

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

DATE: August 13-17, 2018

VENUE: University of Los Andes, Bogotá, Colombia

WEB: <https://mptg-cbp.github.io/teaching/mem-fe-2018/>

ORGANIZER:
 Max Planck Tandem Group in
 Computational Biophysics



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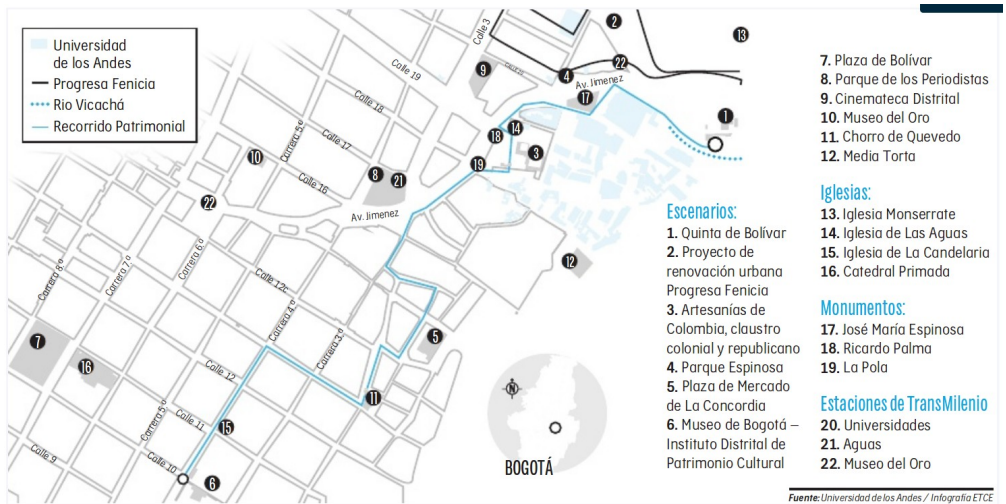
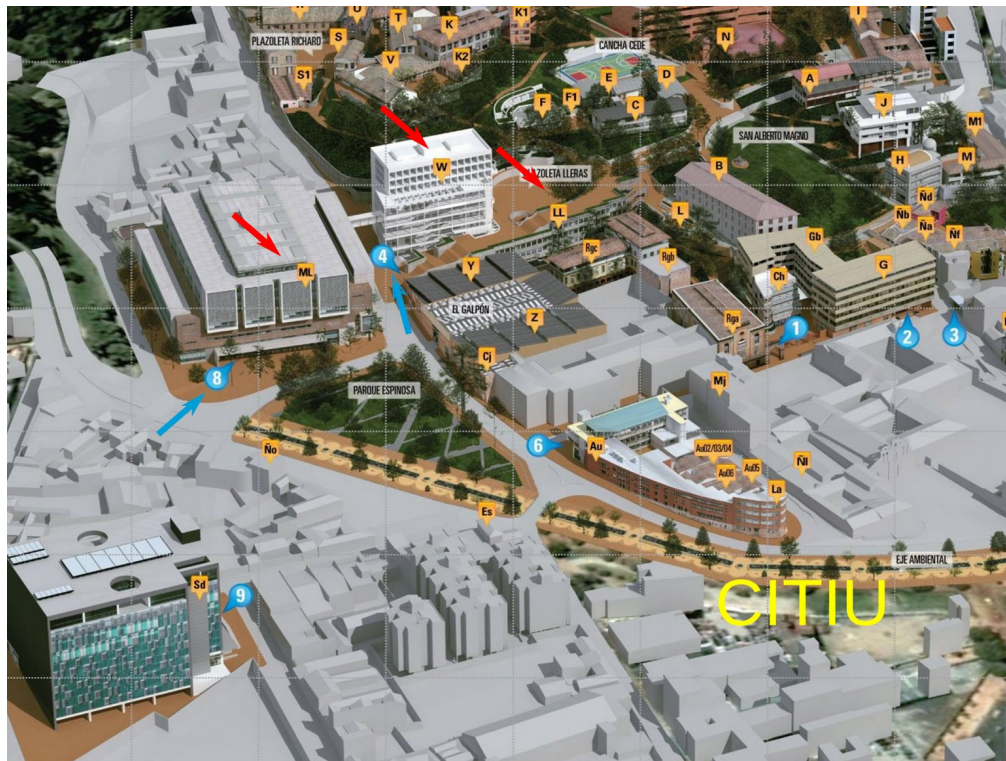
MAPS

Buildings (red arrows): W, ML, and LL

Entrances (blue arrows):

Entrance 4. “Lleras” Address: Calle 19A N° 1 - 37 Este

Entrance 8. “Mario Laserna” Address: Cra. 1 Este N° 19A - 40



PROGRAM OVERVIEW (ROOM)

