



SCIENTIFIC PROGRAM

Scholars International Webinar on

# ADVANCES IN DRUG DISCOVERY AND DEVELOPMENT

28-30 March 2022 | Online | Virtual



Host:

**Craig Smith** | Program Manager

Drug Discovery Webinar 2022 | Scholars Conferences Limited

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<https://scholarsconferences.com/drugdiscovery-webinar/>

# PROGRAM

Day 01 | March 28, 2022 | Virtual | 11:00-18:00 GMT

## KEYNOTE FORUM

11:00-11:10 Opening Ceremony



**11:10-11:45**

**Title:** Challenges in designing the clinical trials for new drugs in women  
**Jayashree Joshi**, Kasturba Health Society- Medical Research Centre, India



**11:45-12:20**

**Title:** Cannabinoid receptor 2 agonists on their way to clinics- Cross-Fertilization of industrial drug discovery and academic research  
**Uwe Grether**, F. Hoffmann-La Roche, Switzerland



**12:20-13:55**

**Title:** Importance of the gut microbiota in the drug development process  
**Andres Ursa**, Instituto de Medicina Integrativa, Spain



**12:55-13:30**

**Title:** Building a new future of drug discovery  
**Bruce E Bloom**, Healx Limited, UK

Networking and Refreshments Break @ 13:30-13:40

## SPEAKERS SESSION



**13:40-14:10**

**Title:** Antiproliferative effects of novel benzothiazole-based compounds in pancreatic and paraganglioma cancer cell lines  
**Alessandra Ammazalorso**, G. d'Annunzio University of Chieti-Pescara, Italy



**14:10-14:40**

**Title:** Drug repurposing with artificial intelligence  
**Diba Dindoust**, The Knowledge Society, Canada



**14:40-15:10**

**Title:** Old wine in a new bottle: Drug repurposing of antipsychotic drugs  
**Jyotirmoi Aich**, DY Patil Deemed to Be University, India

# PROGRAM



**15:10-15:40**

**Title:** Optimising the  $\beta$ -lactam parameters using the force field toolkit  
**Ying-Chih Chiang**, The Chinese University of Hong Kong (Shenzhen), China



**15:40-16:10**

**Title:** Drug repositioning for SARS-CoV-2 with tensor decomposition based unsupervised feature extraction  
**Y-h. Taguchi**, Chuo University, Japan



**16:10-16:40**

**Title:** Prodrugs in drug discovery  
**Mohammed Rashwan**, Coventry University, UK



**16:40-17:10**

**Title:** Method Development, Validation, and Concentration Determination of Metformin Hydrochloride and Atorvastatin Calcium Using UV-Visible Spectrophotometry  
**Udaya K Jayasundara**, Institute of Chemistry Ceylon, Sri Lanka



**17:10-17:40**

**Title:** Single gold nano-bipyramid as a spectroscopic platform for sensing, antennas and plasmonic applications  
**J. Laverdant**, Université de Lyon, France

**B2B Meeting and Panel Discussions @ 17:10-18:00**

Day 01 Ends

# PROGRAM

Day 02 | March 29, 2022 | Virtual | 11:00-18:00 GMT

## KEYNOTE FORUM



**11:00-11:35**

**Title:** Potential combos to neutralize SARS CoV 2 Omicron and future variants  
**Haoneng Tang**, Shanghai Jiao Tong University, China



**11:35-12:10**

**Title:** mRNA translation monitoring as a new strategy in drug discovery  
**Iris Alroy**, Anima Biotech, Israel



**12:10-12:45**

**Title:** Background-free Luminescence Bioassay and Imaging Using Long Lifetime Responsive Probes  
**Run Zhang**, The University of Queensland, Australia

**Networking and Refreshments Break @ 12:45-12:55**



**12:55-13:30**

**Title:** Mass-action law pharmacodynamics (MAL-PD) theory/equation/algorithm based general design, analytical computer-simulation for biomedical research techniques and digital/indexed conclusions  
**Ting-Chao (David) Chou**, Memorial Sloan-Kettering Cancer Center & PD Science LLC, USA



**13:30-14:05**

**Title:** Determination of Uranium, Rare Earths, and Radium in Phosphate Rock, and the Problem of Radon  
**Fathi Habashi**, Laval University, Quebec City, Canada

## SPEAKERS SESSION



**14:05-14:35**

**Title:** Using Raman spectra of teeth for human age and gender determination  
**Ozren Gamulin**, University of Zagreb, Croatia

# PROGRAM



**15:55-16:25**

**Title:** Improved efficiency of pomegranate seed oil administrated nasally  
**Tarik EL OUFY**, Sultan Moulay Slimane University, Morocco



**15:05-15:35**

**Title:** The plant-based active ingredients of some homeopathic medicines in the development of therapeutics effective against snakebite envenomation: Bioinformatics approaches  
**Shyamapada Mandal**, University of Gour Banga, India



**15:35-16:05**

**Title:** DNA Nanotechnology for Modulating the Growth and Development of Neurons  
**Mirza Muhammad Faran Ashraf Baig**, The University of Hong Kong, Hong Kong

**Networking and Refreshments Break @ 16:05-16:15**



**16:15-16:45**

**Title:** TBA  
**Manash K Paul**, University of California, USA



**16:45-17:15**

**Title:** TBA  
**Debmalya Sanyal**, India



**17:15-17:45**

**Title:** Will be updated soon  
**Heinz Wilhelm Siesler**, University of Duisburg-Essen, Germany

**B2B Meeting and Panel Discussions @ 17:45-18:00**

Day 02 Ends

# KEYNOTE PRESENTATIONS (DAY 01)

Joint Event on Scholars International Webinar on Advances in

**DRUG DISCOVERY AND  
DEVELOPMENT & ANALYTICAL AND  
BIOANALYTICAL TECHNIQUES**

28-30 March 2022 | Online | Virtual

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Challenges in designing the clinical trials for new drugs in women**

**Jayashree Joshi**

Kasturba Health Society– Medical Research Centre, India

### **Biography:**

Joshi received a post graduate research fellowship to work on 'Vaginal Cytology in Threatened Abortion' which was the topic for her dissertation. She was selected as ICMR research Fellow and worked in Cama & Albbles Hospitals and Wadia Maternity Hospitals. Later she pursued her clinical research interests at National Institute of the ICMR (NIRRH) on pharmacokinetics and drug interactions with hormonal steroids and drugs commonly used in India using different drug delivery systems to obtain a PhD in Biochemistry. She was awarded a WHO Post-doctoral research fellowship in Clinical Pharmacology, Liverpool, UK in 1980. She has designed, conducted and published clinical Phase 1 to 4 clinical trials related to contraceptives, treatment of women's infections and cervical cancer chemoprevention. After her retirement from ICMR as Deputy Director, she joined Bhavan's SPARC and subsequently continued in MRC-KHS. She has investigated the scientific therapeutic use of Ayurvedic medicinal plants in women's health and kinetics of genistein from soya, genital infections, cervical cancer prevention, menorrhagia and menopausal health through ICMR, DBT and CCRAS research grants. She is trained in gynecologic cytology and was the first to draw attention to the relatively high prevalence of Reproductive Tract Infections (RTIs) in women attending family planning clinics, a low risk population, especially Chlamydia trachomatis infection, by using 4 different types of diagnostic tests. She has guided Mumbai University students for MSc in Life Sciences and PhD in Applied Biology. She has conducted rural clinics and surveys in Primary Health Centre, Kaman, Thane District (NIRRH, ICMR) and later in Balsad (Bhavan's SPARC) and Bhivandi (FPAI) and established cervical cancer screening programmes for underprivileged women. She has more than 115 national and international publications to her credit including 6 chapters and citations in international text books.

