



The 1st International Conference on Natural Products and Drug Discovery

The University of Jordan
September 8 – 10, 2015



Organized by
The University of Jordan
Amman, Jordan
&
ICCBS – Karachi University
Karachi, Pakistan

Abstract Book
The 1st International Conference on
Natural Products and Drug Discovery

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Preface

It is a great honor and privilege to have the patronage of Her Royal Highness Princess Sumaya Bint Al-Hassan for The 1st International Conference on Natural Products and Drug Discovery held at The University of Jordan. The conference is organized by the Faculties of Science and Pharmacy at The University of Jordan and ICCBS- Karachi University in collaboration with the Jordanian Chemical Society (JCS).

The conference aims at emphasizing the importance of natural products in developing new drugs for the economic and health benefits of man kind.

The conference includes key note, plenary and invited lectures which will be given by eminent scientists in the field. This is in addition to oral and poster presentations. Many young scientists will participate in the conference and will have the opportunity to meet and interact with leaders in the field of natural products and learn from their experience. We hope this will also open the doors for mutual cooperation and lead to joint research projects.

The support of The University of Jordan and ICCBS staff during the organization of the conference is highly acknowledged. Also, the financial support from national and international organizations is highly appreciated. We also acknowledge with gratitude the dedicated efforts of the committees' members, and students who helped in organizing this conference.

Prof. Dr. Musa H. Abu Zarqa
Chair of conference

Prof. Muhammad Iqbal Choudhary
Co-Chair of conference

About The University of Jordan

The University of Jordan is both a modern as well as old institution of Higher Education in Jordan. Established in 1962, the University has, since then, applied itself to the advancement of knowledge no less than to its dissemination. In its capacity as a comprehensive teaching, research and community-service institution.

Nowadays, the University of Jordan which lies in the capital Amman gathers diverse students from all over the Kingdom and from other countries to reach about 38,000 students.

At the undergraduate level, students have the choice to select from among 63 different programs in the Arts, Business Administration, Science, Shari'a (Islamic Studies), Medicine, Nursing, Agriculture, Educational Sciences, Engineering and Technology, Law, Physical Education, Pharmacy, Dentistry, Humanities and Social Sciences, Rehabilitation Sciences, Information Technology and, most recently, Arts and Design. For those interested in graduate education, the University offers 30 doctoral programs, 81 Master's programs, 16 programs in Higher Specialization in Medicine, one program in Higher Specialization in Dentistry, 3 Professional Diploma Programs, and 6 interdisciplinary Master's programs across the wide spectrum of academic disciplines.

From an international perspective, the University offers 63 international programs at the undergraduate level, and 130 international programs at the graduate level and in all fields of specializations. All programs offered by the University combine traditional academic lecturing with the more liberal methodologies of instruction which are based on dialogue, research and creative thinking. Theoretical instruction is further assisted with interactive multimedia teaching techniques and computer-based instructional materials to support, and eventually discard, traditional teaching methodologies. Field work, practical training, and applied research are essential components of most of the programs offered by the University. For sometime, UJ has been introducing and implementing the principles of Total Quality Management (TQM). With respect to Information Technologies, UJ is very well-positioned.

For more information about the University of Jordan kindly visit the website: www.ju.edu.jo

About International Center for Chemical and Biological Sciences (ICCBS)

Located in Pakistan's financial centre and largest city, Karachi University's International Center for Chemical and Biological Sciences (ICCBS) is one of the developing world's finest research and training centres in its field.

The large complex, which covers more than 40 hectares, is comprised of 10 research buildings that contain some of the region's most sophisticated laboratory equipment. The complex also includes a residential area with 50 houses, five apartment buildings and an international guesthouse.

ICCBS carries out research, training, product development and service delivery in the chemical, biological and biomedical sciences. The centre also provides diagnostic, analytical and clinical testing for a broad range of clients in both the public and private sectors.

Over the past 40 years, more than 600 students have earned doctorate and master's degrees at the centre. These degree-granting programmes have served as the focal points of ICCBS efforts to provide world-class training to young scientists coming primarily from developing countries, including those belonging to the Organization of Islamic Cooperation (OIC), an international network comprised of 57 Muslim countries.

ICCBS also conducts cutting-edge research for the discovery of clinically important enzymes and antioxidants, explores innovative methodologies for the synthesis of novel proteins, devises effective pharmacological evaluations of bioactive compounds, and seeks to identify new varieties of horticulture plants through applications of biotechnology

Committees

Chair of the Conference: Prof. Musa Abu Zarqa
Co-Chair: Prof. M. Iqbal Choudhary
Secretary: Prof. Amal Al-Aboudi

Advisory Board:

Prof. Atta-ur-Rahman (Chair)
Prof. Musa Nazer
Prof. Salim Sabri
Prof. Adnan Badran
Prof. Marwan Kamal
Prof. Sultan Abu Orabi
Prof. Mustafa Al-Bashir
Prof. Hala Khyami-Horani
Dr. Mohammad Hallaiqa
Dr. Adnan Badwan
Prof. Abeer Al Bawab
Mr. Nabil Ismaeel
Dr. Bassam Al-Bitar

Scientific Committee:

Prof. Jalal Zahra (Chair).
Prof. Fatma Afifi
Prof. Mohammad Hudaib
Prof. Asaad Khalid
Dr. Hala Al-Jaber
Dr. Nuha Swaidan
Dr. Mahmoud Qudah
Dr. Eveen Shalabi

Organizing Committee:

Prof. Raed Al-Qawasmeh (Chair)
Dr. Syed Ghulam Musharraf
Dr. Mohammad Khanfar
Dr. Kamal Swaidan
Dr. Meqdad Al-Habashneh
Dr. Murad Al-Damen
Dr. Fadwa Odeh
Dr. Monther Khanfer
Dr. Mansour Nawasrah
Dr. Mansour Al-Matarneh
Dr. Ehab Al-Shamaileh

Keynote and Plenary speakers



Prof. Atta-ur-Rahman, FRS

Patron-in-Chief of the International Centre for Chemical and Biological Sciences (ICCBS). With more than 970 international publications, including 151 books and 37 international patents, he has the distinction of being the only scientist to be elected Fellow of Royal Society (London) in 2006 in recognition of research contributions carried out within a country in the Islamic world. He is also the only scientist from the Muslim world to have been awarded the UNESCO Science Prize (1999). He was awarded an Honorary Life Fellowship by King's College, University of Cambridge in 2007, an honorary Doctorate of Science by University of Cambridge in 1987, a Doctorate of Education by Coventry University in 2007, a Doctorate of Science by Bradford University in 2010, a Doctor of Philosophy by Asian Institute of Technology, Thailand, in 2010 and honorary Doctor of Science by University of Technology MARA, Malaysia. He was also given the International Cooperation Award, the highest award of the Chinese Academy of Sciences for Institution Building, on 10 January 2014. Prof. Rahman was conferred the highest national award of China, the Friendship Award, at a special ceremony held on 29 September 2014 in Beijing, in recognition of his developing a large number of collaborative programs with China.



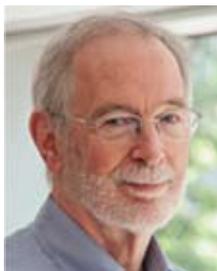
Prof. Adnan Badran

Prof. Badran is currently the Chairman of the Board of Trustees of the University of Jordan, and the Chancellor of University of Petra, with 120 publications,

including 22 books and papers, and patents. He has been awarded honorary doctorates from, Sungkyunkwan University, Seoul (1981); and an Honorary Doctorate in Science from Michigan State University, USA (2007); and West Watkins distinguished Lectureship Award (2009) and the Hall of Fame Alumni Award from Oklahoma State University, USA; Honorary Professorship from L.N. Gumilev Eurasian National University Kazakhstan (2012); an Honorary Doctorate in Business, from Yarmouk University, Jordan (2014).

He was awarded the Arab Thought Foundation Award for best Arab Scientist in higher education research 2005; the TWAS Regional Prize for “Building Scientific Institutions”, Durban, South Africa, Oct. 2009; the World Education Asia award for Outstanding Contribution to education 2011 and the Shoman award for Peer review of young Arab scientists.

Adnan Badran is a former Prime Minister of Jordan (2005) and former Minister of Agriculture and Minister of Education. He joined UNESCO in 1990 as Assistant Director-General for Natural Sciences before serving as Deputy Director-General of UNESCO (DDG) from 1994 to 1998; served as Senator and Chair of the Senate Committee on Science, Education and Culture, and President of the National Centre of Human Rights of Jordan, and President of the Asia-Pacific Forum on human rights, Sidney (2009-2011). He is a Fellow and served as vice-president of the Academy of Sciences for the Developing World (TWAS), and fellow of the Islamic World Academy of Sciences and the Arab Thought Forum, also, President of the Arab Academy of Sciences, and President of the Board of AFED in Beirut.



Prof. Jon C. Clardy

Director of the Infectious Disease Program at the Broad Institute and a professor in the Department of Biological Chemistry and Molecular Pharmacology at the Harvard Medical School, Harvard University, Boston, USA. Prof. Clardy has about 1000 publications in high impact factor journals. His research involves many aspects of biologically active small molecules, especially those known as natural products. Prof. Clardy has received many awards for his research including fellowships from the Alfred P. Sloan Foundation, the Camille and Henry Dreyfus Foundation, and the John Simon Guggenheim Memorial Foundation. He has also received the Ernest Guenther Award and an Arthur C. Cope Scholar Award from the American Chemical Society, and the Research Achievement Award from the American Society of Pharmacognosy. He is a Fellow of the American Academy of Arts and Sciences and the American

Association for the Advancement of Science, and won Cornell's highest award for teaching in the College of Arts and Sciences.



Prof. Muhammad Iqbal Choudhary

H.I., S.I., T.I. Director of the International Centre for Chemical and Biological Sciences (H. E. J. Research Institute of Chemistry) & Dr. Panjwani Centre for Molecular Medicine and Drug Research , University of Karachi, Karachi, Pakistan; is a leading scientist and scholar in the field of organic chemistry . He is renowned for his research in the various areas relating to natural product chemistry. He holds more than 800 researched publications in top international journals with cumulative impact factor of over 1430 and 6000 citations, 25 national and international patents and 32 books published and circulated internationally. He is also the Editor-in-Chief of 4 European science journals and book series. Prof. Choudhary's eminent contributions in the field of Organic Chemistry made him the recipient of civilian awards of different countries nationally and internationally of which are: Tamgha-i-Imtiaz, Sitara-e-Imtiaz , Distinguished National Professor of HEC, Hilal-e-Imtiaz, COMSTECH Award in Chemistry , TWAS Award in 1994, Khwarizmi International Award, Economic Cooperation Organization Award.



Dr. Adnan Badwan

General Director of The Jordanian Pharmaceutical Manufacturing Company in Jordan, Deputy Chairman of DELASS Natural Products and the President of the Board of Directors of The Arab Union of The Manufacturers of Pharmaceutical and Medical Appliances (AUPAM). Dr. Badwan has over 30 years of experience in pharmaceutical R&D management, technology transfer and business development. During his career, he published 130 scientific articles and book chapters, filed more than 70 business-related patents,

established three companies based on locally developed technology and led the first merger in the Jordanian Pharmaceutical Industry in 2004. He received several achievement awards including State Award of Excellence in 2008, by the Ministry of Culture in Jordan, for his work in pharmacy. Businessman of The Year Award in 2006 by the Islamic Corporation for the Development of the Private Sector (ICD). The Field of Invention Award in 2006 by Philadelphia University in Jordan and Arab Technology Entrepreneur of The Year Award in 2005 by the Arab Science & Technology Foundation (ASTF).



Prof. Bilge Sener

Department of Pharmacognosy, Faculty of Pharmacy, Ghazi University, Ankara, Turkey. Prof. Sener has more than 170 publications, 1134 citations with 290 impact points. Her research interests are in development of bioactive compounds from Turkish medicinal plants and marine organisms; evaluation and standardization of Phytopharmaceuticals and Nutraceuticals . Other fields are: Isolation and structure elucidation of alkaloids with biological activity, lignans of *Taxus* species, Fumariaceae and Amaryllidaceae alkaloids, screening of Turkish terrestrial and marine organisms for Anticholinesterase and Antimycobacterial activities and bioassay-guided isolation of active compounds.



Prof. Fatma Afifi

Professor of Pharmacognosy and Phytochemistry Faculty of Pharmacy University of Jordan, Amman, Jordan. She got the “Distinguished Researcher Award” from the University of Jordan for three successive years. Her Research Interests are: Isolation, identification and structure determination of plant constituents - Biological activity of the natural products (antiulcer, hypoglycemic, antiplatelet, anticancer) - Ethnopharmacology and evidence based phytotherapy using local medicinal plants.

Sponsors



Islamic Development Bank Group

The Islamic Development Bank Group (IDB Group) is a South-South multilateral development finance institution established in pursuance of the Declaration of Intent issued by the Conference of Finance Ministers of Muslim Countries held in Jeddah in Dhul Q'adah 1393H, corresponding to December 1973. The Inaugural Meeting of the Board of Governors took place in Rajab 1395H, corresponding to July 1975, and the Bank was formally opened on 15 Shawwal 1395H corresponding to 20 October 1975. The purpose of the Bank is to foster the economic development and social progress of member countries and Muslim communities individually and collectively in accordance with the principles of Shari'ah (Islamic Law). The IDB Group comprises five entities, namely:

- (i) Islamic Development Bank (IDB);
 - (ii) Islamic Research and Training Institute (IRTI);
 - (iii) Islamic Corporation for the Insurance of Investment and Export Credit (ICIEC);
 - (iv) Islamic Corporation for the Development of the Private Sector (ICD);
- and
- (v) International Islamic Trade Finance Corporation (ITFC).

