KEYNOTE SPEAKERS

Kenneth M. Merz, Jr. is currently the Director of the Institute for Cyber Enabled Research (iCER) and the Joseph Zichis Chair in Chemistry at Michigan State University as well as the Editor-in-Chief, Journal of Chemical Information and Modeling, an American Chemical Society publication. One of the pioneers in AMBER Molecular Modeling development team, Dr Merz's research interest lies in the development of theoretical and computational tools and their application to biological problems including structure and ligand based drug design, mechanistic enzymology and methodological verification and validation (i.e., error analysis). He has published ~240 papers and given over 240 lectures worldwide describing his research. Professor Merz was previously a University of Florida Research Foundation Professor, the Edmund H. Prominski Professor of Chemistry, the Colonel Allan R. and Margaret G. Crow Term Professor and a Member of the Quantum Theory Project all at the University of Florida from 2005-2013. Prior to the University of Florida he was an Assistant, Associate and Professor of Chemistry at the Pennsylvania State University from 1989-2005. He also has worked in industry (1998-2001) first as the Senior Director of the Center for Informatics and Drug Discovery (CIDD) at Pharmacopeia, Inc. (now part of Ligand, Inc.) and then as the Senior Director of the ADMET Research and Development Group in the Accelrys software division of Pharmacopeia. He is the founder of the software company QuantumBio, Inc located in State College, Pennsylvania. Dr. Merz carried out postdoctoral training at The University of California, San Francisco (1987-1989, with Peter Kollman) and at Cornell University (1986-1987, with Roald Hoffmann). He received his Ph.D. in Organic Chemistry at The University of Texas at Austin in 1985 (with M. J. S. Dewar) and his B.S. from Washington College, Chestertown, Maryland in 1981. Professor Merz has received a number of honors including, election as the 2013 Chair of the COMP division of the ACS, election as an ACS Fellow, the 2010 ACS Award for Computers in Chemical and Pharmaceutical Research, election as a fellow of the American Association for the Advancement of Science, a John Simon Guggenheim Fellowship and he has held visiting professorships at the Institute for Research in Biomedicine (Barcelona, Spain), Ecole Polytechnique (Paris, France), University of Florence (Florence, Italy), The University of Strasbourg (Strasbourg, France), The University of Oviedo (Oviedo, Spain) and the ETH (Zurich, Switzerland).

Alan Mark is currently a Professor at the School of Chemistry and Molecular Biosciences at The University of Queenland, Australia**.** Dr Alan Mark obtained his PhD from Australian National University in … He also held postdoctoral positions at the RSC (ANU) (1987-1988) and at the University of Groningen (1989-1990). In 1990 he moved with W.F. van Gunsteren to ETH Zurich becoming Oberassistant in 1996. In 1998 Alan was appointed Professor of Biophysical Chemistry, University of Groningen. In 1998 Alan was awarded the Swiss Ruzicka Prize for research in Chemistry. In 2004 he was also awarded an Australian Research Council (ARC) Federation Fellowship and joined The University of Queensland in 2005. In 2011 he was awarded a University of Queensland Vice Chancellor's Senior Research Fellow. Dr Alan Mark is also an affiliate of the Institute of Molecular Biosciences at UQ and the Australian Infectious Diseases Research Centre. Currently, Prof Alan Mark leads a group that focuses on understanding and predicting the macroscopic (experimentally observable) properties of biomolecular systems such as proteins, nucleic acids and lipid aggregates, in terms of the interactions between atoms. In particular our work concentrates on the development of tools (i.e. simulation software, atomic force fields, theoretical models and experimental techniques) that can be used to understand and predict the physico-chemical basis of interactions and dynamic processes within biomolecular systems. Specific areas of interest include structure prediction, protein and peptide folding, the self-assembly of protein/lipid complexes and the calculation of thermodynamic properties such as ligand binding affinities.

INVITED SPEAKERS

Professor Richard Bryce heads up the computational-aided drug design group in the Division of Pharmacy and Optometry. He is a Reader in Biomedicinal Chemistry, having studied chemistry at St. Andrews University (BSc, 1995) and computational chemistry at Manchester University (PhD, 1998). He was a Robert Lincoln MacNeil scholar at the University of Pennsylvania (1992-1993) and a Ramsay Memorial Fellow at the University of Manchester (1999-2001). His work receives support from a variety of sources, including EPSRC, The Wellcome Trust, MRC, BBSRC and the Royal Society. He is a fellow of the Royal Society of Chemistry and member and former chair of the Molecular Graphics and Modelling Society.