### **Abstract:**

Women form 50% of the world population & work force, and therefore in designing clinical trials for new drugs in any population, it is essential to pay attention to certain finer details in the protocols when women are enrolled as patients or participants in drug trials. Additionally the woman and the offspring may face major consequences if she happens to conceive during the trial of a potentially teratogenic drug. Then this concerns 100% of the population because future generations are concerned. From our experience in clinical research on hormonal and nonhormonal contraceptives, drug interactions, vaginal microbicides, antimenorrhagic drugs, menopausal syndrome, Reproductive Tract Infections (RTIs), and standardized plant extracts, we will be highlighting some of the challenges that we had to resolve during clinical trials for women. Recent literature has revealed and highlighted the differences in the drug response in men and women, the need for increasing participation of women in early clinical trials and the risks in pregnant and lactating women. We will briefly review these aspects. In this presentation we also wish to highlight some of the neglected areas in designing the clinical trial protocols and case record forms for women. These can vitiate interpretations on safety and efficacy of Investigational Products (IPs) in women. We recommend that these should be considered in all new drug trials involving women. Individualization of therapy necessitates the consideration of timing of investigations, drugs, and surgical interventions in relation to the menstrual cycle or the physiological phase Eg. prepuberty, pregnancy, lactation, menopause.

Reasons for discontinuation from a clinical trial need to be probed with sensitivity. The importance of a good health educator and a follow up team cannot be overemphasized.

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Cannabinoid receptor 2 agonists on their way to clinics- Cross-Fertilization of industrial drug discovery and academic research**

**Uwe Grether**

F. Hoffmann-La Roche, Switzerland

### **Biography:**

Uwe M. Grether, Expert Scientist, Medicinal Chemistry, F. Hoffmann-La Roche, Ltd. Basel, Switzerland. Uwe received his Ph.D. in chemistry under the direction of Prof. Herbert Waldmann from the University of Karlsruhe in 2000. From 2000-2001 he carried out postdoctoral work in the laboratory of Prof. James D. White at the Oregon State University, Corvallis, OR. In 2001, Uwe joined the Medicinal Chemistry section of F. Hoffmann-La Roche, Ltd. Basel, Switzerland as a research chemist. Over the years he has contributed to a number of drug discovery programs for the treatment of metabolic, cardiovascular, kidney, neuroscience, ophthalmic and inflammatory diseases. Uwe worked as team member and project leader covering both early and late stage research and reaching advanced stages up to phase 3 clinical trials. He is co-author of more than 130 patents, research publications and book chapters.

### **Abstract:**

The type 2 cannabinoid receptor (CB2R) plays an important role in cell migration and immunosuppression and is therefore a promising GPCR drug target for the treatment of tissue injury and inflammation including kidney diseases. During the evolution of Roche's CB2R agonist drug discovery program several challenging scientific questions appeared which could efficiently be addressed by teaming up with academic partners, leading to mutually rewarding collaborations. The presentation will highlight some of them and will illustrate different snapshots of Roche's CB2R program. Both, early aspects such as target validation and hit generation as well as advanced stages including lead optimization and in depth in vitro and in vivo pharmacology profiles of advanced molecules will be covered. In addition, the generation and application of novel CB2R probes will be presented, to illustrate the importance of chemical probes at all stages of drug discovery programs starting from receptor localisation and trafficking studies toward biomarker applications.



# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Importance of the gut microbiota in the drug development process**

**Andres Ursa**

Instituto de Medicina Integrativa, Spain

### **Biography:**

Andrés J. Ursa Herguedas is the Director of the Naturist Clinic and Institute of Integrative Medicine in Valladolid. Teaching official of the Junta de Castilla y León. Care, teaching and research activity. Graduated in Medicine and Surgery from the University of Valladolid in 1983. Rotating services in Gastroenterology, Pulmonology, Traumatology, Obstetrics and Gynecology and Rehabilitation at the Hospital Clínico Universitario de Valladolid. Internal medicine at the Dr. Villacián de Valladolid Assistance Center (former Psychiatric Hospital. Military service with performance in transmissions (for being an electronics technician) and as a doctor in Villanubla (Valladolid). Higher Technician in Acupuncture (1983-85). Naturist Clinician 1985, which I combined with work in Primary Health Care (rural medicine, pediatrics, emergencies). Teaching in private and public health sciences (interim health area of the Junta de Castilla y León). Doctor of Medicine and Surgery "cum laude" from the Complutense University of Madrid in 1992. President of the Spanish-Leonese Society of Acupuncturists, Homeopaths and Naturists, based at the Valladolid College of Physicians, from 1995 to 2014, with the performance of 14 scientific events (seminars, congresses, courses, conferences, etc. ) at the University of Valladolid, College of Physicians of Valladolid, Balneario Palacio de las Salinas in Medina del Campo (Valladolid), etc., with the participation of professors and professors from the University of Valladolid and foreign universities. Accredited courses in Primary Health Care, Gerontology, Advanced CPR, Electrocardiography, Digestive System, Pulmonology, etc. University of Zaragoza: Naturopathic Medicine (1996-98). University of Valladolid: University Specialist in Homeopathy (1994-96). University of Barcelona: Master in Phytotherapy (2007-2009). Spanish Association of Naturopathic Physicians (AEMN): several years on the board of directors. I have given more than 15 lectures to date, in the respective congresses, in various medical colleges and universities in Spain. Spanish Society of Homeopathic Medicine. European Society of Classical Naturopathic Medicine. Teaching official of the health area, specializing in health processes , of the Junta de Castilla y León, being the number one in the opposition. In 2010 he created the Institute of Integrative Medicine , as a teaching activity attached to the clinic, in Valladolid, in order to channel the teaching of Health Sciences. Doctor at the Palacio de Las Salinas Spa , in Medina del Campo (Valladolid) from 2007 to 2013. About 30 publications in national and foreign scientific journals, with research topics, history of medicine, prevention, therapy, medical hydrology, hydrotherapy, geotherapy, heliotherapy, mind-body medicine, environmental medicine, ecology and environment. Editor of Mednaturis, dictionary of concepts in naturopathic medicine, offered by the AEMN website for free. AEMN award in the 1995 edition for the work: "Influence of the medical act on the evolution and progression of diseases".

