conferenceseries.com

14th World Congress on Medicinal Chemistry and Drug Design

June 10-11, 2019
Edinburgh, Scotland

SCIENTIFIC PROGRAM

DAY 1
Monday, 10th June

08:30-09:00 **Registrations**

09:00-09:30 **Introduction**

09:30-09:50 COFFEE BREAK

09:50-11:50 Meeting Hall 01 **KEYNOTE LECTURES**

11:50-13:10

MEETING HALL 01

Sessions:

- Anti-Infective Agents in Medicinal Chemistry
- Anticancer Agents in Medicinal Chemistry
- Applied Medicinal Chemistry
- Bioorganic Medicinal Chemistry

13:10-13:15 GROUP PHOTO

13:15-14:00 LUNCH BREAK

14:00-16:00

MEETING HALL 01

Sessions:

- Medicinal Biochemistry
- Medicinal Chemical Research
- Medicinal Organic Chemistry
- Advances in Medicinal Chemistry
- Medicinal Chemistry Aspects of Drug Action and Drug Metabolism

16:00-16:20 COFFEE BREAK

MEETING HALL 01 (16:20-17:00)	MEETING HALL 01 (17:00-18:00)
Young Researchers in Medicinal Chemistry and Drug Design	Workshop

DAY 2
Tuesday, 11th June

09:00-10:30 Meeting Hall 01 — **KEYNOTE LECTURES**

10:30-10:50 COFFEE BREAK

MEETING HALL 01

10:50-12:50 **Sessions:**

- Medchem-Antimicrobial And Infectious Agents
- Advanced Medicinal Chemistry
- ADME- Drug Chemistry
- Advanced Trends in Organic Chemistry
- Computer Aided Drug Designing

12:50-13:35 LUNCH BREAK

MEETING HALL 01

13:35-15:55 **Sessions:**

- Chemical Biology
- Diagnostic Medicinal Chemistry
- Medical Devices for Drug Delivery
- Targeted Drug Delivery System-TDDS (Smart Drug Delivery)
- Drug Delivery Chemistry

15:55-16:15 COFFEE BREAK

MEETING HALL 01 (16:15-17:00)	MEETING HALL 01 (17:00-18:00)
Poster Presentations	Workshop

conferenceseries LLC Ltd

14th World Congress on Medicinal Chemistry and Drug Design

June 10-11, 2019 Edinburgh, Scotland

AGENDA

Abstract

Title: Synthesis and Cytotoxicity Evaluation of Novel Amide and Sulfonimide PPAR Antagonists

Alessandra Ammazzalorso

Peroxisome Proliferator-Activated Receptors (PPARs) have been widely studied in the last decades, and they attracted the attention of scientists as promising therapeutic targets. Intensive efforts by researchers produced a wide panel of drugs targeting the three PPAR subtypes (PPAR□, PPAR□, PPAR□) able to modulate important metabolic functions. PPAR activation is involved in several physiologic pathways, as lipid and glucose metabolism, insulin sensitivity, energy homeostasis, and cell differentiation.

Title: Isomers and diastereomers of C-methylated spermidine and spermine

Alex R. Khomutov

The polyamines, spermidine (1,8-diamino-4-azaoctane, Spd) and spermine (1,12- diamino-4,9-diazadodecane, Spm) are ubiquitous organic polycations present in all eukaryotic cells in μM-mM concentrations and involved in the regulation of numerous vital processes including the differentiation and growth of cells1. Disturbances of polyamines metabolism are associated with the development of many diseases, including malignant tumors, decreased immune response, some types of pancreatitis, Snyder-Robinson's syndrome, and even type 2 diabetes1.

Title: Design and synthesis of DapE inhibitors as potential antibiotics with a new mechanism

Daniel P. Becker

There is an urgent need for antibacterial agents with new cellular mechanisms of action, and the bacterial enzyme N-succinyl-L,L-diaminopimelic acid desuccinylase (DapE) offers an excellent target for the eventual development of new antibiotics. DapE is in the succinylase pathway, which is the primary biosynthetic pathway for producing meso-diaminopimelate (m-DAP) and lysine in all Gram-negative and most Gram-positive bacteria, and is not expressed in mammals, making it a very important bacterial enzyme to study.

