Saturday, 27/10

17:00-20:00 Registration at Seagull hotel

Sunday, 28/10

8:00-8:45 Registration at the conference site

8:45-9:00 Opening

Protein folding and beyond

Chair: Mai Suan Li

9:00-9:35 **I1.** Robert Best, Co-evolutionary fitness landscapes for sequence design

9:35-9:55 **C1**. Pawel Krupa, Studies of proteins with disulfide bonds with molecular modeling tools

9:55-10:30 **I2.** Johan Aqvist, Entropy and Enzyme Adaptation

10:30-11:00 *Tea Break*

Chair: Edward P. O'Brien

11:00-11:35 **I3.** Changbong Hyeon, Energetic costs, precision, and transport efficiency of molecular motors

11:35-12:10 **I4.** Marek Cieplak, Folding of knotted proteins under nascent conditions and unfolding of entangled neurotoxic polypeptydes in proteasomes

12:10-14:00 *Lunch and Poster Session*

Posters are displayed throughout the conference

Protein aggregation and folding in vivo

Chair: Marek Cieplak

14:00 -14:35 **I5.** Tamir Tuller, Modeling and analyzing the flow of molecular machines in gene expression

14:35-15:10 **I6.** Trinh Xuan Hoang, Protein escape at the ribosomal exit tunnel

15:10-15:45 **I7.** Edward P. O'Brien, Domain topology, stability, and translation speed determine co-translational folding force generation on the ribosome

15:45-16:15 *Tea Break*

Chair: Philippe Derreumaux

16:15-16:50 **I8.** Mai Suan Li, Protein aggregation and neurodegenerative diseases

16:50-17:25 **I9.** Paul Robustelli, Improved physical models enable the investigation of molecular recognition in intrinsically disordered proteins at atomistic resolution

Monday, 29/10

IDPs and Amyloid

Chair: Yuji Sugita

8:30-9:05 **I10.** Giovanni La Penna, Transition metal ions reactivity in disordered biological systems: The perspective of modeling

9:05-9:25 **C2.** Nguyen Truong Co, Impact of surface roughness on aggregation process: Lattice model study

9:25-10:00 **I11.** Hishashi Okumura , Molecular dynamics study of amyloid-β aggregates

10:00-10:20 **C3.** George Pantelopulos, Understanding Intrinsically Disordered Membrane Proteins in Alzheimer's Disease via Molecular Simulation

10:20-10:50 *Tea Break*

Chair: Robert Best

10:50-11:25 **I12.** Phuong H Nguyen, Development and application of nonequilibrium molecular dynamics simulation methods

11:25-12:00 **I13.** Philippe Derreumaux, Folding and self-assembly of peptides using coarse-grained on-lattice and off-lattice simulations

12:00-14:00 *Lunch*

14:00-20:00 *Excursion*

Tuesday, 30/10

IDPs and beyond

Chair: Garegin Papoian

8:30-9:05 **I14.** Shoji Takada, Chromatin and transcription factor dynamics via coarse-grained molecular simulations

9:05-9:40 **I15.** Sebastian Kmiecik, New tools for fast modeling of protein flexibility and protein-peptide docking

9:40-10:00 **C4.** Mateusz Kurcinski, Flexible peptide docking using CABS-dock

10:00-10:30 *Tea break*

Chair: Changbong Hyeon

10:30-10:50 **C5.** Pham Dang Lan, A topological order parameter for describing folding free energy landscapes of proteins

10:50-11:25 **I16.** Akia Kitao, Computational approach to investigate protein complex formation and dissociation

12:00-14:00 *Lunch*

Large scale modeling

Chair: Johan Aqvist

14:00-14:35 **I18.** Garegin Papoian, Towards Simulating Eukaryotic Cells at Single Molecule Resolution

14:35-14:55 **C6.** Lam Nguyen, Multi-scale modeling of cell biology

14:55-15:30 **I19.** Yuji Sugita, Protein-Drug Interaction in Dilute Solution and Cellular Environments

15:30-16:00 *Tea break*

Chair: Akia Kitao

16:00-16:20 **C7.** Pavel Semenyuk, Modeling of protein interaction with charged polymers: from model polymers and nucleic acids to posttranslational modifications of amyloid proteins

16:20-16:55 **I20.** Toan T Nguyen, Recent computational biomedicine and biophysical research at the VNU Key Laboratory on Multiscale Simulation of Complex Systems

16:55-17:10 *Closing*

18:00-22:00 Conference dinner

List of Posters

P1. Hoang Linh Nguyen (ICST, Vietnam), Erythromycin leads to differential protein expression through differences in electrostatic and dispersion interactions with nascent proteins.

P2. Pham Hong An (ICST, Vietnam), Erythromycin, Cethromycin and Solithromycin Exhibit Similar Binding Affinities to the E. coli's Ribosome.

P3. Duc Toan Truong (ICST, Vietnam), Probing Binding Affinity by Jarzynski's Non-equilibrium Binding Free Energy and Rupture Time.

P4. Phan Minh Truong (ICST, Vietnam), Picosecond melting of peptide nanotubes using an infrared laser: A nonequilibrium simulation study.

P5. Nguyen Quoc Thai (Dong Thap University, Vietnam), Protocol for fast screening of multi-target drug candidates: Application to Alzheimer's disease

P6. Tran Thi Minh Thu (ICST, Vietnam), Molecular insight of how Aβ42-G37V reduces toxicity: An in vitro and in silico study

P7. Kiet Ho (ICST, Vietnam), Screening potential inhibitors for cancer target LSD1 from natural products by steered molecular dynamics

P8. Pham Dinh Quoc Huy (IP PAS, Poland), Fullerenol $C_{60}(OH)_{16}$ prevents amyloid fibrillization of $A\beta_{40}$ – *in vitro* and *in silico* approach

P9. Mori Takaharu (RIKEN, Japan), Cryo-EM flexible fitting for large bimolecular systems

P10. Duy Tran (University of Technology, HCM city, Vietnam),In silico study of Bombyx Mori Fibroin N Terminal Domain by Graphene