

SCHOOL:
COMPUTER SIMULATIONS OF BIOLOGICAL MEMBRANES
&
FREE ENERGY CALCULATIONS OF BIOMOLECULAR SYSTEMS

VENUE: University of Los Andes, Bogotá, Colombia

DATE: August 13-17, 2018

PROGRAM OVERVIEW

	Monday (13.08)	Tuesday (14.08)	Wed. (15.08)	Thursday (16.08)	Friday (17.08)
8:00 – 9:00	Registration				
9:00 – 9:30	Welcome				
9:30 - 10:30	Bert de Groot	Thomas Walz (webinar) ML-C	Chad Leidy	Gian Pietro Miscione	Bert de Groot ML-C
				Contributed talk 4	
10:30 – 11:00	Coffee break				
11:00 – 12:00	Helgi Ingólfson	Gerhard Hummer ML-C	Contributed talk 2	Esteban Vohringer- Martínez	Vytas Gapsys ML-C
			Contributed talk 3		
12:00 – 14:00	Lunch		Free program	Lunch	
14:00 – 15:00	Gerhard Hummer	Bert de Groot ML-C		Andrés González	Hands on ML-C
15:00 – 15:30	Vytas Gapsys ML-C	Helgi Ingólfson ML-C		Coffee break	
15:30 – 16:00	Contributed talk 1 ML-C			Contributed talk 5	Closing remarks & departure ML-C
16:00 – 16:30	Coffee break			Contributed talk 6	
16:30 – 17:00	Heading to computer room			Heading to computer room	
17:00 – 19:00	Hands on	Hands on ML-C		Poster session	

PROGRAM IN DETAIL

PART 1: COMPUTER SIMULATIONS OF BIOLOGICAL MEMBRANES			
Monday, August 13			
Time	Room		
8:00 – 9:00		Registration	
9:00 – 9:30		Welcome	
9:30 – 10:30		Bert de Groot (MPIBPC, Göttingen)	The molecular dynamics of solute permeation through biological membranes and membrane proteins
10:30 – 11:00		Coffee break	
11:00 – 12:00		Helgi Ingólfson (LLNL, Livermore)	Coarse-grained simulations: introduction and application to membranes
12:00 – 14:00		Lunch	
14:00 – 15:00		Gerhard Hummer (MPIB, Frankfurt)	tba
15:00 – 15:30		Vytautas Gapsys (MPIBPC, Göttingen)	tba
15:30 – 16:00		Contributed talk 1: Florian Franz (IWR, Heidelberg)	Stability of Biological Membranes upon Mechanical Indentation
16:00 – 16:10		Photo	
16:10 – 16:40		Coffee break	
16:40 – 17:00		Heading to computer room	
17:00 – 19:00		Hands on: all-atom MD simulations of biological membranes	
19:00 –		Invited speakers dinner	
Tuesday, August 14			
9:30 – 10:30		Webinar, Thomas Walz (Rockefeller, New York)	Electron Microscopy Approaches to Studying Lipid-Protein Interactions
10:30 – 11:00		Coffee break	
11:00 – 12:00		Gerhard Hummer (MPIB, Frankfurt)	tba
12:00 – 14:00		Lunch	
14:00 – 15:00		Bert de Groot (MPIBPC, Göttingen)	Permeation, selectivity and gating of ion channels studied by computational electrophysiology
15:00 – 16:00		Helgi Ingolfson (LLNL, Livermore)	Capturing biological membranes in silico at different compositional complexity
16:00 – 16:40		Coffee break	
16:40 – 17:00		Heading to computer room	
17:00 – 19:00		Hands on: coarse-grained MD simulations of biological membranes	
Wednesday, August 15			
9:30 – 10:30		Chad Leidy (UANDES, Bogotá)	Integrating Computational and Experimental Approaches to InvestigateAntimicrobial Peptide Activity in Membranes
10:30 – 11:00		Coffee break	
11:00 – 11:30		Contributed talk 2:	Exponential consensus ranking improves outcome in docking and