Title: Diazeniumdiolates as HNO/NO donors: Synthesis and biological activity

Daniela Andrei

Diazeniumdiolate ions, also known as NONOates, are extensively used in biochemical, physiological and pharmacological studies due to their ability to slowly release nitric oxide (NO.) and/or their congeneric nitroxyl (HNO). NONOates of secondary amines have traditionally been used as NO donors and have become the standard for NO donating compounds in chemistry and biology. However, primary amine diazeniumdiolates have been less studied, and essentially IPA/NO and a few alicyclic amine diazeniumdiolates are the only representatives of this class of compounds.

Title: Novel phenyldiazenyl fibrate analogues as PPAR agonists

Letizia Giampietro

Peroxisome Proliferator-Activated Receptors (PPARs) are nuclear hormone receptors expressed especially in metabolically active tissues. Three different isoforms namely PPAR, PPAR and PPAR are identified; they play important roles in lipid and glucose homeostasis. The research of dual PPAR/□ and pan PPAR α/γ/δ agonists could be useful to treat simultaneously dyslipidemia and type 2 diabetes mellitus, reducing side effects of selective PPAR agonists.

Title: Polyamides as multifaceted molecules for medicinal chemistry

James K.Bashkin

We describe the biophysical behavior of polyamides active against human papillomavirus (HPV) types 16, 18, and 31. The MWs of active polyamides are high, and we observed active uptake for human keratinocytes infected with HPV. We have measured binding constants for a group of active anti-HPV compounds on viral DNA, largely but not exclusively in the long control region (LCR). All of our most active polyamides to date contain guanidine and tetramethylguanidine N-termini, in partial mimicry of the natural product netropsin.

Title: Polyamides as multifaceted molecules for medicinal chemistry

James K. Bashkin

We describe polyamides active against human papillomavirus (HPV), vesicular stomatitis virus (VSV), and the ETS superfamily transcription factor PU.1. The MWs of active polyamides range from high to low, and cell uptake by an active mechanism was observed for human keratinocytes infected with HPV. In the case of VSV, X-ray crystallography revealed a polyamide bound to both the viral negative strand RNA genome and the nucleocapsid proteins, and biophysical studies showed changes to the melting temperature of the nucleocapsid-like particle (NLP) in the presence of the active compound, which protected cells from virally induced lysis.

Title: Approach to GABA-A receptor isoform-selective allosteric agonists

Karol S. Bruzik

Heteropentameric GABA-A receptor is a principal drug target whose function is allosterically modulated by general anesthetics, sedatives and anticonvulsants, such as propofol, etomidate, barbiturates and neurosteroids. The current clinically used general anesthetics have numerous disadvantages including low potency, low receptor-type selectivity among the various Cys-loop receptors, low receptor isoform selectivity and resulting therefrom low therapeutic indices. Determining the locations and structures of modulator sites and the mechanisms that trigger conformational changes to the receptor is essential to the design and development.

Title: Synthesis, spectroscopic characterization, molecular docking and theoretical studies

Lubna Rasheed

Statement of the Problem: A mutual prodrug of ibuprofen and sulphanilamide has been synthesized with dual activity and improved toxicity profile. The synthesized compound has been characterized by elemental analysis, FT-IR, 1HNMR, 13CNMR and ESI-MS. The molecular geometry of the compound was optimized using density functional theory (DFT/B3LYP) method with the 6-311G (d, p) basis sets in ground state. Geometric parameters (bond lengths, bond angles, torsion angles), vibrational assignments, chemical shifts and thermodynamics of the compound has been calculated theoretically and compared with the experimental data.

Title: Synthesis, molecular docking and theoretical studies

Lubna Rasheed

A mutual prodrug of ibuprofen has been synthesized with dual activity and improved toxicity profile. The synthesized compound has been characterized by elemental analysis, FT-IR, 1HNMR, 13CNMR and ESI-MS. The molecular geometry of the compound was optimized using density functional theory (DFT/B3LYP) method with the 6-311G(d, p) basis sets in ground state. Geometric parameters (bond lengths, bond angles, torsion angles), vibrational assignments, chemical shifts and thermodynamics of the compound has been calculated theoretically and compared with the experimental data.