Activities of the Group

IDB Group is engaged in a wide range of specialized and integrated activities such as:

- Project financing in the public and private sectors;
- Development assistance for poverty alleviation;
- Technical assistance for capacity-building;
- Economic and trade cooperation among member countries;
- Trade financing;
- SME financing;
- Resource mobilization;
- Direct equity investment in Islamic financial institutions;
- Insurance and reinsurance coverage for investment and export credit;

- Research and training programs in Islamic economics and banking;
- Awqaf investment and financing;
- Special assistance and scholarships for member countries and Muslim communities in non-member countries;
- Emergency relief; and
- Advisory services for public and private entities in member countries.



Petra University

Located in West of Amman, University of Petra is a home to seven faculties in a friendly campus, housing seven thousand students of undergraduate and graduates: Arts and Sciences, Administrative & Financial Sciences, Pharmacy & Medical Sciences, Information Technology, Architecture & Design, law, Mass Communication.

The University is a hub of creating knowledge through research, in developing skills, in applying knowledge to new technologies and in technology transfer. Therefore, the university has a friendly-use campus to unleash the minds of men and women to new horizons of thought, philosophy and logic. It provides an intriguing environment of freedom of thought, inquiry, interactive and blended learning and R&D facilities. It is aggressive in developing an outreach program for community development and engaging in regional and international science for bridging with other scientists, journals, symposia to bring science to solve social problems and open new opportunities of employment and eradicate poverty.

To be able to do that, the university has achieved the ISO 9001 of managements for supporting higher education certificate, and certificate of quality assurance of the Higher Education Accreditation Commission, in addition the university is ranked 1st runner in the QS ranking of private universities. The university is working toward quality, relevance and alignment in terms of teaching and research, bridging with industry, public and private sectors and community at large.

UOP with the development of e-learning, e-library and high speed communication facilities, is turning into a smart campus, where students and faculty interact with knowledge to develop their state of the art skills to develop entrepreneurship, innovation and creativity.



Arab Academy of Sciences

The Arab Academy of Sciences is a non-profit scientific non-governmental organization supported by UNESCO. It functions through the UNESCO regional Office in Beirut that hosts its Secretariat. The Academy has a Council headed by the President of the Academy HE Dr Adnan Badran.

The Academy undertakes different types of initiatives aimed at contributing to the reform of scientific research, enhancing the development of knowledge, encouraging excellence in sciences and their applications, promoting the culture of sciences and increasing scientific awareness in the Arab society.

The Academy published the four volumes of the Arabic Encyclopedia on “Knowledge for Sustainable Development”, in collaboration with UNESCO and with the support of EOLSS. In addition to general introduction, these volumes deal with environmental, economic and social dimensions of sustainable development. In collaboration with UNESCO and ALECSO, the Academy was involved in the publication of the indicators of science and technology in the Arab World.

The Academy was involved in the organization of several regional conferences and training sessions on science, technology and innovation. Among the international conferences organized by the Academy during the last 12 years are:

- 1) Economic Growth: The Involvement of Biotechnology and the Modern Bioindustries
- 2) Bioethics: how to Adapt Biotechnology to Culture and Values
- 3) Drug Biotechnology and Medicinal Plants
- 4) Nanoscience and its Impact on renewable energy and medicine
- 5) Integrated Water Resources Management in the Arab Region
- 6) Science Parks for the Developing World as Engines of Economic and Social Growth
- 7) Training of Science Park Managers
- 8) Bridging digital divide in Developing Countries
- 9) Alternative and Renewable Sources of Energy
- 10) Water and Energy in Sustainable Food Security
- 11) Water-Energy Nexus and Waste Management for a Sustainable Arab World
- 12) Energy and Water Sustainability
- 13) Sustainable Energy and Water Resource Management for Food Security in the Arab Middle East



Delass Natural Product Ltd.

Delass Natural Product Ltd. was launched in 1999 as a JPM subsidiary with the objective of developing and commercializing medicines, dietary supplements, functional foods, skincare products, and cosmetics derived from natural sources.

Delass production adheres to GMP and its market reach has expanded to include Jordan, Turkey, Saudi Arabia, Syria, Lebanon, Kazakhstan, Uzbekistan, Bosnia, Azerbaijan, Tunisia, Algeria, Sudan and Egypt among others. Delass also offers technical knowhow to other pharmaceutical companies.

Delass products cover a wide range of herbal medicines, dietary supplements, and functional foods. These include natural health care products, cardio vascular, intestinal, respiratory and cough syrups, phytoestrogens, musculoskeletal, genitourinary, immuno stimulants, antioxidants, and dermatological products.



Amman Chamber of Industry (ACI)

Amman Chamber of Industry (ACI) was established in 1962 as a non-profit organization which represents the industrial sector in Jordan. ACI's membership totals around 8000 varying in size from large, medium and small enterprises. The (ACI) also forms and develops a framework to crystallize the industrial point of view of its members in economic issues in general and industrial issues, in particular, where the Chamber cooperates with the ministries and relevant government economic planning, especially with regard to industry, in coordination with the Jordan Chamber of Industry. The Chamber contributes in the membership of boards of trustees and in the management of many institutions involved in economic and social development, training and scientific research.



Jordan Carbonate Company

Jordan Carbonate Company (JCC), situated in Amman, is a privately owned company, which was established in 1979. The company employs a total of 350 Jordanian staff and its board is chaired by Mr. Ayman Hatahet. JCC is specialized in mining, manufacturing and exporting Calcium Carbonate with highest standards of quality, purity, and prompt delivery, which made the company a pioneer in its field. JCC products are exported to 35 countries in Asia, Africa, Europe and Latin America.

JCC invest (5%) of its yearly turnover in research committed to developing product specifications, introducing new applications & conducting market research.



Jordan Chamber of Industry (JCI)

Jordan Chamber of Industry (JCI) was founded by the Chambers of Industry Law number 10 for the year 2005 as a national entity that embodies under its umbrella the three local chambers of industry in Jordan, located in Amman, Irbid and Zarka. The Jordan Chamber of Industry aims at achieving the following:

- To increase the competitiveness of the Jordanian industry.
- To participate in drawing the general policy for the industry and setting the necessary strategies and plans required for implementation.
- Safeguarding the interests of all industrial and micro enterprises.
- Enhancing cooperation with Federations and Arab and Foreign Chambers of Industry.
- Building capacity of the local chambers of industry and coordinating their efforts.

For more information kindly visit the website: Website: www.jci.org.jo



Abdul Hameed Shoman Foundation

The Abdul Hameed Shoman Foundation Established by the Arab Bank in 1978. The Abdul Hameed Shoman Foundation (AHSF) is a non-profit organization dedicated to investing in cultural and social innovation to positively impact the communities it serves through Thought Leadership, Arts and Literature, and Employment and Innovation.



Royal Society of Chemistry

The Royal Society of Chemistry With more than 51,000 members and an international publishing and knowledge business The Royal Society of Chemistry (RSC) is the world's oldest chemical society with more than 175 years of history. RSC as a publisher produces 42 journals, 100 books per year, and 6 databases. As per the 2014 Journal Citation Reports our average Impact Factor (IF) is 5.68 for all our journals, we are among the best quality chemistry publishers in the world where 85% of our journals now have an IF above 3, the highest IF is 33.38 and the lowest is 1.82. RSC is a not-for-profit organization inverts all the revenue back to the scientific community, part of our not-for-profit activities is producing open access databases like ChemSpider (the world's largest free chemical compounds database with more than 34 Million compounds) and Learn chemistry (the free chemical education database). Besides being a top chemistry publisher, we have many other programs like: the RSC international academic accreditation, and RSC industrial accreditation program.



Target Chemicals

Target Chemicals is one of the leading companies in the Levant region that is specialized in the fields of distribution and the trading of chemical raw materials for industrial clients operating in the fields of pharmaceutical, agrochemical, Feed, veterinary, food, personal care, home care, Institutional and construction & coating industries.

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Spectrum light & sound

Spectrum light & sound is your destination for a full audio and automation solution. As exclusive distributors of Bose and authorized dealers of Crestron, we work closely with our partners to customize the right solution that reflects the technological superiority of our products while at the same time meeting your demands as a top priority.

We cherish strong relationships with our clientbase to ensure its a mutual learning experience.

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Jordanian Chemical Society

Jordanian Chemical Society (JCS) was established in 1976 and it is a member in the IUPAC, FACS and UACS, and its objectives include the following:

- 1) Strengthening the relationship among the Jordanian Chemists themselves and among their chemist colleagues.
- 2) Introduce the role of chemistry to relevant fields of the community.
- 3) Contribute in supporting scientific research in different fields of chemistry.
- 4) Communicate with the Arab and International Chemistry organizations, institutions and societies in order to attain the above stated objectives.
- 5) Perform activities that promote chemistry and serve the Jordan community in particular and the Arab community in general.

**The 1st International Conference on Natural Products &
Drug Discovery Venue: Ahmad Al-Lozi Auditorium
King Abdullah II School for Information Technology
The University of Jordan, Amman, Jordan
September 8 – 10, 2015
Program
Day 1 : 08/09/2015**

8:00 - 9:00	Registration	
9:00 - 10:00	Inauguration Ceremony	
10:00 - 10:20	Group Photo and Reception	
Session 1	Chair	Prof. Adnan Badran
10:20 - 11:20	KN-1	Adventures in natural products chemistry and higher education Prof. Atta-ur-Rahman (ICCBS, Pakistan)
Session 2	Chair	Prof. Hala Khyami-Horani & Prof. Rula Darwish
11:20 - 12:10	KN-2	Role of science, technology and innovations in pharmaceutical industry Prof. Adnan Badran (University of Petra, Jordan)
12:10 - 12:50	PL-1	Drug lead discovery from nature: case study I Prof. Muhammad Iqbal Choudhary (ICCBS, Pakistan)
12:50 - 1:20	IL-1	Extensive integrative drug discovery: Using Africa medicinal plants for fighting African endemic neglected diseases Prof. Asaad Khalid (Jazan University, Saudi Arabia)
1:20 - 1:40	OP-1	In vitro modulation of pancreatic insulin secretion and extrapancreatic insulin action, enzymatic starch digestion and protein glycation by <i>Terminalia chebula</i> extracts Dr. Violet Kasabri (The University of Jordan, Jordan)
1:40 – 2:00	OP-2	Two novel cardenolides from <i>Calotropis procera</i> Dr. Nuha Swaidan (University of Petra, Jordan)
2:00 – 3:00	Lunch	
Participants are invited to join session 7 of the NASIC Workshop on “Herbal Drug Development for Socio-Economic Uplift in Developing World” Venue: Ahmad Al-Lozi Auditorium King Abdullah II School for Information Technology		

Session 3	Chair	Prof. Sultan Abu Orabi & Prof Musa Abu Zarqa
3:00 – 3:40	PL-2	Natural Products and Drug Discovery Prof. Jon Clardy (Harvard Medical School, USA)
3:40 – 4:10	IL-2	Plasmodium prolyl tRNA synthetase - a druggable next generation dual-stage target for Malaria elimination Prof. Ralph Mazitschek (Center for Systems Biology, Massachusetts General Hospital, USA)
4:10 – 4:40	IL-3	Application of structural chemistry and structural biology in drug discovery Dr. Atia Tulwahab (ICCBS, Pakistan)
4:40 – 5:30	Concluding Remarks of the workshop & Certificate Distribution Ceremony	

Day 2: 09/09/2015		
Session 4	Chair	Prof. Musa Nazer & Prof. Amal Al-Aboudi
9:00- 10:00	KN-3	Chemistry, genetics, and fungus-growing ants Prof. Jon Clardy (Harvard Medical School, USA)
10:00-10:30	IL-4	Optimization of supercritical fluid extraction of major γ-pyrones from <i>ammi visnaga</i> fruits Prof. Osama Salama (Future University, Egypt)
10:30-11:00	IL-5	Screening of antibiotic resistant inhibitors from local plant materials against MRSA Prof. Rula Darwish (The University of Jordan, Jordan)
11:00- 11:20	Posters and Coffee Break	
Session 5	Chair	Dr. Mohammad Halaiqa & Prof. Abeer Al Bawab
11:20 - 12:00	PL-3	Drug lead discovery from nature- case study II Prof. Atta-ur-Rahman (ICCBS, Pakistan)
12:00 - 12:40	PL-4	Wholistic approach to herbal products quality case study: Identification of Thyme markers Dr. Adnan Badwan (Delass Natural Products Company, Jordan)
12:40 - 1:10	IL-6	Jordanian medicinal plants in drug discovery- where we are standing, establishing a future vision Prof. Talal Aburjai (The University of Jordan, Jordan)
1:10 – 1:40	IL-7	A tale of three medicinal plants from Jordan Prof. Suleiman Al-Khalil Olaimat (The University of Jordan, Jordan)
1:40- 2:30	Lunch	

