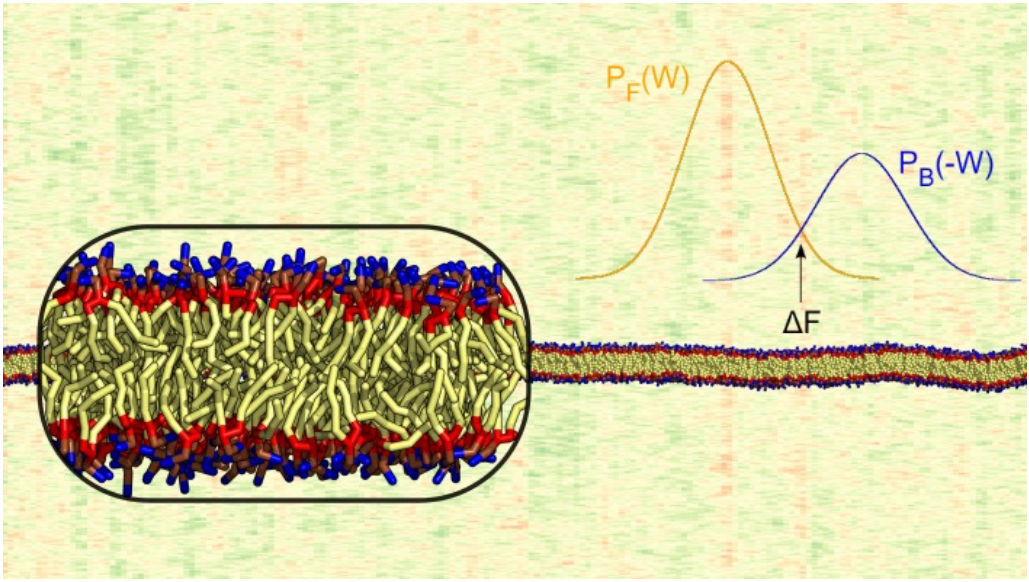


SCHOOL:
COMPUTER SIMULATIONS OF BIOLOGICAL MEMBRANES
&
FREE ENERGY CALCULATIONS OF BIOMOLECULAR SYSTEMS

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

Universidad de los Andes

SPONSORS:

Universidad de los Andes

MAX-PLANCK-GESELLSCHAFT

bioexcel

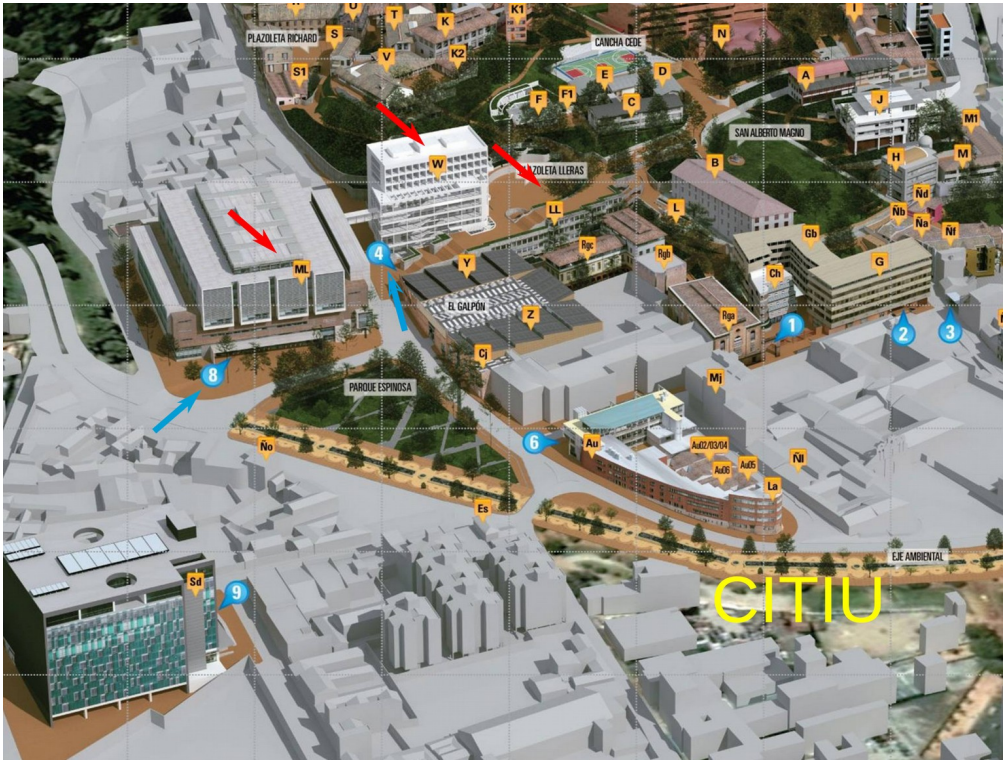
MAPS

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

Entrances (blue arrows):

