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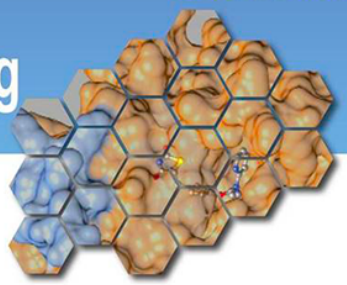
The 2021 ISQBP President's Meeting



June 29th - July 1st, 2021

Online meeting, Strasbourg - France

Tuesday, June 29, 2021[1]	
16:00	**Opening comments**
	Roland H. Stote, IGBMC, CNRS - France
16:15	**Free-Energy Calculations Guide Drug Discovery for SARS-CoV-2**
	William Jorgensen, Department of Chemistry, Yale University - United States
16:45	**Molecular elucidation of the antibiotic resistance mechanism of New Delhi metallo-β-lactamase 1**
	Alessio Prunotto, Institute of Bioengineering, École Polytechnique Fédérale de Lausanne, and Department of Oncology, Ludwig Institute for Cancer Research, University of Lausanne - Switzerland
17:00	Pause
17:15	**The structure, dynamics and chloride conductance of WT and mutant CFTR as gleaned from MD simulations**
	Hanoch Senderowitz, Department of Chemistry, Bar-Ilan University - Israel
17:30	**Structural analysis of the interaction between the SARS-CoV-2 Spike protein and the human ACE2 receptor and druggable pockets identification to inhibit the SARS-CoV-2 viral entry**
	Mariem Ghoula, Unité de Biologie Fonctionnelle et Adaptative -- INSERM U1133, CNRS UMR 8251, Université de Paris - France
17:45	**Gilda Loew Award Lecture** **Studies of ion channel activation and modulation using computational approaches**
	Carmen Domene, Department of Chemistry, University of Bath - United Kingdom
18:30	GROUP PHOTO
18:30	Break, Poster and Networking session
20:00	**Path sampling methodology for membrane permeability simulations**
	Ana Ghysels, IBiTech - Biommeda Group, Ghent University - Belgium
20:15	**Accelerated Molecular Dynamics to Explore Binding of Transition Metals to Amyloid-β**
	Jamie Platt, School of Chemistry, Cardiff University - United Kingdom
20:30	**Alzheimer's is an Autoimmune Disease: An In Silico Study**
	Don Weaver, Krembil Brain Institute, University of Toronto - Canada
20:45	Pause
21:00	**Modelling the Peculiar Reactivity of the Molecular Chaperone Trap1**
	Stefano Serapian, University of Pavia - Italy

21:15	**Syk association with immune receptors, a unique entropy-driven mechanism to regulate protein interactions by phosphorylation**
	Carol Post, Purdue University, West Lafayette, IN - United States
22:00	Close for the day
Wednesday, June 30, 2021	
16:00	**Multiscale simulation for chemical biology: from enzyme evolution to interactive drug design in virtual reality**
	Adrian Mulholland, Centre for Computational Chemistry, School of Chemistry, University of Bristol - United Kingdom
16:30	**Biodegrading plastic and other mechanistic studies**
	Maria Ramos, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto - Portugal
17:00	Pause
17:15	**Moving pictures: Reassessing docking experiments with a dynamic view of protein interfaces**
	Sophie Sacquin-Mora, Laboratoire Biochimie Théorique CNRS UPR9080 (LBT) – CNRS – IBPC - France
17:30	**Computational Biology Award Lecture** **CHARMM Additive and Drude Polarizable Force Fields: The Long and Winding Road....to....Hey Jude**
	Alex MacKerell, Computer-Aided Drug Design Center, Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland - United States
18:00	Break, Poster and Networking session
19:45	**Component Thermodynamics in Phase Separations**
	Montgomery Pettitt, The University of Texas Medical Branch - United States
20:15	**Challenges in Protein Sequencing using 2-D MoS2 Nanopores : Answers from all-atom Molecular Dynamics**
	Adrien Nicolaï, Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), UMR 6303 CNRS - Université de Bourgogne Franche-Comté - France
20:30	Pause
20:45	**Nanocapsule Designs for Antimicrobial Resistance**
	Franca Fraternali, Randall Centre for Cell and Molecular Biophysics, King's College London - United Kingdom
21:15	**High-throughput free energy methods for ligand discovery and design using multi-site λ-dynamics**
	Charles L. Brooks, III, Departments of Chemistry and Biophysics, University of Michigan - United States
22:00	Close for the day
Thursday, July 1, 2021	
16:00	**Simulating epigenetic variants of DNA**
	Modesto Orozco, University of Barcelona - Spain
16:30	**Recent successes in the simulation of nucleic acid structures**
	Thomas E. Cheatham, University of Utah - United States