Session 6	Chair	Dr. Adnan Badwan & Prof. Jalal Zahra
2:30-3:10	PL-5	Quality control and regulatory issues of phytopharmaceutics for global health care Prof. Bilge Sener (Gazi University, Turkey)
3:10- 3:40	IL-8	Novel ligand-based and structure-based drug design approaches developed at the Faculty of Pharmacy- The University of Jordan Prof. Mutasem Taha (The University of Jordan, Jordan)
3:40- 4:10	IL-9	Phytochemical investigation of some selected plants belonging to the Mediterranean region Dr. Hala Al-Jaber (Al-Balqa Applied University, Jordan)
4:10 – 4:40	IL-10	Diastereoselective Design of Privileged Structures: Forward Chemical Genetics for Phenotypic Screening of Chemical Probes Prof. Taleb Al-Tel (University of Sharjah, UAE)
4:40- 5:00	OP-3	Discovery of new human epidermal growth factor receptor-2 (HER2) inhibitors for potential use as anticancer agents via ligand-based pharmacophore modeling Hiba Zalloum (The University of Jordan, Jordan)
5:00 – 5:30	Posters and Coffee Break	

Day 3: 10/09/2015		
Session 7	Chair	Prof. Salim Sabri & Dr. Hala Al-Jaber
9:00-9:40	PL-6	Phytochemical and biological evaluation of some common and rare <i>Salvia</i> species from Jordan Prof. Fatma Afifi (The University of Jordan, Jordan)
9:40- 10:10	IL-11	Identification of novel interleukin-2 inhibitors from natural products: a computational and molecular modeling perspective Dr. Zaheer Al-Haq Qasmi (ICCBS, Pakistan)
10:10- 10:40	IL-12	Drug development and clinical trial challenges for natural products-based drug candidates Prof. Abeer Al-Ghananeem (Sullivan University,USA)
10:40- 11:10	IL-13	How to get your paper published in high impact journals Mr. Wesam Abu Saif (The Royal Society of Chemistry)

11:10-11:30	OP-4	Biogenetic conversion of antifungal phytoalexin wyerone into wyerone epoxide from <i>Vicia faba</i> plant cotyledons Dr. Nedhal Al – Douri (Philadelphia University, Jordan)
11:30-11:50	Posters and Coffee Break	
Sessions 8	Chair	Prof. Osama Salama & Prof. Mohammad Hudaib
11:50 - 12:20	IL-14	Nutraceuticals as a source of bioactive molecules for drug discovery Dr. Mayyada Shhadeh (The University of Jordan, Jordan)
12:20 - 12:50	IL-15	The anti-spermatogenic effects of <i>Taraxacum officinale</i> and <i>Orchis anatolica</i> in male rodents Dr. Lubna Tahtamouni (The Hashemite University, Jordan)
12:50 - 1:10	OP-5	Identification of Rab8b protein inhibitors through homology modeling and virtual screening Mr. Aboubakr Abdelmonsef (Osmania University, India)
1:10- 2:30	Lunch	
Session 9	Chair	Prof. Talal Aburjai & Dr. Meqdad Al-Habashneh
2:30 – 3:00	IL-16	The Plant-derived Molecule Thymoquinone inhibits Self-renewal Capacity of Colorectal Cancer Stem Cells Prof. Hala Gali-Muhtasib (American University of Beirut, Lebanon)
3:00 - 3:30	IL-17	Mass spectrometric dereplication approach for plant extract and plant powder: a case study on <i>Withania somnifera</i> Dr. Syed Ghulam Musharraf (ICCBS, Pakistan)
3:30 – 3:50	OP-6	Elaborate libdock docking, dbcica Implementation and in silico screening reveal new potent acetylcholinesterase inhibitors Maha Habash (Applied Science Private University, Jordan)
3:50 - 5:00	Concluding remarks of the conference & certificate distribution ceremony	

Scientific Program

Day 1: 08/09/2015

- Session 1**
10:20 - 11:20
Chair: Adnan Badran
(KN-1) Adventures in natural products chemistry and higher education
Atta-ur-Rahman
- Session 2**
11:20 - 12:10
Chair: Hala Khyami-Horani & Rula Darwish
(KN-2) Role of science, technology and innovations in pharmaceutical industry
Adnan Badran
- 12:10 - 12:50
(PL-1) Drug lead discovery from nature: case study I
Muhammad Iqbal Choudhary
- 12:50 - 1:20
(IL-1) Extensive integrative drug discovery: Using Africa medicinal plants for fighting African endemic neglected diseases
Asaad Khalid
- 1:20 - 1:40
(OP-1) In vitro modulation of pancreatic insulin secretion and extrapancreatic insulin action, enzymatic starch digestion and protein glycation by *Terminalia chebula* extracts
Violet Kasabri
- 1:40 - 2:00
(OP-2) Two novel cardenolides from *Calotropis procera*
Nuha Swaidan
- Session 3**
3:00 - 3:40
Chair: Sultan Abu Orabi & Musa Abu Zarqa
(PL-2) Natural Products and Drug Discovery
Jon Clardy
- 3:40 - 4:10
(IL-2) Plasmodium prolyl tRNA synthetase - a druggable next generation dual-stage target for Malaria elimination
Ralph Mazitschek
- 4:10 - 4:40
(IL-3) Application of structural chemistry and structural biology in drug discovery
Atia Tulwahab

Day 2: 09/09/2015

- Session 4**
9:00- 10:00 **Chair: Musa Nazer & Amal Al-Aboudi**
(KN-3) Chemistry, genetics, and fungus-growing ants
Jon Clardy
- 10:00-10:30 **(IL-4) Optimization of supercritical fluid extraction of major γ -pyrones from *ammi visnaga* fruits**
Osama Salama
- 10:30-11:00 **(IL-5) Screening of antibiotic resistant inhibitors from local plant materials against MRSA**
Rula Darwish
- Session 5**
11:20 - 12:00 **Chair: Mohammad Halaiqa & Abeer Al Bawab**
(PL-3) Drug lead discovery from nature: case study II
Atta ur-Rahman
- 12:00 - 12:40 **(PL-4) Wholistic approach to herbal products quality case study: Identification of Thyme markers**
Adnan Badwan
- 12:40 - 1:10 **(IL-6) Jordanian medicinal plants in drug discovery- where we are standing, establishing a future vision**
Talal Aburjai
- 1:10 – 1:40 **(IL-7) A tale of three medicinal plants from Jordan**
Suleiman Al-Khalil Olaimat
- Session 6**
2:30-3:10 **Chair: Adnan Badwan & Jalal Zahra**
(PL-5) Quality control and regulatory issues of phytopharmaceutics for global health care
Bilge Sener
- 3:10- 3:40 **(IL-8) Novel ligand-based and structure-based drug design approaches developed at the Faculty of Pharmacy-The University of Jordan**
Mutasem Taha
- 3:40- 4:10 **(IL-9) Phytochemical investigation of some selected plants belonging to the Mediterranean region**
Hala Al-Jaber
- 4:10 – 4:40 **(IL-10) Diastereoselective Design of Privileged Structures: Forward Chemical Genetics for Phenotypic Screening of Chemical Probes**
Taleb Al-Tel
- 4:40- 5:00 **(OP-3) Discovery of new human epidermal growth factor receptor-2 (HER2) inhibitors for potential use as anticancer agents via ligand-based pharmacophore modeling**
Hiba Zalloum

Day 3: 10/09/2015

- Session 7**
9:00-9:40 **Chair: Salim Sabri & Hala Al-Jaber**
(PL-6) Phytochemical and biological evaluation of some common and rare *Salvia* species from Jordan
Fatma Afifi
- 9:40- 10:10 **(IL-11) Identification of novel interleukin-2 inhibitors from natural products: a computational and molecular modeling perspective**
Zaheer Al-Haq Qasmi
- 10:10- 10:40 **(IL-12) Drug development and clinical trial challenges for natural products-based drug candidates**
Abeer Al-Ghananeem
- 10:40- 11:10 **(IL-13) How to get your paper published in high impact journals**
Wesam Abu Saif
- 11:10-11:30 **(OP-4) Biogenetic conversion of antifungal phytoalexin wyerone into wyerone epoxide from *Vicia faba* plant cotyledons**
Nedhal Al-Douri
- Sessions 8**
11:50 - 12:20 **Chair: Osama Salama & Mohammad Hudaib**
(IL-14) Nutraceuticals as a source of bioactive molecules for drug discovery
Mayyada Shhadeh
- 12:20 - 12:50 **(IL-15) The anti-spermatogenic effects of *Taraxacum officinale* and *Orchis anatolica* in male rodents**
Lubna Tahtamouni
- 12:50 - 1:10 **(OP-5) Identification of Rab8b protein inhibitors through homology modeling and virtual screening**
Aboubakr Abdelmonsef
- Session 9**
2:30 – 3:00 **Chair: Talal Aburjai & Meqdad Al-Habashneh**
(IL-16) The Plant-derived Molecule Thymoquinone inhibits Self-renewal Capacity of Colorectal Cancer Stem Cells
Hala Gali-Muhtasib
- 3:00 - 3:30 **(IL-17) Mass spectrometric dereplication approach for plant extract and plant powder: a case study on *Withania somnifera***
Syed Ghulam Musharraf
- 3:30 – 3:50 **(OP-6) Elaborate libdock docking, dbcica implementation and in silico screening reveal new potent acetylcholinesterase inhibitors**
Maha Habash

Poster Presentations

- (PO-1) **In Vitro evaluation of the antiproliferative activity of some medicinal plants traditionally used against cancer in Jordan**
Eman Y. Abu-rish
- (PO-2) **Phytochemical, Anti-acetylcholinesterase, -Oxidant, and -Inflammatory Properties of Selected Jordanian Medicinal Plants**
Sawsan Abuhamdah
- (PO-3) **Photochemical Investigation of Antimicrobial Seed Extracts of Citrus Aurantifolia**
Rehab Mohammed
- (PO-4) **A green Biosynthesis of Silver Nanoparticles (AgNPs) using Maltose and Plant Leaf Extract**
Muna A. Abu-Dalo
- (PO-5) **Phytochemical Analysis and Evaluation of Antimicrobial, Antiangiogenic and Antiproliferative (Against Different Breast Cancer Cell Lines) Activities of the Leaves of Elaeagnus angustifolia.**
Aman Ishaqat
- (PO-6) **Towards Solving Khat Addiction Controversy: Metabolomic, biological and toxicity profiles of various cultivars of khat Plant**
Asaad Khalid
- (PO-7) **Isolation and Identification of the Chemical Constituents of Scabiosa prolifera**
Mahmoud A. Al-Qudah
- (PO-8) **Activity of Some new Iminoxime ligands and their Nickel Complexes**
Manahil Mohammed
- (PO-9) **Characterization of Phytochemical Constituents from the Butanol Crude Extract of Salvia Judaica and Its Antioxidant activity**
Ethar Fattah Khlaifat
- (PO-10) **The Electronic Spectrum of BH₂ Radical**
Mohammed Gharaibeh
- (PO-11) **A prodrug approach to enhance azelaic acid percutaneous absorption**
Sara AlMarabeh
- (PO-12) **Antiproliferative activity of the combination of Quercetin/ Doxorubicin on breast cancer cell line: New method for studying cytotoxicity**
Nirmeen Elmadany
- (PO-13) **Effect of in vitro Slow Growth Conservation of Wild Mint (Ziziphora tenuior L.) on Oil Production and Pulegone Concentration in the Conserved Plants**
Tamara S. Al-Qudah
- (PO-14) **Nanoflora- A New Approach Toward Activity Enhancement of Natural Products**
Dima Khater

Keynote Lectures (KN)
Plenary Lectures (PL)
Invited Lectures (IL)
Oral Presentations (OP)
Posters (PO)

Some Adventures in Natural Product Chemistry and Higher Education

Atta-ur-Rahman, FRS

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Abstract

We have investigated several hundred terrestrial and marine plants for their chemical and biological significance and isolated and identified over 2,000 compounds of which some 600 turned out to be new and novel constituents with interesting biological activity profiles. In order to optimize the chances of finding novel leads, extensive primary biological screenings and activity-guided fractionation and purification were carried out. State-of-the-art spectroscopic techniques, especially modern multi-dimensional NMR techniques, were utilized to elucidate the structures of bioactive natural molecules, rapidly and accurately. The results have been truly exciting as we have identified several new classes of potent enzyme inhibitors. In many cases, chemical structural modifications and microbial transformations were carried out to study the structure-activity relationships. A selection of these results illustrated by their potential application to treat neuronal diseases such as epilepsy as well as others such as leishmania will be described.

Pakistan has made remarkable progress during the period 2000-2008 under my charge as Federal Minister of Science/Higher Education which has directly impacted scientific research. The increase in scientific research output is nothing short of spectacular—1000 per cent increase in scientific publications in international journals and a similar increase in citations in the same period, after decades of stagnation. The Chairman, UN Commission on Science, Technology & Development, Prof. Michael Rode made the following comment about the transformation of the higher education landscape of Pakistan under my charge: *“Around the world when we discuss the status of higher education in different countries, there is unanimity of opinion that the developing country that has made the most rapid progress internationally in recent years is Pakistan. In no other country has the higher education sector seen such spectacular positive developments as that in Pakistan”*. These developments will also be presented.

Role of Science, Technology and Innovations in Pharmaceutical Industry

*Adnan Badran **

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Pharmaceutical industry is a research-based knowledge economy in the development of vaccines and medicines. Global pharmaceutical sale is \$856 billion in 2010, and billions of dollars are invested by thousands of scientists in R&D technology and innovations. Nowadays, the cost of developing a single drug amounts to \$1.5 billion, as compared to \$138 million in 1975. Eighty percent of Pharma R&D is done in U.S (\$51.3 billion, 2005) while 20% is done mostly in Europe.

