Welcome Message

On behalf of the Centre for Natural Products Discovery (CNPD), Liverpool John Moores University and the Organising Committee, I am delighted to invite you to participate in the 2nd Annual CNPD Conference 2021 on 'Natural Products in COVID-19', which will be held virtually on 13-14 May 2021.

This will be a unique two day conference showcasing the best in phytochemical research centred on the theme of "contemporary issues in phytochemical research relevant to Covid-19". The conference itself will take the format of 16 invited speakers who will deliver their latest research in 20 minutes, focusing on what matters most. The spotlight of the conference will then move to young scientists (PhD students and Postdocs) who will also present their work.

The conference will be held virtually as a consequence of the ongoing pandemic, but will be hosted by the Centre for Natural Products Discovery (CNPD) in conjunction with Liverpool John Moores University (LJMU). The CNPD conducts externally-funded natural products research with the aim of discovering new high-value natural products that will contribute to tackling current and future societal and global challenges in health and well-being, socio-economic growth, natural conservation and environmental sustainability.

The CNPD is based in the School of Pharmacy and Biomolecular Sciences at LJMU, which is the second oldest Pharmacy education provider in the UK, and has a rich history of natural products research.

I look forward to welcoming you to this exciting conference. Pls Join us and have a great time with our CNPD.....!!!

Prof Satya Saker
President of the CNPD Organizing Committee
Director of School of Pharmacy & Biomoleular Sciences
Liverpool John Moores University, UK

Programme

Day 1: Thursday 13 May

8.30 – 9.00: **Conference opening and welcome**

Professor Satya Sarker
(Founding Head of the Centre for Natural Products Discovery)

Professor Keith George
(Pro-Vice-Chancellor, Liverpool John Moores University)

9.00 – 10.30: **Session 1**

Chairs: Professor Robert Nash and Dr Francesca Giuntini
Professor Mingquan Guo (China)
Professor Shaikh Jamal Uddin (Bangladesh)
Professor Glyn Hobbs (UK)

10.30 – 11.00: **Break**

11.00-12.30: **Session 2**

Chairs: Professor Randolph Arroo and Dr Amos Fatokun
Dr Didem Şöhretoğlu (Turkey)
Dr Kenny Ritchie (UK)
Dr Jose Prieto-Garcia (UK)

12.30 – 14.00: **Lunch Break**

14.00-15.00: **Session 3**

Chair: Dr Jose Prieto-Garcia
Professor Karel Smejkal (Czech Republic)
Professor Khalid Rahman (UK)

15.00 – 15.30: **Break**

15.30 - 16.30: **Session 4: Short presentations**

Chair: Dr Kenny Ritchie
Flash presentations from PhD students and postdocs

Day 2: Friday 14 May

9.00 – 10.30: **Session 5**
Chairs: Professor Anca Miron and Professor Khalid Rahman
Dr Norazah Basar (Malaysia)
Dr Anupam Das Talukdar (India)
Dr Azhar Rasul (Pakistan)

10.30 – 11.00: **Break**

11.00-12.30: **Session 6**
Chairs: Chairs: Prof Glyn Hobbs and Dr David Bruno
Dr Amos Fatokun (UK)
Dr Touraj Ehtezazi (UK)
Dr Sonia Malik (France)

12.30 – 14.00: **Lunch Break**

14.00-15.00: **Session 7**
Chairs: Professor Satya Sarker and Professor Glyn Hobbs
Dr Olumayokun Olajide (UK)
Dr Fyaz Ismail (UK)

15.30-16.30: **Closing remarks**
Professor Satay Sarker (Founding Head of CNPD)
Professor Khalid Rahman (Head of CNPD)

Abstracts: Invited talks

Session 1

Chairs: Prof Robert Nash and Dr Francesca Giuntini

- **Prof Ming-Quan Guo**

  Chinese Academy of Sciences, Wuhan, China

  "Screening and Identification of Bioactive candidates from Natural Products Employing Multi-Target Affinity Ultrafiltration and LC-MS"

- **Prof Shaikh Jamal**

  Khulna University, Khulna, Bangladesh

  "Antiviral potential of garlic (Allium sativum) and its organosulfur compounds: An update of pre-clinical and clinical data"

- **Prof Glyn Hobbs**

  Liverpool John Moores University, Liverpool, UK

  "Opportunities to find new antibiotics from old friends"

Speaker's Profile

Prof Ming-Quan Guo

Professor Guo is currently a professor in medicinal chemical biology of Chinese Academy of Sciences (CAS), and also the deputy director of the CAS Key Laboratory of Plant Germplasm Enhancement and Specialty Agriculture. His current research interests include but not limited to medicinal biological chemistry and food chemistry, and especially involve the development of a variety of chemical-biology and bio-affinity ultrafiltration based strategies for the quick screening of bioactive small molecules against various drug targets from natural products in the context of targeted new drug discovery and development. He obtained his Ph.D. from Changchun Institute of Applied Chemistry of CAS in 2004, and then moved to USA as a research scientist, and worked successively at National Institutes of Health (MD), UC-Berkeley, and University of Southern California from 2004 to 2012. After that, he joined Wuhan Botanical Institute of CAS as a full professor. By far, he has published over 100 peer-reviewed SCI articles and been acting as Guest Editor or Editorial Board Member for a number of international journals, such as Current Analytical Chemistry, Asian Journal of Chemistry, and Phytochemical Analysis, and Journal of Analysis and Testing. In addition, he has presented over 30 keynote or invited talks at various international/national conferences since 2012.

Screening and Identification of Bioactive candidates from Natural Products Employing Multi-target Affinity Ultrafiltration and LC-MS

Ming-Quan Guo [a,b,c*]

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Various enzymes in our body could play crucial and differential roles in human health and diseases, and many of them have been explored as drug targets. More strikingly, nearly half of the small molecular drugs on the market are enzyme inhibitors with a significant portion of them derived from herbal medicines, resulting in an increasing quest for natural enzyme inhibitors with higher potential for better specificity, lower toxicity and reduced side effects compared with synthesized drugs currently in use. However, to fast screen and identify potential inhibitors from natural products is always a thorny challenge due to complex and diversified chemical composition in minute amounts present in their complex crude extracts. To address these tough challenges, multiple enzymes especially as known drug targets were coupled with bio-affinity-mass spectrometry (MS) to be developed due to their high sensitivity, high resolution, and wide applicability for complex extracts of natural products. In our efforts, the above strategies using different target enzymes (like topoisomerase I and II, COX-1, α-glycosidase, protein kinases and so on) to screen for a wide array of natural inhibitors with diversified chemical structures (such as alkaloids, flavonoids, and saponins, etc.) from various herbal medicines against those targets above have been achieved. For example, an alkaloid from Lycoris radiata was screened out, and exhibited good dose-dependent inhibition against Top I with IC50 at 7.25 ± 0.20 μg/mL comparable to CPT at 6.72 ± 0.23 μg/mL; and also strongly inhibited the proliferation of HT-29 and Hep G2 cells in an intuitive dose-dependent manner with the IC50 values at 3.98 ± 0.29 μg/mL and 11.85 ± 0.20 μg/mL, respectively. These efforts could also be very helpful to unravel the mechanisms of action regarding some traditional herbal medicines through the complex but subtle interactions between their diversified active natural compounds and multiple drug targets. To this end, these strategies have played a crucial role, and will continue to have great potential in providing the direct scientific evidences for traditional natural medicines to take their efficacy in a multiple-component and multiple-target manner.

Speaker's profile

Prof Shaikh Jamal Uddin

Prof Shaikh Jamal Uddin is currently working as a Professor in Pharmacy Discipline, Khulna University, Bangladesh. He started his academic career in 2005 as a lecturer of Pharmacy Discipline, Khulna University. He completed BPharm (Hons.) from Khulna University in 2004 with President and Prime Minister Gold Medal awards. He completed his PhD on natural product chemistry and pharmacology in 2011 from Griffith University, Australia. He was an Erasmus Mundus postdoctoral fellow in Department of Medicinal Chemistry, Uppsala University, Sweden in 2015. His main field of interest are ethnopharmacology and drug discovery from Bangladeshi natural sources. He also working as an adjunct researcher for faculty of pharmacy, Ton Duc Thang University, Vietnam. He has published more than 80 papers and 3 book chapters in international journals. Prof Uddin's current h-index 24 and total citations >2000 (source: Google scholar).

