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			Gian Pietro Miscione	Bert de Groot ML-C
9:30 - 10:30	Bert de Groot	Thomas Walz (webinar) ML-C	Chad Leidy	Contributed talk 4	
10:30 – 11:00	Coffee break				
11:00 – 12:00	Helgi Ingólfson	Gerhard Hummer ML-C	Contributed talk 2 / Contributed talk 3	Esteban Vohringer-Martínez	Vytas Gapsys ML-C
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	Coffee break			Coffee break	
15:30 – 16:30	Vytas Gapsys ML-C	Helgi Ingólfson ML-C		Contributed talk 5	
	Contributed talk 1 ML-C			Contributed talk 6	Closing remarks & departure ML-C
16:30 – 17:00	Heading to computer room			Heading to posters	
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 – 15:10		Photo
15:10 – 15:30		Coffee break
15:30 – 16:10		**Vytautas Gapsys (MPIBPC, Göttingen)**	*tba*
16:10 – 16:40		**Contributed talk 1: Florian Franz (IWR, Heidelberg)**	*Stability of Biological Membranes upon Mechanical Indentation*
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 – 15:30		Coffee break
15:30 – 16:30		**Helgi Ingolfson (LLNL, Livermore)**	*Capturing biological membranes in silico at different compositional complexity*
16:30 – 16:45		Heading to computer room
16:45 – 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)	*receptor ensemble docking*
11:30 – 12:00		**Contributed talk 3: Sergio Mares-Samano (UNAM, México City)**	*Molecular dynamics studies of the solvation effects of water and trifluoroethanol on the peptides pandinin-2 (pin2) and pin2-GVG*
12:00 –		free program	

PART 2) FREE ENERGY CALCULATIONS OF BIOLOGICAL SYSTEMS			
Thursday, August 16			
9:00 – 10:00		**Gian Pietro Miscione (UANDES, Bogotá)**	*Mechanism of L-Tryptophan Prenylation, Catalyzed by FgaPT2: a Computational Study*
10:00 – 10:30		**Contributed talk 4: Hugo J. Bohórquez (FIDIC, Bogotá)**	*The frozen molecule approach in peptide-protein binding energies*
10:30 – 11:00		Coffee break	
11:00 – 12:00		**Esteban Vohringer-Martínez (CONCEPCIÓN, Concepción)**	*Force field improvement with ab-initio methods*
12:00 – 14:00		Lunch	
14:00 – 15:00		**Andrés González (UANDES, Bogotá)**	*tba*
15:00 – 15:30		Coffee break	
15:30 – 16:00		**Contributed talk 5: Angélica Sandoval (UANDES, Bogotá)**	*Specific at one side unspecific at the other: the interaction of blood proteins with extracellular DNA*
16:00 – 16:30		**Contributed talk 6: Stefany Botero Rodríguez (UNAL, Bogotá)**	*Computational Tracing of Protein and ncRNA epitopes inside Dengue Virus*
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)**	*Introduction to alchemical free energy calculations*
10:30 – 11:00		Coffee break	
11:00 – 12:00		**Vytas Gapsys (MPIBPC, Göttingen)**	*tba*
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)**	*In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor.*
2	**Carlos Pinilla UNORTE, Barranquilla**	*FeS all0ys at conditions of the Earth Interior*
3	**Juan David Orjuela UANDES, Bogotá**	*Effect of the lipid-protein interaction on the assembly of the platelet Glycoprotein-IB*
4	**Markus Kurth Heidelberg U. Heidelberg**	*Probing the lipid environment of the Metabotropic glutamate receptor 2*
5	**Laura Pinto Herrera UANDES, Bogotá**	*Effect of particulate matter on the lung surfactant at a high altitude city: Review*
6	**Johann Bedoya Cardona UNAL, Medellín**	*Applicability of some force field parameters of biomolecules to model the surface tension of hexadecane*
7	**Yaritza Fortaleché Rodríguez UNAL, Bogotá**	*Agonist, antagonist or super-activator effect of different ligands in the receptor-ligand interaction of the TraR protein*
8	**Paula Giraldo Hincapie UNAL, Medellín**	*Understanding insecticide peptides: Modeling peptide-membrane interactions with Molecular Dynamics*
9	**Jessica Martinez UAN, Bogotá**	*Does Using Virtual Sites in Proteins Affect the Protein Fold?*
10	**Juan Zarate Moreno SENA, Bogotá**	*Kinetic models for chitosan membranes on biological systems, a computational approach.*
11	**Cesar Quintana Cataño UANDES, Bogotá**	*Force spectroscopy of T4 bacteriophage adhesion during infection.*
12	**Santiago Agudelo Gómez UDEA, Medellín**	*Preferred sites of glycosaminoglycans in the envelope protein of the Zika virus*
13	**Alberto Mario Castillo UBJTL, Bogotá**	*Spring Network Model of Trypanosoma Cruzi bloodstream trypomastigote*
14	**Gesivaldo Santos State U. Bahia**	*Autism Spectro Disorder & Alzheimer Disease: different conditions linked by mTOR pathway*
15	**Helman Amaya Espinosa UANDES, Bogotá**	*Cooperative dynamics of self-interacting Biopolymers in blood elucidated by Coarse-Grained Brownian Dynamics Simulations*
16	**Valeria Mejía Restrepo UANDES, Bogotá**	*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.*
17	**Andrés Cifuentes López UDISTRITAL, Bogotá**	*In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor*
18	**Jhoan Ortiz Giron UDEA, Medellín**	*A novel methodology for cryo-EM map validation*
19	**Adrian Orjuela UNAL, Bogotá**	*tba*