



The 23rd International Annual Symposium on Computational Science and Engineering: Expanding Your Mind

Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai Province, Thailand
June 27 - 29, 2019

Session: Computational Biology, Bioinformatics, Biochemistry, and Biophysics (BIO)

Wednesday, June 26, 2019		
Expected all participants arrive in Chiang Mai and check-in at hotels		
Thursday, June 27, 2019		
08.00 – 09.00	Registration	
09.00 – 09.30	Opening Ceremony	
09.30 – 10.15	The XYG3 Type of Doubly Hybrid Density Functionals: From Molecular Systems to Extended Solids <i>Plenary Lecture: Prof. Xu Xin from Fudan University, China</i>	
10.15 – 10.35	eHPC: Current Status of Thailand HPC Infrastructure <i>Special Talk: Dr. Piyawut Srichaikul from NECTEC, Thailand</i>	
10.35 – 11.00	Coffee Break	
<i>Chairman: Thanyada Rungrotmongkol</i>		
11.00 – 11.30	BIO-I-01	First-Principle-Based and Data-Driven Design of Therapeutics <i>Prof. Lee-Wei Yang</i>
11.30 – 12.00	BIO-I-02	Molecular Dynamics Simulations of Full-length Amyloid-β Peptides <i>Prof. Hisashi Okumura</i>
12.00 – 13.00	Lunch	
<i>Chairman: Seiji Mori and Jitrayut Jitonnorn</i>		
13.00 – 13.30	BIO-I-03	Machine Learning for Property Prediction and Molecular Design <i>Prof. Deva Priyakumar</i>
13.30 – 14.00	BIO-I-04	Theoretical Study on the Singly-bonded Dimanganese Coordination Complexes and Metalloprotein Analogues <i>Prof. Jen-Shiang K. Yu</i>
14.00 – 14.30	BIO-I-05	Understanding Biological Processes in Solution Based on the Statistical Mechanics Theory of Liquids <i>Prof. Norio Yoshida</i>
14.30 – 15.00	BIO-I-06	Multiple Binding Configurations of Fis Proteins on DNA Underlie their Dissociation Pathways <i>Prof. Min-Yeh Tsai</i>
15.00 – 15.15	BIO-O-01	Insight into the Mechanism of the Hydration Structure and Interaction Energy of Sorbitan Monostearate (Span60) in the Gas and Aqueous Phases: A QM/MM Calculations Study



		<i>Mr. Nikorn Shinsuphan</i>
15.15 – 15.30	BIO-O-02	Effect of Surface Functionalization of Aunps on the Internalization into Mammalian Cell <i>Mr. Thodsaphon Lunnoo</i>
15.30 – 15.50	<i>Coffee Break</i>	
<i>Chairman: Jen-Shiang K.Yu</i>		
15.50 – 16.20	BIO-I-07	Theoretical Studies on Reaction Mechanisms of Metalloenzymes:QM/MM analyses <i>Prof. Yasuteru Shigeta</i>
16.20 – 16.35	BIO-O-03	Finite Element Modeling of Vaccine Delivery Using Microneedles: Roles of Microneedle Shape and Antigen Diffusion Rate <i>Mr. Pikkanet Suttirat</i>
16.35 – 16.50	BIO-O-04	Computational Design of Bacillus licheniformis RN-01 levansucrase for Control of the Chain Length of Levan-type Fructooligosaccharides <i>Mr. Pongsakorn Kanjanatanin</i>
17.15 – 18.30	Poster Session (All Poster Presentation)	
18.45	<i>Welcome Dinner</i>	
Friday, June 28, 2019		
09.00 – 09.45	Experimental and Computational Approaches for Elucidating Glycofunctional Mechanisms <i>Plenary Lecture: Prof. Koichi Kato from Institute of Molecular Science, Japan</i>	
09.45 – 10.05	Applications of Synchrotron-based X-ray Absorption Spectroscopy on Advanced Functional Materials <i>Special Talk: Dr. Pinit Kidkhunthod from Synchrotron Light Research Institute, Thailand</i>	
10.05 – 10.25	Combined Experimental Computational Multi-Scale Studies in Catalysis <i>Special Talk: Dr. Supareak Prasertdam from Catalyst Group, Chulalongkorn University, Thailand</i>	
10.25 – 11.00	<i>Coffee Break</i>	
<i>Chairman: Panida Surawatanawong</i>		
11.00 – 11.30	BIO-I-08	Computational Solvation Analysis of Biomolecules in Aqueous Ionic Liquid Mixtures <i>Prof. Christian Schröder</i>
11.30 – 12.00	BIO-I-09	Decomposition of Mechanical Properties in Biomolecules <i>Prof. Jih-Wei Chu</i>
12.00 – 13.00	<i>Lunch</i>	
<i>Chairman: Yasuteru Shigeta and Nuttee Suree</i>		
13.00 – 13.30	BIO-I-10	Bridges between Experiment and Theory on Catalytic Functions <i>Prof. Seiji Mori</i>



13.30 – 14.00	BIO-I-11	Aggregation Process of Amyloid-β Peptides by the Coulomb Replica-Permutation Method <i>Prof. Satoru Itoh</i>
14.00 – 14.30	BIO-I-12	Cheminformatics as a useful tool to search for novel Anti-Alzheimer from Thai Natural Products Database <i>Prof. Supa Hannongbua</i>
14.30 – 14.45	BIO-O-05	Classification and Variable Selection in Large p Small n with Imbalanced Data Problems using Regularized AUC <i>Mr. Tanawat Horsirimanon</i>
14.45 – 15.00	BIO-O-06	Computational Analysis on the Formation and Properties of the Dimeric Zirconocene Complex: The Substituent Effect <i>Ms. Natchayatorn Keawkla</i>
15.00 – 15.20	<i>Coffee Break</i>	
<i>Chairman: Deva Priyakumar</i>		
15.20 – 15.50	BIO-I-13	Computational Enzymology: Methods and Applications <i>Prof. Jitrayut Jitonnorn</i>
15.50 – 16.20	BIO-I-14	Towards a Cure for AIDS: An Integrated Drug Discovery Model Targeting Viral-Host Interactions <i>Prof. Nuttee Suree</i>
16.35 – 17.00	Closing conference with Poster and Oral Presentation Award announcement	
Saturday, June 29, 2019		
07.15 – 16.00	Excursion: Mountain Tour (optional)	
16.00 – 22.00	Saturday walking street market (optional)	
Sunday, June 30, 2019		
Depart from Chiang Mai Province		