**Rosetta Software:**

Rosetta development began in the laboratory of Dr. David Baker at the University of Washington as a structure prediction tool but since then has been adapted to solve common computational macromolecular problems.The Rosetta software suite includes algorithms for computational modeling and analysis of protein structures (https://www.rosettacommons.org/software)

**Amber molecular dynamic Package:**

"Amber" refers to two things: a set of molecular mechanical force fields for the simulation of biomolecules (which are in the public domain, and are used in a variety of simulation programs); and a package of molecular simulation programs which includes source code and demos AMBER software suite provides a set of programs to apply the AMBER forcefields to simulations of biomolecules (http://ambermd.org/)

**El curso se realizará en el Auditorio Victor Villon. Facultad de Química**

**Inscripciones:** https://docs.google.com/forms/d/1RSEILkcXq52tHMretsrCAFCeYqc-C8i4Z9NrA2Cf-cQ/prefill.

**Consultas:** afierroh@uc.cl; jcampusano@bio.puc.cl

**Workshop Organizado por:**

**Dra. Angélica Fierro H.**, Departamento de Química Orgánica, Facultad de Química

Nuestro grupo se enfoca en estudio, mediante simulación molecular, de las interacciones y mecanismos involucrados en el reconocimiento de compuestos orgánicos por macromoléculas del sistema monoaminérgico. Se trabaja en el diseño de nuevos ligandos y la obtención de antecedentes de mecanismos de reacción en proteínas.

**Dr. Jorge Campusano**. Departamento de Biología Celular y Molecular, Facultad de Ciencias Biológicas.

En nuestro laboratorio estudiamos el papel que cumplen los sistemas neuronales de aminas biogénicas en la generación de comportamientos. Para ello utilizamos como modelo la mosca Drosophila melanogaster, un animal que presenta importantes semejanzas con modelos vertebrados y que cuenta con grandes ventajas en términos genéticos.

Workshop realizado con el aporte de la Vicerrectoría de Investigación de la Pontificia Universidad Católica de Chile y proyecto Fondecyt 1161375.

# WORKSHOP DE SIMULACIÓN MOLECULAR

29-31 de Marzo y

24-26 de Abril 2017

## "ESTUDIO ESTRUCTURAL Y TERMODINÁMICO DE MACROMOLÉCULAS"

"Structural and Thermodynamic Study of Macromolecules"

**DR. VLADIMIR YAROV-YAROVOY (UCDAVIS)**

My research interests and expertise encompass neuroscience, protein structure, computational biology, and evolution. Main focus of my research group is on structure and function studies of voltage-gated ion channels, computational design and chemical synthesis of subtype-specific modulators of voltage-gated ion channels, development of computational methods for membrane protein structure prediction and design, and analysis of evolution of human voltage-gated ion channels.

**DR. DONALD HAMELBERG (GEORGIA STATE UNIVERSITY)**

The research in our group focuses on the application and development of theoretical and computational methods with the intent of gaining an in-depth understanding of biomolecular switches. Many interactions in cell signaling pathways are mediated by intricate networks of interacting proteins and RNAs. Deregulation of these pathways could trigger cellular transformation, oncogenesis, and a host of other diseases.

## Miércoles 29 de Marzo

**11:00 h** Registro

**11:15 h Inauguración**

**Seminario:**

**11:30 h** Auditorio Victor Pillon, Campus san Joaquin.

**17:00 h** Auditorio Abate Molina, Casa Central.

**"Design of novel ion channel modulators using Artificial Intelligence"**

(*En caso de ser necesario los participantes del Workshop pueden habilitar sus computadores personales en el auditorio V. Pillon a las 15:00 h)

## Jueves 30 de Marzo

**9:00-12:30/14:00-17:00 h** Theoretical and practical computational modeling course focused on Foldit (Rosetta based video game for protein structure prediction and design)

## Viernes 31 de Marzo

**9:00-12:30/14:00-15:30 h** Theoretical and practical computational modeling course focused on Rosetta computational modeling

**15:30-16:30 h** Presentación de Póster,

**16:40-17:00 h Término Parte I Workshop**

## Lunes 24 de Abril

**11:00 h** Registro

**Seminario:**

**11:30 h** Auditorio Victor Pillon, Campus san Joaquin.

**17:00 h** Auditorio Abate Molina, Casa Central.

**"Atomistic insights into coupled dynamics in protein allosteric mechanisms"**

## Martes 25 de Abril

**9:00-12:30/14:00-17:00 h**

Theoretical background of Molecular Dynamics, Setting up MD simulations with AMBER. Solvating, neutralizing and equilibration.

## Miércoles 26 de Abril

**9:00-12:30/14:00-17:00 h** Theoretical and practical computational modeling course focused on Running long molecular dynamics simulations. Basic analyses. Free energy calculations and pKa shift calculations.

**17:00-17:30 h** Presentación de Póster,

**17:30-18:00 h Término Workshop**