Antiviral potential of garlic (Allium sativum) and its organosulfur compounds: An update of pre-clinical and clinical data

Shaikh J. Uddin[1,2*], Razina Rouf[3], Jamil A. Shilpi[1], Lutfun Nahar[4] and Satyajit D. Sarker[5]

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[3]*Department of Pharmacy, Faculty of Life Science, Bangabandhu Sheikh Mujibur Rahman Science & Technology University, Gopalganj-9300, Bangladesh.*
[4]*Laboratory of Growth Regulators, Institute of Experimental Botany ASCR & Palacký University, Olomouc, Czech Republic*
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Garlic (*Allium sativum* L.) is a common herb consumed worldwide as functional food and traditional remedy for the prevention of infectious diseases since ancient time. Garlic and its active organosulfur compounds (OSCs) have been reported to alleviate a number of viral infections in pre-clinical and clinical investigations. However, so far no update on its antiviral effects and the underlying molecular mechanisms exists. In this project we have summarized pre-clinical and clinical investigations on antiviral effects of garlic and its OSCs as well as to further analyse recent findings on the mechanisms that underpin these antiviral actions. Pre-clinical data demonstrated that garlic and its OSCs have potential antiviral activity against different human, animal and plant pathogenic viruses through blocking viral entry into host cells, inhibiting viral RNA polymerase, reverse transcriptase, DNA synthesis and immediate-early gene 1(IEG1) transcription, as well as through downregulating the extracellular-signal-regulated kinase (ERK)/mitogen activated protein kinase (MAPK) signaling pathway. The alleviation of viral infection was also shown to link with immunomodulatory effects of garlic and its OSCs. Clinical studies further demonstrated a prophylactic effect of garlic in the prevention of widespread viral infections in humans through enhancing the immune response. As a conclusion, garlic possesses significant antiviral activity and can be used prophylactically in the prevention of viral infections.

Speaker's profile

Prof Glyn Hobbs

My first degree was in Microbiology from University College Cardiff I then went on conduct my Ph.D in the same institution funded by the Ministry of Defence working on the biochemistry of hydrocarbon degradation. On completion of my PhD I joined the University of Manchester Institute of Technology (UMIST) where I worked as a Research Associate on antibiotic producing bacteria. In 1992 I joined Liverpool John Moores University as a lecturer in Microbiology. Today I am a Professor of Applied Microbiology at LJMU. During my time at LJMU I have worked with numerous commercial companies, producing antibiotics, enzymes, developing biofilm models. One of my current interests is rapid diagnostics for pathogens.

Opportunities to find new antibiotics from old friends

Glyn Hobbs* and Ismini Nakouti

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One of the greatest challenges we face is the emergence of drug resistant microbial pathogens. The incidence of newly isolated resistant bacteria is increasing in an exponential fashion world wide. We face the fact that at some point in the future we will not have antibiotics to treat them. Our ability to find new classes of antibiotic has declined and the reasons will be discussed but suffice to say we need new antibiotics. Whole genome sequencing over the past two decades has shown us that the genus of Streptomyces have the capacity to synthesis many more antibiotics than we can actually get them to produce. The presence of these “cryptic” genes present us with potentially many “new” antimicrobials. All we have to do is discover how to get them to express. We will discuss how the genes for the antibiotic methylenomycin can be switched on in Streptomyces coelicolor using an environmental signal of decreasing pH. We will then discuss the way forward in new antibiotic discovery.

Session 2

Chairs: Prof Randolph Arroo and Dr Amos Fatokun

- **Dr Didem Şöhretoğlu**

  Hacettepe University, Ankara, Turkey

  "Importance of immunomodulatory potential of triterpenes in Covid-19 era"

- **Dr Kenny Ritchie**

  Liverpool John Moores University, Liverpool, UK

  "Natural product inhibitors of SARS-CoV-2 via regulation of the Nrf2 pathway"

- **Dr Jose Prieto Garcia**

  Liverpool John Moores University, Liverpool, UK

  "COVID-19, Herbal Medicines and Clinical Protocols in a Global World"

Speaker's profile

Dr Didem Şöhretoğlu

Dr Didem Şöhretoğlu studied Pharmacy, at Hacettepe University, Ankara, Turkey. She received her Master of Science degree in Pharmacognosy, Hacettepe University and her PhD degree in a sandwich program between Hacettepe University, Turkey and Lund University, Sweden. She worked as a post-doc in the Department of Organic Chemistry, Lund University, Sweden for a short term. She was a visiting associate professor at the Biochemistry and Molecular Biology Department in Louisiana State University, Shreveport, LA, USA for one year. Presently, she works as an associate professor in Department of Pharmacognosy, Hacettepe University, Ankara (Turkey). Her research interests are focused on the isolation, structure elucidation and biological activities of secondary metabolites, as well as anticancer (autophagy, apoptosis, proliferation, cell cycle and mTOR pathway) and enzyme inhibitory (β-glucosidase, tyrosinase, topoisomerase) activities of natural products. She is Pharmacognosy section editor of *Journal of Research in Pharmacy* and also in the editorial board of *Phytochemical Analysis* and *Frontiers in Pharmacology*.

Importance of immunomodulatory potential of triterpenes in Covid-19 era

Didem Şöhretoğlu[1]* and Gülin Renda[2]

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Covid-19 has had devastating effects globally since 2019. Since total eradication of the virus seems unlikely in foreseeable future, it seems that we need to learn how to live with this disease despite vaccine rollouts and development of different treatment protocols. Boosting the immune system with natural immunomodulators may be an option in this regard. Immunomodulators have the ability to stimulate, suppress or modulate any aspect of the immune system and boost or suppress the host defence response. They are important not only for preventive use in Covid-19 infection, but also for its treatment in combination with antivirals. Triterpenes exhibit immunomodulatory properties by many different mechanisms. Different triterpenes, including components of commonly consumed plants, can promote some protection and alleviation of the disease symptoms as well as promoting overall well-being. In this presentation, immunostimulatory potential of triterpenes will be discussed.

Speaker's profile

Dr Kenny Ritchie

Dr Kenny Ritchie received his undergraduate degree in Pharmacology from the University of Aberdeen, and his PhD from the University of Cardiff. To gain experience in transgenic models he then undertook a postdoctoral research position in the Scripps Research Institute, San Diego, California with Professor Dong-Er Zhang. Upon returning to the UK, Dr Ritchie combined his interests of toxicology and transgenics by conducting research within the Cancer Research UK Molecular Pharmacology Unit, headed by Professor Roland Wolf and based within the University of Dundee. In 2009, Dr Ritchie accepted a lectureship in toxicology at Liverpool John Moores University (LJMU). Whilst at LJMU Dr Ritchie has worked closely with Professor Satya Sarker, Director of the School of Pharmacy and Biomolecular Sciences, to develop his interest in phytochemical research. He has also contributed to the establishment of the Centre for Natural Products Discovery (CNPD) in which he is the lead scientist in the toxicology section. Dr Ritchie also plays an active role in the wider phytochemical community and as such is currently the treasurer of the Phytochemical Society of Europe (PSE).

Natural product inhibitors of SARS-CoV-2 via regulation of the Nrf2 pathway

Kenny Ritchie*

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Chemoprevention was first used as a term in the context of preventing cancer *in vivo*. Since that point the term has become widely used and can be broken down into two distinct areas; blocking agents that prevent DNA damage from occurring and supressing agents that are generally aimed at reducing the progression of the initiated (mutated) cell to clinically defined cancer. Central to this response is the ability of natural products to induce enzyme based cellular defence mechanisms with much of that research focussed on the master regulator molecule of antioxidant gene induction, Nrf2 (nuclear erythroid 2-related factor). In addition to its role in preventing carcinogenesis, which is the focus of our work here at LJMU, Nrf2 is also known to reduce inflammation specifically through regulation of *IL6* and *IL1B.* Further lung biopsies from COVID-19 patients (the disease caused by SARS-CoV-2) have been found to be lacking in proteins associated with Nrf2 activation and Nrf2 inducers have been found to inhibit the replication of SARS-CoV-2 and its associated inflammatory response. In this presentation recent research which has investigated the ability of specific natural products to induce Nrf2 and their consequent ability to inhibit SARS-CoV-2 will be considered.

Speaker's profile

Dr Jose Prieto-Garcia

Dr Jose M. Prieto is Associated Professor in Natural Products (Phytochemistry) at Liverpool John Moores University. He obtained BPharm (Hons) and MPharm degrees in Pharmacy from the University of Valencia (Spain) where he also completed a PhD in Pharmacology. Prior to his current employment, he also held EU Research Fellowships at the University of Pisa (2000-2004) and University of London (2005-2006). As a a lecturer at University College London he applied advanced techniques to the analysis and pharmacological effects of complex natural products, coordinated an MSC in Medicinal Natural Products and Phytochemistry, acted as advisor of the British Medicines Agency and consultant to the Herbal Industry. He is a Member of the Royal Society of Chemistry and Fellow of the Higher Education Academy since 2010. His research focuses on anticancer and anti-inflammatory properties of phytochemicals. His new research interest is in computational phytochemistry. He has over 70 publications including the reference book "Fundamentals in Pharmacognosy and Phytotherapy" (Elsevier).

