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

10:30 - 11:00	Monday, August 13 8:00 - 9:00 9:00 - 9:30 9:30 - 10:30	Registration Welcome Bert de Groot The molecular dynamics of solute permeation through biological membranes and membrane proteins
14:00 – 15:00 Gerhard Hummer tba 15:00 – 15:30 Coffee break. 15:30 – 16:30 Webinar by Thomas Walz tba 16:30 – 16:45 Heading to computer room 16:45 – 19:00 Hands on Tuesday, August 14 9:30 – 10:30 9:30 – 10:00 Capturing biological membranes in silico at different compositional complexity 10:30 – 11:00 Coffee break 11:00 – 12:00 Bert de Groot Permeation, selectivity and gating of ion channels studied by computational electrophysiology 12:00 – 14:00 Lunch 14:00 – 15:00 Gerhard Hummer tba 15:30 – 16:10 Vytautas Gapsys tba 16:10 – 16:40 Contributed talk 1 16:40 – 17:00 Heading to computer room		Coffee break. Helgi Ingolfson
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9:30 – 10:30 Chad Leidy	9:30 - 10:30	Chad Leidy
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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
	tba
10:15 - 11:00	Esteban Vohringer-Martínez
	Force field improvement with ab-initio methods
11:00 - 11:30	Coffee break
11:30 – 12:00	Contributed talk 1
12:00 – 14:00	Lunch
14:00 - 15:00	Bert de Groot
	<i>Introduction to alchemical free energy calculations</i>
15:00 - 15:30	Coffee break
15:30 - 16:30	Vytas Gapsys
	tba
16:30 - 16:45	Heading to poster room
16:45 - 19:00	Poster session
Friday, August 17	
9:15 – 10:00	Andrés González
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10:00 - 10:30	Coffee break
10:30 – 11:00	Contributed talk 2
11:00 – 11:30	Contributed talk 3
11:30 - 13:00	Lunch
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13:00 - 15:00	Hands on
15:00 – 15:30	Coffee break
15:30 – 16:30	Gerhard Hummer tha
16:30 – 17:00	
10.30 - 17:00	Closing remarks and departure