17:15	Pause
17:30	**Simulations of hERG PAS Domain**
	Lennart Nilsson, Karolinska Institutet - Sweden
18:00	**An Asymmetric Mechanism in a Symmetric Molecular Machine**
	Marco Cechinni, Institut de Chimie de Strasbourg – UMR7177 – University of Strasbourg - France
18:30	Break, Poster and Networking session
20:00	**Enhanced Antibody-Fc Receptor Interactions Revealed by Antibody Glycoengineering and Replica Exchange Simulations**
	Gene Chong, University of Maryland Baltimore - United States
20:15	**Breaths, twists, and turns of atomistic nucleosomes with or without interaction partners**
	Vlad Cojocaru, Hubrecht Institute - Netherlands
20:30	**Antibodies exhibit multiple paratope states influencing VH–VL domain orientations**
	Klaus Liedl, University of Innsbruck - Austria
21:00	Closing comments
22:00	

[1] The program is based on the Strasbourg local time (UTC+2)

Posters will accessible outside of session hours over the course of the meeting.

Poster Presentations June 29, 2021

Investigations of immune stimulatory single stranded DNA by biomolecular simulations and NMR, Barna Tóth [et al.]

Homo- and heterodimers bHLH transcription factors induce different deformation of supercoiled DNA: a potential transcriptional regulation mechanism, Johanna Hörberg [et al.]

Deeprank-GNN: A Graph Neural Network Framework to Learn Interaction Patterns from Protein-Protein Interfaces, Manon Réau [et al.]

Accurate receptor-ligand binding free energies from QM conformational chemical space sampling,Matthias Stein [et al.]

Insights into antibiotic breakdown by class D β-lactamases through multiscale simulations,Viivi Hirvonen [et al.]

A Machine Learning Classifier to Select Water-Ligand Interactions to Facilitate Empirical Force Field Optimization, Frank Horrigan [et al.]

Multiscale Simulations of Radical Cation Guanine in the Nucleosomal DNA, Elise Dumont [et al.]

Shark Antibody Variable Domains Rigidify Upon Affinity Maturation - Under- standing the Potential of Shark Immunoglobulins as Therapeutics, Clarissa Amanda Seidler [et al.]

Implicit Solvent Model for the Polarizable Drude Force Field and its application forpKaprediction, Alexey Aleksandrov [et al.]

How contribution of higher-order proximal distribution functions influence the solvent structure, Razie Yousefi

Conformational changes regulate the half-life of proteins of the Bcl-2 family, Luis Alberto Caro-Gómez [et al.]

Ensembles in solution as a new paradigm for antibody structure prediction and design, Monica Fernandez-Quintero [et al.]

Coarse-grained modelling of ionic and DNA transport through nanopores, Nathalie Basdevant [et al.]

Intermolecular Electrostatic Interactions in the Short Range: a Quantum Chemical Topology Analysis, Fernando Jiménez-Grávalos [et al.]

The directional vinculin-actin catch-bond: a molecular mechanism of biomechanical properties under force, Aubin Ramon [et al.]

Ion and Water Interactions with a Biomimetic Nanopore: Molecular Dynamics with Effective Polarization, Linda X. Phan [et al.]

Structural and Conformational study of FMN-containing miniSOG, Oksana Azpitarte [et al.]

Structural mechanism of Fab domain dissociation as a measure of interface stability, Nancy Pomarici [et al.]

Solvation Thermodynamics in Ionic Solution: an Extension of Grid Inhomogeneous Solvation Theory Predicts Salting-Out Coefficients, Franz Waibl [et al.]

Development of the Site-Identification by Ligand Competitive Saturation (SILCS) Methodology for Targeting RNAs with Small-molecules, Abhishek A. Kognole [et al.]

The importance of 29RAPRKKG35 linker region for HIV-1 virion structure and infectivity: a molecular dynamic study, Nedjoua Drici

A single-point mutation in the aminoglycoside-regulated riboswitch affects its dynamics and activity, Piotr Chyży [et al.]

AGIST for All, Johannes Kraml [et al.]

Poster Presentations June 30, 2021

Thermosensitive Hydration – Solvation Entropy Determines Conformational Ensemble, Patrick K. Quoika [et al.]

Amino acids intercalated into bioinorganic clays: molecular understanding of binding modes in ananoconfined aqueous environment, Vishal Kumar Porwal [et al.]

Étude des propriétés dynamiques et des interactions du domaine effecteur (dimère) de la protéine NS1 du virus de l'influenza A, Sarah Naceri [et al.]

Path sampling methods for protein-ligand binding kinetics, Wouter Vervust [et al.]

Structural analysis and conformational rearrangement of the human Insulin Degrading Enzyme, Mariem Ghoula [et al.]

Evaluation of AutoDock and AutoDock Vina on the CASF-2013 benchmark, Thomas Gaillard

Molecular dynamics simulations of hydrophobic gating in the TMEM175 channel: the effect of polarisability and water model, Charlotte Lynch [et al.]

DNA packaging in bacteriophages: The effect of DNA – capsid interactions, Cecilia Bores [et al.]

Investigating Ion-Exchange Adsorption of Proteins through Experiments and Molecular Dynamics Simulations, Marine Tournois [et al.]