COVID-19, Herbal Medicines and Clinical Protocols in a Global World

Jose Prieto-Garcia*

Centre for Natural Products Discovery, School of pharmacy and Biomolecular Sciences, Liverpool John Moores University.

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Current recommendations for the self-management of SARS-Cov-2 disease (COVID-19) include self-isolation, rest, hydration, and the use of NSAID in case of high fever only. It is expected that many patients will add other symptomatic/adjuvant treatments, such as herbal medicines. This has prompted both scientist and healthcare professionals to discuss whether modern phytotherapy and clinical practices around the World may safely and effectively work together in this context.

Herbal practitioners across China have been working along with regular medical doctors to control the COVID-19 disease. The meta-analyses of the results led the Chinese National Health Commission to integrate Traditional Chinese Medicine in the treatment of COVID-19 patients (Xu et al., 2020) (Li et al., 2020). In India, Ayurveda Practitioners are setting clear protocols with a rationale consistent with their millenary system. Clinical settings and regulations of research on COVID-19 through Ayurveda, Unani, Siddha, and Homeopathy systems have already been published by the Indian Ministry of Ayush (INDIA, 2020). The clinical benefits/risks of European and Latin-American herbal medicines listed by the WHO and EMA for use in respiratory conditions have been recently assessed and some of them present safety margins superior to those of reference drugs (Silveira et al., 2020).

While these herbal medicines will not cure or prevent respiratory infections, they may both improve general patient well-being and offer opportunities to personalize the therapeutic approaches in the context of the current and future coronavirus outbreaks.

Session 3

Chair: Dr Jose Prieto-Garcia

- **Prof Karel Šmejkal**

  Masaryk University, Brno, Czech Republic

  "Prenylated phenolics as lead compounds for Covid-19 therapeutics?"

- **Prof Khalid Rahman**

  Liverpool John Moores University, Liverpool, UK

  "Nutraceuticals and Covid-19: Food for Thought?"

Speaker's profile

Prof Karel Šmejkal

Prof Karel Šmejkal recently moved to the Department of Natural Drugs in the Faculty of Pharmacy at Masaryk University. Besides heading the Department of Natural Drugs, he became vice-dean for External Relations and Internationalization of Faculty of Pharmacy.

Associate Professor Šmejkal is interested in phytochemistry – especially separation and identification of natural substances. He works especially with prenylated phenols from Moraceae plants, Amaryllidaceae alkaloids, and lignans of Schisandra chinensis. He routinely works with different chromatographic methods and provides identification of metabolites (IR, CD, MS, NMR). Secondary aim of his interest are bioassays of natural compounds– in particular anticancer (effect on cell cycle), anti-inflammatory (COX inhibitors, NF-κB), antibacterial activity (anti MRSA).

His publication record shows 85 publications according to WOS, H-index according to WOS 20. He is author or co-author of at least 70 conference papers, active attendant of 30 conferences.

Prenylated phenolics as lead compounds for Covid-19 therapeutics?

Karel Šmejkal*,[1], Martina Fojtíková[2], Josef Mašek[2], Jan Hošek[2,3], Milan Malaník[1], Lenka Molčanová[1] and Jakub Treml[3]

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Viral diseases are caused by infections of the body with pathogenic viruses. Many viruses (including SARS-Cov-2) cause serious illness with different symptoms: from respiratory diseases, diarrhea, dermatotoxicity, liver damage, to immune failure. Organisms can respond to a viral infection by activating the immune system, which paradoxically can be inappropriate and can damage the body's own tissues. Treatment of viral infections is often symptomatic (includes e. g., antipyretics, analgesics) or, if available, antivirals are given. If a severe inflammatory reaction develops, anti-inflammatory agents may also be administered. Viral infection can be complicated by secondary bacterial infection and then antibiotics are also applied.

Natural substances often have a pleiotropic effect and can affect several cellular processes in parallel. They can have parallel anti-inflammatory and antibacterial effects, together with the current antiviral effect. Their mechanism of action is complex. However, the problem of natural substances is often their limited solubility and consequently also problematic bioavailability.

As part of the lecture, we will introduce the isolation and identification of prenylated phenols with potential antiviral and anti-inflammatory effects, we will describe their bioactivity, their formulations to increase solubility, and will describe the possibilities of their further development.

The work of J.H. was also supported by the Ministry of Education, Youth and Sports of the Czech Republic under the project “FIT” CZ.02.1.01/0.0/0.0/15_003/0000495, and Czech Ministry of Agriculture grant no. RO0518.

Speaker's profile

Prof Khalid Rahman

I am currently employed as a Professor in the School of Pharmacy and Biomolecular Sciences, at Liverpool John Moores University. I am the Deputy Head of the Centre for Natural Product Discovery and my research interests are in the usage of nutraceuticals in the prevention of chronic diseases, mainly cardiovascular disease. I have investigated the medicinal properties of nutraceuticals both at an academic and commercial level. Currently, I have research collaboration with groups based in UK, China and Kuwait. Traditional medicine therapies can have profound effects on health and thus need scientific validation and their usage may have a positive impact on health budgets. I have published over 175 papers, written reviews, and chapters for books and presented my work at various International Conferences. I am a member of The Biochemical Society and The Speciality Committee of Traditional Chinese Pharmacognosy affiliated to World Federation of Chinese Medicine Society (WFCMS). I am a serving editorial board member of the Evidence-Based Complementary and Alternative Medicine, World Journal of Cardiology, Kuwait Journal of Science and The EC Nutrition journals.

Nutraceuticals and Covid-19: Food for Thought?

Khalid Rahman and Gordon Lowe

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Covid-19 is one of the deadliest pandemics of the century. It is a viral disease that affects the epithelial cells of the respiratory system and causes inflammation of the mucosal membrane, causing alveolar damage and eventually pneumonia. This disease has made everyone realise the policy of “Prevention is better than cure”. Most guidelines for containing the pandemic are focussed on personal hygiene and prevention of the spread of virus. Only minimal focus has been given towards the role of immunity and more importantly the role of nutrition in supporting immunity. WHO has stated that the global burden of nutritional deficiency is very high and this gap is filled by nutraceuticals, which are foods or components of food, which provide medical or health benefits, including the prevention and treatment of diseases. Optimum functioning of the immune system requires optimal nutrition, which allows immune cells to carry out effective responses against pathogens. We have investigated several nutraceuticals including garlic and green tea extract. Garlic was given to healthy volunteers and displayed antioxidant properties as judged by an increase in total antioxidant status, inhibition of LDL oxidation and prevented platelet aggregation, a complication of Covid-19 infection. Neutrophils play a defensive role against bacterial infections by oxygen dependent and independent pathways. Neutrophils were isolated from healthy volunteers and primed and activated with formyl peptide fMethionine-Leucine-Phenylalanine (fMet-Leu-Phe) and lactoferrin and myeloperoxidase was measured as well as water-soluble antioxidant status. Green tea extract was then given to volunteers and the assays repeated; increase in lactoferrin, myoperoxidase and water-soluble antioxidants was observed. This presentation will summarise the data from our laboratory and highlight other nutraceuticals, which may enhance immunity in Covid-19 infected patients.

Session 5

Chairs: Prof Anca Miron and Prof Khalid Rahman

- **Dr Norazah Basar**

  Universiti Teknologi Malaysia, Johor, Malaysia

  "Ultrasound Assisted Extraction of Phytochemicals Using Response Surface Methodology in Commercial Moringa oleifera Lam Leaves"

- **Dr Anupam Das Talukdar**

  Assam University, Assam, India

  "Understanding and Targeting TMPRSS2: a step towards combating COVID-19"

- **Dr Azhar Rasul**

  Government College University, Faisalabad, Pakistan

  "Hesperidin: A promising drug candidate against COVID-19"

Speaker's profile

Dr Norazah Basar

Dr Norazah Basar obtained her B.Sc (Hons) in Industrial Chemistry in 2000 and Master degree by Research in Chemistry (2002) from Universiti Teknologi Malaysia (UTM), Malaysia. Her MSc research was in the area of Natural Products Chemistry. She completed her PhD in Organic synthesis at the Universiti Teknologi Malaysia (UTM) in 2009. Part of the PhD work was carried out at the School of Chemistry, Manchester University, UK. Upon completing her PhD research, she expanded her experience working as Research/Postdoctoral Fellowship at the School of Pharmacy and Biomolecular Science, Liverpool John Moores University, U.K for one year (April 2013) under supervision of Prof Satyajit D Sarker in the area of Phytochemistry. Dr Basar started her career as a tutor at the Department of Chemistry, Faculty of Science, UTM in July 2000 and after finishing her MSc, she started working as a lecturer in October 2001. Currrently, she is a Senior Lecturer at the Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, Johor Bahru since August 2010. She actively involved in research and teaching activities in Chemistry. With successful research collaboration supported with research grants have resulted in 35 indexed publications (ISI and Scopus), 15 non-index and two organic chemistry textbooks.

