**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**

<table>
<tr><th></th><th>Monday (13.08)</th><th>Tuesday (14.08)</th><th>Wed. (15.08)</th><th>Thursday (16.08)</th><th>Friday (17.08)</th></tr>
<tr><td>8:00 – 9:00</td><td>Registration</td><td colspan="3" rowspan="2"></td><td rowspan="3">Bert de Groot<br>MLC</td></tr>
<tr><td>9:00 – 9:30</td><td>Welcome</td><td rowspan="2">Gian Pietro Miscione</td></tr>
<tr><td>9:30 - 10:30</td><td>Bert de Groot</td><td>Thomas Walz<br>(webinar) MLC</td><td>Chad Leidy</td><td>CT4: Hugo J. Bohórquez</td></tr>
<tr><td>10:30 – 11:00</td><td colspan="5">Coffee break</td></tr>
<tr><td>11:00 – 12:00</td><td>Helgi Ingólfsson</td><td>Gerhard Hummer<br>MLC</td><td>CT2: Karen Palacio Rodríguez<br>CT3: Sergio Mares-Samano</td><td>Esteban Vohringer-Martínez</td><td>Vytas Gapsys<br>MLC</td></tr>
<tr><td>12:00 – 14:00</td><td colspan="2">Lunch</td><td rowspan="7">Free program</td><td colspan="2">Lunch</td></tr>
<tr><td>14:00 – 15:00</td><td>Gerhard Hummer</td><td>Bert de Groot<br>MLC</td><td>Andrés González</td><td rowspan="5">Hands on<br>MLC<br><br>Closing remarks & departure<br>MLC</td></tr>
<tr><td>15:00 – 16:00</td><td>Vytas Gapsys /<br>Camilo Aponte /<br>CT1: Florian Franz</td><td>Helgi Ingólfsson<br>MLC</td><td>Coffee break<br>CT5: Angélica Sandoval</td></tr>
<tr><td>16:00 – 16:30</td><td colspan="2">Coffee break</td><td>CT6: Stefany Botero Rodríguez</td></tr>
<tr><td>16:30 – 17:00</td><td colspan="2">Heading to computer room</td><td>Heading to computer room</td></tr>
<tr><td>17:00 – 19:00</td><td>Hands on</td><td>Hands on<br>MLC</td><td>Poster session<br>MLAB</td></tr>
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**PROGRAM IN DETAIL**

| **PART 1: COMPUTER SIMULATIONS OF BIOLOGICAL MEMBRANES** | | | |
|---|---|---|---|
| ***Monday, August 13*** | | | |
| Time | Room | | |
| 8:00 – 9:00 | | Registration | |
| 9:00 – 9:30 | | Welcome | |
| 9:30 – 10:30 | | **Bert de Groot**<br>**MPIBPC, Göttingen** | *The molecular dynamics of solute permeation through biological membranes and membrane proteins* |
| 10:30 – 11:00 | | Coffee break | |
| 11:00 – 12:00 | | **Helgi Ingólfsson**<br>**LLNL, Livermore** | *Coarse-grained simulations: introduction and application to membranes* |
| 12:00 – 14:00 | | Lunch | |
| 14:00 – 15:00 | | **Gerhard Hummer**<br>**MPIB, Frankfurt** | ***tba*** |
| 15:00 – 15:20 | | **Vytautas Gapsys**<br>**MPIBPC, Göttingen** | *Grid-based methods for the analysis of MD simulations of biological membranes I: g_lomempro* |
| 15:20 – 15:40 | | **Camilo Aponte**<br>**UANDES, Bogotá** | *Grid-based methods for the analysis of MD simulations of biological membranes II: GROMaρs* |
| 15:40 – 16:00 | | **Contributed talk 1:**<br>**Florian Franz**<br>**IWR, Heidelberg** | *Stability of Biological Membranes upon Mechanical Indentation* |
| 16:00 – 16:10 | | Photo | |
| 16:10 – 16:40 | | Coffee break | |
| 16:40 – 17:00 | | Heading to computer room | |
| 17:00 – 19:00 | | **Hands on: all-atom MD simulations of biological membranes** | |
| 19:00 – | | Invited speakers dinner | |
| ***Tuesday, August 14*** | | | |
| 9:30 – 10:30 | MLC | **Webinar, Thomas Walz**<br>**Rockefeller, New York** | *Electron Microscopy Approaches to Studying Lipid-Protein Interactions* |
| 10:30 – 11:00 | | Coffee break | |
| 11:00 – 12:00 | MLC | **Gerhard Hummer**<br>**MPIB, Frankfurt** | ***tba*** |
| 12:00 – 14:00 | | Lunch | |
| 14:00 – 15:00 | MLC | **Bert de Groot**<br>**MPIBPC, Göttingen** | *Permeation, selectivity and gating of ion channels studied by computational electrophysiology* |
| 15:00 – 16:00 | MLC | **Helgi Ingolfson**<br>**LLNL, Livermore** | *Capturing biological membranes in silico at different compositional complexity* |
| 16:00 – 16:40 | | Coffee break | |
| 16:40 – 17:00 | | Heading to computer room | |
| 17:00 – 19:00 | MLC / XXX | **Hands on: coarse-grained MD simulations of biological membranes**<br>**Introductory (room MLC) Advanced (room XXX)** | |
| *Wednesday, August 15* | | | |
| 9:30 – 10:30 | | **Chad Leidy**<br>**UANDES, Bogotá** | *Integrating Computational and Experimental Approaches to InvestigateAntimicrobial Peptide Activity in Membranes* |

