



北京大学定量生物学中心
CENTER FOR QUANTITATIVE BIOLOGY

The 3rd Worldwide Chinese Computational Biology Conference

第三届世界华人计算生物学大会

Online Meeting

August 3-6, 2020



Website



Webcast





北京大学定量生物学中心
CENTER FOR QUANTITATIVE BIOLOGY

Host:

Center for Quantitative Biology (CQB) at Peking University (<http://cqb.pku.edu.cn/en/>)

Organization Committee:

Chair: Luhua Lai, Chao Tang

Secretary-general: Chen Song

Members: Fangting Li, Zhiyuan Li, Zhirong Liu, Jianfeng Pei, Letian Tao, Changsheng Zhang, Lei Zhang

Contact:

Dr. Chunmei Li

Email: qbio@pku.edu.cn

Tel: +86-10-62759599

Fax: +86-10-62759595

Academic Committee:

Zexing Cao, Qiang Cui, Yong Duan, Weihai Fang, Jiali Gao, Yiqin Gao, Tingjun Hou, Xuhui Huang, Hualiang Jiang, Luhua Lai, Guohui Li, Xiaoqiao Lin, Haiyan Liu, Haibin Luo, Rui Luo, Qi Ouyang, Yibing Shan, Chao Tang, Yuhai Tu, Renxiao Wang, Wei Wang, Wenning Wang, Guanghong Wei, Guowei Wei, Yundong Wu, Xin Xu, Shengyong Yang, Wei Yang, Weitao Yang, Changguo Zhan, Yingkai Zhang, Zenghui Zhang, Huanxiang Zhou, Ruhong Zhou, Yaoqi Zhou

Conference Website:

<https://qbio.pku.edu.cn/CB2020>

Sponsors:

Peking-Tsinghua Center for Life Sciences

Beijing Bioinformatics Research Society

Biophysical Society of China-Academic Committee of Bioinformatics and Theoretical Biophysics



北京大学定量生物学中心
CENTER FOR QUANTITATIVE BIOLOGY

Webcast:

<https://www.koushare.com/live/liveroom?islive=0&lid=394&roomid=132792>



Conference Website and Program Download

<https://qbio.pku.edu.cn/CB2020>



Monday, August 3rd

8:15-8:30	Opening: ZHANG, Zenghui & LAI, Luhua	
Session 1 (Chair: LI, Zhiyuan)		
8:30-9:10	TANG, Lei-Han Hong Kong Baptist University	Calibrated Intervention and Containment of the COVID-19 Pandemic
9:10-9:50	DONG, Hao Nanjing University	A stochastic particle dynamics model for predicting epidemics
9:50-10:15	ZHU, Huaqiu Peking University	TBA
Break		
Session 2 (Chair: DONG, Hao)		
10:25-11:05	DING, Qiang Tsinghua University	Functional and Genetic Analysis of Viral Receptor ACE2 Orthologs Reveals a Broad Potential Host Range of SARS-CoV-2
11:05-11:45	LUO, Haibin Sun Yat-Sen University	Free energy perturbation-based virtual screening against COVID-19 and clinical validation
11:45-12:10	ZHANG, Lu Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences	Role of 1'-Ribose Cyano Substitution for Remdesivir to Effectively Inhibit both Nucleotide Addition and Proofreading in SARS-CoV-2 Viral RNA Replication
Break		
Session 3 (Chair: WANG, Yibo)		
13:30-14:10	LAI, Luhua Peking University	Prediction of targeted cancer drug resistance
14:10-14:50	OUYANG, Defang University of Macau	Integrated computer-aided formulation design: A case study of andrographolide/ cyclodextrin ternary formulation
14:50-15:15	XIA, Kelin Nanyang Technological University	Topology Data Analysis (TDA) Based Machine Learning Models for Drug Design
15:15-15:40	WU, Ruibo Sun Yat-Sen University	GM-DockZn: A Geometry Matching based Docking Algorithm for Zinc Proteins
Break		
Session 4 (Chair: WU, Ruibo)		
15:55-16:35	WEI, Dongqing Shanghai Jiao Tong University	人工智能与精准药物发现：大数据时代的个性化药物设计
16:35-17:15	YANG, Yuedong Sun Yat-Sen University	Effective Deep Learning for Protein-drug interactions
17:15-17:40	LI, Zhe Sun Yat-Sen University	Development of FEP-ABFE method and its applications in drug discovery
17:40-18:05	WANG, Yibo Changchun Institute of Applied Chemistry, Chinese Academy of Sciences	靶向跨膜蛋白-蛋白相互作用的药物发现
Break		
Session 5 (Chair: XIA, Kelin)		
19:30-20:10	ZHAN, Changguo University of Kentucky	Power of computational design in drug discovery and development: A journey from in silico to clinical studies
20:10-20:50	ZHANG, Yingkai New York University	Integrating Machine Learning and Molecular Modelling for Drug Design
20:50-21:30	PEI, Jianfeng Peking University	AI-Assisted Drug Design