Ultrasound Assisted Extraction of Phytochemicals Using Response Surface Methodology in Commercial Moringa oleifera Lam Leaves

Norazah Basar* and Nuridayu Yusmaidi

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Moringa oleifera Lam is a rich source of phenolic and flavonoid compounds that act as antioxidant, antibacterial and anti-inflammatory agents. M. oleifera is one of the species belong to Moringa genus from the Moringaceae family. This research was carried out to optimize the ultrasound-assisted extraction (UAE) of the extract from commercial sample of M. oleifera leaves by using response surface methodology (RSM). Box-Behnken design (BBD) was used to design the 17 experiments using three variables which were extraction temperature (40, 50, 60°C), time (25, 30, 35 min) and methanol composition as solvent (60, 70, 80%). The effect of parameters on the responses of extraction yield, quantification of quercetin and chlorogenic acid, as well as DPPH (2,2-diphenyl-1-picrylhydrazyl) assay for antioxidant were determined. Quantification of quercetin and chlorogenic acid in the extracts was done using reversed-phase high-performance liquid chromatography coupled with a diode array detector. It was discovered that both compounds were present in the optimized extracts. The highest percentage of yield (48.99%) and the concentration of chlorogenic acid (31.07% w/w) were found at the extraction temperature of 50°C, time of 30 minutes and 70% of methanol. The highest antioxidant activity was also found in this condition with the IC_{50} value of 31.77 µg/ml. The highest concentration of quercetin (5.40% w/w) was discovered when the extraction was carried out at 50°C for 35 minutes and 80% of methanol concentration.

Speaker's profile

Dr Anupam Das Talukdar

Dr Anupam Das Talukdar is currently working as Senior Assistant Professor (Stage – III), in the Department of Life Science & Bioinformatics, Assam University, Silchar, Assam, India. He has 17 years of teaching and research experience in Computer Aided Drug Designing, Bioinformatics, Ethnobotany and Phytochemistry. In his current research area, he has successfully completed four research projects and two projects are ongoing till date, funded by the various National funding agency of India as a Principal Investigator. He has produced eight PhD and six MPhil scholars till date. Currently, four PhD scholars are working under his guidance. He has published 80 international research article, 24 book chapters and four books. He also awarded gold medal twice in his early academic periods for obtaining the first class first position in his Bachelor and Master degree and also awarded prestigious DBT – Overseas Associateship for his post-doctoral studies. Dr Das Talukdar has obtained his PhD degree from The Assam University, Silchar, Assam, India, in collaboration with Bose Institute, Kolkata, India, in the year 2010.

Understanding and Targeting TMPRSS2: a step towards combating COVID-19

Anupam Das Talukdar*

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COVID-19 has become a major humanitarian catastrophe. The culprit, SARS-CoV2 virus, has already claimed more than 260,000 lives within each passing 4 months from its time of inception and this is exponentially increasing in each coming days. SARS-CoV2 utilizes very efficiently its spike protein(S) to bind with human ACE2 for host cell entry. And ACE2 receptor needs a specialized serine protease enzyme, TMPRSS2 for its activation. This activation aids in the attachment of the spike protein to the host cell. Understanding the pattern of the interaction of this enzyme and their behavior in the system has become urgency. We thus in this piece of work design attempt has been made to model this serine protease enzyme, TMPRSS2 and target with the known FDA drugs, an initiative of drug repurposing. Modeling of the protein is carried followed by various PROCHECK analysis. Further high throughput virtual screening is accomplished to target this enzyme significantly. The small molecules and the drugs which can mask the catalytic triad of the enzyme will be selected and the best molecule will be subjected to pharmacophore modeling. This will not only bring-forth a novel approach in understanding an therapeutic target enzyme but also will give a direction in the target treatment.

Speaker's profile

Dr Azhar Rasul

Dr Azhar Rasul is an Assistant Professor at Faculty of Life Sciences, Government College University Faisalabad. He received MSc and M. Phil degree in Biology from Bahauddin Zakariya University, Multan, Pakistan. He obtained PhD fellowship jointly awarded by Ministry of Education (MOE), Pakistan and China Scholarship Council (CSC), China and completed his Ph.D. in Cell Biology (Chemical Cancer Biology) from Northeast Normal University, China. He later received China postdoctoral fellowship in 2012, Japanese Society for Promotion of Science (JSPS) Postdoctoral fellowship in 2013, and subsequently Tokyo Biochemical Research Foundation (TBRF) fellowship in 2015. He has published over 119 peer-reviewed articles with cumulative impact factor over 262 and with over 2254 citations. He also has published eleven book chapters. He has presented several invited talks at National and International level. He has attended more than 20 International conferences in Japan, China, South Korea, Dubai, Sri Lanka, Qatar, Turkey, Thailand, Malaysia and France. Under his supervision, thirteen MPhil students completed their research work. Three PhD and two MPhil students are currently working under his supervision. He has obtained several national and international research grants (HEC-Pak Turk Mobility Grant, ISSESCO RG, HEC-NRPU RG(s), The Nagai Foundation Tokyo RG(s) and COMSTECH-TWAS RG). His lab is actively engaged in interdisciplinary research on novel tumor biomarkers, cancer-related health disparities, identification of non-toxic anti-cancer compounds for various hallmarks of cancer (cancer stem cells, cancer cell metabolism, and tumor hypoxia) from natural sources and development of highly efficient green extraction methodologies for preparation of active constituent enriched-bioactive extracts libraries. He is reviewer and editorial board member of several well-reputed journals.

Hesperidin: A promising drug candidate against COVID-19

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SARS CoV-2, a rapidly spreading new strain of coronavirus, has affected almost all the countries of world and received worldwide attention. The lack of specific drugs or vaccines against SARS CoV-2 is a major hurdle towards the prevention and treatment of COVID-19. Thus, there is an urgent need to boost up research for the development of effective therapeutics against COVID-19. The crystallized form of SARS CoV-2 main protease (Mpro) was demonstrated by a Chinese researcher Liu et al. (2020) which is a novel therapeutic drug target. This study was conducted to evaluate the efficacy of customized dietary-nutrients based virtual library against COVID-19 virus Mpro by molecular docking study. Molecular docking investigations were performed by using Molegro Virtual Docker 7 to analyze the binding interactions of these compounds against COVID-19 virus Mpro. COVID-19 virus Mpro (PDB ID: 6LU7: Resolution 2.16 Å) was docked with 80 flavonoid compounds and the binding energies were obtained. According to obtained results, hesperidin, rutin, diosmin, and apiin have been found as more effective against COVID-19 virus Mpro than nelfinavir (positive control). This study will hopefully pave a way for doing advanced experimental research to evaluate the real medicinal potential of these compounds to cure COVID-19.

Session 6

Chairs: Dr David Bruno and Dr Fyaz Ismail

- **Dr Amos Fatokun**

  Liverpool John Moores University, Liverpool, UK

  "Natural product inhibitors of poly (ADP-ribose) polymerase (PARP) as potential treatments for COVID-19"

- **Dr Touraj Ehteazi**

  Liverpool John Moores University, Liverpool, UK

  "The Potential Use of Cyclosporine Inhaler in the Treatment of SARS-CoV-2"

- **Dr Sonia Malik**

  University of Orleans, Orleans, France

  "Bioactive essential oils from *Artemisia vulgaris* L."

