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

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

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 – 16:30		**Webinar, Thomas Walz (Rockefeller, New York)**	***tba***
16:30 – 16:45		Heading to computer room	
16:45 – 19:00		**Hands on: all-atom MD simulations of biological membranes**	
19:00 –		Invited speakers dinner	
Tuesday, August 14			
9:30 – 10:30		**Helgi Ingolfson (LLNL, Livermore)**	*Capturing biological membranes in silico at different compositional complexity*
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 – 16:10		**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: 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

Diego Gomez Hernandez (UDISTRITAL, Bogotá)	*In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor.*
Carlos Pinilla UNORTE, Barranquilla	*FeS all0ys at conditions of the Earth Interior*
Juan David Orjuela UANDES, Bogotá	*Effect of the lipid-protein interaction on the assembly of the platelet Glycoprotein-IB*
Markus Kurth Heidelberg U. Heidelberg	*Probing the lipid environment of the Metabotropic glutamate receptor 2*
Laura Pinto Herrera UANDES, Bogotá	*Effect of particulate matter on the lung surfactant at a high altitude city: Review*
Johann Bedoya Cardona UNAL, Medellín	*Applicability of some force field parameters of biomolecules to model the surface tension of hexadecane*
Yaritza Fortaleché Rodríguez UNAL, Bogotá	*Agonist, antagonist or super-activator effect of different ligands in the receptor-ligand interaction of the TraR protein*
Paula Giraldo Hincapie UNAL, Medellín	*Understanding insecticide peptides: Modeling peptide-membrane interactions with Molecular Dynamics*
Jessica Martinez UAN, Bogotá	*Does Using Virtual Sites in Proteins Affect the Protein Fold?*
Juan Camilo Zarate Moreno SENA, Bogotá	*Kinetic models for chitosan membranes on biological systems, a computational approach.*
Cesar Quintana Cataño UANDES, Bogotá	*Force spectroscopy of T4 bacteriophage adhesion during infection.*
Santiago Agudelo Gómez UDEA, Medellín	*Preferred sites of glycosaminoglycans in the envelope protein of the Zika virus*
Alberto Mario Castillo UBJTL, Bogotá	*Spring Network Model of Trypanosoma Cruzi bloodstream trypomastigote*
Gesivaldo Santos State U. Bahia	*Autism Spectro Disorder & Alzheimer Disease: different conditions linked by mTOR pathway*
Helman Amaya Espinosa UANDES, Bogotá	*Cooperative dynamics of self-interacting Biopolymers in blood elucidated by Coarse-Grained Brownian Dynamics Simulations*
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.*
Andrés Cifuentes López UDISTRITAL, Bogotá	*In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor*
Jhoan Ortiz Giron UDEA, Medellín	*A novel methodology for cryo-EM map validation*
Adrian Orjuela UNAL, Bogotá	*tba*