### **Abstract:**

Since the Human Microbiome project started in the first decade of this century, there have been many discoveries that have been revealed thanks to current technology. Not without reason is the intestinal microbiota (IM) considered an organ with digestive, metabolic, immunological, endocrine, psychoneurological, and purifying functions. These functions are achieved if there is eubiosis, with a good ratio between different species of bacteria and microbial diversity. Due to these properties, IM has been taken into account for years in drug development. Because commonly used drugs are potentiated, degraded or altered by IM, more time and financial resources should be allocated to expand the information on each active ingredient in this regard in order to increase the efficacy and safety of these drugs.

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Building a new future of drug discovery**

**Bruce E Bloom**  
Healx Limited, UK

### **Biography:**

Bruce Bloom is Chief Collaboration Officer of Healx, a Cambridge UK biotech using AI and drug redevelopment to create novel therapies for rare disease patients. He founded and lead the global charity Cures Within Reach that brought over a dozen redeveloped drug therapies to patients through proof-of-concept clinical trials, and developed CureAccelerator®, the online drug redevelopment collaboration marketplace. Dr. Bloom is an Ashoka Social Entrepreneur Fellow, the Patient Advisory Board Chair for the Institute for Translational Medicine, Board member of the Rare Disease Company Coalition, member of the Vanderbilt Institute for Clinical and Translational Research External Advisory Board, Executive Board member of Mission: Cure, and is on the Science Advisory Boards of the Dr. Ralph and Marian Falk Medical Research Trust Awards Programs, the Findacure Fundamental Disease Charity, the Rare Disease Research Hub of the Westchester Biotech Project, ReBootRx, and the editorial board of ASSAY and Drug Development Technologies.

### **Abstract:**

The traditional drug discovery model is not working as well as it could. It is lengthy, expensive and risky - with the chances of achieving a successful treatment woefully low. Due to this, pharmaceutical companies tend to focus on blockbuster drugs aimed at large disease populations that can help recoup the costs of development for not only the successes but also the many, many failures. This approach often leaves smaller patient populations out of scope and out of reach of treatments that could potentially improve their lives. Technology and a new focus on the patient voice can augment the current industry paradigm and drive the discovery of new treatments for rare diseases - 95% of which shockingly do not have an approved treatment. This talk will discuss three aspects of this paradigm change, 1) Reduce risk and complexity with Artificial Intelligence tools, 2) Speed up the process with by starting with drugs, nutraceuticals and human safe shelved compounds, and 3) Embed the patient voice throughout the drug discovery process.



# SCIENTIFIC SESSIONS (DAY 01)

Joint Event on Scholars International Webinar on Advances in

**DRUG DISCOVERY AND  
DEVELOPMENT & ANALYTICAL AND  
BIOANALYTICAL TECHNIQUES**

28-30 March 2022 | Online | Virtual

# Featured Speaker

## Drug Discovery Webinar 2022



### **Title: Antiproliferative effects of novel benzothiazole-based compounds in pancreatic and paraganglioma cancer cell lines**

**Alessandra Ammazalorso**

G. d'Annunzio University of Chieti-Pescara, Italy

#### **Biography:**

Alessandra Ammazalorso obtained her PhD in Pharmaceutical Sciences from the University of Chieti (Italy) in 2001. Since 2004 she is Assistant Professor at Pharmacy Department of University of Chieti. Her research interests include the design, synthesis and biological evaluation of novel small molecules, mainly compounds targeting Peroxisome Proliferator-Activated Receptors, aromatase and nitric oxide synthase.

#### **Abstract:**

For their multiple biological activities, benzothiazoles represent privileged scaffolds in medicinal chemistry, useful in drug discovery programs to modulate biological activities of lead compounds. A large body of knowledge about benzothiazoles has been reported in scientific literature, describing their antimicrobial, anticonvulsant, neuroprotective, anti-inflammatory, and antiproliferative effects. Recently, we reported the identification of N-acylsulfonamides containing a benzothiazole scaffold able to antagonize the effect of the PPAR $\alpha$  agonist GW7647 at low micromolar concentration. Notably, some of them significantly reduced viability in pancreatic and colorectal cancer cells. Starting from these results, we synthesized novel derivatives by modifying the structure of the previously reported sulfonimide derivative AA452. In the new series of compounds, the Nacylsulfonamide group was replaced by a secondary amide, substituted by alkylic, aromatic, or arylalkylic residues. These novel compounds did not retain a remarkable activity as PPAR $\alpha$  antagonists, but they induced significant antiproliferative effects in three pancreatic cancer cell lines, and in two in vitro models of paraganglioma, PTJ64i and PTJ86i. Structure-activity relationship studies were carried out, identifying the major structural requirements ensuring a good antiproliferative effect. Computational studies are also ongoing to identify putative targets responsible for the antiproliferative effects of this class of benzothiazole derivatives.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Drug repurposing with artificial intelligence**

**Diba Dindoust**

The Knowledge Society, Canada

### **Biography:**

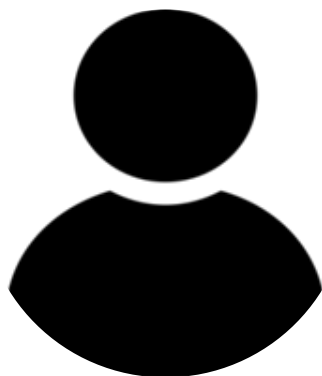
Diba Dindoust is a 17-year-old innovator and visionary who is excited about building the future of biotechnology. She has built projects in the fields of gene editing, synthetic biology and computational drug discovery. Her work has been showcased on IBM's CASCON x Evoke and the TEDx stage. While attending high school, she enjoys publishing STEM-related articles on her Medium blog and Youtube channel, as well as working on her newly-released podcast Biotech Mafia alongside other young innovators to discuss the future of biotechnology.

