



III *International conference on*

CLINICAL SCIENCES & DRUG DISCOVERY



**November 09-11
2017**



Sheraton Reston Hotel
11810 Sunrise Valley Dr, Reston
VA 20191
USA

Day-1 | November 09, 2017

08:00 - 08:30 Introduction

Keynote Session

08:30 - 09:00 **New paradigms in GPCR drug discovery**

Kenneth A. Jacobson, NIH, MD, USA

09:00 - 09:30 **Targeted imaging and therapeutic agents for cancer, autoimmune and inflammatory diseases**

Philip S. Low, Purdue University, West Lafayette, IN, USA

09:30 - 10:00 **The comprehensive solution to characterise and treat every disease**

Ram Samudrala, University at Buffalo, NY, USA

10:00 - 10:30 **Chemistry and health: Now is the time for a comprehensive approach**

Stephen Matlin, Imperial College London, UK

10:30 - 10:50 *Coffee Break*

10:50 - 12:50 Technical Session I

Session - Ram Samudrala, University at Buffalo, NY, USA

Chairs Philip S. Low, Purdue University, West Lafayette, IN, USA

10:50 - 11:10 **Evaluating CNS pharmacology to improve drug delivery to brain tumors**

Sadhana Jackson, NCI/NIH, MD, USA

11:10 - 11:30 **Novel computational chemogenomics knowledge bases target hunter for system pharmacology drug discovery and translational research**

Xiang-Qun (Sean) Xie, NIH/NIDA, MD, USA

11:30 - 11:50 **Normalizing urine exosome biomarkers: a second look at hidden gems**

Peter Yuen, NIH/NIDDK, MD, USA

11:50 - 12:10 **Non-inhibitory pharmacological chaperones of glucocerebrosidase for the treatment of gaucher's and parkinson's disorders**

Juan Jose Marugan, NCATS/NIH, MD, USA

12:10 - 12:30 **Antiviral nucleoside phosphonate prodrugs: Potency amplifiers**

Charles McKenna, University of Southern California, CA, USA

12:30 - 12:50 **Safety of current cancer drugs and vaccines and future perspectives for a healthier society**

Mahin Khatami, NIH, MD, USA

12:50 - 13:40 *Lunch*

13:40 - 17:40 Technical Session II

Session - *Harold C. Smith, University of Rochester, NY, USA*
Chairs *Brent E. Korba, Georgetown University, Washington, DC, USA*

13:40 - 14:00 **New structure based drug discovery opportunities for GPCRs and Transporters**
Sid Topiol, 3D-2Drug LLC, NJ, USA

14:00 - 14:20 **Toward a functional cure for HIV/AIDS: Regulatory interactions between RNA and the HIV restriction factor APOBEC3G**
Harold C. Smith, University of Rochester, NY, USA

14:20 - 14:40 **Hydrogen/deuterium ratio is a key regulator of cell proliferation and metabolism – Drug development on submolecular basis**
Somlyai Gabor, HYD Pharma Inc., Hungary

14:40 - 15:00 **Bisphosphonates: bones and beyond**
Graham Russell, Oxford University, UK

15:00 - 15:20 **New drug candidates for liposomal delivery identified by computer modeling of liposomes' remote loading and leakage**
Amiram Goldblum, The Hebrew University of Jerusalem, Israel

15:20 - 15:40 Coffee Break

15:40 - 16:00 **Privileged structures: a versatile concept to explore new chemical space with medicinal chemistry utility**
Jorg Benningshof, Mercachem, The Netherlands

16:00 - 16:20 **Understanding human norovirus nucleotidylation: Potential target for intervention?**
Brent E. Korba, Georgetown University, Washington, DC, USA

16:20 - 16:40 **Novel treatment strategies for smooth muscle disorders: Targeting Kv7 potassium channels**
Kenneth L. Byron, Loyola University Chicago, IL, USA

16:40 - 17:00 **Antiplasmodial activity and cytotoxicity of lapachol and synthetic related naphthoquinones**
Alaíde Braga de Oliveira, Universidade Federal de Minas Gerais – UFMG, Brazil

17:00 - 17:20 **Targeted nanotherapies for neuroinflammation: novel therapeutics for CNS disorders**
Kannan Rangaramanujam, Johns Hopkins School of Medicine, MD, USA