The innovation gap crises in pharma R&D is growing. New molecular entities (NMEs) approved drugs remained flat in the past decade. In the 1990's, eleven new drugs had reached the "top 100 drugs" while in 2000-2004 only two new drugs approved made it to the top 100 revenue generation. R&D cost is on the rise due to a lengthy clinical trials by FDA for safety. Only one drug candidate out of 13 preclinical candidates is passed (8%). It takes 10-15 yrs for the FDA to pass a new drug.

Basic scientific research is lacking in pharma-research. If there is no new science, there is nothing to apply. The industry is often after a short-term gains. They have no interest in lengthy basic research for new discovery which would open a new space for technology and innovations to multiply. Easy wins in pharmaceuticals have already been made. Low hanging fruits have already been picked and more difficult ones are the remains. Now the challenge is how to deal with more complex diseases and malfunctions. There is a decline of new drugs and the new drugs are derived from already marketed drugs each year. The pharma R&D pipeline is drying up, and pharma industry is in crisis. Huge layoffs were made by thousands in drug discovery to cut down on costs and exposure to risk.

Restructuring through large scale merger, acquisitions and risk sharing partnership is underway. Also, shifting R&D from small molecules in

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chemistry to large molecules of biology has triggered layoffs of thousands of chemists by big pharma companies. Growth of drug discovery in the future is seen in small pharma and biotech, and not in big pharma. Expiring green chip patents, and cut down on R&D for drug discovery are the biggest threat to big pharma against collapse and being to be replaced by newer smaller pharma.

The use of computer assisted design and biotechnology will speed up drug discovery. While Intellectual Property Rights (IPR) enhances technology advancement in the industry.

Most pharma-research in the past decade was focusing on four major problems: CNS, cancer, cardiovascular and infectious disease. Human genome discovery has opened a new horizon for R&D in DNA and RNA genetic diseases and disorders, and stem cells research.

For developing countries, particularly the BRICS * emerging countries there is a potential to grow in pharma-industry, due to:

- a) Economy of scale of dense population.
- b) Cheaper in conducting R&D particularly basic research due to lower wages and less costly. Big companies are outsourcing R&D to supplement their internal chemistry-biology capacity outside U.S and Europe particularly in Asia, and helping out developing countries to get to FDA standard.
- c) The big patent cliffs, making use of expiring patents of major drugs by developing countries- in the US patents exclusivity of 110 products expired in 2012-2014.
- d) Harvesting medicinal natural products of their wealthy wild flora biodiversity.

But the main challenge in developing countries remains in reforming their education system, particularly higher education, to deliver excellence of scientists and scientific research, and to incubate the R&D outcome and transfer to technology, to be marketed, to industry in a business-like-fashion.

* Brazil, Russia, India, China and South Africa.

**Chemistry, genetics, and fungus-growing ants
How is this?**

Jon Clardy

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Abstract

Four types of animals – humans, ants, termites and beetles – have highly derived agricultural systems, and this talk will focus on the chemical ecology that regulates the multilateral symbioses of fungus-farming ants. These molecules not only regulate symbiotic relations; they can also be exploited to discover antibiotics and anticancer agents. The lecture begins by describing the various participants in the system: the ant farmers, their fungal crop, the specialized fungal pathogens, and the symbiotic bacteria, and then discuss the chemical defenses supplied by the bacterial symbionts. Since the ant system has evolved from a single beginning in the Amazon 50-60 million years ago to include over 200 species, the chemical diversity included in this system is both large and poorly explored. What could be gained by trying to systematically characterize this chemical diversity? Opportunities include: 1) discovery of new chemotypes, new biosynthetic pathways, and potentially useful therapeutic agents, 2) understanding of how biosynthetic pathways, which are arguably provide ideal case studies for multigenic phenotypes, evolve, and 3) potential approaches to uncovering cryptic metabolites.

Drug Lead from Nature: Case Study I

Muhammad Iqbal Choudhary and Atta-ur-Rahman

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Abstract

Modern drug development is expensive and lengthy which requires over \$ 1.8-2.0 billion worth of investments and focused work of a large interdisciplinary team of scientists involving years of efforts and screening of thousands of compounds. This level of investments and human resources are only available with the large multinational conglomerates. Unfortunately this situation has outnumbered and out-resourced the academic institutions and pharmaceutical R&D of developing nations. The role of academic institutions, in drug development, particularly in developing world, is gradually diminishing. Ironically, the decision of developing a drug by multinational companies is largely commercial, rather than human-need based. As a result, a large number of diseases affecting the lives of poor population of the Africa and South Asia remains untreated. This situation demands a major re-thinking by pharmaceutical scientists who wish to serve the humanity through the skill they possess. During last two decades we have been focusing on natural products. This has led to the identification of novel lead molecules with potent activities against various disease-related targets.

The emerging gap among the rising incidence of diseases that are caused by MDR bacterial strains and the rapid reduction in the development of novel drugs is now pushing us back into pre-antibiotic era. Although there are many antimicrobials and chemotherapeutic agents available for the treatment of a wide range of infectious diseases, the emerging antimicrobial resistance demands the continuous discovery of new classes of antimicrobial agents. The antibiotic resistance is a serious threat for health and it requires an alternative approach for its management. The outbreak of methicillin-resistant *Staphylococcus aureus* (MRSA) is now widespread throughout the world. *S. aureus* is the most common bacterial pathogen which cause skin, soft-tissue and endovascular infections, pneumonia, septic arthritis, endocarditis, osteomyelitis, and sepsis. Based on this new drugs and novel approaches have to be developed to meet the challenge of bacterial resistance.

During our recent study, we discovered several novel and potent inhibitors of MDR *S. aureus* (EMRSA-17, EMRSA-16, MRSA-252 and Pak clinical

isolates) and *Pseudomonas aeruginosa* from natural and synthetic sources. These active and reproducible inhibitors have the potential to possibly block the efflux pumps, alters the membrane potential, revert the multidrug resistance, and induce the ROS production in MDR *S. aureus*. Effect of newly identified inhibitors in the presence of blood medium (*ex-vivo*), and synergistic effects of these compounds in combination with existing antibiotics showed significant results.

Similarly due to high prevalence of leishmaniasis in our region and associated morbidity, we conducted a systemic study on folk medicines used against leishmaniasis in Pakistan. We have isolated antileishmanial agents of natural origin and conducted *in vitro* screening as well as animal toxicity assays. We also conducted human clinical trials on leishmaniasis patients by applying topical applications of new ointment based formulations. A total of 110 patients were recruited with clinical leishmaniasis, diagnosed by smear examination on lesions. The results of this clinical study unambiguously established the efficacy, safety and cost effectiveness of the *Physalis minima* extracts-based topical gel against cutaneous leishmaniasis.

During this presentation, underlying philosophy and approach of our research on cost-effective discovery of drug molecules will be presented.

Natural Products and Drug Discovery

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Abstract

This talk addresses a seemingly simple question: Why have natural products been so successful as therapeutic agents? Natural products are a very tiny fraction of known molecules, yet they have contributed the majority of useful antibiotics, anticancer, and immunomodulators. Many researchers have investigated the structural properties of natural products in an effort to understand what makes a molecule ‘natural product-like’, and while there are clear general differences between naturally-occurring and synthetic molecules, efforts to translate these differences into molecular libraries for drug screening have generally been disappointing. The important distinguishing feature of natural products is their evolutionary history; they have one and synthetic molecules do not. The talk will cover the early prebiotic history of naturally occurring small molecules and some of the more spectacular tactics that have evolved to confer selective and potent biological activity.

Drug Lead Discovery from Nature: Case Study II

Atta-ur-Rahman and Muhammad Iqbal Choudhary

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Abstract

Biodiversity is an outward manifestation of chemical diversity. Plants contain a fascinating array of highly evolved, specific, and effective gene products. Their diverse structural and stereochemical characteristics make them valuable templates for exploring novel manifestations of molecular diversity. Nature has been the first source of cure for diseases and discomforts, which have led to the foundation of many empirical therapeutic systems. Even today over 50% of prescription drugs owe their origin to natural sources. Therefore, the need for systematic scientific research on folk remedies is essential for the future development of integrated healthcare systems and provision of affordable medicines for poor man's diseases. During this presentation, a case study of the discovery and early phase development of a potent anti-epileptic agent from an indigenous natural remedy will be described in a step by step manner.

Epilepsy is a group of chronic nervous system disorders, characterized by recurrence of seizures which are caused by uncontrolled repetitive electrical firing of neurons in different parts of the brain, leading to abnormal body movements. About 50 million people worldwide suffer from epilepsy; with almost 90% of these people being in developing countries. Epilepsy is a non-curable disease, but it can be controlled and managed with medications. Unfortunately most of the anticonvulsant drugs available in the market, synthetic in nature, are associated with severe side effects and have to be used for the whole life to control the seizures. Through extensive studies on medicinal plants of the family Ranunculaceae, anticonvulsant natural products, isoxylitones, were discovered from the medicinal plant *Delphinium denudatum*, and also detected in the non-alkaloidal aqueous extracts of *Aconitum cochleare*, *Aconitum laeve*, and *Delphinium nordhagenii*.

Extracts of *Delphinium denudatum* were found to exhibit good anticonvulsant activity in in vivo animal models of epilepsy. Bioassay-guided isolation studies on the roots of this plant, afforded a non-toxic and non-alkaloidal aqueous extract, which exhibited strong anticonvulsant activities in *in vivo*

animal models of epilepsy, such as MEST test, scPTZ, scBIC, scPTX, and scSTN tests. Further purification of the aqueous extracts led to the isolation of a strongly anticonvulsant isomeric mixture of E/Z isoxylitones. A library of derivatives were then synthesized to investigate their anticonvulsant activities in in vitro and in vivo tests of epilepsy. Studies have shown potent anti-epileptogenic activity of isoxylitones in scPTZ-induced kindling model in mice and they were also found to affect some of the underlining molecular changes that are induced following the seizures. Isoxylitones (E/Z) blocked the Na⁺ current in a concentration dependent manner (IC₅₀ = 184.9 nM). These compounds were also subjected to various toxicological studies and did not exhibit LD₅₀ up to the dose of 1,000 mg/kg. They were found to be harmless in model animals with higher potency as antiepileptic compounds than the currently available drugs. US patents have been obtained and the compounds are presently in phase 2 clinical trials in Canada.

Wholistic Approach to Herbal Products Quality Case study: Identification of Thyme Markers

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Abstract

The comeback of natural herbal products to position itself as first line prophylactic agents for many ailments is recognized globally.

The debate to use the whole plant versus the use of its extract or some of the plant component is going on. Whether a whole plant or its extracts are used the necessity for quality products cannot be ignored.

Consequently, manufacturers with regulators in different countries are in continuous process for developing specifications and standards for these products. This shall satisfy safety and quality in these products.

The first step of using plants starts from planting and harvesting which must be totally controlled. Periods of water deprivation, harvesting and drying conditions must be identified. Once the extraction process is started the nature and concentration of solvents must be observed to guarantee the production of reproducible qualities of the extracts with similar qualities.

The components characteristics must be identified and determined for every extraction step. Different kinds of markers can be differentiated and the use of certain markers must serve the needed purpose. It is advisable to use chemical, pharmacological and biomarkers to ascertain the reproducibility of these preparations

Quality Control and Regulatory Issues of Phytotherapeutics for Global Health Care

Bilge ŞENER

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Abstract

Herbal medicinal products have been playing an important role in the primary health care of the people around the world, specially in the developing countries. In order to treat health problems with the modern medicines, the production of safe and effective herbal medicinal products in a standardized way is essential.

Assessment of the quality, safety and efficacy of herbal medicinal products are an important issue. Standardization of raw materials, intermediates and final product of herbal medicines are the main issue for the quality control of herbal medicinal products. All of the supporting evidence behind the use of phytomedicines has been on use of standardized extracts of the plant material to ensure reproducibility in the clinical setting.

With the growing interest for alternative approaches in treating diseases, herbal medicinal products have also an important role for the development of new therapeutic agents. For this issue, researches can be focused by

- characterization of phytomedicines in terms of chemical composition and biofunctional activity
- studying the effects of certain processing and extraction methods and parameters on the chemical characteristics of phytomedicines source materials
- development of chemo-based and bio-based standardization methods for phytomedicines.

Herbal medicinal products named as “Phytomedicines” exhibit a variety of biological activities on human health. These range from the control of regulatory processes by Health Authorities is essential for human life. Therefore, herbal medicinal products are also subject to the same legislative controls as other medicines.

The overview of the herbal medicinal products in the worldwide along with current registration guidelines and criteria for the control and market situation of herbal medicinal products in Turkey will be highlighted.

Phytochemical and biological evaluation of some rare *Salvia* species from Jordan

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Abstract

Salvia is the predominant genus in the family Lamiaceae. In Jordan, the occurrence of 19 indigenous species of *Salvia* is reported; mainly in the Mediterranean and Irano-Turanian biogeographic zones of the country. Several *Salvia* species are closely linked to Jordanian traditional medicine in the treatment of multiple ailments.

The aim of this work was to screen two rare *Salvia* species, namely *S. multicaulis* and *S. judaica* phytochemically and evaluate their dual alpha-amylase /alpha glucosidase and pancreatic lipase inhibitory activities as well as their antiproliferative potential. HPLC-DAD-MS analysis and quantification of the ethanol extracts of both *Salvia* species revealed the presence of flavonoids, coumarins and plant acids. Also the composition of the essential oils isolated from the aerial parts of *S. multicaulis* and *S. judaica* - using Solid Phase Micro-Extraction (SPME) method - was determined by GC and GC-MS and the composition of the fresh and dry specimens were compared. Monoterpenoid compounds were detected as the dominant components of both volatile oils. Antiproliferative activities were investigated using SRB assay against a panel of breast cancer cell lines with Doxorubicin positive control. *In vitro* enzymatic starch digestion was evaluated with Acarbose as the reference drug. Pancreatic lipase catalytic activity was determined colorimetrically and compared to Orlistat.