### **Abstract:**

An overview of the current state of drug repurposing and how artificial intelligence (AI) is applied as a tool. One cost-effective way of finding therapies for diseases is the repurposing of approved or investigational drugs for new targets. Examples of repurposed drugs are remdesivir for COVID-19 and thalidomide for multiple myeloma. The cost of drug repurposing is lower than de novo drug discovery because repurposing does not require preclinical testing if there is dose compatibility between the original and new targets. AI has been applied in drug repurposing in the processes of target and leads identification to reduce the rate of failure in human trials. AI had been used to identify multiple repurposed drugs for COVID-19 other than remdesivir. AI models that have been employed are deep learning models and classifiers alongside molecular docking. In my project, I looked at repurposing drugs with lower costing APIs for HIV with the goal of reducing the cost of local production of antiretroviral therapy in African countries. My prototype identified glyburide - a diabetes drug - as a potential candidate for HIV from a small sample group.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Old wine in a new bottle: Drug repurposing of antipsychotic drugs**

**Jyotirmoi Aich**

DY Patil Deemed to Be University, India

### **Abstract:**

Cancer is a complex disease affecting millions of people around the world. Breast cancer is one of the most frequently diagnosed cancer and the leading cause of cancer related deaths among women. Despite advances in surgical and radiation therapy, chemotherapy continues to be an important therapeutic option for the treatment of cancer. The current treatment is expensive and has several side effects. Also, over a period of time cancer cells develop resistance to the chemotherapeutic drugs due to which there is a demand for new drugs. Drug repurposing is a novel approach that focuses on finding new applications for the old clinically approved drugs. The process of drug repurposing has been facilitated by current advances in the field of proteomics, genomics and computational biology. Drug Repurposing approach not only provides cheaper, effective and safe drugs with less side effects but also fastens the process of drug development. The aim of the present study is to identify a potential Antipsychotic drug that can be repurposed for the treatment of breast cancer based on the in silico and in vitro studies. A list of Antipsychotic drugs having anticancer potential was obtained through literature survey and by using the ReDO database. Molecular docking studies were performed for all these drugs with the receptors upregulated in breast cancer using AutoDock Vina. Brexpiprazole, an atypical antipsychotic drug, showed high binding affinity towards all the receptors. In vitro cytotoxicity study of Brexpiprazole was performed on the MCF-7 Breast cancer cell line. The IC<sub>50</sub> value for Brexpiprazole was found to be 10.14  $\mu$ M. Significant morphological alterations were observed when MCF-7 cells were treated with different concentrations of Brexpiprazole. Therefore, based on the in silico and in vitro studies it can be concluded that Brexpiprazole is a promising drug candidate for repurposing in breast cancer.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Optimising the  $\beta$ -lactam parameters using the force field toolkit**

**Ying-Chih Chiang**

The Chinese University of Hong Kong (Shenzhen), China

### **Biography:**

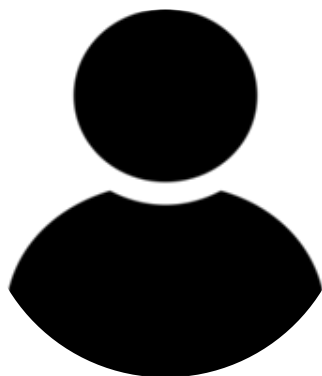
Ying-Chih Chiang graduated from National Taiwan University with a M. Sc. degree in Chemistry in 2006. After two years of work, she obtained a scholarship from International Max-Planck Research School for Quantum Dynamics and joined the Theoretical Chemistry Group in Heidelberg, Germany, under the supervision of Prof. L. S. Cederbaum. One year after obtaining her Ph. D. in 2012, she joined Prof. Y. Wang's biophysics group in The Chinese University of Hong Kong. Since 2018 she joined Prof. J. W. Essex's group in Southampton University as a Newton International Fellow. Starting from 2020 March she became an assistant professor at the Chinese University of Hong Kong – Shenzhen. Her research interests focus on using MD simulations and free energy calculations to reveal the resistance mechanism of antibiotics.

### **Abstract:**

Benefiting from the development of highly accurate force fields and the increase of computational power, molecular dynamics (MD) simulations are now frequently used in drug design. Often used all atom force fields include CHARMM, Amber, and OPLS-AA. However, while the associated ligand force fields such as CGenFF and GAFF are provided, accurate ligand force field parameters are not always readily available for drug molecules, and the users must optimise these parameters prior to the MD simulations. We examined the parameters of  $\beta$ -lactam antibiotics, and discovered that the parameters of their core structures are labeled with high penalties by ParamChem, a web server that automatically generates CHARMM compatible parameters (CGenFF) for molecules. Therefore, a thorough optimization is needed. We performed this force field parameter optimisation for various  $\beta$ -lactams using the Force Field Toolkit (FFTK) and Gaussian calculations. Two problems that users are likely to encounter when optimising other drug molecules are identified. First, inappropriate CGenFF parameters without penalty prediction could cause a difficulty in optimisation. Second, multiple dihedral parameter sets may produce the same molecular mechanics (MM) potentials of similar quality, raising the question on how to choose the right parameter set as the best solution. A systematic protocol incorporating molecular dynamics simulations and a principle for selecting the dihedral phase shifts are introduced. Using this protocol, we then successfully optimised both neutral and anionic forms of penam and of cephem. Our results highlight the importance of selecting proper phase shifts during the dihedral optimisation, and the protocol proposed in this work is beneficial to other users.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Drug repositioning for SARS-CoV-2 with tensor decomposition based unsupervised feature extraction**

**Y-h. Taguchi**

Chuo University, Japan

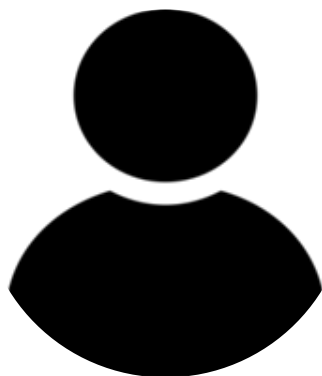
### **Abstract:**

In order to develop effective drug for SARS-CoV-2, various kind of attempts were performed. Among them, drug repositioning is one of effective ways, since known drug can be used for SARS-CoV-2 without considering other factors, e.g., side effects. We have applied recently proposed tensor decomposition based unsupervised feature extraction to gene expression profiles of cell lines infected by SARS-CoV-2. Identified genes are coincident with known human genes supposed to interact with SARS-CoV-2 proteins. Drugs targeting these genes include many know anti-virus drugs that are supposed to be effective to SARS-CoV-2.



# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Prodrugs in drug discovery**

**Mohammed Rashwan**  
Coventry University, UK

### **Biography:**

Mohammed Rashwan is awarded an MSc in Pharmacology and Drug Discovery with distinction from Coventry university. In both my bachelor and masters, I have focused on the potential chemopreventive properties of three different subclasses of flavonoids on breast cancer cell lines. My humble time (10 weeks between both degrees) in research have taught me how to utilize different assays to determine the potential of the chemical to inhibit cancer development & progression. I plan on going into research and working closely in drug discovery.