Dr. Asif Khan is currently appointed as the Director of the Perdana University Center for Bioinforomatics (PU-CBi), Assistant Professor to the faculty of the Perdana University Graduate School of Medicine (PUGSOM) and School of Postgraduate Studies (PU-SPS), Malaysia and Visiting Scientist to the Department of Pharmacology and Molecular Sciences, Johns Hopkins University School of Medicine (JHUSOM), USA.

Dr. Khan's broad research interests are in the area of biological data warehousing and applications of bioinformatics to the study of immune responses, vaccines, venom toxins, drug design, and disease biomarkers. Specifically, he is interested in understanding the human-pathogen interactome, defined as the pathogen and human genetic sets (DNA, RNA, Protein) that are directly or indirectly involved in the complex, dynamic interactions between the two, relevant for the survival of each other. He has authored/co-authored a total of 38 published articles (http://bit.ly/1xDXelB) in various international journals, conferences, and books, and has presented his work at numerous international conferences. His scientific contributions include development of several novel bioinformatics methodologies, tools, and specialized databases, and currently has three patents filed.

Professor Fumio Hirata completed the Doctor thesis from Hokkaido University. He started the postdoctoral work at Prof. H. Friedman's lab in 1978 in the State University of New York at Stony Brook. When about one year was past at Stony Brook, Prof. P. Rossky, who then was also a postdoc of Friedman's group, was offered a tenure track position in the University of Texas, and asked him to join his group as a postdoc. After two years of stay in Texas, he decided to go back to Japan in order to release the stress from insecurity. After a stint in Japan working in Fujitsu, he moved to Rutgers, to work with Prof. R. Levy. In Rutgers, he started to apply the extended RISM theory to realistic problems in aqueous solutions, including biophysical phenomena. Professor Hirata was also offered an associate professor position at the chemistry department of Kyoto University in 1989, where they were searching a theorist in the field of biophysics. Currently, he is an emeritus Professor at Fumio Hirata Toyota Physical & Chemical Research Institute, Japan.

Professor Kam Zhang is currently a Team Leader at the Center for Life Science Technologies, RIKEN, Japan. His main research interests are on protein design and drug design. His lab is using computational tools in the structure-based drug discovery for various protein targets. His lab has discovered small molecular inhibitors for sumoylation enzymes, epigenetic regulators, chitinases and protein-protein interactions. Prior to joining RIKEN, he was the Director of Structural Biology at Plexxikon Inc. in Berkeley, USA, where he established the scaffold-based drug discovery platform. He has contributed to the discovery of several drug candidates that are currently in various stages of clinical trials. One of them, Zelboraf, has been approved by FDA for the treatment of metastatic melanoma. He was a faculty member at the Fred Hutchinson Cancer Research Center, and University of Washington, Seattle, USA. He obtained a BSc in Chemistry from Peking University, China and a PhD in Physics from the University of York, UK. He did his postdoctoral training at the Molecular Biology Institute, UCLA, USA.

Professor Norio Yoshida is currently an Associate Professor at Department of Chemistry Faculty of Science, Kyushu University. His main research interest is in Theoretical study on the electronic structure of solvated molecule and biomolecule combined with statistical mechanics.

Prof. Mohd Basyaruddin is currently the Dean of Faculty of Science, Universiti Putra Malaysia and also a Fellow of Academy of Sciences Malaysia. He obtained his Bachelors double degree in Chemistry and Computer Science with Education at Universiti Teknologi Malaysia in 1995 and his PhD at University of Southampton in 1999. He served on the Editorial Board of The Open Catalysis Journal (Bentham), Journal of Chemical Biology & Therapeutics (OMICS), and JSM Enzymology and Protein Science (JSciMedCentral). His research interests are catalysis chemistry, chemical biology and computational chemistry. He received Top Research Scientist Malaysia award in 2012, Outstanding Academic Young Scientist, World Economic Forum award in 2009, and Young Chemists Award, IUPAC in 2007.