	PART 1: membranes			PART 2: free energy	
	Monday (13.08)	Tuesday (14.08)	Wed. (15.08)	Thursday (16.08)	Friday (17.08)
8:00 – 9:00	Registration W101				
9:00 – 9:30	Welcome W101				
9:30 - 10:30	Bert de Groot W101	Thomas Walz (webinar) MLC	Chad Leidy W101	CT4: Hugo J. Bohórquez / W101	Coffee break
10:30 – 11:00	Coffee break				Hands on LL002 W504
11:00 – 12:00	Helgi Ingólfsson W101	Gerhard Hummer MLC	CT2: Karen Palacio CT3: Sergio Mares-Samano W101	Esteban Vohringer-Martínez W101	
12:00 – 14:00	Lunch		Free program	Lunch	
14:00 – 15:00	Gerhard Hummer W101	Bert de Groot MLC		Andrés González W101	
15:00 – 16:00	Vytas Gapsys / Camilo Aponte / CT1: Florian Franz W101	Helgi Ingólfsson MLC		Coffee break	Vytas Gapsys MLC
16:00 – 16:40	Coffee break			CT5: Angélica Sandoval CT6: Stefany Botero Rodríguez W101	Closing remarks & departure MLC
16:40 – 19:00	Hands on LL001 LL002	Hands on LL001 LL002		Poster session Hall ML AB	

PROGRAM IN DETAIL

PART 1: COMPUTER SIMULATIONS OF BIOLOGICAL MEMBRANES

Monday, August 13

Time	Room		
8:00 – 9:00	W101	Registration	
9:00 – 9:30		Welcome	
9:30 – 10:30	W101	Bert de Groot MPIBPC, Göttingen	<i>The molecular dynamics of solute permeation through biological membranes and membrane proteins</i>
10:30 – 11:00		Coffee break	
11:00 – 12:00	W101	Helgi Ingólfsson LLNL, Livermore	<i>Coarse-grained simulations: introduction and application to membranes</i>
12:00 – 14:00		Lunch	
14:00 – 15:00	W101	Gerhard Hummer MPIB, Frankfurt	<i>Large finite-size effects in molecular dynamics simulations of membranes</i>
15:00 – 15:20	W101	Vytautas Gapsys MPIBPC, Göttingen	<i>Grid-based methods for the analysis of MD simulations of biological membranes I: <u>g_lomempro</u></i>
15:20 – 15:40	W101	Camilo Aponte UANDES, Bogotá	<i>Grid-based methods for the analysis of MD simulations of biological membranes II: <u>GROmars</u></i>
15:40 – 16:00	W101	Contributed talk 1: Florian Franz IWR, Heidelberg	<i>Stability of Biological Membranes upon Mechanical Indentation</i>
16:00 – 16:10		Photo	
16:10 – 16:30		Coffee break	
16:30 – 16:40		Heading to computer room	
16:40 – 19:00	LL001/ LL002	Hands on: all-atom MD simulations of biological membranes Introductory (LL001) – Advanced (LL002)	
19:00 –		Invited speakers dinner	

Tuesday, August 14

9:30 – 10:30	MLC	Webinar, Thomas Walz Rockefeller, New York	<i>Electron Microscopy Approaches to Studying Lipid-Protein Interactions</i>
10:30 –		Coffee break	

11:00			
11:00 – 12:00	MLC	Gerhard Hummer MPIB, Frankfurt	<i>Molecular dynamics simulations of proteins that sense the composition and state of lipid membranes</i>
12:00 – 14:00		Lunch	
14:00 – 15:00	MLC	Bert de Groot MPIBPC, Göttingen	<i>Permeation, selectivity and gating of ion channels studied by computational electrophysiology</i>
15:00 – 16:00	MLC	Helgi Ingolfson LLNL, Livermore	<i>Capturing biological membranes in silico at different compositional complexity</i>
16:00 – 16:30		Coffee break	
16:30 – 16:40		Heading to computer room	
16:40 – 19:00	LL001/ LL002	Hands on: coarse-grained MD simulations of biological membranes Introductory (LL001) – Advanced (LL002)	
Wednesday, August 15			
9:30 – 10:30	W101	Chad Leidy UANDES, Bogotá	<i>Integrating Computational and Experimental Approaches to Investigate Antimicrobial Peptide Activity in Membranes</i>
10:30 – 11:00		Coffee break	
11:00 – 11:30	W101	Contributed talk 2: Karen Palacio Rodríguez UDEA, Medellín	<i>Exponential consensus ranking improves outcome in docking and receptor ensemble docking</i>
11:30 – 12:00	W101	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	W101	Gian Pietro Miscione UANDES, Bogotá	<i>Mechanism of L-Tryptophan Prenylation, Catalyzed by FgaPT2: a Computational Study</i>
10:00 – 10:30	W101	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	W101	Esteban Vohringer-Martínez	<i>Force field improvement with ab-initio methods</i>

		UCONCEPCIÓN, Concepción	
12:00 – 14:00		Lunch	
14:00 – 15:00	W101	Andrés González UANDES, Bogotá	Applications of product design departing from free energy calculations
15:00 – 15:30		Coffee break	
15:30 – 16:00	W101	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	W101	Contributed talk 6: Stefany Botero Rodríguez UNAL, Bogotá	Computational Tracing of Protein and ncRNA epitopes inside Dengue Virus
16:30 – 16:40		Heading to poster room	
16:40 – 19:00	Hall ML AB	Poster session (with wine and finger food)	
Friday, August 17			
9:00 – 10:00	MLC	Bert de Groot MPIBPC, Göttingen	Introduction to alchemical free energy calculations
10:00 – 10:45		Coffee break	
10:45 – 12:45	LL002 W504	Hands on: Free energy calculations Introductory (LL002) – Advanced (W504)	
12:45 – 15:00		Lunch	
15:00 – 16:00	MLC	Vytas Gapsys MPIBPC, Göttingen	Application of the alchemical free energy calculations to proteins, nucleic acids and ligands
16:00 – 16:30	MLC	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>