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|---|---|---|---|
| 10:30 – 11:00 | | Coffee break | |
| 11:00 – 11:30 | | **Contributed talk 2:**<br>**Karen Palacio Rodríguez**<br>**UDEA, Medellín** | *Exponential consensus ranking improves outcome in docking and receptor ensemble docking* |
| 11:30 – 12:00 | | **Contributed talk 3:**<br>**Sergio Mares-Samano**<br>**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 | | **Gian Pietro Miscione**<br>**UANDES, Bogotá** | *Mechanism of L-Tryptophan Prenylation, Catalyzed by FgaPT2: a Computational Study* |
| 10:00 – 10:30 | | **Contributed talk 4:**<br>**Hugo J. Bohórquez**<br>**FIDIC, Bogotá** | *The frozen molecule approach in peptide-protein binding energies* |
| 10:30 – 11:00 | | Coffee break | |
| 11:00 – 12:00 | | **Esteban Vohringer-Martínez**<br>**UCONCEPCIÓN,**<br>**Concepción** | *Force field improvement with ab-initio methods* |
| 12:00 – 14:00 | | Lunch | |
| 14:00 – 15:00 | | **Andrés González**<br>**UANDES, Bogotá** | *Applications of product design departing from free energy calculations* |
| 15:00 – 15:30 | | Coffee break | |
| 15:30 – 16:00 | | **Contributed talk 5:**<br>**Angélica Sandoval**<br>**UANDES, Bogotá** | *Specific at one side unspecific at the other: the interaction of blood proteins with extracellular DNA* |
| 16:00 – 16:30 | | **Contributed talk 6:**<br>**Stefany Botero Rodríguez**<br>**UNAL, Bogotá** | *Computational Tracing of Protein and ncRNA epitopes inside Dengue Virus* |
| 16:30 – 17:00 | | Heading to poster room | |
| 17:00 – 19:00 | MLAB | **Poster session (with wine and finger food)** | |
| *Friday, August 17* | | | |
| 9:30 – 10:30 | MLC | **Bert de Groot**<br>**MPIBPC, Göttingen** | *Introduction to alchemical free energy calculations* |
| 10:30 – 11:00 | | Coffee break | |
| 11:00 – 12:00 | MLC | **Vytas Gapsys**<br>**MPIBPC, Göttingen** | *Application of the alchemical free energy calculations to proteins, nucleic acids and ligands* |
| 12:00 – 14:00 | | Lunch | |
| 14:00 – 16:00 | MLC<br>/XXX | **Hands on: Free energy calculations**<br>**Introductory (room MLC) Advanced (room XXX)** | |
| 16:00 – 17:00 | | Closing remarks and departure | |

**POSTERS**

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|---|---|---|
| **1** | **Diego Gomez Hernandez**<br>**UDISTRITAL, Bogotá** | *In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor.* |
| **2** | **Carlos Pinilla**<br>**UNORTE, Barranquilla** | *FeS all0ys at conditions of the Earth Interior* |
| **3** | **Juan David Orjuela**<br>**UANDES, Bogotá** | *Effect of the lipid-protein interaction on the assembly of the platelet Glycoprotein-IB* |
| **4** | **Markus Kurth**<br>**Heidelberg U. Heidelberg** | *Probing the lipid environment of the Metabotropic glutamate receptor 2* |
| **5** | **Laura Pinto Herrera**<br>**UANDES, Bogotá** | *Effect of particulate matter on the lung surfactant at a high altitude city: Review* |
| **6** | **Johann Bedoya Cardona**<br>**UNAL, Medellín** | *Applicability of some force field parameters of biomolecules to model the surface tension of hexadecane* |
| **7** | **Yaritza Fortaleché Rodríguez**<br>**UNAL, Bogotá** | *Agonist, antagonist or super-activator effect of different ligands in the receptor-ligand interaction of the TraR protein* |
| **8** | **Paula Giraldo Hincapie**<br>**UNAL, Medellín** | *Understanding insecticide peptides: Modeling peptide-membrane interactions with Molecular Dynamics* |
| **9** | **Jessica Martinez**<br>**UAN, Bogotá** | *Does Using Virtual Sites in Proteins Affect the Protein Fold?* |
| **10** | **Juan Zarate Moreno**<br>**SENA, Bogotá** | *Kinetic models for chitosan membranes on biological systems, a computational approach.* |
| **11** | **Cesar Quintana Cataño**<br>**UANDES, Bogotá** | *Force spectroscopy of T4 bacteriophage adhesion during infection.* |
| **12** | **Santiago Agudelo Gómez**<br>**UDEA, Medellín** | *Preferred sites of glycosaminoglycans in the envelope protein of the Zika virus* |
| **13** | **Alberto Mario Castillo**<br>**UBJTL, Bogotá** | *Spring Network Model of Trypanosoma Cruzi bloodstream trypomastigote* |
| 14 | **Gesivaldo Santos**<br>**State U. Bahia** | *Autism Spectro Disorder & Alzheimer Disease: different conditions linked by mTOR pathway* |
| **15** | **Helman Amaya Espinosa**<br>**UANDES, Bogotá** | *Cooperative dynamics of self-interacting Biopolymers in blood elucidated by Coarse-Grained Brownian Dynamics Simulations* |
| **16** | **Valeria Mejía Restrepo**<br>**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**<br>**UDISTRITAL, Bogotá** | *In silico evaluation of the potential afinity of anandamide analogues for CB1 receptor* |
| **18** | **Jhoan Ortiz Giron**<br>**UDEA, Medellín** | *A novel methodology for cryo-EM map validation* |