

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 (TENTATIVE)****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 Ingolfson <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 Ingolfson <i>Capturing biological membranes in silico at different compositional complexity</i>
10:30 – 11:00	Coffee break
11:00 – 12:00	Bert de Groot <i>Permeation, selectivity and gating of ion channels studied by computational electrophysiology</i>
12:00 – 14:00	Lunch
14:00 – 15:00	Gerhard Hummer <i>tba</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>
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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

9:30 – 10:15	Gian Pietro Miscione <i>tba</i>
10:15 – 11:00	Esteban Vohringer-Martínez <i>Force field improvement with ab-initio methods</i>
11:00 – 11:30	Coffee break
11:30 – 12:00	Contributed talk 1
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 2
16:00 – 16:30	Contributed talk 3
16:30 – 16:45	Heading to poster room
16:45 – 19:00	Poster session

Friday, August 17

9:15 – 10:15	Bert de Groot <i>Introduction to alchemical free energy calculations</i>
10:15 – 10:45	Coffee break
10:45 – 12:45	Hands on
12:45 – 15:00	Lunch
15:00 – 16:00	Vytas Gapsys <i>tba</i>
16:00 – 16:30	Closing remarks and departure