

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*

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| 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

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| 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

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| 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

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| 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 | Bert de Groot <i>Introduction to alchemical free energy calculations</i> |
| 15:00 – 15:30 | Coffee break |
| 15:30 – 16:30 | Vytas Gapsys <i>tba</i> |
| 16:30 – 16:45 | Heading to poster room |
| 16:45 – 19:00 | Poster session |

Friday, August 17

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| 9:15 – 10:00 | Andrés González <i>tba</i> |
| 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 |
| 13:00 – 15:00 | Hands on |
| 15:00 – 15:30 | Coffee break |
| 15:30 – 16:30 | Gerhard Hummer <i>tba</i> |
| 16:30 – 17:00 | Closing remarks and departure |