17:20 - 17:40 **A rapid-evolving small RNA based immune system targeting avian leukosis virus in chickens**
Xin Li, University of Rochester, NY, USA

17:40 - 18:30 Poster Presentations

09:00 - 12:40 Technical Session III

Session - *Graham Russell, Oxford University, UK*
Chairs - *Somlyai Gabor, HYD Pharma Inc., Hungary*

09:00 - 09:20 **Hydralazine induces stress resistance and extends lifespan in *C. elegans* via Nrf2/SKN-1 pathway**
Hamid Mirzaei, UT Southwestern Medical Center, TX, USA

09:20 - 09:40 **Can lipid nanoparticles improve intestinal absorption?**
Carla Vitorino, University of Coimbra, Portugal

09:40 - 10:00 **A trisaccharide analog that Acts as a TLR-4 agonist: A potential vaccine adjuvant?**
Cecilia H. Marzabadi, Seton Hall University, NJ, USA

10:00 - 10:20 **Tissue models for drug screening against cancer stem cells**
Esmail Jabbari, University of South Carolina, SC, USA

10:20 - 10:40 **The essential role of pharmacology in discovery translational research**
Giora Z. Feuerstein, Temple University, PA, USA

10:40 - 11:00 Coffee Break

11:00 - 11:20 **Delineating ligand binding to the human cytochrome P450 3A4**
Maria Kontoyianni, Southern Illinois University Edwardsville, IL, USA

11:20 - 11:40 **Neutrophil gelatinase-associated lipocalin in urine as a non-clinical safety biomarker for acute kidney injury**
Kiyonori Kai, Daiichi Sankyo Co., Ltd., Japan

11:40 - 12:00 **High levels of serum lipid peroxides and protein carbonyls in mild dengue fever verses severe dengue**
Sunil Premawansa, University of Colombo, Sri Lanka

12:00 - 12:20 **Advanced machine learning to boost the accuracy of scoring function**
X. Simon Wang, Howard University College of Pharmacy, Washington, DC, USA

12:20 - 12:40 **Anti-cancer effects of Marijuana and Hemp**
Wasana Sumanasekera, Sullivan University College of Pharmacy, Louisville, KY, USA

12:40 - 13:30 Lunch

13:30 - 15:50 Technical Session IV

Session - *Charles McKenna, University of Southern California, CA, USA*
Chairs *Jorg Benningshof, Mercachem, The Netherlands*

- 13:30 - 13:50 **Discovery of novel reactivators for DFP-inhibited acetylcholinesterase using in silico pharmacophore modeling**
Apurba K Bhattacharjee, Georgetown University, Washington, DC, USA
- 13:50 - 14:10 **Study design and analysis for multistage clinical proteomic studies**
Irene Suilan Zeng, University of Auckland, New Zealand
- 14:10 - 14:30 **Discovery of novel small molecules and targets for neuro-degenerative diseases through yeast based phenotypic screening**
Bhaumik Pandya, Yumanity Therapeutics, MA, USA
- 14:30 - 14:50 **Novel phosphatidylinositol 4-kinase IIIb inhibitors as potential therapeutics**
Radim Nencka, Gilead Sciences & IOCB Research Centre, Czech Republic
- 14:50 - 15:10 **Herbal remedies for mandibular fracture healing**
Shadab Mohammad, King George's Medical University, India
- 15:10 - 15:30 **Chemoecology guided discovery of drug leads from south china sea marine invertebrates**
Yue-Wei Guo, Chinese Academy of Sciences, China
- 15:30 - 15:50 **A Chemist's view of animal disease models for drug screening**
Takashi Tsukamoto, Johns Hopkins University, MD, USA

15:50 - 16:10 Coffee Break

16:10 - 17:25 Young Researchers Forum

- 16:10 - 16:25 **Modulating supramolecular nanostructures cross-linked by hyaluronic acid derivatives for drug delivery**
Tania. F .G. G. Cova, University of Coimbra, Portugal
- 16:25 - 16:40 **Extended release of venlafaxine hydrochloride using Montmorillonite based excipients as a delivery vehicle**
Shilpa Jain, University of Delhi, India
- 16:40 - 16:55 **Bioanalytical method development, validation & pharmacokinetics study of 5-Fluorouracil loaded nanoparticles**
Saurabh Srivastava, King George's Medical University, India
- 16:55 - 17:10 **The facial-Re(CO)₃ core based luminophores as non-toxic bio-imaging agents**
Deepak Gupta, University of Delhi, India
- 17:10 - 17:25 **Drug Addiction and Oral Health Complications in India**
Sana Farooqui, King George's Medical University, India