Tuesday, August 4th

Session 1 (Chair: WANG, Binju)		
8:30-9:10	ZHOU, Huanxiang University of Illinois at Chicago	Correlated Segments and Fuzzy Membrane Association of Intrinsically Disordered Proteins
9:10-9:50	LIU, Yajun Beijing Normal University	Tuning Color and Activity of Calcium-regulated Photoprotein Luminescence
9:50-10:15	MEI, Ye East China Normal University	Adaptive QM/MM via the Reference-Potential Method
Break		
Session 2 (Chair: MEI, Ye)		
10:25-11:05	MU, Yuguang Nanyang Technological University	OnionNet: a multiple-layer inter-molecular contact based convolutional neural network for protein-ligand binding affinity prediction
11:05-11:45	ZHAO, Yilei Shanghai Jiao Tong University	Specific Regio- and Enantioselectivity of Fluostatin Conjugation
11:45-12:10	WANG, Binju Xiamen University	Deciphering the Enigmatic Oxygen Activation and Methane Oxidation Mechanisms by Particulate Methane Monooxygenase
Break		
Session 3 (Chair: ZHU, Tong)		
13:30-14:10	GAO, Yiqin Peking University	From dinucleotide to chromatin, a domain segregation perspective for chromatin structure change in development, differentiation, senescence and certain diseases
14:10-14:50	LI, Guohui Dalian Institute of Chemical Physics, Chinese Academy of Sciences	生物体系多尺度理论研究的方法发展及应用
14:50-15:15	HAN, Wei Peking University Shenzhen Graduate School	Bottom-Up Derived Flexible Water Model with Dipole and Quadrupole Moments for Multiscale Molecular Simulations
15:15-15:40	XIU, Peng Zhejiang University	A novel multiscale scheme to accelerate atomistic simulations of bio-macromolecules by adaptively driving coarse-grained coordinates
Break		
Session 4 (Chair: HAN, Wei)		
15:55-16:35	ZHANG, Zenghui NYU Shanghai	蛋白质相互作用及自由能计算研究
16:35-17:15	ZHANG, Linfeng Beijing Institute of Big Data Research	Learning assisted modeling for molecular simulation
17:15-17:40	ZHU, Tong East China Normal University	Force Field Development for Metalloproteins with Artificial Neural Networks
17:40-18:05	ZHANG, Zhiyong University of Science and Technology of China	Phase Separation of FUS-LC investigated by Multiscale Modeling
Break		
Session 5		
19:30-21:30	Flash Talk and Poster	