Characterizing Immunoglobulin Inter-Domain Orientations, Valentin Hoerschinger

Surprisingly Fast Interface and Elbow Angle Dynamics of Antigen-Binding Fragments, Katharina Kroell [et al.]

Molecular dynamics as a supporting tool for refinement of the new MC4R Cryo-EM active

structure, Fabrizio Fierro [et al.]

The simulation of amyloid-beta (Aβ) aggregation considering in vivo conditions, Hebah Fatafta [et al.]

Towards better understanding of sweet-tasting molecules, Yaron Ben Shoshan-Galeczki [et al.]

Deep learning protein conformational space with convolutions and latent interpolations, Samuel Musson [et al.]

Discovering three-dimensional biomolecular shapes for a small number of two-dimensional XFEL diffraction patterns, Sandhya Tiwari [et al.]

New Quinolines Derivatives for Antimalarial activity: Docking, ADMET and Drug-likeness Studies, Khadidja Bellifa [et al.]

Averting side effects and improving specificity and efficacy of novel μ-opioid receptor (MOR) agonists guided by Site Identification by Ligand Competitive Saturation (SILCS), Payal Chatterjee [et al.]

Irreversible Cu(I) Transfer From Atx1 to Ccc2 Protein: A Theoretical Study, Rajapandian Varatharaj

Design of a Novel Multi Epitope-Based Vaccine for Pandemic Coronavirus Disease (COVID-19) by Vaccinomics and Probable Prevention Strategy against Avenging Zoonosis, Syed Sikander Azam

Inhibiting RNA:Protein Interactions using an Integrative Computational and Experimental Approach: Application to Y Box Binding Protein 1, Krystel El Hage [et al.]

Determination of Vibrational Circular Dichroism spectra of biomolecules through a classical dynamic approach using polarisable force fields, Jessica Bowles [et al.]

Divalent Cations and Ribozyme Catalysis : a Molecular Dynamics Study, Julie Puyo

Poster Presentations July 1, 2021

Missense mutations modify the α-helix and β-sheet content of the conformational ensemble of α-synuclein monomer which exhibits a two-phase characteristic, Adrien Guzzo [et al.]

Parameterization Made Easy With ParaMol, João Morado [et al.]

Effect of Resonance Width in the Investigation of Dissociative Electron Attachment Cross–Section to Some Bio Molecules, Manabendra Sarma

Capturing Water Networks During Ligand Binding with the Site-Identification by Ligand Competitive Saturation Approach, Himanshu Goel [et al.]

Inhibitors of human neutrophil elastase against proteinase 3: A multisite lambda dynamics

(MSLD) study, Parveen Gartan [et al.]

Quantum and classical effects in DNA point mutations: Watson-Crick tautomerism in AT and GC basepairs, Louie Slocombe [et al.]

Modelling DNA in complex 3D rearrangements, Agnes Noy

Enhanced Sampling Molecular Dynamics, Maximum Entropy Reweighing, and HDX-MS Guided Ensemble Modeling: an approach to characterize the structure and dynamics of the cytoplasmic heme binding protein PhuS., Kyle Kihn [et al.]

Additive CHARMM36 Force Field for Nonstandard Amino Acids, Anastasia Croitoru [et al.]

SerraNA/SerraLINE: Programs for analysing structural and flexibility properties of nucleic acids from simulation data, Victor Velasco

Flexibility of homotetrameric pteridine reductase 1 enzyme from trypanosomatid human parasites in the complex with ligands, studied by molecular dynamics techniques., Joanna Panecka-Hofman [et al.]

CHARMM General Force Field (CGenFF) Compass: A Lexical Dictionary Bridge from Functional Groups to their Atom Types., Suliman Sharif

Structural analysis of Odorant-Binding Proteins for gas sensing, Arménio Barbosa [et al.]

Functionalization of the alkaline earth metal oxide BeO, MgO, CaO with alkaline metal oxide - the acid-base catalytic properties, Faron Dawid [et al.]

Specificity of Loxosceles α clade Phospholipase D enzymes for choline-containing lipids: role of a conserved aromatic cage, Emmanuel E. Moutoussamy [et al.]

Exploring the effects of the F310S mutation on the structural dynamics of the PPARγ nuclear receptor, Ana Milinski [et al.]

Rapid and accurate estimation of protein–ligand relative binding affinities using site-identification by ligand competitive saturation, Himanshu Goel [et al.]

Rational design of modulators of skeletal myosin, Anna Katarina Antonovic [et al.]

Application of molecular dynamics to elucidation of the mechanism of glucose net and exchange transport via GLUT1, Saul Gonzalez [et al.]

Differential electrostatic properties of reaction model as a tool for prediction and reverse design of catalytic properties, Paweł Kedzierski [et al.]

Towards the elucidation of a glucocorticoid and mineralocorticoid receptor ligand binding domain common dimerization interface, Laurent Bianchetti [et al.]