Title: Antibacteria, antiparasitic and *in silico* studies of Dichapetalum madagascariense

Mary Anti Chama

Dichapetalum madagascariense (Dichapetalaceae) is used to treat bacterial infections, jaundice, urethritis and viral hepatitis. Its root has been investigated to contain broad spectrum biologically active dichapetalins. To evaluate the plant's antibacterial and antiparasitic potentials coupled with in silico methods, we isolated and identified the known dichapetalins A and M from the roots. Both dichapetalins were tested together with the leaf (DML) and root ethanol extracts on six ATCC bacteria strains (Shigella flexneri, Bacillus cereus, Salmonella paratyphi B, Listeria monocytogenes, Escherichia coli, Staphylococcus aureus) and three parasites; Trypanosoma brucei brucei, Leishmania donovani.

Title: Aryl-sulfonylthiosemicarbazides as anticancer agents and COX-2 inhibitors

Muhammed Ihsan Han

Among the sulfur, oxygen and nitrogen containing compounds, thiosemicarbazides have potential pharmacological activities such as antibacterial, antifungal, analgesic, anti-inflammatory, and antitumor activities1-3. Of last years, the attention has been rapidly growing in gaining insight into the properties of thiosemicarbazides and their derivatives due to their antioxidant and anticancer activities4-5. On the basis of these findings, we led us interested in synthesis and biological evaluation of sulfonylthiosemicarbazide derivatives.

Abstract

Title: Ecofriendly benign and productive synthesis protocol for the formation of biopotent complexes of heterocycles

Neha Mathur

Bio-potent materials synthesised by heterocycles are one of the most important of classes for the new generation. The demand of the present era is the formation of the novel co-ordination complexes, which may be fruitful to fulfill the requirements of the society. They make us open the new vistas of upcoming researches. One of the ways of restoring the activity of organic moieties is to modify and tailor the structure by introducing a potent and active species.

Title: Some aspects of medicine distribution in Sudan

Abdeen Omer

The strategy of price liberalisation and privatisation had been implemented in Sudan over the last decade, and has had a positive result on government deficit. The investment law approved recently has good statements and rules on the above strategy in particular to pharmacy regulations. Under the pressure of the new privatisation policy, the government introduced radical changes in the pharmacy regulations. To improve the effectiveness of the public pharmacy, resources should be switched towards areas of need, reducing inequalities and promoting better health conditions.

Title: A knowledge-based approach for drug target and bioactivity prediction

Orazio Nicolotti

Pairing novel compounds to specific drug targets or repositioning old drugs to apparently unrelated diseases is a fascinating and challenging theme of rational drug discovery. In this scenario, we developed an easy-to-run in silico tool for drug target and quantitative bioactivity prediction implementing a multi-fingerprint similarity search algorithm, whose acronym is MuSSeL. Predictions were derived by exploiting a large collection of highly curated experimental bioactivity data available from ChEMBL (version 22.1) and combining results based on similarity search screening employing 13 different molecular fingerprints.

Abstract

Title: Calcium-mediated KRAS allosteric modulation: Implications in cancer drug discoverv

Patrick DePaolo

For decades, KRAS, a small GTPase, has been implicated in cancer research. Many have attempted to synthesize small-molecule inhibitors that have the capacity to interrupt the constitutively active, GTP-bound state of KRAS which causes an overstimulated oncogenic pathway. Burhman (2015) solved KRAS X-ray structure in the presence of calcium, a breakthrough suggesting the existence of allosterically-mediated changes not previously hypothesized.

Title: Sandalwood, an Indian medicinal plant attenuates the microbial growth and influence up/down regulation of the metabolites

Sadaf Fatima

Santalum album (sandalwood) is an Indian medicinal plant with various pharmacological properties and being used traditionally in cosmetics and therapeutics. Sandalwood has several ethnomedicinal applications; hence we have performed the present study to explore its antibacterial potential and phytocompound detection. The methanolic extract of sandalwood (SwME) was prepared by soxhlet apparatus and the antibacterial assay was performed. Further, the metabolite profiling of SwME and lysates of E. coli and E. coli grown in the presence of SwME was generated.

Title: Combined prodrugs: Dual action against HIV and HCMV

Anastasia Khandazhinskaya

Since the discovery of AIDS, coinfections became one of the clinical problems and HCMV (human cytomegalovirus) is among the most common opportunistic infectious agent observed in HIV-infected persons.1 HCMV infects people of all ages, but it is not overly pathogenic in immunocompetent people. However, in HIV-infected individuals, HCMV is associated with a wide range of serious diseases, such as retinitis, pneumonitis, colitis and other end organ disease, as well as with more rapid progression of HIV and increased occurrence of AIDS-related events.2,3 Recently, HCMV has also been associated with a higher risk of HIV transmission.