Speaker's profile

Dr Amos Fatokun

Dr Amos Fatokun is currently the Section Lead for Natural Products Pharmacology within the Centre for Natural Products Discovery (CNPD) of Liverpool John Moores University, UK. He obtained a first degree in Pharmacy (Obafemi Awolowo University, Nigeria) and a PhD in Pharmacology and Neuroscience (University of Glasgow, UK), and undertook prestigious postdoctoral fellowships in the US (Johns Hopkins School of Medicine) and the UK (University of Nottingham), and a visiting fellowship in Australia (University of Sydney). His current, externally funded research explores the cellular and molecular mechanisms underpinning cell death in cancers and neurodegeneration and the development of novel, targeted therapeutics for treating the conditions. A key target he is working on is the nuclear enzyme poly (ADP-ribose) polymerase (PARP), against which he has identified small-molecule inhibitors. He also seeks to scientifically validate, at the interface of biology and chemistry, ethnobotanical uses of natural products. Dr Fatokun's laboratory uses methods and techniques in pharmacology, drug discovery, cell and molecular biology and fluorescence imaging to identify small-molecule hits for molecular (drug) targets and conduct hit-to-lead characterisation, with the goal of translation to clinical utility. He has published several papers in high-impact journals and supervises MSc and PhD students and postdoctoral fellows.

Natural product inhibitors of poly (ADP-ribose) polymerase (PARP) as potential treatments for COVID-19

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The current COVID-19 pandemic (caused by the SARS-CoV-2 coronavirus) has taken an unprecedented and incalculable toll on humanity, from which recovery might be long, hard, and tortuous. While thankfully there are now some vaccines and therapeutic agents that combat the disease, in several regions of the world vaccine roll out is still quite deficient and access to relevant therapeutic agents is largely limited. In addition, to date, many aspects of the symptomatology and pathophysiology of the disease are not well known. It is, therefore, critically important that concerted efforts continue in expanding the therapeutic armamentarium against COVID-19, including with regard to treating its long-term sequelae and complications, such as 'long COVID'. Natural products are a proven source of effective medicines and have been reported to be deployed against COVID-19. One of the identified targets for drug development against COVID-19 is the enzyme poly (ADP-ribose) polymerase (PARP), a DNA damage sensor beneficially involved in the DNA damage response and whose inhibitors (PARPi) are used in the clinic to treat certain germline-mutation cancers and have also been proposed to be repositioned to treat some other diseases. Our work has identified natural product PARP inhibitors, including 4'-methoxyflavone and 3',4'-dimethoxyflavone, which can be investigated for efficacy against COVID-19. This invited oral presentation will discuss the relevance of PARP to the pathophysiology and treatment of COVID-19, including associated mechanisms such as preventing oxidative stress, inflammation and DNA damage. It will then showcase natural product inhibitors of PARP as potential anti-COVID-19 treatments.

Speaker's profile

Dr Touraj Ehtezazi

Dr Touraj Ehtezazi graduated from School of Pharmacy, University of Tabriz, Iran and acquired his PhD from School of Pharmacy, University of Nottingham in 1997. Dr Ehtezazi has worked as formulation scientist in world leading pharmaceutical companies, and lecturer in University of Leicester from 2000-2003. Currently, Dr Ehtezazi is Senior Lecturer, at School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University. His research interest includes pharmaceutical inhalers, 3D printing, and brain targeting drug delivery systems. Touraj has supervised PhD students a Postdoc in the field of drug delivery systems. Touraj also has established collaborations with the Department of Clinical Neurosciences, University of Cambridge for the development of novel brain targeting drug delivery systems for the treatment of multiple sclerosis and ischemic stroke. Dr Ehtezazi was awarded a grant by The Royal Society of Chemistry in developing 3D printed light-activated wound dressings. Also, Dr Ehtezazi was awarded a grant by the Liverpool John Moores University in 2020 in response to COVID-19 to develop protocols to minimise aerosol levels in dental clinics to minimise contraction of COVID-19 for both clinical staff and patients. Dr Ehtezazi published this research paper in 2021. Touraj also is leader of drug delivery formulation section in Centre for Natural Product Discovery at Liverpool John Moores University.

The Potential Use of Cyclosporine Inhaler in the Treatment of SARS-CoV-2

Touraj Ehtezazi*

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Cyclosporine A is a natural product produced by fungi such as *Tolypocladium inflatum* and *Aspergillus terreus*. Cyclosporine A belongs to a group of Cyclosporines, which are cyclic peptides composed of 11 amino acids. Cyclosporine A is the major component of the cyclosporines, which distinguishes from other cyclosporines by the type of amino acid at carbon number 2. It is the only member of this group used clinically for the prevention and treatment of graft-versus-host reactions. Cyclosporine A has shown remarkable antiviral activities against SARS-CoV-2 by inhibiting the Cyclophilin A, a key component in the replication of SARS-CoV-2. Cyclosporine A is a drug that has been used for the treatment of COVID-19 with improved survival rate of patients, but with parenteral doses above 300 mg per day, which led to observing side effects such as acute renal failure. Fortunately, inhalation therapy of cyclosporine A has been tolerated in clinical trials of patients with lung transplants. As COVID-19 serious respiratory problems start when the virus reaches the alveolar level; then a solution pressurised metered dose inhaler of cyclosporine A would have substantial benefits in the treatment of COVID-19. In this work, I will present the work so far with cyclosporine inhalers and next steps required to take cyclosporine A as inhaler to clinical trials of COVID-19.

Speaker's profile

Dr Sonia Malik

Dr Sonia Malik has obtained her doctoral degree in Plant Biotechnology from CSIR-Institute of Himalayan Bioresource Technology, Palampur, India in 2009. Her basic area of research is plant secondary metabolites and genetic manipulation and she did work on several medicinal plants. After her post-doctoral studies at University of Campinas, Brazil and Palacky University, Czech Republic. Dr Malik has worked as an Assistant Professor (tenure track position) in Biology at Biological and Health Sciences Center, Federal University of Maranhão, Sao Luis, Brazil. For contributions in teaching and research during this period, she got Junior Researcher award from FAPEMA. She visited many world's leading cross-disciplinary research and teaching institutions including University of California, USA, Southern Regional Research Center, USDA-ARS, USA, De Montfort University, Leicester, UK and University of Adelaide, Australia as a visiting researcher. At present, she is working as a senior researcher at University of Orleans, France.

Dr Malik has published more than 30 research articles in reputed journals. She has authored 8 book chapters and edited four books as a sole editor from Springer International Publisher. She is editorial board member and reviewer of many International scientific journals.

Bioactive essential oils from *Artemisia vulgaris* L.

Sonia Malik[1,2]*, Ludmilla Santos Silva de Mesquita[3], Carolina Rocha Silva[4], José Wilson Carvalho de Mesquita[3], Emmeline de Sá Rocha[3], Patricia de Maria Silva Figueiredo[3] and Livio M. Costa-Júnior[4]

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The genus Artemisia is among the most widely distributed and largest genera of family Asteraceae. *Artemisia vulgaris* L., commonly known as mugwort has a long history of its use in traditional systems of medicine in different parts of the world. Essential oils from this plant species are known to possess various biological activities including anti-parasitical, insecticidal, anticancer, anti-inflammatory, antimicrobial and anti-helminthic properties. Various mugwort genotypes growing in different geographic areas showed varied components fraction. Biological activities of these essential oils are mainly attributed to volatile compounds, such as α-pinene, camphor, caryophyllene, camphene, germacrene D, 1,8-cineole, and α-thujone. These chemical compounds and their composition vary depending upon on geographic origin, environmental conditions as well as plant growth stages. Knowing the exact chemical composition of mugwort oil is critical to identify its biological properties This talk will present an overview on the essential oils from *A. vulgaris* and the authors' own findings on the chemical profile of EOs from A. vulgaris cultivated in Brazil and their biological activities. The results indicate the potential for using essential oil from *A. vulgaris* as disinfectants and preservatives against microorganisms.

Session 7

Chairs: Prof Satya Sarker and Prof Glyn Hobbs

- **Dr Olamayokun Olajide**

  University of Huddersfield, Huddersfield, UK

  "Inhibition of exaggerated cytokine production by natural products from African plants in cellular models of SARS-CoV-2 spike glycoprotein S1-stimulated PBMCs and RAW264.7 macrophages"

- **Dr Fyaz Ismail**

  Liverpool John Moores University, Liverpool, UK

  "Natural products *vs*. rational drug designed molecules against SarsCoV-2 targets: Nature *vs*. artificial intelligence guided synthesis"

Speaker's profile

Dr Olumayokun Olajide

Dr Olumayokun Olajide is a Reader in Biochemical Pharmacology in the Department of Pharmacy, University of Huddersfield where he leads the natural products research group. He This was followed by Humboldt Postdoctoral Research Fellowships in the Pharmaceutical Biology Research Group, Department of Pharmacy, University of Munich, and the Neurochemistry Research Laboratories, University of Freiburg Medical School, Germany. His research programme focuses on the Molecular Pharmacology of Phytochemicals with anti-inflammatory activity and has authored 60 publications in this field. He is currently investigating phytochemicals which inhibit neuroinflammation as potential leads in the discovery of new therapeutics for Alzheimer's disease. His pioneering study on the potential benefits of pomegranate polyphenols in Alzheimer's disease has resulted in an ongoing human intervention study.