Wednesday, August 5th

Session 1 (Chair: YU, Jin)		
8:15-8:55	CUI, Qiang Boston University	Functional plasticity and evolutionary adaptation of allosteric regulation
8:55-9:35	HUANG, Xuhui The Hong Kong University of Science and Technology	Memory Kernels of Protein Conformational Dynamics
9:35-10:00	ZHU, Lizhe The Chinese University of Hong Kong (Shenzhen)	Assessing the performance of Travelling-salesman based Automated Path Searching (TAPS) on complex biomolecular systems
Break		
Session 2 (Chair: ZHU, Lizhe)		
10:10-10:50	SHAN, Yibing D.E.Shaw Research	Structural modeling of large biomolecular assemblies--case studies on full-length JAK2 kinase and on Ras-Raf signalosome
10:50-11:30	MA, Jianpeng Fudan University	TBA
11:30-11:55	LI, Jianing The University of Vermont	Targeting Stress-Related GPCRs for Next-Generation Pain Treatments
11:55-12:20	YU, Jin University of California, Irvine	Simulating Protein Stepping along DNA
Break		
Session 3 (Chair: ZHAO, Suwen)		
13:30-14:10	LI, Shuhua Nanjing University	TBA
14:10-14:50	CHEN, Haifeng Shanghai Jiao Tong University	Environmental Specific Precise Force Field for Intrinsically Disordered and Ordered Proteins
14:50-15:15	DUAN, Mojie Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences	The Regulation of Phosphorylation on the Structures and Interactions of Intrinsically Disordered Proteins
15:15-15:40	WANG, Beibei University of Electronic Science and Technology of China	Release of empty nanodiscs from charged droplets in the electrospray ionization process: A molecular dynamics study
Break		
Session 4 (Chair: DUAN, Mojie)		
15:55-16:35	MA, Jing Nanjing University	A Data-Driven Accelerated (DA2) Sampling Method for Searching Functional States of Proteins
16:35-17:15	LIU, Haiyan University of Science and Technology of China	Statistical energy functions for de novo protein design
17:15-17:40	ZHAO, Suwen ShanghaiTech University	Discovery of universal activation mechanism of class A GPCRs by residue-residue contact score
17:40-18:05	WANG, Yong University of Copenhagen	Integrative Ensemble Modeling of a Mitochondria Chaperone-Membrane Protein Complex Using Incomplete and Ambiguous Experimental Information
Break		
Session 5 (Chair: SONG, Chen)		
19:30-20:10	YANG, Wei Florida State University	Energy Sampling of Long-Timescale Biomolecular Dynamics: the Energy Flow Viewpoint
20:10-20:50	CHENG, Yuan-Chung National Taiwan University	Theoretical study on the dynamics of light harvesting in the Photosystem II
20:50-21:30	WEI, Guanghong Fudan University	Molecular simulation study of peptide self-assembly and amyloid fibril inhibition by natural small molecules

Session 1 (Chair: GONG, Haipeng)		
8:30-9:10	ZHOU, Yaoqi Griffith University	Identifying molecular recognition features in intrinsically disordered regions of proteins by transfer learning
9:10-9:50	XU, Jinbo Toyota Technological Institute at Chicago	Latest development of deep learning for protein folding
9:50-10:15	GONG, Xinqi Renmin University of China	Multimer protein complex structure prediction by machine learning
Break		
Session 2 (Chair: GONG, Xinqi)		
10:30-11:10	XU, Xin Fudan University	New insights into the ion- π interactions
11:10-11:50	GONG, Haipeng Tsinghua University	Protein inter-residue distance prediction and enhanced sampling
11:50-12:15	YUAN, Shuguang Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences	Enhancing the Signaling of GPCRs via Orthosteric Ions
Break		
Session 3 (Chair: ZHANG, Lei)		
13:30-14:10	LI, Hao University of California, San Francisco	Deciphering the Genetic Determinants of Complex Human Traits through an Integrative Analysis of GWAS and Intermediate Molecular Trait Data
14:10-14:50	HAO, Nan University of California, San Diego	Divergent trajectories of single-cell aging
14:50-15:30	OUYANG, Qi Peking University	The free energy cost of oscillator synchronization
Break		
Session 4 (Chair: LI, Zhiyuan)		
15:45-16:25	LIU, Chenli Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences	Expanding at the right speed: an evolutionary stable strategy to colonize spatially extended habitats
16:25-17:05	ZHANG, Lei Peking University	Network design principle for dual function of adaptation and noise attenuation
17:05-17:30	WANG, Weikang University of Pittsburgh	Reconstruct cellular dynamics from single cell data
17:30-18:10	LIN, Jie Harvard University	Evolution of microbial traits under serial dilution
Break		
Session 5 (Chair: LIU, Chenli)		
19:30-20:10	CHEN, Luonan Shanghai Institute of Biochemistry and Cell Biology, Chinese Academy of Sciences	Constructing single cell specific networks
20:10-20:50	TANG, Chao Peking University	Oscillation, phase locking and Arnold tongues in pancreatic islets
20:50-21:00	Closing: TANG, Chao	