Professor Stephen Doughty is currently the Chief Executive Officer and President of Penang Medical College, a position he held since 2015. Prior to that Prof. Doughty was the Vice-Provost (Teaching and Learning) at the University of Nottingham Malaysia Campus in Kuala Lumpur. He obtained a first-class degree in Chemistry from the University of Essex and a DPhil in Chemistry from Oxford University. In 2005, he moved to the Malaysia Campus to establish the School of Pharmacy at UNMC and became the Dean of the Faculty of Health & Biological Sciences, later renamed to the Faculty of Science. In 2008, in recognition of his contribution to teaching on the MPharm degree and the student experience at UNMC, he became the first member of staff based at the Malaysia Campus to be awarded the Dearing Award for Excellence in Teaching. He has had extensive experience helping to guide the strategic direction of UNMC and continues to drive new teaching and learning initiatives in order to keep pace with developments in learning technologies and student expectations. His research interests are focused on modeling and computer-aided drug design with a particular interest in modeling membrane-bound proteins. Particular emphasis upon anti-cancer drug design, including using novel techniques such as QM/MM hybrid approaches to model the conversion of harmless pro-drugs in to anti-cancer therapeutic drugs. Also, modeling membrane-bound proteins such as GPCRs and ion channels for drug design.

Professor Muchtaridi is a full professor and Departmental Chair of Pharmaceutical Analysis and Medicinal Chemistry of Faculty of Pharmacy, Universitas Padjadjaran, Indonesia. He obtained his PhD from School of Pharmaceutical Sciences, Universiti Sains Malaysia in 2013 under the supervision of Prof. Dr. Habibah A. Wahab. His main research interest is drug discovery of natural products and that includes bio-guide assay isolation combining in silico i.e virtual screening and design against anti-breast cancer and anti-influenza. His current research is Potential activity of some natural products compounds as Neuraminidase inhibitors based on molecular docking simulation and in vitro test.

Professor Jutti Levita is a full professor and researcher in Department of Pharmaceutical Analysis and Medicinal Chemistry of Faculty of Pharmacy, University of Padjadjaran, Indonesia. She obtained her PhD at School of Pharmacy, Bandung Institute of Technology, Indonesia in 2011. In 2011 to 2014, she served as the Managing Editor for Indonesian Journal of Applied Sciences. Her major research interests are in the field of natural products and in silico studies pertaining anti-inflammatory drug design. She is actively involved in the research on natural products such as Selliguea feei (pakis tangkur), Zingiber officinale (ginger), Andrographis paniculata (sambiloto), Myristica fragrans Houtt (nutmeg) and Hibiscus sabdariffa. Her latest work is on virtual screening of co-formers for ketoprofen cocrystallization and the molecular properties of the co-crystal.

Associate Professor Vannajan Lee (Universiti Malaya, Malaysia) Asst. Prof. Dr. Vannajan Sanghiran Lee received her BSc (1994) in Chemistry from Chiang Mai University, Thailand and PhD (2001) in Pharmaceutical Sciences and Physical Chemistry from University of Missouri-Kansas City, USA under the scholarship from the Institute of Promotion and Development Science and Technology Project, Thailand. After that she received the Post Doctoral Scholarship (2002) from the Thailand Research Fund and worked at the Computational Chemistry Unit Cell (CCUC), Chulalongkorn University, Thailand. Presently, she is working as a lecturer and researcher in Computational Simulation and Modeling Laboratory (CSML), Department of Chemistry and Center for Innovation in Chemistry, Chiang Mai University, Chiang Mai, Thailand. In 2010, she has joined the school of pharmaceutical sciences, University Sains Malaysia as a visiting researcher. She has recently worked as a senior lecturer at Department of chemistry, University of Malaya. Her present research interest includes computer-aided molecular modeling and computational chemistry using Molecular Dynamics (MD), Monte Carlo Simulations (MC) and Quantum Mechanics (QM) in diverse research and development fields such as biomolecular/material design.

Dr. Choong Yee Siew (INFORMM, Malaysia) Yee Siew is a lecturer in Institute for Research in Molecular Medicine (INFORMM), Universiti Sains Malaysia. Her research emphasis on the modeling, structural studies and scFv design against biomarkers of enteric and parasite diseases from the developing and under-developed countries. Besides that, she is also interested to look into the effects of human cytochrome P450s variants on drug binding.