### **Abstract:**

In the past, prodrugs were considered a last resort strategy to improve the available therapies at the time. Prodrugs are now an essential aspect considered at drug research and development initiation stages. 10% of the drugs available on the market are prodrugs. Around 15% of all newly FDA approved drugs in the last decade were prodrugs, becoming a potentially effective solution to over physicochemical hurdles. The insight into prodrugs shows a promising glimpse of the drug development pipeline. Prodrugs are bioreversible, inactive derivatives that enhance a parent drug's biopharmaceutic, pharmacodynamic or pharmacokinetic profile. Although prodrugs are a new chemical entity, they are still favourable to novel drugs. They require less financial backing, cutting down on time consumed and overall efforts on the project. Here, we will discuss the different strategies employed to design a favourable drug, investigating different examples of prodrugs and their pharmaceutical properties & challenges that need to be considered.

# Featured Speaker

## Drug Discovery Webinar 2022



### Title: Method Development, Validation, and Concentration Determination of Metformin Hydrochloride and Atorvastatin Calcium Using UV-Visible Spectrophotometry

**Udaya K Jayasundara**

Institute of Chemistry Ceylon, Sri Lanka

#### Biography:

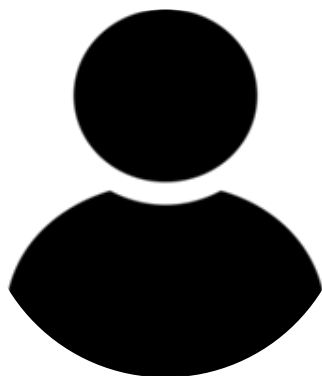
Udaya K Jayasundara received his BSc Honours degree in Chemistry from the University of Peradeniya Sri Lanka in 2004 and Ph.D. in Chemistry from the University of Nevada Reno USA in 2011. He conducted his doctoral research based on molecular dynamics where he was involved in laser and molecular spectroscopic studies. After graduating, he worked as an adjunct instructor in a community college and as a scientist in a contract research organization in the USA. Currently, he is working as a senior lecturer in chemistry and as a laboratory safety consultant where he delivers lectures and provide consultancy to upgrade the quality of laboratory workers. He has published several peer-reviewed articles in photochemistry, laboratory safety, wastewater treatment, development and validations of analytical methods, and oxalate content in vegetables and fruit items. He has received professional training in areas related to chemical management and chemical safety. He is a member of several scientific forums such as American Chemical Society and Division of Chemical Health and Safety.

#### Abstract:

The usage of pharmaceutical products has been significantly increased since the beginning of 2020 due to the prevailing situation in the world. Hence, the drug manufacturers are engaged in large-scale production to meet the demand and it is essential to have simple but fast analytical procedures to determine the active pharmaceutical ingredient (API) concentrations in those drug substances before reaching patients. The goal of this study is to develop simple but accurate and fast analytical methods to determine the API concentrations of metformin hydrochloride (MH) and atorvastatin calcium (AC) using simple ultraviolet-visible spectroscopy (UV-Vis). The wavelengths with maximum absorbance ( $\lambda_{max}$ ) for MH and AC were determined and methods were developed according to the International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH) guidelines and validated using the acceptance criteria of main validation parameters. Five-point calibration curves were obtained within a concentration range of 2-10 ppm ( $R^2 \geq 0.999$ ) for MH and 5-15 ppm range ( $R^2 \geq 0.998$ ) for AC. The accuracy was tested with the spike recovery method which showed the mean recoveries ranged from 92.14% to 95.04% for MH and 90.10% to 102.90% for AC, respectively. The sample analysis demonstrated that API of MH ranged from 382.70 to 454.19 mg per 500 mg tablet while 9.00 to 9.88 mg per 10 mg tablet for AC. The study demonstrated that the working curves had stabilities at room temperature and refrigerated conditions for up to seven days. Therefore, sample analysis can be conducted for seven days without additional standard preparations which could be beneficial for the industrialists as it is a cost-effective process.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Single gold nano-bipyramid as a spectroscopic platform for sensing, antennas and plasmonic applications**

**J Laverdant**

Université de Lyon, France

### **Biography:**

Udaya K Jayasundara received his BSc Honours degree in Chemistry from the University of Peradeniya Sri Lanka in 2004 and Ph.D. in Chemistry from the University of Nevada Reno USA in 2011. He conducted his doctoral research based on molecular dynamics where he was involved in laser and molecular spectroscopic studies. After graduating, he worked as an adjunct instructor in a community college and as a scientist in a contract research organization in the USA. Currently, he is working as a senior lecturer in chemistry and as a laboratory safety consultant where he delivers lectures and provide consultancy to upgrade the quality of laboratory workers. He has published several peer-reviewed articles in photochemistry, laboratory safety, wastewater treatment, development and validations of analytical methods, and oxalate content in vegetables and fruit items. He has received professional training in areas related to chemical management and chemical safety. He is a member of several scientific forums such as American Chemical Society and Division of Chemical Health and Safety.

### **Abstract:**

Metallic nanostructures based on noble metals have attracted many researches due to the existence of surface plasmon resonances. These resonances appear at the interface between the metal and the surrounding dielectric. Due to the high sensitivity to the local environment, surface plasmons show enormous potential as sensors and miniaturized photonic components. In this presentation, we will present the case of gold nano-bipyramids (AuBP) that possess sharp tips. These elongated nanoparticles are very promising as a platform for many applications due a strong plasmon resonance. Different optical experiments have been performed on AuBP at the single level. To demonstrate sensing applications, AuBP have been deposited on a silanized glass substrate. This enable a robust and stable system to study the evolution of the AuBP resonance with different refractive indices with storage over many months. Furthermore, AuBPs may also act as oriented nanoantennas. Their orientations have been investigated using polarimetric analysis of their scattering.

Different perspectives will be presented such as the utilization of AuBPs to interact and launch surface plasmon waves on a gold mirror.



# KEYNOTE PRESENTATIONS (DAY 02)

Joint Event on Scholars International Webinar on Advances in

**DRUG DISCOVERY AND  
DEVELOPMENT & ANALYTICAL AND  
BIOANALYTICAL TECHNIQUES**

28-30 March 2022 | Online | Virtual

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Potential combos to neutralize SARS CoV 2 Omicron and future variants**

**Haoneng Tang**

Shanghai Jiao Tong University, China

### **Biography:**

I have participated in drug discovery program “Developing SARS-CoV-2 Neutralizing Antibody from Convalescent Patients B Cells” since the outbreak of COVID-19. We have discovered and developed a broad ultra-potent neutralizing antibody 2G1 (published in Cell Discovery DOI: <https://doi.org/10.1038/s41421-022-00381-7>), and now this antibody 2G1 have been approved for clinical trial by National Medical Products Administration (NMPA).