Title: Anecdotal Studies

James K Bashkin

Approximately 5,000 women die each year in the US from cervical cancer, and the worldwide mortality is 300,000 per year, yet this is only one type of cancer caused by human papillomavirus (HPV). In addition to the broad use of vaccines, anti-HPV drugs are needed for those who are already infected. Off-label, non-blinded clinical studies performed with formulations of the active pharmaceutical ingredient chloroquine, a well-known antimalarial, showed strong anti-HPV activity and restored normal skin tissue health to patients with both high- and low-risk HPV diseases.

Title: Design, synthesis and molecular modeling of isothiochromanone hybrids

Jinyi Xu

Alzheimer's disease (AD), which is characterized by dementia, memory loss, cognitive impairment and ultimately death, is a progressive neurodegenerative disease. It is estimated that over 132 million elderly people will be affected by AD at 2050. Although considerable researches have been devoted to the pathogenetic mechanisms of AD, the etiology of AD still remain unclear. Several pathological hallmarks including acetylcholinesterase (AChE) have been verified to play vital roles in the pathogenesis of AD.

Title: Development of a solid-phase catch-reles linker system for cysteine alkylation

Manal Alanazi

The modification of proteins with chemical species provides a wide range of opportunities to study, alter or exploit protein function. For example, antibody-drug-conjugates are currently receiving significant attention as tools to allow the selective delivery of therapeutic agents to specific cell types. The selective modification of proteins represents a significant chemical challenge because the reaction must modify the targeted residue selectively in the presence of other competing unprotected polypeptide side chains .

Abstract

Title: Structure-guided identification of a small molecule that inhibits anaerobic choline metabolism by human gut bacteria

Maud Bollenbach

The human body is colonized by trillions of microorganisms (the human microbiota), the majority of which are present in the gut. These microorganisms can produce a wide variety of small-molecule metabolites that may influence host health. Indeed, metabolomics experiments have showed strong correlations between levels of human serum metabolites made or modified by gut microbes and both health and disease states. Anaerobic choline metabolism by gut microbes exemplifies the challenges involved in studying microbial activities.

Title: Design, synthesis and pharmacological assessment of novel arylaldoxime nitroimidazole/morpholine hybrids

Mudasir Nabi Peerzada

Microtubule Affinity-Regulating Kinase 4 (MARK4) is an important drug target in the anticancer drug discovery paradigm due to its direct involvement in the regulation of microtubule dynamics and over expression in cancerous cells. In order to find out the novel MARK4 inhibitors, two libraries of arylaldoxime based nitroimidazole/morpholine hybrids were designed and synthesized following the pharmacophoric hybridization approach. The compounds 20 (IC50=1.47 μM) and 28 (IC50=3.17 μM) emerged as the potent MARK4 inhibitors as validated by the fluorescence binding and molecular docking studies.

Title: Synthesis and anti-tumor evaluation of C-23 modified novel 23-hydroxybetulinic acid derivatives

Shengtao Xu

23-Hydroxybetulinic acid (23-HBA) is an anticancer polycyclic triterpenoid isolated from the root of Pulsatilla chinensis. In this study, a series of C-23 modified novel 23-HBA derivatives were synthesized and evaluated for their antiproliferative activity against a panel of cancer cell lines (A2780, A375, B16, MCF-7 and HepG2). The biological screening results showed that all of the derivatives exhibited more potent antiproliferative activity than the parent compound 23-hydroxybetulinic acid, and compound 6e exhibited the most potent activity with IC50 values of 2.14 μM, 2.89 μM and 3.97 μM against A2780 cells, B16 cells, MCF-7 cells.

Abstract

Title: New derivatives of monoazaphenothiazine: Synthesis, *in silico* and antibacterial evaluation

Okafor Sunday N

Phenothiazines and its derivatives have shown various pharmacological activities including psychotropic, anticancer, and have found use as building blocks in organic synthesis for designing pharmaceuticals. In this study, we reported the synthesis and characterisation of new derivatives of monoazaphenothiazine.

Title: Synthesis and Biological of newoxazepin -4-7-dion of Pyrazine

Moayad Mohmmad

Nucleoside as the buliding blocks of RNA and DNA play an imprtant role in the molecular mechanism of conservation , replicion and tranxrination of the genitic information. Organic chemist have been activitely involoved in the synthesis of nucleoside analogues clinical antiviral drugs, clinical anti-Aids drugs and clinical anti cancer drugs . Synthesis Nucleosides derivative having schiff buses at position (-3) 1,2,5,6 –di-O-isoproplidene α-D-gluco furanose with theophylin or second type synthesis of schiff bases from oxazoles.