Inhibition of exaggerated cytokine production by natural products from African plants in cellular models of SARS-CoV-2 spike glycoprotein S1-stimulated PBMCs and RAW264.7 macrophages

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Since the first report of the emergence of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), there has been a widespread appearance of coronavirus disease 2019 (COVID-19). Acute respiratory distress syndrome (ARDS) and multi-organ damage in severe SARS-CoV-2 infection have been linked to cytokine storm and the accompanying exaggerated release of pro-inflammatory cytokines such as interleukin-6 (IL-6), interleukin-1 beta (IL-1β), and tumour necrosis factor (TNFα), which damage the lung and other organs. Studies have shown that the S1 sub-unit of the SARS-CoV-2 spike glycoprotein is a target for the host immune responses, including excessive production of pro-inflammatory cytokines. In cellular models for investigating natural products with potential pharmacological/therapeutic potentials in reducing SARS-CoV-2 cytokine storm, human peripheral blood mononuclear cells (hPBMCs) and RAW264.7 mouse macrophages were stimulated with a recombinant SARS-CoV-2 spike glycoprotein S1 sub-unit (100 ng/mL) for 24 h. Analyses of culture supernatants showed significant elevation in the production of TNFα, IL-6, IL-1β, and IL-8. Furthermore, pre-treatment of both cells with dexamethasone (100 nM) resulted in significant reduction of S1-induced increased production of TNFα, IL-6, IL-1β, and IL-8. This talk will present results of our investigations on the effects of extracts and some phytochemicals obtained from *Garcinia kola* (seeds), *Zanthoxylum zanthoxyloides* (root bark) and *Azadiractha indica* (leaves) on SARS-CoV-2 spike glycoprotein S1-induced increased production of TNFα, IL-6, IL-1β, and IL-8 in PBMCs and RAW264.7 macrophages.

Speaker's profile

Dr Fyaz Ismail

Dr Fyaz Ismail completed his PhD in Physical Organic Chemistry (of vitamin E and related compounds) in 1989 (Salford University with Professor Roger H. Bisby) and then went onto"green" the highly polluting Kelly process (by converting it from batch to flow; Monsanto Research Fellow at Reading University with Dr Neal Stuart Isaacs: High-Pressure Chemistry Unit). After a decade as a senior lecturer in Spectroscopy and Medicinal Chemistry (University of Hertfordshire), he became a subject leader at the School of Pharmacy (LJMU till 2005). His research interests include modulating free radical processes in disease by perfecting weakly active substance (inspired by natural products) into clinically useful medicines using rational drug design, especially natural products such as artemisinin and cryptolepine using NMR and DFT. For the last decade, he and his colleagues have used DFT, spectroscopic and spectrometric methods (ion mobility) to discover that Quinine and Chloroquine drugs act at the heme Plasmodial receptor through hydrogen bonding interactions, followed by fast electron transfer and scission of the porphyrin ring and eventually causing Plasmodial death through ferroptosis. Currently, he is the section lead for: The synthesis of Natural Products at the Centre for Natural Product Discovery, LJMU, Liverpool.

Natural products *vs.* rational drug designed molecules against SarsCoV-2 targets: Nature *vs.* artificial intelligence guided synthesis

Fyaz Ismail*

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The current Covid-19 pandemic has mobilized both the pharma sector and government-industry-academic partnerships to rapidly-produce effective vaccines, currently able to diminish the severity of against SARS-CoV-2 infections. Protection in clinical studies has ranged from 95% for mRNA vaccines to ~70% for adenovirus-based vaccines diminishing severity of infections and hospitalizations. Apart from vaccine sceptics, in some patients vaccines may be contraindicated, or ineffective due to the appearance of resistant mutants virus strains. Since high resolution atomic resolution cryo-em structures of SARS-CoV-2 virus target proteins are publicly available in protein databases, rational drug design of viral proteases covalent inhibitors, especially 3ClPro has accelerated [2]. For instance, the oral antiviral clinical candidate PF-07321332 (Fig. 1a), a SARS-CoV2-3CL protease inhibitor, reveals potent anti-viral activity in vitro against SARS-CoV-2, as well as activity against other coronaviruses [3].

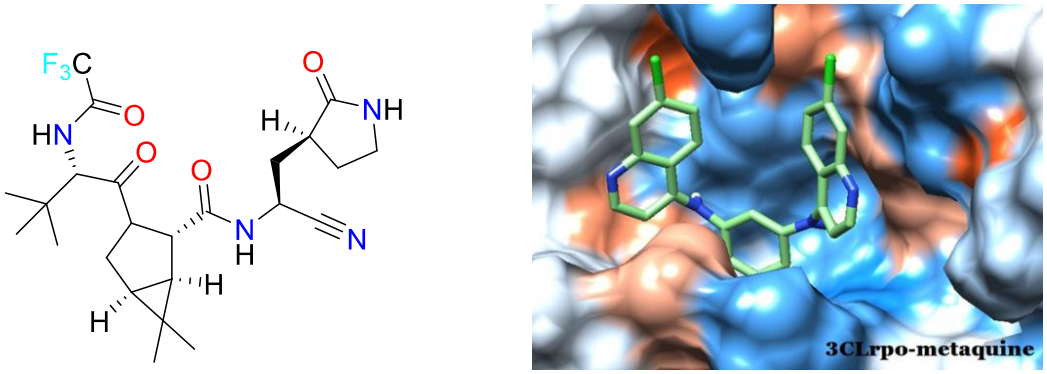

Figure 1 (a) PF-07321332; (b) Metaquine docked in 3Clpro

Synthetic compounds surveyed from published work range from weakly active lead compounds to those that could serve as clinically useful compounds [1]. In parallel, various natural products have also been screened mostly in vitro and in silico (against protein targets) providing a wealth of information. Consequently, promising compounds including will be highlighted [2], together with synthetic compounds which appear promising, such as metaquine; [Fig 1b] as lead compounds which we are developing in conjunction with Brazilian colleagues [5] and The Oswaldo Cruz Foundation, Brazil against resistant variants of SarsCoV2.

Session 4

3-minutes oral presentations

Chair: Dr K Ritchie

Speakers: 3-minutes oral presentations

- **Mr Kevser Tavan Agça**
  "Flavonoids as potential natural compounds against COVID-19"
- **Dr Debib Aicha**
  "Possible bioactive substances with antiviral activity (anti SARS-CoV-2) from green cypress *Cupressus sempervirens* L"
- **Ms. Ankita Chandwani**
  "Development of a novel phyto combination for common respiratory ailments"
- **Ms. Vinisha Dudhat**
  "An effervescent tablet preparation from herbs with docking study against COVID-19"
- **Ms. Asma Hakem**
  "*Juncus acutus*, a potential remedy for coronaviruses"
- **Mr Debojyoti Halder**
  "A Review on Possible Treatment of Symptoms of COVID-19 by *Justicia adhatoda* (Vasaka Leaf)"
- **Ms. Reema Jaiswal**
  "Development and validation of stability indicating HPTLC method for simultaneous estimation of metformin hydrochloride and remogliflozin enabonate in pharmaceutical dosage form"
- **Ms. Anne-Sophie Paguet**
  "Study of the diversity of wild hops in French Flanders on the chemical and genetic aspects in the perspective of developing a local hop"
- **Dr Vaibhav Patel**
  "Curative effect of *Macrotyloma uniflorum* seeds in EG induced urolithiasis in rats"
- **Ms. Risfa Samanudeen**
  "Neutralizing effect of different extracts of the whole plant of *Eclipta prostrata* using in vitro methods"
- **Dr Rajni Sharma**
  "*Glycyrrhiza glabra* extract and quercetin reverses cisplatin-resistance in triple-negative MDA-MB-468 breast cancer cells via inhibition of cytochrome P450 1B1 enzyme"
- **Ms. Priyanka Yadav**
  "Investigation of cytotoxic potential of *Crataeva nurvala* against benign prostate hyperplasia"

Flavonoids As Potential Natural Compounds Against COVID-19

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Natural resources are of great importance in human civilization in treating various diseases, including viral infections. Among the natural resources, medicinal plants are stand out with their widespread use and their chemical compounds. Flavonoids are a secondary metabolite group with benzo-γ-pyron skeleton in higher plants. They are responsible for a variety of pharmacological activities such as antioxidant, hepatoprotective, antibacterial, anti-inflammatory, anticancer, and antiviral. Viral infections take a large place in acute infectious diseases. New types of viruses often appear with high incidence and mortality rates as viruses are generally mutated. For the treatment and prevention of epidemic diseases, natural products could be good options thanks to their fewer side effects, wide therapeutic window, and low cost. COVID-19, the new coronavirus disease, first appeared in December 2019 and spread worldwide. This disease caused an international outbreak of acute respiratory disorder and WHO declared that COVID-19 can be characterized as a pandemic. In the current pandemic of COVID-19, specific drug development studies are continuing for disease prevention and treatment. At this point, natural resources draw attention to their potential antiviral activity. In this review, *in vitro*, *in vivo*, and *in silico* studies on flavonoid type compounds and plant extracts containing these constituents will be summarized in terms of their potential in COVID-19.