### **Abstract:**

**Background:** Objective s and Goals Immune evasion has become a major problem due to the emerging circulating SARS CoV 2 variants like Omicron. Efforts are being made in developing combination strategies to mitigate this issue.

**Methods:** Here we comprehensively evaluated combinations of ACE2 Fc and neutralizing antibodies (NABs) that target diverse epitopes on the SARS CoV 2 spike receptor binding domain.

**Expected Results/ Conclusion / Contribution:** NAb+ACE2 Fc combinations efficiently neutralized HIV based pseudovirus carrying the spike protein of the Delta or Omicron variants. Then using a replication competent VSV SARS CoV 2 S virus that we established we found NABs without combo with ACE2 Fc were escaped by this virus within six passages. But all the NAb+ACE2 Fc combinations had no escape after fifteen passages, revealing a great potential to neutralize future variants. These findings provided important implications for future strategy design to combat the emerging SARS CoV 2 variants including Omicron and future variants. Different perspectives will be presented such as the utilization of AuBPs to interact and launch surface plasmon waves on a gold mirror.

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: mRNA translation monitoring as a new strategy in drug discovery**

**Iris Alroy**  
Anima Biotech, Israel

### Biography:

Iris Alroy has broad background and more than 20 years of experience in small molecule drug discovery, preclinical development, and development of IND-enabling studies. Dr. Alroy was VP of Discovery at Proteologics, where she established several research programs for the identification of small molecules inhibiting the activity of E3 ubiquitin ligases in HIV-1 and Cancer. Subsequently, she was VP R&D at Pharmos Corp., in which she managed organic and medicinal chemistry, biology and pharmacology groups. Under her guidance efficacy animal models were set up, validated and used for testing lead molecules in pain and inflammation up to Phase I study in inflammatory pain.

Dr. Alroy was entrepreneur and CEO of startup biotech companies, Fusimab, Ltd., ProMining Therapeutics Ltd., developing bispecific antibodies and small molecules, respectively. Dr. Alroy successfully managed drug discovery and development projects (e.g. staffing, patent protections, budget), collaborated with researchers in academia and large pharmaceutical companies, and produced peer-reviewed publications.

### Abstract:

mRNA translation is a highly regulated process which can respond to external cues. Once an mRNA is transcribed it is bound by various regulatory proteins which determine its fate. The regulators, RNA binding proteins (RBPs), bind indirectly or directly to the mRNA via cis elements that reside mainly in the UTRs. RBPs are classified to; splicing factors, that determine which exons are to be retained; transport proteins, that determine mRNA localization in the cell; proteins that regulate translation efficiency; and proteins that determine mRNA decay or stabilization

Anima Biotech has developed a mRNA translation monitoring platform, TranslationLight, which uses high content image capture and image and big data analyses, to discover drugs that regulate mRNA translation in a gene, cell and tissue specific manner. Anima has identified drug-like compounds which downregulate Collagen Type I translation in response to external stimuli in activated fibroblasts, specifically in lung fibroblasts. Three structurally different leads have been discovered which regulate collagen-I translation by three distinct modes of action and through different targets – affecting collagen-I mRNA polyadenylation site usage or its ability to be recognized by ribosomes. In Anima's Oncology project, compounds which regulate c-Myc mRNA localization, decay, or polyadenylation site usage, have been identified. In both projects, cell-based activity has been successfully translated to animal models and lead compounds are ready to start preclinical development. In neurobiology, Anima's discovery platform identified compounds which downmodulate the translation of Tau mRNA, showing activity in neuronal cell lines and in iPSC-derived neurons.

# Keynote Speaker

## Drug Discovery Webinar 2022



### Title: Background-free Luminescence Bioassay and Imaging Using Long Lifetime Responsive Probes

**Run Zhang**

The University of Queensland, Australia

#### Biography:

Run Zhang is a Senior Research Fellow and Biosensing and Imaging Team Leader at the Australian Institute for Bioengineering and Nanotechnology, The University of Queensland (AIBN UQ). He received his PhD of Analytical Chemistry from the Dalian University of Technology in 2012. He was a Postdoc Researcher at the Department of Physics and Astronomy in Macquarie University (MQ) in 2012, then a Macquarie University Research Fellow at the Department of Chemistry and Biomolecular Science in 2013-2015. He joined the AIBN UQ in 2016, and here, he was awarded the Australian Research Council Discovery Early Career Researcher Award (ARC DECRA) in 2017 and the National Health and Medical Research Council (NHMRC) Investigator in 2020. His team is working on developing responsive molecules and nanomaterials for bioassay, imaging, early disease diagnosis and treatment.

#### Abstract:

Rapid advances in the chemical and biomedical studies stimulate the design of new bioanalytical probes for precise and accurate sensing and bioimaging of specific disease biomarkers. These analytical probes enable detection and visualization of the physiological and pathological functions of key biomarkers in living cells and organisms, thus contributing to early diagnosis of diseases and monitoring of their treatments. Of various approaches, luminescent molecular-/nano-probes that can specifically detect and visualize biomolecules have been recognized as one of the most promising technologies due to their high sensitivity and selectivity in sensing and high spatiotemporal resolution in bioimaging. Nevertheless, conventional molecule and nanoparticle-based probes for biomarker detection is readily interfered by autofluorescence from complicated biological environments, leading to false positive/negative signals. The high reactivities of disease's reactive biomarkers (such as reactive oxygen/nitrogen species with less than one second lifetime) necessitates the development of new bioanalytical probes for background-free detection these unstable and highly reactive biomarkers in situ. In our research, we found that the optical output signals can be easily modulated to eliminate the autofluorescence signals via three strategies, including anti-Stokes upconversion luminescence, time-gated luminescence, and photoswitchable "double-checked" luminescence. In this presentation, I will introduce our responsive bioanalytical probes for accurate and background-free luminescence detection and imaging of reactive biomarkers in vitro and in vivo.

# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Mass-action law pharmacodynamics (MAL-PD) theory/equation/algorithm based general design, analytical computer-simulation for biomedical research techniques and digital/indexed conclusions**

**Ting-Chao (David) Chou**

Memorial Sloan-Kettering Cancer Center & PD Science LLC, USA

### Biography:

Prof. Ting-Chao Chou, theoretical biologist, pharmacologist and cancer researcher, was born in Taiwan. He received Ph.D. in Pharmacology from Yale University and Post-Doc. at Johns Hopkins University School of Medicine. He was a Member at Memorial Sloan-Kettering Cancer Center (MSKCC) and Professor of Pharmacology at Cornell University Graduate School of Medical Sciences in 1988. He retired from MSKCC in 2013 and established PD Science LLC.