The screening of the rare species of the widely used indigenous plants for different biological activities is essential for inspiration of new drug discovery and development.

Extensive Integrative Drug Discovery: Using Africa Medicinal Plants for Fighting African Endemic Neglected Diseases

Asaad Khalid

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Abstract

Natural products are characterized by their unorthodox and often unanticipated chemical structures that offer novel leads of clinically useful drugs. Studies have demonstrated that the hit rate of natural products is on average 3-10%, compared with ~ 0.03% of that of compounds from synthetic origin.

The road to the discovery of successful drug from medicinal plants could be full of challenges and adventures. The myriad of structurally diverse compounds found in nature makes them play an important role as a unique source for drug discovery, but they always play hide-and-seek and more often hard-to-get. Even though, most of the FDA approved drugs are either natural products or natural product-derived compounds.

Drug discovery could follow any of the two approaches i.e. cell-based and/or target-based. Enzymes represent the major class of drug targets. Recent reports show that about 50% of small molecule drugs are enzyme inhibitors. This lecture will give an overview of our target and cell-based research on the inhibition of neglected diseases-related enzymes. This multidisciplinary integrative research has led to the identification of very interesting drug properties of some Sudanese medicinal plants, to be highlighted.

**Plasmodium Prolyl tRNA Synthetase - a Druggable
Next Generation Dual-stage
Target for Malaria Elimination**

Ralph Mazitschek

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The sustained availability of efficacious drugs is requisite for the renewed worldwide efforts to successfully eradicate malaria. However, the emergence of clinical resistance is a major limitation for the use of current antimalarials and constitutes a major public health issue. Thus the discovery of novel druggable targets and pathways including those that are critical for multiple life stages is a major challenge for the development of next-generation therapeutics. Within our efforts to address this challenge we have applied an integrated chemogenomic approach combining drug-resistance selection, whole genome sequencing and an orthogonal yeast model, which validated the *Plasmodium falciparum* cytoplasmic prolyl-tRNA synthetase (PfcPRS) as the biochemical and functional target of the natural product febrifugine, the active principle of a traditional Chinese herbal malaria remedy, and its synthetic derivatives. Our group has developed halofuginol, a novel halofuginone analog, which is highly active against both liver and asexual blood stage of malaria and unlike halofuginone and febrifugine, is well tolerated at efficacious doses in *P. berghei* malaria mouse models.

Application of Structural Chemistry and Structural Biology in Drug Discovery

Atia-tul-Wahab, M. Iqbal Choudhary

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Abstract

The emergence of methicillin-resistant *Staphylococcus aureus* (MRSA) is causing a tremendous pressure on the healthcare system, and causing major suffering to the patients. The antibiotic resistance is a serious threat for health and it requires an alternative approach for its management. The outbreak of methicillin-resistant *Staphylococcus aureus* (MRSA) is now widespread throughout the world. *S. aureus* is the most common bacterial pathogen which cause skin, soft-tissue and endovascular infections, pneumonia, septic arthritis, endocarditis, osteomyelitis, and sepsis. MRSA isolates have developed resistance to a wide-range of antibiotics, which include macrolides, lincosamides, aminoglycosides, β -lactams, penicillins, and cephalosporins. The mechanisms through which bacteria reveal resistance to variety of drugs include drug inactivation, target site alteration, modification of metabolic pathway and decreased antimicrobial accumulation. Epidemiologic studies indicate the infections due to MDR *S. aureus* are highly associated with increased burden on healthcare resources with increased morbidity and mortality. The emerging gap among the rising incidence of diseases that are caused by MDR bacterial strains and the rapid reduction in the development of novel drugs is now pushing us to investigate new drug targets. Based on this new drugs and novel approaches have to be developed to meet the challenge of bacterial resistance.

The bacterial cell division protein FtsZ is an attractive target and an under developed research domain for the discovery of new antibacterial agents. Inhibiting the division process can broaden existing molecular lead(s) inventory and can also be used in combination with existing antibiotics, aiming to lower administered doses with same therapeutic effects. During our studies we have cloned, expressed and purified FtsZ, which was further investigated for GTPase activity *in vitro* we have screened libraries of natural-product and small-molecules against FtsZ activity *in vitro*. This lead to identification several new and novel chemical classes of inhibitors.

The bacterial phosphoenolpyruvate-dependent sugar phosphotransferase system (PEP-PTS) is an important bacterial multi-protein system for transportation and phosphorylation of various types of sugars and their derivatives and thus help in regulation of cellular metabolism. In prokaryotic cells the phosphate group originates from PEP instead of ATP like in mammalian cells and finally transfer to the sugar moiety through five successive steps. The first two steps of phosphate transfer from PEP to EI (enzyme I) and from EI to HPr (histidine-containing phospho carrier protein) are similar for all sugars while the subsequent three steps i.e. transfer of phosphate from HPr to functional domains of the permease enzyme II (EIIA and EIIB) then finally to sugar are sugar specific. The three-dimensional structure information. As a result of our work, the complete three-dimensional dynamic structure of the PTS subunit IIB from *Staphylococcus aureus* was determined by using biological NMR spectroscopy. CYANA was used for the structure calculation of the protein. The protein showed a well-defined globular structure comprising a parallel β -sheet, and three α -helices.

Optimization of Supercritical Fluid Extraction of Major γ -Pyrone from *Ammi Visnaga* Fruits*

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Abstract

Ammi visnaga belongs to the family Apiaceae. Ancient records revealed various medicinal properties of *A. visnaga* as a popular source to cure variety of different ailments. The fruits are used specifically for the treatment of kidney stones. The active chemicals of that plant work as a calcium channel blocker-type antispasmodic helping to relax ureters tissue. In this way small stones are passed through the passages easier. The fruits as whole or its extract or even pure γ -pyrones are used for the production of a number of herbal medicines used in the cure of renal colic, ureteric stones, angina pectoris, and asthma. Its activity is mainly correlated to its γ -pyrones contents, mainly khellin and visnagin. The supercritical fluid extraction technique of khellin and visnagin was investigated and the operating conditions for their extraction were optimized. The effect of different pressure (150, 200, 300, 400 and 500 bars), temperature (35, 40, 45, 50 and 55°C), and particle sizes of the raw material (0.5 mm, 1.4 mm and entire fruits) on the extract yield was studied under dynamic conditions for extraction for a run time of 90 minutes. The extracts were analyzed by both HPTLC and HPLC. Optimum supercritical extraction condition was found to be 200 bars at 45°C, and optimum particle size was found to be 1.4 mm. The yield is yellowish white bitter powder and measures 1.74% w/w relative to the dried weight of the fruits containing 38.41% w/w average γ -pyrones content of which 29.40% w/w khellin, and 9.01% w/w visnagin.

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Screening of Antibiotic Resistant Inhibitors from Local Plant Materials Against MRSA

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Abstract

Staphylococcus aureus is one of the five most common causes of hospital-acquired infections. Methicillin resistant *S. aureus* (MRSA) is one of a number of greatly feared strains of *S. aureus* that have become resistant to most β -lactam antibiotics. It is most often found associated with institutions such as hospitals, but is becoming increasingly prevalent in community-acquired infections.

The inhibitory effects of methanolic extracts of 19 Jordanian plants and their combinations with seven antibiotics, on the resistance of (MRSA), which was isolated from patient and a standard strain of *S. aureus* were evaluated using a broth microdilution method. Our results showed that there are variations in the effect of some combinations used on the resistant and the standard strains. In general the results showed that combinations of gentamicin and chloramphenicol could be improved by the use of plant materials, whereas nalidixic acid activity cannot be improved when combined with plant materials.

This study probably suggests possibility of concurrent use of these antibiotics and plant extracts in treating infections caused by MRSA or at least that the simultaneous administration may not impair the antimicrobial activity of these antibiotics.

Jordanian Plants in Drug Discovery - Establishing a Future Vision

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Abstract

During the past decade, traditional systems of medicine have become a topic of global importance. Current estimates suggest that, in many developing countries, a large proportion of the population rely heavily on traditional practitioners and medicinal plants to meet primary health care needs. Although modern medicine may be available in these countries, herbal medicines (phytomedicines) have often maintained popularity for historical and cultural reasons. Concurrently, many people in developed countries have begun to turn to alternative or complementary therapies, including medicinal herbs. The practices of traditional medicine are based on hundreds of years of belief and observations, which predate the development and spread of modern medicine. It is well known that old civilizations have flourished in the Middle East and used the natural plants for various daily needs, such as food, shelter, clothes and medicine. Jordan is a relatively small country but well known for the great variation in wild plants due to the geographical diversity and climatic circumstances. Around 2500 plant species (of which 100 species (2.5%) are listed as endemic) were recorded. The floral species in Jordan also include medicinal and herbal species as well as aromatic and spices species. From these plants, 485 species from 99 different families are categorized as medicinal plants. These species have a wide distribution in the country.

Drug Discovery: a Tale of Three Medicinal Plants from Jordan

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Abstract

Fresh rhizomes (tubers) of *Asphodelus microcarpus*, have been collected during the flowering period. Different chromatographic methods led to the isolation of the active constituents, ramosin being the major one and the extract of the plant is standardized according to the percentage of ramosin as a reference standard.

The use of *Paronychia argentea* for kidney stones have folkloric bases in Jordainian traditional medicine. An HPLC method for standardization of *P. argentea* was developed, depending on vanillic acid as a main efficacious active constituent in the plant.

Various chromatographic techniques show that extracts of *Inula viscosa* possess a high contents of flavonoids. The plant extract is standardized according to the percentage of ilicic acid as a reference standard.

Novel Ligand-Based and Structure-Based Drug Design Approaches Developed At he Faculty of Pharmacy-University of Jordan

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Abstract

Drawbacks of receptor-based computer-aided drug discovery methods prompted us to devise two interesting and novel modelling methodologies for discovery and optimization of new bioactive hits:

(i) A ligand-based computational approach that is carried out over two subsequent stages. Firstly, the pharmacophoric space of the targeted enzyme is extensively explored. The resulting binding models are then allowed to compete via QSAR context driven by multiple linear regression or k nearest neighbour analysis. We reported the successful use of this combination to probe the induced fit flexibilities of activated factor X and towards the discovery of new inhibitory leads against glycogen synthase kinase-3 β , bacterial MurF, protein tyrosine phosphatase, DPP IV, hormone sensitive lipase, influenza neuraminidase, estrogen receptor β , cholesteryl ester transfer protein, β -secretase, cycline dependent kinase, β -D-glucosidase, and β -D-galactosidase, heat shock protein, renin, PPAR γ , fungal N-myristoyl transferase, glycogen phosphorylase, Ca²⁺/calmodulin-dependent protein kinase II, Rho Kinase, endothelial nitric oxide synthase, inducible nitric oxide synthase, transition state β -secretase, mammalian target of rapamycin, migration inhibitory factor, urokinase plasminogen activator, human neutrophil elastase, acetylcholinesterase, phosphoinositide 3-kinase gamma (PI3K γ), and glucokinase activators.

(ii) A structure-based approach, namely, docking-based Comparative Intermolecular Contacts Analysis (dbCICA). This novel approach is based on the number and quality of contacts between docked ligands and amino acid residues within the binding pocket. It assesses a particular docking configuration based on its ability to align a set of ligands within a corresponding binding pocket in such a way that potent ligands come into contact with binding site spots distinct from those approached by low-affinity ligands and vice versa. Optimal dbCICA models can be translated into valid pharmacophore models that can be used as 3D search queries to mine structural databases for new bioactive compounds. dbCICA was implemented to search for new inhibitors of candida N-myristoyl transferase, 32 glycogen phosphorylase (GP), Hsp90 α , check point kinase 1, and glucokinase activators.

Phytochemical Investigation of Some Selected Plants Belonging to the Mediterranean Region

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Abstract

Based on altitude – Jordan can be classified into three parallel regions, the Rift Valley, Mountain ranges and the Eastern Desert, all of which comprising the four bio-geographical regions including the Mediterranean, Irano-Turanian, Saharo-Arabian and Tropical regions. Its unique location and remarkable climatic variations allowed astonishing biodiversity. The total number of plant species recorded in Jordan exceeds 2500 species (belonging to 150 families and 700 genera) of which 100 are endemic.

Our group has always been interested in the isolation, characterization of the chemical constituents and bioactivity evaluation of medicinal plants belonging to the Flora of Jordan.

In a continuous effort conducted for investigating the chemical composition of the volatile and nonvolatile constituents of Jordanian medicinal plants and evaluation of their bioactivity, we present here a summary of our results concerning the characterization of the chemical constituents of *Salvia dominica*. growing wild in Jordan. Moreover, a summary of our recent findings concerning the chemical and biological evaluation of some other medicinal plants will be also presented.

