected.

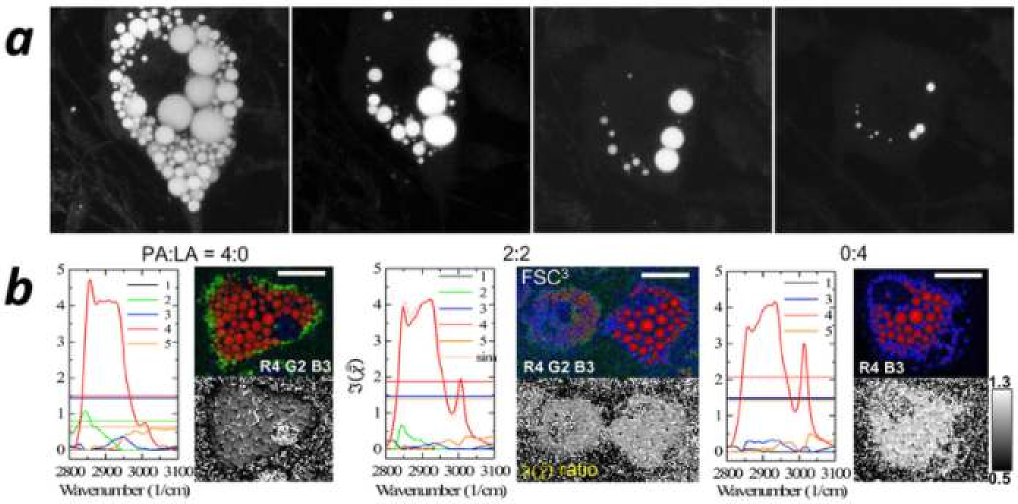
A Coherent Anti-Stokes Raman Scattering (CARS) signal was first recorded in the mid-1960s. At that time, it was called “Three wave mixing experiment”. After ten years, first applications on biological samples were shown. CARS spectroscopy is used to get detailed information of molecules or identification of components within a sample, because of the structural fingerprint

CARS – Microscopy is an imaging method which is based on the intrinsic vibrational contrast of certain molecules and thus allows a high-resolution representation of structures. Using two laser beams with a certain difference of the two frequencies, vibrational states of molecules can be probed. To differentiate between vibrational states, one of the beams, Pump or Stokes, must be tunable. The resulting inelastic scattering of blue-shifted photons (Anti-Stokes or CARS – Signal) are used for imaging.

While fluorescence microscopy is more sensitive, CARS – Microscopy offers a higher resolution at lower power level due to the multi-photon process, without the need of complex preparation of the sample with dyes (label free) that can influence the sample and the results of the experiment. In respect to this, this method is suitable for studies on living samples (in vivo), whereby the sample remains virtually unaffected.



Scheme of the experimental apparatus used for coherent anti-Stokes Raman scattering and stimulated Raman scattering



Applications using coherent anti-Stokes Raman scattering (CARS) microscopy. (a, left to right) Time-course CARS imaging of cellular lipid depletion in 3T3-L1 adipocytes. (b) CARS spectra with hyperspectral CARS images (red, green, blue) [5]

References

1. Wang, Xiang, et al. "Tip-enhanced Raman spectroscopy for surfaces and interfaces." *Chemical Society Reviews* 46.13 (2017): 4020-4041
2. Anderson, Mark S. "Locally enhanced Raman spectroscopy with an atomic force microscope (AFM-TERS)". *Applied Physics Letters*. **76** (21) (2000)
3. Berweger, Samuel, et al. "Optical nanocrystallography with tip-enhanced phonon Raman spectroscopy." *Nature Nanotechnology* 4.8 (2009): 496-499.
4. Kurouski, Dmitry. "Advances of tip-enhanced Raman spectroscopy (TERS) in electrochemistry, biochemistry, and surface science." *Vibrational Spectroscopy* 91 (2017): 3-15
5. Zhang, Chi, Delong Zhang, and Ji-Xin Cheng. "Coherent Raman scattering microscopy in biology and medicine." *Annual review of biomedical engineering* 17 (2015): 415-445.
6. https://www.ape-berlin.de/en/coherent-anti-stokes-raman-scattering/