Dr. Chou pioneered the Mass-Action-Law based Pharmacodynamics (PD) General Theory (median-effect equation, algorithm and plot), and the Combination Index (CI) theorem, which quantitatively determine synergy as  $CI < 1$  by computer simulation. His article (1984) introducing the MAL-PD/CI method has 7,371 citations in over 1,420 biomedical journals internationally. Dr. Chou's published 375 papers have garnered over 38,000 citations with an h-index of 74. Currently, he advocates for MAL based quantitative, cost-effective biomedical R&D/Precision Translational Medicine, and PD/BD-based modernization of basic guidelines-and-regulations for new drug evaluations.

### Abstract:

Specific-biomedical R&D techniques such protein assay and DNA sequencing are broadly used internationally. Due to complexity and diversity of biological system, the unified general/basic physical, chemical and mathematical principle of the MAL-PD is need as the largest common-denominator to simplify and integrate the complex bio-systems. This paper shares and illustrates that MAL-PD as indicated by (A) the unified median-effect eq. and plot, (MEE and MEP), which also called Doctrine of the Median, DoM) that provides potency ( $D_m$ ) and shape ( $m$ ) PD-parameters for individual drugs; and by (B) the general combination index equation (CIE), algorithm, and automated computer simulation, where  $CI < 1$ ,  $= 1$ , and  $> 1$  determined synergism, additive-effect, and antagonism, respectively. Since each terms of both MEE and CIE are "relativity ratio" (dimensionless), therefore, the MAL-PD and CI theory/method is regardless of mechanisms, units, and whether the studies are carried out in vitro (molecular, cellular), in animals or in clinical trial protocol design/data analysis, thus bridging basic sciences with clinical studies under the same theory/principle. In addition, MEP linearizes all PD dose-effect curves (DEC), which lead to the "Minimum Two Dose-data Points Theory" (MTDPT) of MAL-PD and CI, which is especially valuable in animal studies and in clinical trials, where dose-range and dose-density are practically limited. Thus MAL-PD/CI provide new paradigm for general principle/method for simple, efficient, cost-effective, computer simulation automation and digital/indexed conclusions. MTDPT indicates that single dose of any drug can not satisfy PD studies (i.e., a single point has no shape), and thus impossible to determine synergism or antagonism. Because of simple, flexible features of MAL-PD/CI theory/method, three articles are highly and broadly cited for (i) Original PD/CI theory (TC Chou & P. Talalay, Adv.Enz.Regul. 22:27-55.1984), (ii) General review (TC Chou, Pharmacol.Rev. 58:621-681.2006) and (iii) Perspectives (TC Chou, Can.Res.70:440-446.2010) with a total of 15,866 citations as of October 20,2021..



# Keynote Speaker

## Drug Discovery Webinar 2022



**Title: Determination of Uranium, Rare Earths, and Radium in Phosphate Rock, and the Problem of Radon**

**Fathi Habashi**

Laval University, Quebec City, Canada

### **Abstract:**

Uranium in solution of phosphoric acid is determined spectroscopically using arsenazo 1 after separation by an anionic exchanger Amberlite IRA 400. After pH adjustment and solvent extraction by tributyl phosphate, rare earths and calcium are precipitated as oxalates. Knowing the amount of calcium by atomic absorption it is possible to calculate the amount of rare earths by difference. Radium was determined in phosphate rock by the emanation method. The problem of radon generated during the treatment of phosphate rock by sulfuric acid to produce fertilizers can be solved by using nitric acid instead of sulfuric acid. In this case, radium which is the source of radon, goes into solution and can be precipitated by a controlled method.



# SCIENTIFIC SESSIONS (DAY 02)

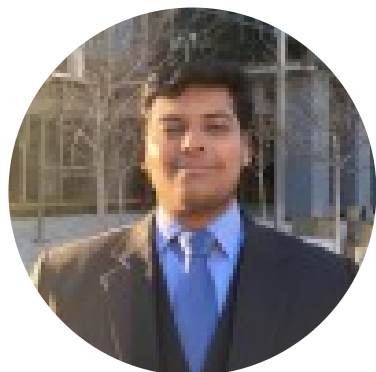
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28-30 March 2022 | Online | Virtual

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Using Raman spectra of teeth for human age and gender determination**

**Ozren Gamulin**  
University of Zagreb, Croatia

### **Biography:**

Ozren Gamulin was born in Zagreb, Croatia. He received his PhD in Solid State Physics from the University of Zagreb, Croatia. He is the author and co-author of more than 70 papers in international journals, conference proceedings and books. More than 50 published papers were cited in Current Contents database. Published papers are in the field of semiconductor physics, biophysics, Raman spectroscopy, Fourier transform infrared spectroscopy and application of data mining and statistics in spectroscopy signal processing. Currently, he is an associate professor and department head of the Department of Physics and Biophysics in the School of Medicine at University of Zagreb.

### **Abstract:**

Raman spectra were recorded from male and female molars and premolars on three distinct sites, tooth apex, crown and neck. The sample of 71 teeth was obtained from donors aged from 11 to 76 years. No particular selection criteria were applied; teeth affected with various pathological processes were deliberately included to simulate a realistic forensic scenario. Recorded spectra were sorted into suitable datasets and initially analyzed. For gender determination first, we apply principal component analysis which showed separation between spectra of male and female teeth. Then, reduced datasets with scores of the first 20 principal components were formed and two classification algorithms, support vector machine and artificial neural networks were applied to form classification models for gender recognition. Obtained results showed that gender recognition with Raman spectra of teeth is possible but strongly depends both on the tooth type and spectrum recording site.

For age determination whole recorded spectra (3500 – 200  $\text{cm}^{-1}$ ) were used for principal component analysis (PCA) and building of the age determination model using PCR. The predictive capabilities of the obtained age determination models varied according to the spectra collection site. Optimal age determination was attained by using Raman spectra collected from the cementum at the root apex ( $R^2$  values of 0.84 and 0.71 for male and female donors, respectively).