Possible bioactive substances with antiviral activity (anti SARS-CoV-2) from green cypress *Cupressus sempervirens* L

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The novel coronavirus disease 2019 (COVID-19) pandemic starting from December 2019 has cast unprecedented threat to public health worldwide with over 109.19 million infection cases and 2.4 million death till February 15, 2021, and the case number is still soaring (WHO, 2021). COVID-19 is caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), a member of beta-coronaviruses family. The fight against this virus is becoming a major global public health issue which requires the development of both preventive and curative strategies. Although to date there is no specific drug recommended to prevent or treat the novel coronavirus", traditional herbal medicine approaches, including oral administration of preventative formulas, have always been recommended for prevention and treatment of infectious diseases, even during the current COVID-19 epidemic. Based on previous studies, natural products can be introduced as preventive and therapeutic agents in the fight against coronavirus. In this presentation, we will be interested in this prospering medicine and more particularly in the properties of the green cypress (*Cupressus sempervirens*) extracts rich in bioactive molecules against SARS-CoV-2.

Development of a novel phyto combination for common respiratory ailments

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Common respiratory diseases are the infections caused in any part of the respiratory tract with symptoms such as cough, fever, cold, etc. and in more severe cases difficulty in breathing. A novel combination of herbal drug sis formulated in form of mouth dissolving tablet for above mentioned use. Molecular docking approach was employed for selection of active ingredients. Herbal drugs opted for the study has bronchodilatory effect and they also boost immune system, facilitating prevention of major symptom of the disease in due course of time. This phytomedicine targets all the areas of which are prone to get infection. It is an herbal formulation so no toxicity and side effects would occur. Since drug will get absorbed from mouth/ buccal mucosa reduction in first pass metabolism in liver. We may get rapid and more drug release, therefore rapid onset of drug action. As we can arrest the entry of the virus from the mouth and the first pass metabolism is also bypassed. These mouth dissolving tablets were analysed for various parameters such as hardness, friability, weight variation, wetting test, disintegration time and uniformity of content. Optimized formulation was also evaluated by accelerated stability study. Developed combination possessed good physicomechanical properties and disintegration time. Phytochemical assays were performed and the formulation significantly passed all the limits. It was also found stable under elevated stress conditions. This phyto combination may work as a frontline barrier against the entry of the infectious organism like a ray of boon in the dark.

An effervescent tablet preparation from herbs with docking study against COVID-19

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As there is need of immunity potentiation against COVID-19 infection, many poly herbal formulas are coming up with preventive way of dealing with such immunity impairing virus. Recent studies of computational research on phyto-constituents by in-silico analysis against SARS CoV2 test system is a very helpful tool for judging post infection therapy potential of well-known medicinal plants. Taking this tool to select such plants and design an appropriate formulation for the same is approach of this research. Four Indian traditional plants were selected having phytoconstituents like rutin, epigenin, leuteolin, oleanolic acid, piperine etc. and were studied for docking on the target proteins [5RGJ, 6WLC, 7BVL, 6W6Y, 6LZG etc] of SARS CoV 1 and 2 using Auto Dock VINA software. A herbal effervescent tablet was prepared using the plant extracts by direct compression method and evaluated for quality and stability. The optimized and assessed formulation could be very convenient and effective formulation for adjuvant therapy of Corona virus infection.

Juncus acutus, a potential remedy for coronaviruses

Asma Hakem[1]*, Lowiese Desmarets[2], Ramla Sahli[3], Rawen Ben Malek[1], Nathan François[2], Gabriel Lefèvre[1], Jennifer Samaillie[1], Sophie Moureu[1], Jean Dubuisson[2], Sandrine Belouzard[2], Sevser Sahpaz[1], Riadh Ksouri[3], Karin Séron[3] and Céline Rivière[1]*

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Research for therapeutic solutions against coronaviruses, in particular against the new emerging SARS-CoV-2, is a challenging task to different healthcare actors and to the scientific community. At the beginning of COVID-19 pandemic crisis, the repositioning of marketed drugs (remdesivir, umifenovir, hydroxychloroquine...) were deployed but until now results are not satisfactory. Fortunately, a number of vaccines have been developed over a very short period of time and are very effective against the original strain of SARS-CoV-2. However, the search for new antiviral efficient treatments remains a major challenge. One of the strategies of research focuses on the identification of natural substances from plants. Our previous study has demonstrated the antiviral potential of phenanthrenes produced by *Juncus* species. In particular, we demonstrated that dehydrojuncusol isolated from *Juncus maritimus* was an inhibitor of hepatitis C virus replication. In this context, we explored the antiviral potential of several *Juncus* species against two coronaviruses: HCoV-229-E and SARS-CoV-2. Antiviral activity against HCoV-229E was observed for ethyl acetate and aqueous sub-extracts of several *Juncus*. During the presentation, purification steps will be displayed only for the selected plant: *Juncus acutus*.

A review on possible treatment of symptoms of COVID-19 by *Justicia adhatoda* (Vasaka Leaf)

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COVID-19, caused by novel corona virus (SARS CoV 2) is now a pandemic and global outbreak. No specific treatment is available till date, except few vaccines are on trials. So, treatments are being done on the symptomatic basis – several antimicrobial agents and antipyretic drugs are used for the treatment of COVID positive patients. *Adhatoda vasaka* (Vasaka) belonging to the family “Acanthaceae” is a plant used in the indigenous system of medicine and a potent expectorant and antitussive agent in the Ayurvedic and Unani medicine. For immediate application of the treatment of COVID-19 positive patients, in which few common drug-molecules are tested as protease inhibitor and replicase inhibitor of COVID-19 virus. It is observed that anisotine and vasicoline of Justicia adhatoda are very good inhibitors. Extracts of various parts of the plants such as bark, root, leaf, flower, fruit and many a times, the whole plants are used in the management of pain, inflammation, asthma, cold, cough, diabetes, bronchitis, diarrhoea, dysentery and other upper respiratory diseases and it is also used to heal wounds. In asthma and acute stages of bronchitis, the extract of Vasaka offers an amazing result by decreasing the thickness of the sputum. According to the present day studies the alkaloids such as vasicinone, vasicine, and oxyvasicine which are present in *A. vasica* are responsible for most of the activities. But extensive studies need to be conducted to understand the constituent responsible for the treatment of symptoms of Covid 19 activity.

Development and validation of stability indicating HPTLC method for simultaneous estimation of metformin hydrochloride and remogliflozin enabonate in pharmaceutical dosage form

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A novel and quick HPTLC-densitometric method was developed for the simultaneous determination of Metformin Hydrochloride and Remogliflozin Enabonate. Chromatographic separation of the drugs was performed on precoated silica gel aluminium plate 60F254, (20×10) 100µm thickness; using Methanol: Ethyl Acetate: Acetic Acid (6:3.5:0.5v/v) as mobile phase. A TLC scanner set at 245 nm was used. The two drugs were satisfactorily resolved with Rf values Rf 0.23 for MET and Rf 0.83 for REMO respectively. Calibration curves were polynomial in the range concentration range of 200-1200ng/band for Remogliflozin Enabonate and 1000-6000ng/band for Metformin Hydrochloride. Correlation coefficients (r) values were 0.9999, 0.999 for Metformin Hydrochloride and Remogliflozine Enabonate respectively. A low relative standard deviation (< 2%) was found for both precision and robustness study showing that the proposed method was precise and robust. The method had an accuracy of 98.82%, 98.42% of Metformine Hydrochloride and Remogliflozin Enabonate were validated according to ICH guidelines. The percentage recovery ranges from 98-101%. Forced degradation conditions of hydrolysis (neutral, acidic and alkaline), oxidation, photolysis and thermal stress, as suggested in the ICH guideline Q1A (R2).