09:00 - 12:40 Technical Session V

Session - *Kenneth L. Byron, Loyola University Chicago, IL, USA*

Chairs *Apurba K Bhattacharjee, Georgetown University, Washington, DC, USA*

09:00 - 09:20 **High throughput screening identifies an anti-ebola lead compound**

Ryan P. Bennett, OyaGen, Inc., NY, USA

09:20 - 09:40 **Hypoxia inducible factor 1: A urinary biomarker of kidney disease**

Movafagh S, Shenandoah University, VA, USA

09:40 - 10:00 **Neointimal caveolin-1 loss may in part facilitates metabolic shift in pulmonary arterial hypertension**

Rajamma Mathew, New York Medical College, NY, USA

10:00 - 10:20 **p-coumaric acid, main active compound isolated from Bambusae Caulis in Taeniam suppresses cigarette smoke-induced lung inflammation**

Jinju Kim, Kyung Hee University, Republic of Korea

10:20 - 10:40 **Stability and activity of nano-crystalized camptothecin**

James Liang, Stevens Institute of Technology, NJ, USA

10:40 - 11:00 Coffee Break

11:00 - 11:20 **The clinical implementation of molecular biomarkers in Glioma**

Jessica L. Fleming, The Ohio State University, OH, USA

11:20 - 11:40 **Restoring FMRP expression: an alternative treatment strategy for fragile X syndrome**

Daman Kumari, NIDDK/NIH, MD, USA

11:40 - 12:00 **Synthesis of Ofornine mimics from natural product 1-Vasicine as anti-hypertensive agents**

Abdul Rouf, University of Florida, FL, USA

12:00 - 12:20 **Synthesis and biological evaluation of some novel N-methylenebenzenamine**

Sushant Kumar Shrivastava, Indian Institute of Technology (BHU), India

12:20 - 12:40 **Surveillance for hepatitis B virus surface antigen in a northern Nigerian population: An advocacy for aggressive vaccination**

Mukhtar Dauda, Bayero University, Nigeria

12:40- Lunch & Departure

Poster Presentations

- P-01 **Consensus comparative modeling to construct structural models of human C-C Chemokine Receptor 4 (CCR4) to discover small-molecule therapeutics to treat cancer metastasis**
Jeffery J. Bullock, Howard University, Washington, DC, USA
- P-02 ***In vitro* efficacy of a novel RNA-dependent RNA polymerase inhibitor against a broad range of RNA viruses**
Elena Postnikova, NIH, MD, USA
- P-03 **Transition metal and photocatalyst-free perfluoroalkylation reactions of organic sulfides with relevant biological activity**
Damian E. Yerien, Universidad de Buenos Aires, Argentina
- P-04 **Ferumoxytol nanoparticles enable imaging of brain tumor-associated neuro inflammation**
Heather L. McConnell, Oregon Health and Science University, Oregon, USA
- P-05 **A genome-wide screening of antifungal drug target genes in fission yeast**
Sol Lee, Chungnam National University, South Korea
- P-06 **Protein kinase selectivity analysis based on the topological water networks**
Myeong Hwi Lee, Chungnam National University, South Korea
- P-07 **Enhancement of expression level and stability of hEC-SOD3 by conjugating human serum albumin**
Eun Yeong SONG, Chungnam National University, South Korea
- P-08 ***In vitro* glucuronidation of icaritin by human liver microsomes, human intestine microsomes and expressed UDP-glucuronosyltransferase enzymes: contribution of individual enzymes, reaction kinetics and activity correlation**
Zhihong Yao, Jinan University, China
- P-09 **Identification of ESE-1 as a tumor suppressor in lung cancer**
Zhiyuan Lou, University of Maryland, MD, USA
- P-10 **Pharmacokinetics of Tafamidis in Rats**
Jong-Woo Jeong, Chungnam National University, South Korea

We wish to see you at CSDD-2018



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