Entrance 4. “Lleras” Address: Calle 19A Nº 1 - 37 Este

Entrance 8. “Mario Laserna” Address: Cra. 1 Este Nº 19A - 40



Escenarios:

1. Quinta de Bolívar
2. Proyecto de renovación urbana Progresa Fenicia
3. Artesanías de Colombia, claustro colonial y republicano
4. Parque Espinosa
5. Plaza de Mercado de La Concordia
6. Museo de Bogotá – Instituto Distrital de Patrimonio Cultural
7. Plaza de Bolívar
8. Parque de los Periodistas
9. Cinemateca Distrital
10. Museo del Oro
11. Chorro de Quevedo
12. Media Torta

Iglesias:

13. Iglesia Monserrate
14. Iglesia de Las Aguas
15. Iglesia de La Candelaria
16. Catedral Primada

Monumentos:

17. José María Espinosa
18. Ricardo Palma
19. La Pola

Estaciones de TransMilenio

20. Universidades
21. Aguas
22. Museo del Oro

Fuente: Universidad de los Andes / Infografía ETCE

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			Gian Pietro Miscione W101	
9:30 - 10:30	Bert de Groot W101	Thomas Walz (webinar) MLC	Chad Leidy W101	CT4: Hugo J. Bohórquez / W101	Bert de Groot MLC
10:30 – 11:00	Coffee break				
11:00 – 12:00	Helgi Ingólfsson W101	Gerhard Hummer MLC	CT2: Karen Palacio CT3: Sergio Mares-Samano W101	Esteban Vohringer-Martínez W101	Vytas Gapsys MLC
12:00 – 14:00	Lunch		Free program	Lunch	
14:00 – 15:00	Gerhard Hummer W101	Bert de Groot MLC		Andrés González W101	**Hands on** LL002 W504
15:00 – 16:00	Vytas Gapsys / Camilo Aponte / CT1: Florian Franz W101	Helgi Ingólfsson MLC		Coffee break	
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**	*The molecular dynamics of solute permeation through biological membranes and membrane proteins*
10:30 – 11:00		Coffee break	
11:00 – 12:00	W101	**Helgi Ingólfsson LLNL, Livermore**	*Coarse-grained simulations: introduction and application to membranes*
12:00 – 14:00		Lunch	
14:00 – 15:00	W101	**Gerhard Hummer MPIB, Frankfurt**	*Large finite-size effects in molecular dynamics simulations of membranes*
15:00 – 15:20	W101	**Vytautas Gapsys MPIBPC, Göttingen**	*Grid-based methods for the analysis of MD simulations of biological membranes I: g_lomempro*
15:20 – 15:40	W101	**Camilo Aponte UANDES, Bogotá**	*Grid-based methods for the analysis of MD simulations of biological membranes II: GROmars*
15:40 – 16:00	W101	**Contributed talk 1: Florian Franz IWR, Heidelberg**	*Stability of Biological Membranes upon Mechanical Indentation*
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**	*Electron Microscopy Approaches to Studying Lipid-Protein Interactions*
10:30 –		Coffee break	

11:00			
11:00 – 12:00	MLC	**Gerhard Hummer MPIB, Frankfurt**	*Molecular dynamics simulations of proteins that sense the composition and state of lipid membranes*
12:00 – 14:00		Lunch	
14:00 – 15:00	MLC	**Bert de Groot MPIBPC, Göttingen**	*Permeation, selectivity and gating of ion channels studied by computational electrophysiology*
15:00 – 16:00	MLC	**Helgi Ingolfson LLNL, Livermore**	*Capturing biological membranes in silico at different compositional complexity*
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**	*Integrating Computational and Experimental Approaches to InvestigateAntimicrobial Peptide Activity in Membranes*
10:30 – 11:00		Coffee break	
11:00 – 11:30	W101	**Contributed talk 2: Karen Palacio Rodríguez UDEA, Medellín**	*Exponential consensus ranking improves outcome in docking and receptor ensemble docking*
11:30 – 12:00	W101	**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	W101	**Gian Pietro Miscione UANDES, Bogotá**	*Mechanism of L-Tryptophan Prenylation, Catalyzed by FgaPT2: a Computational Study*
10:00 – 10:30	W101	**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 –	W101	**Esteban Vohringer-**	*Force field improvement with ab-initio methods*

12:00		**Martínez 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	HallM LAB	**Poster session (with wine and finger food)**	
Friday, August 17			
9:30 – 10:30	MLC	**Bert de Groot MPIBPC, Göttingen**	*Introduction to alchemical free energy calculations*
10:30 – 11:00		Coffee break	
11:00 – 12:00	MLC	**Vytas Gapsys MPIBPC, Göttingen**	*Application of the alchemical free energy calculations to proteins, nucleic acids and ligands*
12:00 – 14:00		Lunch	
14:00 – 16:00	LL002 W504	**Hands on: Free energy calculations Introductory (LL002) – Advanced (W504)**	
16:00 – 17:00	MLC	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*