Diastereoselective Design of Privileged Structures: Forward Chemical Genetics for Phenotypic Screening of Chemical Probes

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Phenotype-based screening is a favored methodology for the encounter of first-in-class drugs in the arenas of chemical biology and medicinal chemistry, because new bioactive chemical entities can be identified through the monitoring of phenotypic changes in living cells or whole organisms. A latest analysis shown that more than half of 50 first-in-class small-molecule drugs approved by the U.S. Food and Drug Administration between 1999 and 2008 were discovered using a phenotype-based approach, which endorses phenotypic screening as the most effective approach for discovering novel therapeutic agents with new modes of action. In this regards, molecular diversity is particularly important for the successful discovery of novel small-molecule ligands using phenotypic screening. Therefore, in this presentation, the focus will be shifted toward the design of quality compounds with privileged structures (Figure 1). Furthermore, preliminary studies in our labs indicated that these privileged molecular architectures possess the attributes as potential anticancer lead candidates.

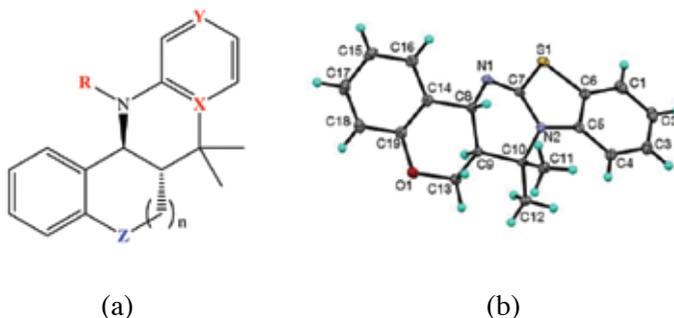


Figure 1. General structure of privileged motifs and ORTEP drawing of benzopyrane polycyclic scaffold.

Identification of Novel Interleukin-2 Inhibitors by Using Natural Products: A Computational and Molecular Modelling Perspective

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Bioactive natural products have been an essential part of sustaining civilizations because of their medicinal properties. Past discoveries of natural products have greatly relied on luck. Drug discovery has encountered significant challenges during the past decade. In recent years the pharmaceutical industry has placed low emphasis on natural-product-based drug discovery efforts because of an increasing reliance on newer technologies including computer based drug discovery. However, natural products with therapeutic potential are abundantly available in nature and some of them are beyond exploration by conventional methods. The effectiveness of computational approaches as versatile tools for facilitating drug discovery and development has been well recognized. In the current era, scientists are bombarded with data produced by advanced technologies. Thus, rendering these data into knowledge that is interpretable and meaningful becomes an essential issue. In this regard, computational approaches utilize the existing data to generate knowledge that provides valuable understanding for addressing current problems and guiding the further research and development of new natural-derived drugs. Furthermore, several medicinal plants have been continuously used in many traditional medicine systems since antiquity throughout the world, and their mechanisms have not yet been elucidated. Therefore, the utilization of computational approaches including SBDD and LBDD would yield great benefit to improving the drug discovery campaign. Here, we will discuss some exciting results from our ongoing research work.

Drug Development and Clinical Trials Challenges for Natural Products-Based Drug Candidates

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Abstract

Natural products have historically been an extremely productive source for new medicines with great therapeutic potential and continue to deliver a great variety of structural templates for drug discovery and development.

Drug development in pharmaceutical industry can range from only a few to as many as 20 years. For natural products it tends toward the longer timespan in development due to many challenges mainly with sources, purity, regulatory, and consequently commercial market supplies.

Clinical development has its own challenges as more Code of Federal Regulations (CFR) guidelines and rules are created. The recognition of a clinical drug study has to be approved by IRB or an Independent Ethics Committee (IEC). The clinical trials aspects of safety/tolerability, efficacy, Pharmacokinetics, Pharmacodynamics, and risk-benefit evaluation has more challenges with natural products-based drugs.

Regulatory marketing registration process starts by preparing Common Technical Document (CTD) Harmonised format for applications in the three ICH regions (Europe, Japan, and USA) or the format per the application and marketing region Food and Drug Administration (FDA). Natural product-based drug registration dossier prepared through the CTD documentation illustrates five modules. The complete CTD would then be filed as a New Drug Application (NDA) with EMEA (Europe), FDA (USA), or the marketing authorization entity at the country of submission.

Even with all those challenges, out of the anti-cancer agents developed and approved over the last seven decades, almost 40% of those were natural products or directly derived from natural products. In fact the interest in natural sources to obtain pharmacologically active compounds has recently been regenerated with improved access to a broader base of sources (i.e. new microbial and marine origins) and advanced analytical methods.

How to get your paper published in high impact journals

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Abstract

With more than 70% rejection rate and an average impact factor of 5.9 for the 42 Royal Society of Chemistry journals ranging from 1.938 (the lowest impact factor) to 33.38 (the highest), many researchers think it is very difficult to publish with RSC. The seminar will shade more light on the article acceptance process and give detailed information on how to get the article accepted. Most of the reasons for article rejections can be overcome by very simple procedure. The aim is to avoid mistakes in writing the scientific article.

Nutraceuticals as a source of bioactive molecules for drug discovery

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Abstract

The term nutraceuticals is used to describe a range of pharmaceutical products of concentrated, purified food or nutrient that provide health and medical benefits, both in prevention and treatment of diseases. Global market has been estimated to be approximately US\$ 30-60 billion in the past year 2014. Therefore, part of the on-going research has been directed towards the scientific evaluation of selected Jordanian traditional food and herbal remedies for antimicrobial, anti-inflammatory, anti-coagulant and hypoglycemic activity both in vivo and in vitro. Preliminary results indicated that selected *Salvia* species inhibited the growth of *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans*. In addition, different *Salvia* species reduced dermal inflammation induced by croton oil in mice. Popular *Hibiscus sabdariffa* drink inhibited collagen-induced platelet aggregation from human blood. *Punica granatum* (pomegranate) seeds' extract reduced blood sugar in tested mice. Research results indicated that nutraceuticals might provide us with a new drug lead to treat microbial infections, inflammation, platelet aggregation and hyperglycemia. Further research to identify and isolate active principles is essential. Results of the scientific research support the recommendation to consider biologically active traditional food and drinks as complementary to medical treatment.

The Anti-spermatogenic Effects of *Taraxacum Officinale* and *Orchis Anatolica* in Male Rodents

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Abstract

For centuries, plants have been the base of medicinal treatment. Modern medicine has recognized phytochemicals as an alternative therapy; but it is still widely used without strict scientific evidence. Though some people do not believe in using plant-derived recipes to improve fertility and sexuality, many others used them throughout history to improve their fertility and libido. In Jordan, *Taraxacum officinale* and *Orchis anatolica* are used to enhance male fertility and sexual drive, respectively.

Our results show that the aqueous extract of *T. officinale* whole plant, leaves or roots decreases male rat fertility *in vivo*. In particular, the root aqueous extract decreased sperm concentration, motility and normal morphology. It also caused germ cell hypoplasia and absence of interstitial cells. The differentiation of spermatogonial stem cells was impaired in the root-treated groups causing early maturation arrest.

In regards to the effect of the ethanolic extract of *O. anatolica* leaves on male fertility parameters, our findings are contradictory to what local people and traditional herbalists believe; the leaves of this orchid have anti-fertility effects.

Our future work involves the identification of the biologically active constituents in these two plants that cause male infertility.

Traditional herbal medicine is a common practice in Jordan. However, most of the traditional herbalists are not licensed or properly trained for handling herbal medicine. Thus, the need for extensive research to validate the use of each plant used traditionally is indeed pressing. Otherwise, the improper use of herbal medicine could lead to acute or chronic toxicity.

The Plant-derived Molecule Thymoquinone inhibits Self-renewal Capacity of Colorectal Cancer Stem Cells

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Abstract

Thymoquinone (TQ) is a promising anticancer molecule that inhibits cancer cell growth and progression in numerous cancer systems both *in vitro* and *in vivo*. Here we evaluated whether TQ affects the self renewing capacity of colorectal cancer stem cells using two isogenic HCT116 human colon cancer cell lines that differ in their p53 status (p53^{+/+} and p53^{-/-} cells). Sphere-formation and propagation assays were used to assess TQ effect on self-renewal potential of enriched cancer stem cells populations. We also investigated the relevance of stem cell markers profiling in 2-dimensional (2-D) monolayer cultured cells versus 3-dimensional (3-D) colonospheres.

We showed that 10-fold lower concentrations of TQ inhibited colonosphere growth in 3-D HCT116 cultures in comparison to 2-D monolayers. Colonospheres which survived TQ treatment at 1 and 3 μ M TQ were propagated from generation 1 to 5 and showed, at every generation, similar dose-dependent decrease in sphere viability upon TQ treatment. Colonospheres treated with 1 μ M TQ showed 50% decrease in sphere viability from generation 1 to 5 regardless of their p53 status. TQ significantly decreased HCT116 p53^{+/+} sphere size at generation 1 but not in HCT116 p53^{-/-} cells. No decrease in sphere size was noted in subsequent generations in both cell lines. We also showed that TQ treatment decreased expression levels of colorectal stem cell markers EpCAM and CD44 in monolayer HCT116 p53^{+/+} and p53^{-/-} cells and in HCT116 p53^{-/-} colonospheres. Altogether, our findings document for the first time TQ's promising effects on colon cancer stem cells and provide insight on the underlying mechanisms of TQ inhibition of colon cancer relapse, information which is essential for clinical translation of this natural anticancer molecule.

Dereplication Studies of Natural Products Based on Advanced Mass Spectrometric Tools: A Case Study on Withanolides

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Plant metabolites can act as drugs for the treatment of a variety of diseases due to their unique skeletal features. A large number of plant metabolites are used as drugs for the treatment of many diseases. High-throughput techniques, such as MALDI-MS and LC-ESI-MS/MS, can be the techniques of choice for rapid dereplication of natural products in plant extract/materials.

This talk will focus on advance mass spectrometric methods that are being utilized for the effective and high-through dereplication of natural products in their complex mixtures. Withanolides (a class of steroidal lactones) will be considered as a case study in this talk. Details of structure-fragmentation relationship (SFR) studies of various withanolides using CID-MS/MS analysis of standard withanolides revealed the important correlation between fragments formed during product ion analysis and the structural features. Validation of results was carried out by the LC-MS/MS analysis of *Withania somnifera* extract. The application of the MALDI-MS for the rapid screening of withanolides and other natural products in plant materials is also developed. A fast and reproducible matrix free approach for the direct detection of UV active metabolites in plant materials with minimum sample preparation was developed. The approach was validated by the characterization of withaferin A and nicotine in the leaves of *Withania somnifera* and *Nicotiana tabacum*, respectively.

A LC-QqQ-MS method for the determination of withanolides in *Withania coagulans* plant extract is developed. The established method can be useful for high throughput routine screening of various withanolides in *W. coagulans* extract and may potentially extend to other herbal formulations derived from *W. coagulans*.

In vitro Modulation of Pancreatic Insulin Secretion and Extrapancreatic Insulin Action, Enzymatic Starch Digestion and Protein Glycation by *Terminalia chebula* Extracts

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Abstract

Traditional plant treatments have been used throughout the world for the therapy of diabetes mellitus. Using multiple in vitro models; this study was designed to investigate the efficacy and mode of action of *Terminalia chebula* Retz. (Combretaceae) used traditionally for treatment of diabetes.

T. chebula aqueous extract stimulated basal insulin output and potentiated glucose-stimulated insulin secretion concentration-dependently in the clonal pancreatic beta cell line, BRIN-BD11 ($p < 0.001$). The insulin secretory activity of plant extract was abolished in the absence of extracellular Ca^{2+} and by inhibitors of cellular Ca^{2+} uptake, diazoxide and verapamil, ($p < 0.001$). Furthermore, the extract increased insulin secretion in depolarised cells and augmented insulin secretion triggered by IBMX, but not by tolbutamide or glibenclamide. T. chebula extract did not display insulin mimetic activity but it enhanced insulin-stimulated glucose transport in 3T3 L1 adipocytes by 280% ($p < 0.001$). At (0.5-5.0mg/mL) concentrations, the extract also produced 22-84% ($p < 0.001$) decrease in starch digestion In vitro and inhibited protein glycation ($p < 0.001$) at 1mg/ml aqueous extract.

This study has revealed that water soluble bioactive principles in T.chebula extract stimulate insulin secretion, enhance insulin action and inhibit both protein glycation and starch digestion. The former actions are dependent on the bioeffective component(s) in the plant being absorbed intact. Future work assessing the use of *Terminalia chebula* as dietary adjunct or as a source of active antidiabetic agents may provide new opportunities for the treatment of diabetes.

Two Novel Cardenolides from *Calotropis Procera*

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Calotropis procera Linn, growing wild from West Africa to South East Asia, belongs to the Asclepiadaceae family. *C. procera* have been used for the treatment of various diseases namely leprosy, ulcers, and diseases of the spleen, liver, and abdomen. It also has anti-bacterial, anti-inflammatory, and analgesic effects. Sterols, triterpenes, flavonoids and cardiac glycosides have been isolated from *C. procera*. Cardenolides (cardiacglycosides) are a class of secondary metabolites that are traditionally used to increase cardiac contractile force in patients with congestive heart failure and cardiac arrhythmias. The above-mentioned importance of *C. procera* as well as the fact that no previous investigation was done on this plant in Jordan, a study of the chemical constituents of the plant was carried out. In Jordan, *C. procera* is locally known as Ishar.