Study of the diversity of wild hops in French Flanders on the chemical and genetic aspects in the perspective of developing a local hop

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French Flanders is a historical region for beer production and for hop cultivation. Female cones are used in brewery for their bitterness and their flavours, as well as for their antimicrobial properties. Because of several factors, this local production is declining since the middle of the XXè century. However, in recent years, a new dynamism is observed partly explained by a renewed interest in aromatic and craft beers. As a result, microbreweries are widely developing, using local and sustainable ingredients. To answer to this consumption shift, hops production is adapting. Especially hop growers are looking for hops suitable to local terroir, with good yields but above all, good chemical qualities for brewery. In addition, due to their chemical composition, hops have interesting biological properties, including oestrogenic, sedative, antimicrobial, antiproliferative and anti-inflammatory ones. In particular, hops produce prenylated chalcones including xanthohumol and desmethylxanthohumol as well as acylpholoroglucinol derivatives with alpha and beta acids. The bitterness searched by brewers is due to alpha acids, whereas flavours come from volatile compounds.

In this context of varietal research, we are exploring the chemical and genetic diversity among fifty wild hops collected in September 2019 on several natural sites of the North of France. These fifty wild hops are going to be mapped and compared with ten commercial varieties and three old varieties. Genetic analysis are focused on the study of microsatellites regions; the phytochemical characterization of hops is based on the quantification of their major secondary metabolites: prenylated phenolic compounds (xanthohumol and bitter acids) by UHPLC-UV and volatile compounds by GC-MS. Non targeted metabolomics analysis are also carry out to identify wild hops with an original chemotype which may interested in brewers. These analyses will be filled by morphological characterization of studied hops and their organoleptic qualities. Multivariate data will be correlated by principal component analysis. This talk will especially present the first outcomes of the chemical characterisation of collected hops. Preliminary results show interesting levels of alpha acids in some wild hop comparable to those of commercial varieties.

Curative effect of *Macrotyloma uniflorum* seeds in EG induced urolithiasis in rats

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Macrotyloma uniflorum Linn. (Fabaceae) seeds are widely used for their diuretic and urolithiatic effects in India. The present study investigated the effect of methanolic of *Macrotyloma uniflorum* seeds (MEMU) on ethylene glycol induced urolithiasis in rats. To induce urolithiasis, 0.75% v/v ethylene glycol was administered orally for 14 days. The curative doses of 400 and 800 mg/kg were administered from 15th to 28th day. On the 28th day, 24 hr urine, serum was collected and various biochemical parameters were estimated in urine, serum and kidney homogenate along with histology of kidney. Co-administration of MEMU with ethylene glycol has significantly ($p<0.001$) increased the urine volume and the level of calculus inhibitors like magnesium, citrate and decreased the level of calculus promoters like calcium, oxalate, uric acid and urea. MEMU supplement also prevented the pathological changes in the kidney and increased the glomerulus activity of the kidney. These results indicate that MEMU showed significant activity in urolithiasis which might be due to its diuretic, calcium oxalate crystal formation inhibitory effects and its ability to increase the levels of inhibitors and decrease the level of promoters of urolithiasis.

Neutralizing effect of different extracts of the whole plant of *Eclipta prostrata* using *in vitro* methods

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Eclipta prostrata (Linn.) is a small, branched annual herb, commonly known as 'Trailing Eclipta' in English, 'Keekirindiya' in Sinhala and 'Karippan' in Tamil. *E. prostrata* is used as a remedy for many ailments in traditional medicine. This study evaluates the neutralizing effects of different extracts of whole plant of *E. prostrata* using *in vitro* methods. The end pH of freshly prepared hexane, dichloromethane, ethyl-acetate, methanol and hot water extracts of *E. prostrata* and their neutralizing effect on artificial gastric acid (AGA) were determined and compared with deionized water and reference drugs (Belcid and Eno). The neutralizing capacity of different concentrations of hot water extract was determined *in vitro* using titration method of Fordtran. A modified model of Vatier's artificial stomach was used to determine the duration of consistent neutralization of AGA by therapeutic dose of hot water extract of *E. prostrata.* All the tests were triplicated and results were analyzed using One-way ANOVA, using SPSS 25.0. End pH<3 was considered to have no neutralizing effect. Hexane, dichloromethane, ethyl-acetate, methanol extracts were found to have no neutralizing effect. Hot water extract demonstrated a significant ($p<0.001$) neutralizing effect which was comparable with Belcid and Eno and exhibited dose dependent higher neutralizing capacity and a significantly ($p<0.001$) higher duration of consistent neutralization than deionized water. In conclusion, hot water extract of *E. prostrata* exhibited significant neutralizing effect, justifying its use as an antacid remedy in traditional medicine. Further studies using purified constituents of hot water extracts are needed to understand the complete profile of neutralizing effect.

Glycyrrhiza glabra extract and quercetin reverses cisplatin-resistance in triple-negative MDA-MB-468 breast cancer cells via inhibition of cytochrome P450 1B1 enzyme

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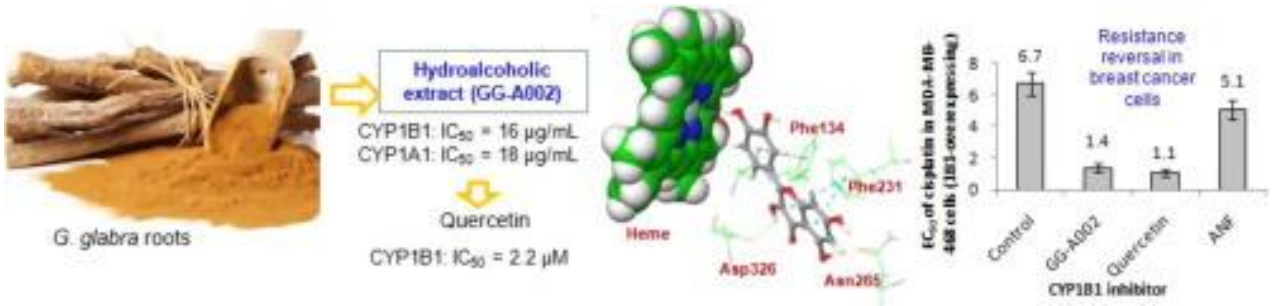
The development of multi-drug resistance to existing anticancer drugs is one of the major challenges in cancer treatment. The over-expression of cytochrome P450 1B1 enzyme has been reported to cause resistance to cisplatin. With an objective to discover cisplatin-resistance reversal agents, herein, we report the evaluation of Glycyrrhiza glabra (licorice) extracts and its twelve chemical constituents for inhibition of CYP1B1 (and CYP1A1) enzyme in Sacchrosomes and live human cells. The hydroalcoholic extract showed potent inhibition of CYP1B1 in both Sacchrosomes as well as in live cells with IC50 values of 21 and 16 µg/mL, respectively. Amongst the total of 12 constituents tested, quercetin and glabrol showed inhibition of CYP1B1 in live cell assay with IC50 values of 2.2 and 15 µM, respectively. Both these natural products were found to be selective inhibitors of CYP1B1 and does not inhibit CYP2 and CYP3 family of enzymes (IC50 > 20 µM). The hydroalcoholic extract of G. glabra and quercetin (4) showed complete reversal of cisplatin resistance in CYP1B1 overexpressing triple negative MDA-MB-468 breast cancer cells. The selective inhibition of CYP1B1 by quercetin and glabrol over CYP2 and CYP3 family of enzymes was studied by molecular modeling studies.



Investigation of cytotoxic potential of *Crataeva nurvala* against benign prostate hyperplasia

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Benign prostate hyperplasia (BPH) is the most common urologic disease in elderly men, encountered by above 40% of 50 years old males. The frequency of BPH might be about 80% when the age reaches to 80 years. It clinically manifests as urinary hesitancy or straining in initiating urination, causing deterioration in urinary function and quality of life. The current treatment available focuses on the symptomatic relief only. Surgical procedure is the only approach for the BPH treatment which is difficult, while in some older men surgical procedure is not possible because of which they have to suffer a lot. *Crataeva nurvala* (Family Capparidaceae), commonly known as 'Varuna', is a medium sized deciduous plant indigenous to India. It is a reputed drug for disorders related to kidney, urinary tract and prostate gland. It is used traditionally as a remedy of benign prostate hyperplasia (BPH), but there is no scientific data for its activity on BPH. Hence, the present research work was an attempt to prepare standardized extracts or fractions from *C. nurvala* stem bark that shows significant therapeutic effect in BPH. The cytotoxic activities were evaluated on androgen sensitive human prostate adrenocarcinoma cell line LnCAP, using *in vitro* MTT assay. The study was further followed by isolation of the bioactives using bioactivity-guided approach and their characterization using chromatographic techniques. The combination of standardized extract or isolated bioactives from the plant may lead to formulation of a promising medicament for the management of BPH in near future.