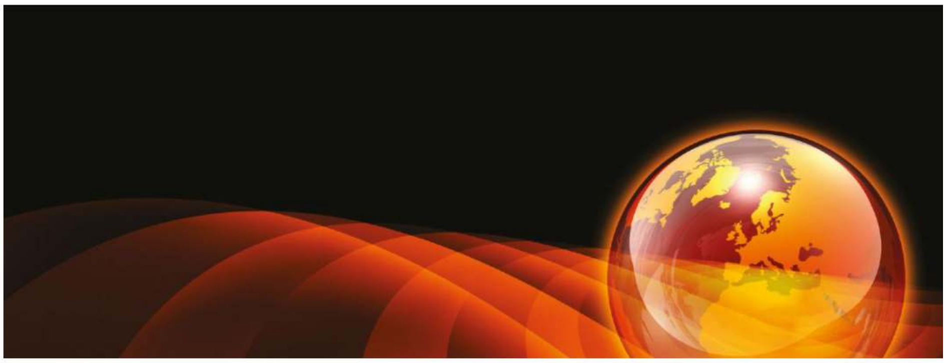
Prepared by:

Elnaz Hosseini, PhD student

Institute of Biochemistry and Biophysics

University of Tehran

New Conferences:



Physics meets Biology 2021

13 Sep 2021 to 15 Sep 2021 09:00 to 16:00
University of Oxford
More information: https://events.iop.org/physics-meets-biology-2021

International Conference on Biophysical Chemistry

June 07-08, 2022 in San Francisco, United States

More information: https://waset.org/biophysical-chemistry-conference-in-june-2022-in-san-francisco

International Conference on Biophysical Chemistry and Biomolecules

August 30-31, 2021 in Sydney, Australia

More information: https://waset.org/biophysical-chemistry-and-biomolecules-conference-in-august-2021-in-sydney

More information: https://www.biophysics.org/2022meeting

ISOBC NEWSLETTER 2021

Volume 16, Number 2

Mourning a loss of a giant of magnetic resonance
"Richard Ernst 1933-2021"

Richard R. Ernst, the 1999 Nobel Prize winner in Chemistry, died June 4 at the age of 87. He was considered the father of nuclear magnetic resonance imaging (MRI). He was an ETH Professor Emeritus who refined the high resolution nuclear magnetic resonance (NMR) spectroscopy, giving rise to the development of MRI technology, which is an imaging method for depicting tissue and organs in the body and a mainstay of medical diagnostics for more than 30 years. The International Electron Paramagnetic Resonance Society tweeted on 8 June that it was 'mourning a loss of a giant of magnetic resonance'. Ernst's work not only made NMR spectroscopy a basic and indispensable tool in chemistry but also extended its usefulness to other scientific fields, including physics, biology, and medicine. One of the most widely known applications of NMR is in diagnostic medicine, in which NMR (now magnetic resonance imaging), is a safe, noninvasive way to visualize the interior of the human body. In this capacity, NMR or MRI is well adapted to differentiating between normal and diseased or damaged tissues. It has proved useful for detecting anatomic abnormalities such as tumors and physiologic abnormalities such as blood-starved tissues.

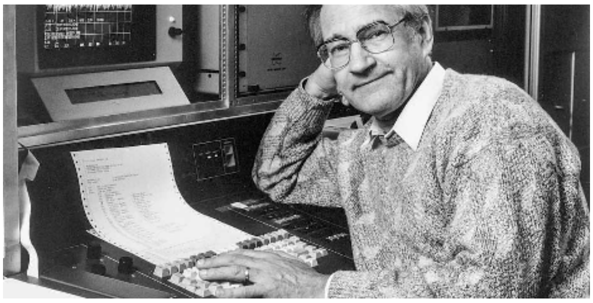
Richard Robert Ernst was born on August 14, 1933, in Winterthur, Switzerland. His family was part of the city's establishment, with a history stretching back at least 500 years. His father taught architecture at the technical high school of Winterthur and was a high-ranking officer in the Swiss army. During his childhood, he was interested in music, playing the violoncello and even considering a career as a musical composer. At 13-years old, Ernst had become interested in chemistry. He found a box of chemicals belonging to his late uncle, a metallurgical engineer, and began doing experiments. So, after completing high school in Winterthur, Ernst enrolled at the Swiss Federal Institute of Technology (ETH) in Zurich, and earned his undergraduate degree in chemistry in the 1950s. He received his PhD in physical chemistry from the same institution in 1962, focusing on NMR technology. He later moved to the USA to work in the private sector. In 1968 he returned to ETH Zurich, to teach and would remain there for the duration of his career. He started as a lecturer and his career developed to Assistant Professor in 1970, Associate Professor in 1972. Since 1976, Richard R. Ernst was Full Professor of Physical Chemistry. Ernst led a research group dedicated to magnetic resonance spectroscopy (NMR).

