

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

Part 1) Computer simulations of biological membranes*Monday, August 13*

8:00 – 9:00	Registration
9:00 – 9:30	Welcome
9:30 – 10:30	Bert de Groot <i>The molecular dynamics of solute permeation through biological membranes and membrane proteins</i>
10:30 – 11:00	Coffee break.
11:00 – 12:00	Helgi Ingólfson <i>Coarse-grained simulations: introduction and application to membranes</i>
12:00 – 14:00	Lunch.
14:00 – 15:00	Gerhard Hummer <i>tba</i>
15:00 – 15:30	Coffee break.
15:30 – 16:30	Webinar by Thomas Walz <i>tba</i>
16:30 – 16:45	Heading to computer room
16:45 – 19:00	Hands on

Tuesday, August 14

9:30 – 10:30	Helgi Ingólfson <i>Capturing biological membranes in silico at different compositional complexity</i>
10:30 – 11:00	Coffee break
11:00 – 12:00	Gerhard Hummer <i>tba</i>

12:00 – 14:00	Lunch
14:00 – 15:00	Bert de Groot <i>Permeation, selectivity and gating of ion channels studied by computational electrophysiology</i>
15:00 – 15:30	Coffee break
15:30 – 16:10	Vytautas Gapsys <i>tba</i>
16:10 – 16:40	Contributed talk 1
16:40 – 17:00	Heading to computer room
17:00 – 19:00	Hands on

Wednesday, August 15

9:30 – 10:30	Chad Leidy <i>tba</i>
10:30 – 11:00	Coffee break
11:00 – 11:30	Contributed talk 2
11:30 – 12:00	Contributed talk 3
12:00 –	free program

Part 2) Free energy calculations of biomolecular systems

Thursday, August 16

9:00 – 10:00	Gian Pietro Miscione <i>tba</i>
10:00 – 10:30	Contributed talk 4
10:30 – 11:00	Coffee break
11:00 – 12:00	Esteban Vohringer-Martínez <i>Force field improvement with ab-initio methods</i>
12:00 – 14:00	Lunch
14:00 – 15:00	Andrés González <i>tba</i>
15:00 – 15:30	Coffee break
15:30 – 16:00	Contributed talk 5
16:00 – 16:30	Contributed talk 6
16:30 – 17:00	Heading to poster room
17:00 – 19:00	Poster session

Friday, August 17

9:30 – 10:30	Bert de Groot <i>Introduction to alchemical free energy calculations</i>
10:30 – 11:00	Coffee break
11:00 – 12:00	Vytas Gapsys <i>tba</i>
12:00 – 14:00	Lunch
14:00 – 16:00	Hands on
16:00 – 16:30	Closing remarks and departure