

**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	Helgi Ingólfson ML-C	Chad Leidy	Gian Pietro Miscione Contributed talk 4	Bert de Groot ML-C
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	<b>Hands on ML-C</b>
15:00 – 15:30	Coffee break			Coffee break	
15:30 – 16:30	Thomas Walz (webinar)	Vytas Gapsys ML-C		Contributed talk 5	
		Contributed talk 1 ML-C		Contributed talk 6	
16:30 – 17:00	Heading to computer room			Heading to posters	
17:00 – 19:00	<b>Hands on</b>	<b>Hands on ML-C</b>		<b>Poster session</b>	

## 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		<b>Bert de Groot (MPIBPC, Göttingen)</b>	<i>The molecular dynamics of solute permeation through biological membranes and membrane proteins</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		<b>Helgi Ingólfson (LLNL, Livermore)</b>	<i>Coarse-grained simulations: introduction and application to membranes</i>
12:00 – 14:00		Lunch	
14:00 – 15:00		<b>Gerhard Hummer (MPIB, Frankfurt)</b>	<i>tba</i>
15:00 – 15:30		Coffee break	
15:30 – 16:30		<b>Webinar, Thomas Walz (Rockefeller, New York)</b>	<i>tba</i>
16:30 – 16:45		Heading to computer room	
16:45 – 19:00		<b>Hands on</b>	
Tuesday, August 14			
9:30 – 10:30		<b>Helgi Ingolfson (LLNL, Livermore)</b>	<i>Capturing biological membranes in silico at different compositional complexity</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		<b>Gerhard Hummer (MPIB, Frankfurt)</b>	<i>tba</i>
12:00 – 14:00		Lunch	
14:00 – 15:00		<b>Bert de Groot (MPIBPC, Göttingen)</b>	<i>Permeation, selectivity and gating of ion channels studied by computational electrophysiology</i>
15:00 – 15:30		Coffee break	
15:30 – 16:10		<b>Vytautas Gapsys (MPIBPC, Göttingen)</b>	<i>tba</i>
16:10 – 16:40		<b>Contributed talk 1: Florian Franz (IWR, Heidelberg)</b>	<i>Stability of Biological Membranes upon Mechanical Indentation</i>
16:40 – 17:00		Heading to computer room	
17:00 – 19:00		<b>Hands on</b>	
Wednesday, August 15			
9:30 – 10:30		<b>Chad Leidy (UANDES, Bogotá)</b>	<i>tba</i>
10:30 – 11:00		Coffee break	
11:00 – 11:30		<b>Contributed talk 2: Karen Palacio Rodríguez (UDEA, Medellín)</b>	<i>Exponential consensus ranking improves outcome in docking and receptor ensemble docking</i>
11:30 – 12:00		<b>Contributed talk 3:</b>	<i>Molecular dynamics studies of the solvation effects of water and</i>

		<b>Sergio Mares-Samano</b> (UNAM, México City)	<i>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		<b>Gian Pietro Miscione</b> (UANDES, Bogotá)	<i>tba</i>
10:00 – 10:30		<b>Contributed talk 4:</b> <b>Hugo J. Bohórquez</b> (FIDIC, Bogotá)	<i>The frozen molecule approach in peptide-protein binding energies</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		<b>Esteban Vohringer-Martínez</b> (CONCEPCIÓN, Concepción)	<i>Force field improvement with ab-initio methods</i>
12:00 – 14:00		Lunch	
14:00 – 15:00		<b>Andrés González</b> (UANDES, Bogotá)	<i>tba</i>
15:00 – 15:30		Coffee break	
15:30 – 16:00		<b>Contributed talk 5:</b> <b>Angélica Sandoval</b> (UANDES, Bogotá)	<i>Specific at one side unspecific at the other: the interaction of blood proteins with extracellular DNA</i>
16:00 – 16:30		<b>Contributed talk 6:</b> <b>Stefany Botero Rodríguez</b> (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	
Friday, August 17			
9:30 – 10:30		<b>Bert de Groot</b> (MPIBPC, Göttingen)	<i>Introduction to alchemical free energy calculations</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00		<b>Vytas Gapsys</b> (MPIBPC, Göttingen)	<i>tba</i>
12:00 – 14:00		Lunch	
14:00 – 16:00		Hands on	
16:00 – 17:00		Closing remarks and departure	

## POSTERS

<b>Diego Gomez Hernandez</b> (UDISTRITAL, Bogotá)	<i>In silico evaluation of the potential affinity of anandamide analogues for CB1 receptor.</i>
<b>Carlos Pinilla</b> UNORTE, Barranquilla	<i>FeS alloys at conditions of the Earth Interior</i>
<b>Juan David Orjuela</b> UANDES, Bogotá	<i>Effect of the lipid-protein interaction on the assembly of the platelet Glycoprotein-IB</i>
<b>Markus Kurth</b> Heidelberg U. Heidelberg	<i>Probing the lipid environment of the Metabotropic glutamate receptor 2</i>

<b>Laura Pinto Herrera</b> UANDES, Bogotá	<i>Effect of particulate matter on the lung surfactant at a high altitude city: Review</i>
<b>Johann Bedoya Cardona</b> UNAL, Medellín	<i>Applicability of some force field parameters of biomolecules to model the surface tension of hexadecane</i>
<b>Yaritza Fortaleché Rodríguez</b> UNAL, Bogotá	<i>Agonist, antagonist or super-activator effect of different ligands in the receptor-ligand interaction of the TraR protein</i>
<b>Paula Giraldo Hincapié</b> UNAL, Medellín	<i>Analysis of Insecticide peptide - membrane interactions by molecular dynamics</i>
<b>Jessica Martinez</b> UAN, Bogotá	<i>Does Using Virtual Sites in Proteins Affect the Protein Fold?</i>
<b>Juan Camilo Zarate Moreno</b> SENA, Bogotá	<i>Kinetic models for chitosan membranes on biological systems, a computational approach.</i>
<b>Cesar Quintana Cataño</b> UANDES, Bogotá	<i>Force spectroscopy of T4 bacteriophage adhesion during infection.</i>
<b>Santiago Agudelo Gómez</b> UDEA, Medellín	<i>Preferred sites of glycosaminoglycans in the envelope protein of the Zika virus</i>
<b>Alberto Mario Castillo</b> UBJTL, Bogotá	<i>Spring Network Model of Trypanosoma Cruzi bloodstream trypomastigote</i>
<b>Gesivaldo Santos</b> State U. Bahia	<i>Autism Spectro Disorder &amp; Alzheimer Disease: different conditions linked by mTOR pathway</i>
<b>Helman Amaya Espinosa</b> UANDES, Bogotá	<i>Cooperative dynamics of self-interacting Biopolymers in blood elucidated by Coarse-Grained Brownian Dynamics Simulations</i>
<b>Valeria Mejía Restrepo</b> 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>
<b>Andrés Cifuentes López</b> UDISTRITAL, Bogotá	<i>In silico evaluation of the potential affinity of anandamide analogues for CB1 receptor</i>
<b>Jhoan Ortiz Giron</b> UDEA, Medellín	<i>A novel methodology for cryo-EM map validation</i>
<b>Adrian Orjuela</b> UNAL, Bogotá	