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: Improved efficiency of pomegranate seed oil administrated nasally**

**Tarik EL OUFY**

Sultan Moulay Slimane University, Morocco

### **Abstract:**

Clay modified carbon paste electrode (CPE-C) its applicability for electroanalysis of N, N'-ethylene-2,2'-bipyridinium (diquat) has been described in the present work. Electrochemical modification was performed by electronic impedance spectroscopy (EIS) and cyclic voltammetry (CV) in the range of -0.6 V to 1.2 V in 0.1M K<sub>2</sub>SO<sub>4</sub> (pH 3). The voltammetric method behavior of DQ is suggested where an anodic and cathodic peak appeared at E<sub>pa</sub>=0.55 V and E<sub>pc</sub>=0.1 V, successively. These peaks obtained from the reversible redox of DQ at the CPE-C surface. The optimal preconcentration time and percentage of clay insert were 10 minutes and 20% respectively. The proposed method exhibits certainly an electro-catalytic success toward DQ redox. The peaks current recorded using cyclic voltammetry has been linearly dependent on the DQ concentration ranging from 1×10<sup>-5</sup> to 5×10<sup>-5</sup> molL<sup>-1</sup>. The detection limit (DL) calculated for the anodic peak is 5.33×10<sup>-8</sup> molL<sup>-1</sup>. Then relative standard deviation for 2×10<sup>-5</sup> molL<sup>-1</sup> diquat has been 4.3% for nine repetitions. The proposed detector has been successfully applied for DQ electroanalysis in a river water sample with a DL of 8.17×10<sup>-8</sup> molL<sup>-1</sup>. W used B3LYP / 6-311G (d, p) to determine the chemical descriptor, the ionization potential (I), the electron affinity (A), the chemical potential (μ), the chemical hardness (η). Nonlinear optical descriptors (NLO) such as dipole moment (μ), polarizability (α), first hyperpolarizability (β) and second hyperpolarizability (γ), 3D maps of HOMO and LUMO orbitals, lengths and Bond angles of ascorbic acid are also determined by both DFT and MP2 (The Møller-Plesset theory of order 2 perturbation). Both DFT and MP2 methods yielded almost the same value of dipole moment. The DFT and MP2 methods gave slightly different values for polarization, hyperpolarizability and second hyperpolarization because of the number of variables taken into consideration in the calculations by each method. The negative and positive regions of ascorbic acid were determined by molecular electrostatic potential.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: The plant-based active ingredients of some homeopathic medicines in the development of therapeutics effective against snakebite envenomation: Bioinformatics approaches**

**Shyamapada Mandal**  
University of Gour Banga, India

### Biography:

Shyamapada Mandal is Professor and Head of the Department of Zoology, and Dean (Science), University of Gour Banga, India. He is interested on infectious diseases, probiotics, and genomics and bioinformatics research. He did pre-PhD, PhD, and post-PhD research under the guidance of Professor Nishith Kumar Pal at Calcutta School of Tropical Medicine, India. He has published 118 articles with eight book chapters. He is life member of IAMM and IASR, India, and fellow member of SASS, India. Eight national academic and research awards have been conferred to him. He has guided 52 post graduate students; supervised three MPhil and three PhD students, and supervising 6 PhD and one MPhil students. Professor Mandal is among the world's top 2% scientists as per the survey of the Stanford University, published in PLOS (Public Library of Science) Biology (October, 2020). He is featured in the top 2% world scientists list for second consecutive time as published by the Stanford University-Elsevier BV (October, 2021).

### Abstract:

Snakebite envenomation causes several critical, acute as well as chronic, public health problem particularly in rural areas of tropical developing countries, with tens of thousands of deaths. Phospholipase A2 (PLA2) activity of snake venoms are myotoxic or neurotoxic leading to inflammation, and thus, this enzyme (PLA2) has been regarded as an important target of modern drug development for snakebite treatment. The current study aims to determine the inhibition capacity of some plant-based homeopathic active ingredients against PLA2 in in silico systems. Molecular docking study revealed good binding affinity of homeopathic medicine active ingredients (ligands): Andrographis paniculata (Andrographis extract; ANP), alkaloid C, from Gelsemium sempervirens (GLS), melandrin (MLD), hypericin (from Hypericum perforatum; HYP) and cedron to PLA2 (target protein from Daboia russelii pulchella) with binding energy ranging from -9.1 kcal/mol to -6.9 kcal/mol, through different hydrogen bond formation and hydrophobic interactions. The 3-dimensional structures of the ligands, which were obtained from PubChem, obeyed Lipinski's rule of five (RO5) and displayed good bioavailability score (0.55 - 0.56). Compared to the above plicatic acid (Thuja plicata extract; TPE) had lower affinity to PLA2 (binding energy: -6.3 kcal/mol) with low bioavailability score (0.11) and one violation of Lipinski's RO5. Thus, plant-based active ingredients are effective against PLA2, and might be useful in the development of biotherapeutics, alternative and/or complementary to antivenom treatment, for snakebite envenomation.

# Featured Speaker

## Drug Discovery Webinar 2022



**Title: DNA Nanotechnology for Modulating the Growth and Development of Neurons**

**Mirza Muhammad Faran Ashraf Baig**  
The University of Hong Kong, Hong Kong

### Biography:

Mirza Muhammad Faran Ashraf Baig is a registered Pharmacist and currently a post-doctoral fellow at the Faculty of Dentistry, The University of Hong Kong under the supervision of Professor Chengfei Zhang. He received his Doctor of Pharmacy (PharmD) and MPhil (Pharmaceutical Chemistry) degrees from the Faculty of Pharmacy, Bahauddin Zakariya University (BZU), Multan, Pakistan, and a Ph.D. degree from the School of Chemistry and Chemical Engineering, Nanjing University (NJU), China under the supervision of Prof. Dr. Xing-Hua Xia. His research work is about Biomedical Engineering, Mechano-Pharmacology, Polymers, Material Chemistry, DNA Nanotechnology, Developmental Biology, Neuroscience, Nano-Therapeutics, Bio-sensing, Bio-imaging, Diagnostics, Biotechnology, Biophysics, and Biochemistry. His current research focus is designing DNA based novel functional & bio-active nanomaterials to apply in Restorative Dentistry, Oral Microbiology & Oncology, Regenerative Therapeutics, Stem Cells Research, Drug Delivery, and Molecular Pharmaceutics. He published in the top journals e.g Nano Letters (ACS, USA), indexed in Harvard University Library Press.

### Abstract:

Late prenatal growth, early postnatal growth, and layering of the neocortical neurons (NC-Ns) play determining roles in the development of the cerebral cortex (CC). Here, we systematically explore the interactive role of neuronal surface receptors (NSRs) on cytoskeleton activation (CA) and the piconewton (pN) force generation (P-FG) and their influence on the proper development, growth, and functioning of neurons using a designed DNA nanomechanical device (DNA-NMD). This DNA-NMD, functioning as a molecular tension probe (MTP), can be used to selectively bind the different NSRs ( $\beta$ -NGFR, Reelin, and Integrin) to mono-, bi-, and trispecifically activate the receptors on the NC-Ns surface for imaging and calculating the P-FG involved in various processes. Measurements in vivo on the brain of newly born Institute of Cancer Research mice (early postnatal) or in vitro after extracting neurons from the fetal brain of pregnant Institute of Cancer Research mice (late prenatal) reveal that there are augmented interactive roles of the  $\beta$ -NGFR with Integrin and Reelin receptors (RR) on the CA and P-FG, resulting in enhanced directional migration of the neuronal endings (M-NEs), layering, and the somal terminal translocation (S-TT) followed by early postnatal growth.

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