We report here the identification of two new cardenolides in addition to 10 known compounds from *C. procera* from the plant growing naturally in Jordan. The methanol extract afforded the new cardenolides, ischarin and ischaridin, together with the known compounds uzarigenin, calotropin, calactin, calotoxin, β -sitosterol glucoside. The butanol extract yielded the known compounds 19 dihydrocalotropagenin, and 3'-O-methyl quercetin-3-O-rutinoside, whereas the methanol extract of the latex gave calotropenyl acetate, β -sitosterol, uscharin, calotropin, calotoxin, and 19-dihydrocalotropagenin. The structure elucidation of all compounds was achieved by their spectral data including ^1H and ^{13}C -NMR data, 2D NMR (COSY, HMQC, and HMBC), and mass spectra.

Discovery of New Human Epidermal Growth Factor Receptor-2 (HER2) Inhibitors for Potential Use as Anticancer Agents via Ligand-Based Pharmacophore Modeling

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Abstract

To discover potential antitumor agents directed toward human epidermal growth factor receptor-2 HER2/ErbB2 overexpression in cancer, we have explored the pharmacophoric space of 115 HER2/ErbB2 inhibitors. These identified 240 pharmacophores which were subsequently clustered into 20 groups and cluster centers were used as 3D-pharmacophoric descriptors in QSAR analysis with 2D-physicochemical descriptors to select the optimal combination. We were obliged to use ligand efficiency as the response variable because the logarithmic transformation of bioactivities failed to access self-consistent QSAR models. Two binding pharmacophore models emerged in the optimal QSAR equation, suggesting the existence of distinct binding modes accessible to ligands within the HER2/ErbB2 binding pocket. The QSAR equation and its associated pharmacophore models were employed to screen the National Cancer Institute (NCI) and Drug Bank databases to search for new, promising, and structurally diverse HER2 inhibitory leads. Inhibitory activities were tested against HER2-overexpressing SKOV3 Ovarian cancer cell line and MCF-7 which express low levels of HER2. In silico mining identified 80 inhibitors out of which four HER2 selective compounds inhibited the growth of SKOV3 cells with IC₅₀ values < 5μM and with virtually no effect in MCF-7 cells. These lead compounds are excellent candidates for further optimization.

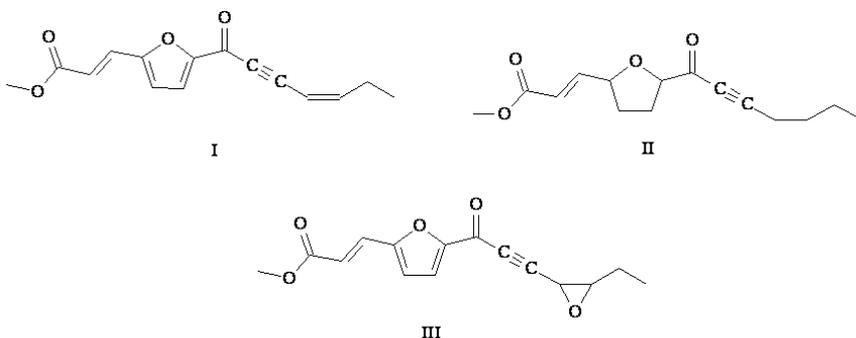
Biogenetic Conversion of Antifungal Phytoalexin Wyerone into Wyerone Epoxide from *Vicia Faba* Plant Cotyledons

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Abstract

The biogenetic conversion between the antifungal phytoalexins in the broad bean plant cotyledons, wyerone (I), 11-12- dihydrowyerone (II), and wyerone epoxide (III) has been investigated Figure 1.



Labeled wyerone and dihydrowyerone were obtained by feeding sodium (2-¹⁴C) acetate to abiotically CuCl₂-induced *Vicia faba* cotyledons, and separation by HPLC. The two titled compounds were then fed to induced bean cotyledons to establish any possible interconversion.

The results in this study indicated clearly that wyerone epoxide was derived from wyerone, and dihydrowyerone transformed into wyerone epoxide quite efficiently, but the epoxidation of wyerone to wyerone epoxide appeared to be more important. It is possible that a metabolic grid existed for these compounds in *V. faba*.

The origin of wyerone biosynthesis in *Vicia faba* was studied previously (Al-Douri, et al., 1986) and the conversion of wyerone to wyeron acid has been demonstrated earlier (Al-Douri, 2014). In the present study the conversion of wyerone into wyerone epoxide using labeled compounds and the potential role of these compounds in the biogenetic relationship has been established.

Identification of Rab8b protein inhibitors through homology modeling and virtual screening

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Abstract

Testicular cancer is a cancer that develops in one or both testicles in young men. Most of testicular cancers begin in germ cells (cells that make sperm) and are called testicular germ tumours. Many of Rab proteins share the same interacting partners and perform unique roles in specific locations. Rab8b is a member of the Rab small G protein family, participates in intracellular trafficking events at the site of the adherens junction dynamics in the testis by regulating the arrangement of cell adhesion proteins, such as cadherins and catenins, during germ cell translocation across the seminiferous epithelium via the cytoskeleton. Overexpression of Rab8b and loss of functioning adherens junction may accelerate tumorigenesis in testis. Thus, computer aided high throughput virtual screening studies were implemented to identify potent leads for human Rab8b protein.

In the present work, the homology model of Rab8b (207 amino acid residues) was developed based on the crystal structure of appropriate template; the structure reveals 6 α - helices and 6 β - strands. The computed model's energy was minimized and validated using ProSA, PROCHECK and Errat tools. The active site was identified using computational active site prediction tools like CASTp, efindsite and SiteMap, which show that the residues (Glu33 to Gln60) are important for binding. The molecular interactions of Rab8b with its natural substrate Rabin8 were examined by protein-protein docking studies using patchDock tool and the results were corroborated with the active site identified from previous computational active site prediction techniques. Virtual screening studies were carried out with ligand databases using glide Schrödinger suite. The ligands which are potential antagonists against the Rab8b protein were prioritized from the results of virtual screening based on glide score, glide energy and acceptable ADME properties.

Elaborate Libdock Docking, dbCICA Implementation and In silico Screening Reveal New Potent Acetylcholinesterase Inhibitors

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Abstract

Acetylcholinesterase enzyme (AChE) inhibitors have been shown to improve neurodegenerative diseases prompting several attempts to discover and optimize new AChE inhibitors. The significant role played by docking algorithms in drug discovery combined with their serious pitfalls prompted us to envisage a novel concept for validating docking solutions, namely, docking-based Comparative Intermolecular Contacts Analysis (dbCICA). We explored the most important contact amino acids within AChE binding site using dbCICA concept and Libdock docking of 85 AChE inhibitors both in ionized and unionized state and in presence and absence of crystallographic water. Optimal dbCICA models can be translated into valid pharmacophore models used as 3D search queries to mine structural databases for new bioactive compounds. dbCICA was implemented to search the NCI database for new AChE inhibitors.

Six low micromolar AChE inhibitors were identified. The most potent gave IC₅₀ value of 2.5 μ M.

In Vitro evaluation of the antiproliferative activity of some medicinal plants traditionally used against cancer in Jordan

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Abstract

Arbutus andrachne L., Chrysanthemum coronarium L., and Teucrium polium L., are three medicinal plants from the Jordanian flora that have been used in traditional medicine against cancer. This study evaluates the antiproliferative activity of the extracts of the three plants against a panel of human tumor cell lines representing the most common types of cancer in Jordan, breast cancer and colorectal cancer, in addition to skin cancer. Methanolic extracts of the aerial parts of the three plants were prepared and assessed for antiproliferative activity against six human tumor cell lines (A375.S2, WM1361A, CACO-2, HRT18, MCF-7, T47D) using MTT cell proliferation assay. At 100 μ g/ml, *C. coronarium* methanolic extract inhibited the proliferation of the 6 examined cell lines, whilst, the extracts of the other two plants exhibited weak activity. The calculated IC₅₀ values of *C. coronarium* methanolic extract against the six cell lines were in the range of 75.8 to 138.5 μ g/ml. Thus, *C. coronarium* methanolic extract might be a potential source of new natural compounds with antineoplastic activity.

Phytochemical, Anti-acetylcholinesterase, -Oxidant, and -Inflammatory Properties of Selected Jordanian Medicinal Plants

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Abstract

The study aimed at evaluating the therapeutic potentials of six traditional medicinal plants used in Jordan for the improvement of memory in old age. The anti-inflammatory, anti-cholinesterase and anti-oxidant properties of the medicinal plant methanol extracts were investigated. Phytochemical analysis, for the total phenolic and flavonoid contents, was also carried out using spectrophotometric methods. AChEI, anti-oxidant, COX inhibitory and metal chelating activities were determined as described previously (n = at least 3 replicate experiments).

A. citrodora and *P. harmala* root and seeds showed modest inhibitory effects on AChE (mean IC₅₀ 68,100 and 93 µg/ml, respectively). *A. microcarpus*, *I. viscosa* and *A. citrodora* displayed COX-1 enzyme inhibitory activity (IC₅₀ 34.9, 3.4 and 3.2 µg/ml, respectively). Potent DPPH radical scavenging activity was demonstrated by all tested plants. Two extracts (mean *A. andrachne* and *A. microcarpus*) exhibited potent NO scavenging activity (IC₅₀ 4.5 and 5.0 µg/ml, respectively). Three extracts *A. citrodora*, *P. harmala* (Root & seed) and *A. microcarpus* exhibited potent metal chelating ability (IC₅₀ 4.5, 6.2, 6.5 and 6.7 µg/ml, respectively).

The reversible interaction against AChE, moderate activity against COX-1, potent antioxidant activity and strong metal chelating ability make them promising new agents for further investigation in vivo, either as total extracts or as single bioactive constituents. *A. andrachne* and *A. microcarpus* extracts should be further evaluated since they exhibited promising nitric oxide (NO) scavenging activities.

The results obtained in this study suggest the potential use of plants in Jordanian traditional medicine for age-related neurological diseases.

**Photochemical Investigation of Antimicrobial Seed
Extracts of *Citrus Aurantifolia***

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Abstract

The seeds of Lime of the family Ructaceae are gaining grounds as important source for treatment in complementary medicine. The Sudanese varieties are one of the best in the market, which prompted investigation of seed extracts. The 96% ethanolic extract exhibited significant antimicrobial activity and highlighted the biological monitoring of activity in order to isolate the active metabolites from the chloroform extract of the seeds.

The presence of sterols and triterpenes, carotenoids, coumarins, alkaloids, saponins, tannins and carbohydrates was confirmed by phytochemical screening of the diethyl ether, methanolic and aqueous extracts of the seeds. Isolation of the antibacterial secondary metabolites was achieved by fractionation of the active chloroform extract by sing, liquid solid column chromatographic technique and biological monitoring of activity of column fractions eluted with chloroform and methanol. The composition of fractions was monitored by analytical and preparative TLC.

A green Biosynthesis of Silver Nanoparticles (AgNPs) using Maltose and Plant Leaf Extract

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Abstract

As the production of silver nanoparticles (AgNP) using various synthesis processes increases, there is a need to determine efficient and environmentally appropriate manufacturing techniques.

A collaborative research group between the Jordan University of Science and Technology (JUST) and the University of Rhode Island (URI) seeks to evaluate different green methodologies for the manufacturing of silver nanoparticles, enhancing the nanoparticles surface, and controlling their shape and size. Tollen's method was used for green silver nanoparticles synthesis using maltose and leaf extracts; Rosemary leaf Extract (RLE), olive leaf extract (OLE). To enhance nanoparticles surface, shape and size, different stabilizers (sodium dodecyl sulfate, Polyvinylpyrrolidon (PVP) and Polyvinyl Alcohol (PVA)), and different leaf extract concentrations were studied at different pH and temperature.

Silver nanoparticles sizes and shapes were determined using UV-vis spectroscopy, Transmission Electronic Microscopy (TEM) and Scanning Electron Microscopy (SEM). The results manifested better AgNPs formation in terms of size, size identification easiness and monodispersity at lower leaf extract concentrations with PVP as coating agent. Average core sizes of 10 ± 3.1 nm and 17 ± 2.6 nm for OLE and RLE were measured by TEM. Increasing synthesis temperature, pH and broth dosage was accompanied with a better reduction and higher yields. OLE was more sensitive to temperature while RLE was more sensitive to solution pH. Antimicrobial testing will be assessed to confirm their usefulness for pharmaceuticals and water purification applications.

Phytochemical Analysis and Evaluation of Antimicrobial, Antiangiogenic and Antiproliferative (Against Different Breast Cancer Cell Lines) Activities of the Leaves of *Elaeagnus angustifolia*.

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Abstract

Elaeagnus angustifolia has a long history of use in ethnopharmacology in Iran, Turkey and Chinese medicine. Some of its parts were studied for their biological activity. However, few studies investigated the potential activities of the leaves. Furthermore, the leaves' chemical composition was not fully investigated before. The chemical composition of the extract of *E. angustifolia* leaves was analyzed and major compounds were identified. Different extracts of the leaves were screened for their antimicrobial, antiangiogenic and antiproliferative activities. Leaves extract obtained by maceration and further extracted with solvents differing in their polarity. Extracts submitted to CC, followed by smaller CC and preparative TLC to isolate major compounds. Those were analyzed using UV-Vis and/or NMR. For different biological activities, leaves were extracted using four solvents; ethanol, ethyl acetate, chloroform and water. Agar diffusion method was used to screen antimicrobial activity against *Escherichia coli*, *Staphylococcus aureus*, *Aspergillus niger* and *Candida albicans*. Rat aortic ring assay was used to screen for antiangiogenic activity. Antiproliferative activity was done against MCF-7 and T-47D breast cancer cell lines using SRB method. One terpene (β -sitosterol) and four flavonoids (chrysin-7-glucoside, rutin, luteolin and kaempferol) were isolated and identified. None of the four extracts was found active against the tested microorganisms. Ethyl acetate extract was found cytotoxic against T-47D breast cancer cell line with $IC_{50} = 23.05 \mu\text{g/mL}$. Potent anti-angiogenic activity of ethanol- ($IC_{50} = 3.039 \mu\text{g/mL}$), ethyl acetate- ($IC_{50} = 6.289 \mu\text{g/mL}$) and water-extract ($IC_{50} = 7.153 \mu\text{g/mL}$) was reported for the first time for *E. angustifolia* leaves.