In 1966, Ernst and a colleague found that NMR spectroscopy could be more effective if the slow sweeping radio waves traditionally used to bombard a sample were replaced by short, intense pulses. They used a computer to perform a complex series of mathematical operations (Fourier transformations) in the received signal. This improved the sensitivity by as much as 100-fold. This change (called Fourier transform NMR) has enabled chemists to study more types of nuclei and small amounts of material. Ernst's second major contribution to the field of NMR spectroscopy was made in the mid-1970s, when he developed 2-dimensional NMR techniques to study exceedingly large molecules. By the 1990s, various NMR techniques were in use to determine the 3-dimensional structure of organic and inorganic compounds and large complex molecules such as proteins; to study the interaction between biological molecules and metal ions, water molecules, drug molecules, and other substances; to identify chemical species; and to study the rates of chemical reactions. He retired in 1998. He participated in the development of medical magnetic resonance tomography, as well as the NMR structure determination of biopolymers in solution collaborating with Professor Kurt Wüthrich. He also participated in the study of intra-molecular dynamics.

Richard Ernst was on a flight over the Atlantic in 1991 when he learnt that he had been awarded the Nobel Prize in chemistry. At some 35,000 feet in the air, he was informed that he was being offered the laureateship “for his contributions to the development of the methodology of high-resolution nuclear magnetic resonance (NMR) spectroscopy”. Ernst is credited with numerous inventions and holds several patents in the field. In addition to the Nobel Prize, He was awarded 17 honorary doctorates as well as numerous other prestigious scientific awards, such as the Benoist Prize and the Louise Gross Horwitz Prize of Columbia University (New York City). Ernst had also received the Wolf Prize in Chemistry in 1991 for ‘revolutionary contributions to NMR spectroscopy, especially

Fourier-transform and two-dimensional NMR'. In 2002, Ghana issued a stamp (Scott No. 2281d) to honor him as a Nobel laureate.

Richard Ernst put the greatest of passion into his research into the fundamentals of chemistry, and was forever thinking of ways it could be applied in our everyday lives. Ernst described himself as a "work-addict". A toolmaker, he liked to provide others with new ways to solve problems. Colleagues and former students remember him as intensely intelligent, hard-working, creative, and generous. He was known to sit in the front row at lectures and take detailed notes, even when the speaker was only a year or two into their PhD work. Yet he also believed that scientists should have a wide range of interests outside their field. In parallel with his spectroscopic interests, Ernst built and studied an extensive collection of antique Tibetan paintings.



Richard Ernst in his laboratory at ETH Zurich in 1991

The Iran Society of Biophysical Chemistry (ISOBC) members extend their condolences to the scientific and chemical community on this great loss. It is hoped that young researchers and chemists will look deeper into science and increment Richard Ernst's achievements.

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3547585/

https://www.nobelprize.org/prizes/chemistry/1991/ernst/biographical/

https://www.nature.com/articles/d41586-021-02040-5

Prepared by:

S. Abedanzadeh, PhD

ISOBC Member and

Assistant Professor at Department of Chemistry,

Kharazmi University, Karaj, Iran

ISOBC NEWSLETTER

2021

Volume 16, Number 2

Iran's Natural Wonders- Mount Damavand

news@isobc.com
Editor: Dr A. Ebrahim-Habibi
Executive Manager: A. Agheli
E-mail: a_agheli@ut.ac.ir
IT Manager: A. Mohsenimehr
Assistant Editor: E. Hosseini