PAST AFFILIATES

PAST AFFILIATES

kAlexei Basnakian
University of Arkansas, USA

Maia Merlani
Tbilisi State Medical University, Georgia

William G Whitford
GE Health Care, USA

Zhongli Gao
Sanofi, USA

Nana Gorgaslidze
Tbilisi State Medical University, Georgia

Monika I Konaklieva
American University, USA

Taosheng Chen
St. Jude Children's Research Hospital, USA

Pierre Falson
IBCP, France

Shoujun Xu
University of Houston, USA

Yanli Wang
National Institutes of Health, USA

Jetze J. Tepe
Michigan State University, USA

Victor J. Hruby
University of Arizona, USA

Marc Le Borgne
University Lyon 1, France

Carsten Detering
BioSolveIT Inc, USA

Bin Xu
Virginia Tech, USA

Pierre Falson
CNRS Research , France

Prabagaran Narayanasamy
University of Nebraska Medical Center, USA

Victor J. Hruby
University of Arizona, USA

Istvan J. Enyedy
Biogen Idec, USA

Debatosh Majumdar
Glycosyn LLC, USA

Yuk Yin Shamr
University of Minnesota, USA

Pierre Falsonr
University of Minnesota, France

Patrick M Woster
Medical University of South Carolina, USA

Gjumrakch Aliev
GALLY International Biomedical Research Consulting, USA

PAST AFFILIATES

PAST AFFILIATES

Mark D Shenderovich
Mol3D Research, USA

Gerard Rosser
Dart Neuroscience, USA

G Sridhar Prasad
CalAsia Pharmaceuticals, USA

Tulay Aygan Atesin
The University of Texas-Pan American, USA

Brian S J Blagg
The University of Kansas, USA

Cesar M Compadre
University of Arkansas for Medical Sciences, USA

Larry Wilson
Emory University, USA

Jianwen Fang
The University of Kansas, USA

Ahmed M. Radwan
PIONEERA HealthCare Group, UK

Ahmed Radwan
Pioneera Health Care Group, UK

Alexander Heifetz
Evotec (UK) Ltd, UK

Andreia Valente
Universidade de Lisboa, Portugal

Alexander Heifetz
Evotec Ltd, UK

Thorsten Nowak
C4X Discovery Holdings PLC, UK

Mire Zloh
University of Hertfordshire, UK

Howard Apler
University of Ottawa, Canada

Dr.Howard Apler
University of Ottawa, Canada

Arvi Rauk
University of Calgary, Canada

Nicolas Moitessier
McGill University, Canada

Mario Ciampolini
Unity of Gastroeneterology in the Pediatric Clinic of Firenze, Italy

Mario Ciampolini
University of Florence, Italy

Bernhard Wünsch
Institute of Pharmaceutical and Medicinal Chemistry, Germany

Concepción González-Bello
Universidade de Santiago de Compostela, Spain

PAST AFFILIATES

PAST AFFILIATES

Horacio Pérez-Sánchez
University of Murcia, Spain

Aditya Bhushan Pant
Indian Institute of Toxicology Research, India

Aditya Bhushan Pant
Indian Institute of Toxicology Research Lucknow, India

Man Singh
Central University of Gujarat, India

Jaya Pandey
Amity University, India

Rakeshwar Bandichhor
Dr. Reddy's Laboratories, India

Leonard Amaral
Universidade Nova de Lisboa, Portugal

Thomas Högberg
LEO Pharma, Denmark

Csaba Hetenyi
Hungarian Academy of Sciences, Hungary

Marjana Novič
Kemijski inštitut, Slovenia

Alessandra Nurisso
University of Geneva, Switzerland

Jiapu Zhang
The University of Ballarat, Australia

Mitsuji Yamashita
Shizuoka University, Japan

Hideharu Shintani
Professor Chuo University, Japan

Tatsuya Takagi
Osaka University, Japan

Abbas Amini
Western Sydney University, Australia

Sameeh A. Mansour
National Committee of Toxicology, Egypt

Glimpses of

Medicinal Chemistry and Drug Design Conferences

Edinburgh Attractions