**Towards Solving Khat Addiction Controversy:
Metabolomic, biological and toxicity profiles of
various cultivars of khat Plant**

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Abstract

Khat abuse is one of the most serious social, economic and security challenges afflicting many African and Middle east countries including Saudi Arabia and neighboring Yemen.

In Saudi Arabia and particularly in Jazan region, it is known that khat is among the most commonly abused substances. Khat used in Saudi Arabia and Yemen is of many cultivars that differ in many pharmacological, behavioral and toxicological effects produced in the user . This indicate differences in the chemical constituents of these khat cultivars.

This poster will try to show a comprehensive and comparative chemical constituent of these khat cultivars. Pharmacological and toxicological profiles will also be highlighted in an attempt to explain chemical-biological relationship on these khat cultivars.

Results of the present study could lay a scientific ground for protecting the society against khat use.

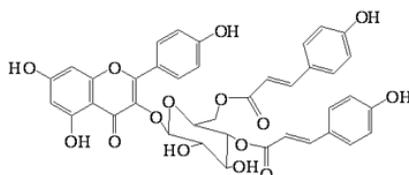
Isolation and Identification of the Chemical Constituents of *Scabiosa prolifera*

Mahmoud A. Al-Qudah, Noor K. Ootom and Sultan T. Abu Orabi

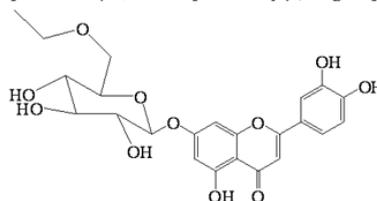
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Abstract

A phytochemical study of *Scabiosa prolifera* led to the isolation of two new flavonoids, Kaempferol-3-O-(4'',6''-di-E-p-coumaroyl)- β -D-glucopyranoside and Luteolin 7-O-(6'-O-ethyl- β -glucopyranoside) along with nine known compounds : β -sitosterol, β -sitosteryl glucoside, ursolic acid, corosolic acid, ursolic acid 3-O- β -D-arabinopyranoside, apigenin, methyl- α -D-glucopyranoside, luteolin-7-O-glucoside and luteolin-6-C-glucoside. Their structures were established using chemical methods and spectroscopic methods namely IR, UV and NMR (1D and 2D). All compounds were isolated for the first time from the plant. Corosolic acid, ursolic acid 3-O- β -D-arabinopyranoside and luteolin-6-C-glucoside were isolated before from natural sources but this is the first report for their isolation from Dipsacaceae family. The antioxidant and antimicrobial activities of the different plant extracts and the new compounds were evaluated.



Kaempferol-3-O-(4'',6''-di-E-p-coumaroyl)- β -D-glucopyranoside



Luteolin 7-O-(6'-O-ethyl- β -glucopyranoside)

Activity of Some new Iminoxime ligands and their Nickel Complexes

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Abstract:

Three new hexadentate Imine-oxime ligands were synthesized (1, 2- diamino benzene- 2, 6-diacetyl pyridine monoxime , 1, 2- diamino ethane-2, 6-diacetyl pyridine monoxime , 1,3-diamino propane-2, 6-diacetyl pyridine monoxime and other one a heptadentate ligand 3-(3-aminopropylimino) butan-2-one Oxime) - 2, 6-diacetyl pyridine). The Nickel complexes with three new variety of hexadentate and a heptadentate ligands of the type $[Ni L-H_2]$, $[Ni L] X_2$, (where $X= Cl^-$ and $L=$ (ligand)) were synthesized. All these four new ligands and their Nickel complexes were characterized by various spectroscopic techniques including melting point, infrared spectroscopy, UV-Vis spectroscopy, and elemental analysis and NMR spectroscopy. The compounds (EL, ProNi, Et.Ni, LL, Ph.Ni and LL.Ni) were tested for their antifungal activity against (*Risophus stolinifer* (R.S), *Calvutaria Lunata* (C.L), *Fusarium Lini* (F.L), *Aspergellius alliaces* (A.A) and *Aspergillus niger* (A.N) fungi, and antibacterial activity against (*Staphylococcus aureus*, *E. coli* and MRSA) bacterial strains by agar disk diffusion method. Most of these compounds have been found to be biologically active. The screening results have shown that the Iminoxime ligands are more active than their Nickel complexes, and 1, 2- diamino ethane-2, 6-diacetyl pyridine monoxime exhibit significantly better activity than the other compounds and have potential use as antibacterial and antifungal agents.

Characterization of Phytochemical Constituents from the Butanol Crude Extract of *Salvia Judaica* and Its Antioxidant activity

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Abstract

The phytochemical constituents of the butanol extract of *Salvia judaica* of Jordanian origin were investigated. Nine compounds have been separated by using chromatographic methods. All compounds are separated for the first time from *Salvia judaica* and one of them, which is Methyl saljudicate (SJB 8) is isolated for the first time from a natural source. Another one is isolated for the first time from *Salvia genus*; which is Methyl isoferuloyl-7-(3,4-Dihydroxyphenyl) lactate (SJB 7). The remaining compounds have been isolated before from *Salvia genus*; these are Luteolin-3'-methyl ether (SJB 1), Indole-3-carboxyaldehyde (SJB 2), p-Hydroxybenzaldehyde (SJB 3), Tricin (SJB 4), Apigenin (SJB 5), Methyl rosmarinate (SJB 6) and Rosmarinic acid (SJB 9).

Structure elucidation of these compounds was achieved using different spectroscopic techniques including IR, UV and NMR (1D and 2D). The antioxidant activity of the extracts of the *S. judaica* as well as all fractions of butanol extract was determined. A high antioxidant activity was observed. In addition, the antioxidant activity of the new compound, Methyl saljudicate, was studied where it showed a high antioxidant activity. It showed 95.19±3.59 DPPH inhibition at 0.8 mg/ml with IC₅₀ of 0.08, and 99.29±0.23 ABTS inhibition at the same concentration with IC₅₀ of 0.04.

The Electronic Spectrum of BH₂ Radical

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Abstract

The A²B₁(Π_u) – X²A₁ linear-bent electronic transition of the BH₂ free radical from 11700 - 14600 cm⁻¹ was previously studied by Girhard Herzberg and Johns in the year 1967. In this work, an extensive LIF and emission studies of the electronic spectrum of jet-cooled ¹¹BH₂, ¹⁰BH₂, ¹¹BD₂, and ¹⁰BD₂ up to 21100 cm⁻¹ is performed. With the aid of the high resolution studies of ¹¹BD₂ and ¹¹BH₂, the ground state geometry is refined and good parameter were obtained. Also ab-initio calculations and variational methods were used to predict the ro-vibronic energy levels of this Renner-Teller system. The results agree very well with the experimental data, confirming and extending our assignments.

A prodrug approach to enhance azelaic acid percutaneous absorption

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Abstract

A prodrug of azelaic acid was synthesized and investigated to improve the percutaneous absorption of azelaic acid throughout the stratum corneum. Partitioning, solubility, chemical stability and enzymatic susceptibility were examined. In addition, permeation of azelaic acid and diethyl azelate (DEA) throughout synthetic membrane and human stratum corneum was studied. Partitioning coefficient ($\log P$) of the prodrug increased up to 3.7 compared to azelaic acid with $\log P$ value of 2.2. In the skin permeation experiment, DEA resulted in a significant increase in absorption compared to azelaic acid throughout the silicone membrane. However, the results were the opposite when human stratum corneum was used. Azelaic acid displayed better permeation to the receptor compartment compared to DEA. This was explained by a reservoir effect of stratum corneum for DEA prodrug. Therefore, a desorption study of DEA from the stratum corneum was implemented to confirm the reservoir behavior of stratum corneum. The results showed a clear sustained release behavior of DEA. As a result, DEA increases azelaic acid penetration towards stratum corneum; thus, a significant enhancement in azelaic acid keratolytic effect is expected. However, clinical studies are required to confirm the keratolytic results.

Antiproliferative activity of the combination of Quercetin/ Doxorubicin on breast cancer cell line: New method for studying cytotoxicity

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Abstract

Breast cancer is one of the most serious types of cancer that affect mainly females but also males in a lesser extent. Statistically breast cancer occupies the first rank over other types of cancer among female in both developed and developing countries.

Doxorubicin (Dox) is the main chemotherapy drug used in advanced breast cancer. It is a neoadjuvant and an adjuvant therapy which has been considered “gold standard” medication for a long time. Unfortunately, Dox exerts serious side effects on the heart, as it is considered cardiotoxic. Quercetin (Quer) is a natural antioxidant that has successfully protected cardiomyocytes in the Dox-induced heart damage models. The challenge is, while protecting heart from Dox-induced cardiotoxicity does Quer affect the antiproliferative activity of Dox?

The aim of this study is to identify the antiproliferative activity on breast cancer cell line, after combining Dox/Quer on the same samples. This can be done by using a new bio-analytical technique for cytotoxicity assay by the means of Fourier-transform infrared micro-spectroscopy (FTIRM).

FTIRM has become a valuable technique for examining the chemical make-up of biological molecules by probing their vibrational motions at a microscopic scale⁽⁴⁾. A key advantage of infrared spectroscopy is that it is sensitive to the structure and concentration of all cell components (proteins, lipids, carbohydrates, phosphates, carbonates, nucleic acids, etc.) present in the sample. This technique is a non-invasive approach in the sense that no extrinsic staining is required to generate the imaging contrast with minimal handling steps and incubation time.

The routine Sulforhodamine B (SRB) cytotoxicity assay was performed as a standard to verify the results obtained by FTIRM. FTIRM measurements were performed by acquisition of Infrared spectra on each sample location. The collected spectra have been merged together and undergo the multivariate data analysis by Principal Component Analysis (PCA).

In the SRB results, the relationship between the percentage of cancerous cells proliferation and Dox concentrations was modified by the addition of Quer in a definite dose. In PCA analysis revealed significant changes in the biochemical structure of control and treated cells, mainly in the DNA, protein and lipid regions of the infrared spectral range.

As conclusion of this study, we noticed that the combination of Dox/Quer seems to be safe and efficient chemotherapeutic regimen in breast cancer treatment. However, more experiments are being carried out at the moment in order to validate this approach by the means of FTIRM.

Effect of *in vitro* Slow Growth Conservation of Wild Mint (*Ziziphora tenuior* L.) on Oil Production and Pulegone Concentration in the Conserved Plants

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Abstract

Ziziphora tenuior L. is one of the important medicinal plant species that belongs to the Lamiaceae family. This plant is distributed in Jordan, particularly in the southern part and it is a rare species which might be extinct totally from wild. So it is very important to keep it for medicinal use. In this study the effect of slow growth conservation using different osmotic agents of sugars (sorbitol, mannitol, and sucrose) and (ABA growth retardant regulator) at different concentrations on the oil production and pulegone concentration of conserved *Ziziphora tenuior* L plants was studied. On the other hand the extracted oil from *in vitro* conserved *Ziziphora tenuior* L plants was compared with those extracted from (*in vivo*) wild plants.

Slow growth conservation of *Ziziphora tenuior* L., microshoots on medium provided with (0.2 M) sucrose or ABA at all levels (3.8, 7.6, 11.4 μ M) were able to reduce the growth, number of subcultures needed and to maintain survival and recovery rates after storage. On the other hand using sorbitol or mannitol with any concentration had lower effect on both survival and recovery after conservation. According to chemical analysis using GC-MS, there were variations in amount of extracted oils yield and pulegone concentrations in both *in vivo* (wild) and *in vitro* stored *Ziziphora tenuior* L. The maximum amount of oil (5%) and pulegone (0.0312 M) were recorded in the *in vivo* plants. Meanwhile about third amount of oil were extracted from *in vitro* stored plant treatments compared to those obtained from *in vivo* plant. Also, the amount of pulegone found in the dried *in vitro* stored samples (0.0041-0.0046 M) was about the same in all concentrations treatments and much lower than those obtained from the *in vivo* samples.

Nanoflora- A New Approach Toward Activity Enhancement of Natural Products

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Abstract

The use of Herbal medicines is accompanied by many difficulties such as low solubility and bioavailability, high toxicity, and limited stability. This situation prevents those phytochemicals from achieving their full potential as pharmaceutical formulations. By nanotechnology and phytochemicals delivery, it becomes possible to overcome these difficulties since Nanotechnology is able to offer many advantages to drug delivery including enhancing solubility and bioavailability, reducing toxicity and side effects, and increasing the stability to be able to resist the harsh conditions along their way to their target. The nanocarriers can be anything from emulsion and microemulsions, dendrimers, fullerenes, liquid crystals, quantum dots, nano-rods, solid lipid nanoparticles (SLN), liposome. This poster introduces nanotechnological approaches related to enhance the bioavailability of herbal medicines.

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Notes

A series of horizontal dotted lines spaced evenly down the page, providing a guide for writing notes. There are 25 dotted lines in total, starting from the top of the page and extending to the bottom.