		Karen Palacio Rodríguez (UDEA, Medellín)	<i>receptor ensemble docking</i>
11:30 – 12:00		Contributed talk 3: Sergio Mares-Samano (UNAM, México City)	<i>Molecular dynamics studies of the solvation effects of water and trifluoroethanol on the peptides pandinin-2 (pin2) and pin2-GVG</i>
12:00 –		free program	
PART 2) FREE ENERGY CALCULATIONS OF BIOLOGICAL SYSTEMS			
Thursday, August 16			
9:00 – 10:00		Gian Pietro Miscione (UANDES, Bogotá)	<i>Mechanism of L-Tryptophan Prenylation, Catalyzed by FgaPT2: a Computational Study</i>
10:00 – 10:30		Contributed talk 4: Hugo J. Bohórquez (FIDIC, Bogotá)	<i>The frozen molecule approach in peptide-protein binding energies</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		Esteban Vohringer-Martínez (CONCEPCIÓN, Concepción)	<i>Force field improvement with ab-initio methods</i>
12:00 – 14:00		Lunch	
14:00 – 15:00		Andrés González (UANDES, Bogotá)	<i>Applications of product design departing from free energy calculations</i>
15:00 – 15:30		Coffee break	
15:30 – 16:00		Contributed talk 5: Angélica Sandoval (UANDES, Bogotá)	<i>Specific at one side unspecific at the other: the interaction of blood proteins with extracellular DNA</i>
16:00 – 16:30		Contributed talk 6: Stefany Botero Rodríguez (UNAL, Bogotá)	<i>Computational Tracing of Protein and ncRNA epitopes inside Dengue Virus</i>
16:30 – 17:00		Heading to poster room	
17:00 – 19:00		Poster session (with wine and finger food)	
Friday, August 17			
9:30 – 10:30		Bert de Groot (MPIBPC, Göttingen)	<i>Introduction to alchemical free energy calculations</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		Vytas Gapsys (MPIBPC, Göttingen)	<i>tba</i>
12:00 – 14:00		Lunch	
14:00 – 16:00		Hands on: Free energy calculations	
16:00 – 17:00		Closing remarks and departure	

POSTERS

1	Diego Gomez Hernandez (UDISTRITAL, Bogotá)	<i>In silico evaluation of the potential affinity of anandamide analogues for CB1 receptor.</i>
2	Carlos Pinilla UNORTE, Barranquilla	<i>FeS alloys at conditions of the Earth Interior</i>
3	Juan David Orjuela UANDES, Bogotá	<i>Effect of the lipid-protein interaction on the assembly of the platelet Glycoprotein-IB</i>
4	Markus Kurth Heidelberg U. Heidelberg	<i>Probing the lipid environment of the Metabotropic glutamate receptor 2</i>
5	Laura Pinto Herrera UANDES, Bogotá	<i>Effect of particulate matter on the lung surfactant at a high altitude city: Review</i>
6	Johann Bedoya Cardona UNAL, Medellín	<i>Applicability of some force field parameters of biomolecules to model the surface tension of hexadecane</i>
7	Yaritza Fortaleché Rodríguez UNAL, Bogotá	<i>Agonist, antagonist or super-activator effect of different ligands in the receptor-ligand interaction of the TraR protein</i>
8	Paula Giraldo Hincapié UNAL, Medellín	<i>Understanding insecticide peptides: Modeling peptide-membrane interactions with Molecular Dynamics</i>
9	Jessica Martinez UAN, Bogotá	<i>Does Using Virtual Sites in Proteins Affect the Protein Fold?</i>
10	Juan Zarate Moreno SENA, Bogotá	<i>Kinetic models for chitosan membranes on biological systems, a computational approach.</i>
11	Cesar Quintana Cataño UANDES, Bogotá	<i>Force spectroscopy of T4 bacteriophage adhesion during infection.</i>
12	Santiago Agudelo Gómez UDEA, Medellín	<i>Preferred sites of glycosaminoglycans in the envelope protein of the Zika virus</i>
13	Alberto Mario Castillo UBJTL, Bogotá	<i>Spring Network Model of Trypanosoma Cruzi bloodstream trypomastigote</i>
14	Gesivaldo Santos State U. Bahia	<i>Autism Spectro Disorder & Alzheimer Disease: different conditions linked by mTOR pathway</i>
15	Helman Amaya Espinosa UANDES, Bogotá	<i>Cooperative dynamics of self-interacting Biopolymers in blood elucidated by Coarse-Grained Brownian Dynamics Simulations</i>
16	Valeria Mejía Restrepo UANDES, Bogotá	<i>The effect of G1324A and G1324S mutations on the complex formed by the von Willebrand factor A1 domain and the glycoprotein Iba-platelet receptor, studied through molecular dynamics simulations and free energy calculations.</i>
17	Andrés Cifuentes López UDISTRITAL, Bogotá	<i>In silico evaluation of the potential affinity of anandamide analogues for CB1 receptor</i>
18	Jhoan Ortiz Giron UDEA, Medellín	<i>A novel methodology for cryo-EM map validation</i>
19	Adrian Orjuela UNAL, Bogotá	<i>tba</i>