# Symposium PROGRAM

## Molecular Interactions in Chemistry and Biology

**Auditorio II, Fac. Cs. Químicas, UdeC**
**4th December 2017**

**Monday, December 4th 2017**

*9.30* Symposium Opening

9.40 *CETCH me if you can - Bringing inorganic carbon into life with novel enzymes and synthetic CO2 fixation*

**Dr. Tobias Erb**, Director of Max-Planck Institute for Terrestrial Microbiology, Marburg, Germany.

10.30 Coffee Break

11.00 *Studying protein-protein interactions through single molecule force microscopy.*

**Dr. Christian Wilson,** Facultad de Bioquímica y Farmacia, Universidad de Chile

11.45 *Southamerican Inititative for a Rapid and Accurate Hamiltonian (SIRAH): toward a biologically complete coarse grained force field for MD simulations.*

**Dr. Sergio Pantano,** Institute Pasteur de Montevideo, Uruguay.

12:30 Lunch Break

15:15 *Insights into protein-ligand interactions from molecular simulations.*

**Dr. David Mobley**, Department of Chemistry, University of California Irvine, EEUU.

16:00 Coffee break

16.30 *Characterizing activation processes through the reaction force analysis and the Marcus equation. (la merveilleuse équation de Marcus)*

**Dr. Alejandro Toro-Labbé**, QTC, Pontificia Universidad Católica de Chile, Santiago.

17:15 *Interactions between molecular fragments: some insights from the generalized dual descriptor and new index based upon the polarized electron density.*

**Dr. Chistophe Morrell,** Frederic Guegan, Institute of Analytical Sciences, Lyon, France.

*18:00 Closing*

*20.00 Dinner Centro Español*

## Workshops for Students

### Tuesday, 5th December, 2017

Workshop on "Free Energy Calculations with Molecular Dynamics Simulations" by **Dr. David Mobley, Department of Chemistry, University of California Irvine, EEUU** and Dr. Esteban Vöhringer-Martinez.

### Wednesday, 6th December 2017

Workshop on "Molecular Dynamics Simulations of Membrane Protein Interactions" by **Dr. Camilo Aponte, Universidad de los Andes, Bogota, Colombia** and Dr. David Saez (webinar).

### Thursday, 7th December, 2017

Workshop on "Intermolecular Interactions: Theory and Electronic Structure Methods" by **Dr. Adelio Matamala and Dr. Stefan Vogt-Geisse, Quantum Chemistry and Molecular Modeling Group, UdeC**.