Mauricio **Esguerra**

COMPUTATIONAL CHEMIST · BIOINFORMATICIAN

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Profile

Experienced researcher with an international background in Sweden, the United States and Colombia. Highly skilled in Structural Molecular Biology, Python, Bioinformatics, Biopolymers, Cluster system administration and full-stack web development. PhD focused in RNA Structure and Bioinformatics from Rutgers, The State University of New Jersey. Expert knowledge on G-Protein Coupled Receptors (GPCR's), RNA structure, the Ribosome, tRNA modifications, and antigene technology via triple helical DNA modifications.

Career Goal

To strenghten my career path in Sweden in science related areas in a broad scope. I have a laid back attitude when interacting with others and know when to and how to react wisely to personal cues with a warm and positive attitude. I am also highly skilled in anything related to a computer, so, continuing a relation with cutting edge computational developments and how to take advantage of them is a passion I want to stay close to and constantly fortify. I also consider myself an avid english reader and enjoy writing and editing english texts and consider myself highly competent at it. In my current job writing is fundamental, specially being creative when one has to convey complex scientific messages to general audiences, this kind of writing I enjoy greatly and would like to continue practicing in my next career step. I also enjoy human interaction and intelectual discussion, solving problems and discussing them thoroughly, and learning from the other which is one of the ingredients I want to constantly have in my career.

Professional Experience

Uppsala University
Uppsala, Sweden

Researcher
Apr. 2015 - PRESENT

- Main focus has been research on the effect of tRNA modifications on initial selection in protein translation.
- Have deployed a ROCKS cluster for the department and helped on its maintenace.
- Constant interaction, project management and collaboration with graduate students.

Uppsala University
Uppsala, Sweden

Carl Tryggers Fellow
Apr. 2013 - Apr. 2015

- Developed a python module for automatic recognition of Ballesteros-Weinstein pairs in GPCR's structures which are used to improve molecular dynamics simulations.
- GPCR webserver full update with the django web framework, full-stack development of front-end and back-end.
- Development of **Q**, creation of github organization, and documentation writing.
- Study of the catalytic mechanisms of β-phosphoglucomutase using the Empirical Valence Bond method and the Molaris software.

Karolinska Institute
Huddinge, Sweden

Post-doctoral Fellow
Oct. 2010 - Apr. 2013

- Worked on analysis of the sequence dependence of helical deformation in a classical parallel triplex.
- Worked on the effect of the sugar modification called LNA in the mechanical properties of the antiparallel triplex, finding that the final effect is that of a concerted increase in the major and minor grooves of B-type DNA.
- Lectured on the principles of nucleic acid structure as understood with Calladine-Drew mechanical rigid-body parameters, and the basic Tinoco-Uhlenbeck based Nusinov algorithm for secondary structure folding predictions of RNA.

Rutgers University
New Brunswick, New Jersey, U.S.A

Teaching Assistant in various chemistry courses
2003 - 2009

- Problem solving sessions.
- Office hours for students.
- Grading.

Universidad de los Andes
Bogota, Colombia

Course instructor in physics for pre-freshman students
2002, 2003

- Developed experiments and wrote guides.
- Taught the course.

Alvaro Castellanos y Cia. *Bogota, Colombia*

Patent Advisor *2001-2002*

- Translate patents.
- Prepare submission to local patent office.
- Prepare replies to local patent office.

Baker & Mackenzie *Bogota, Colombia*

Patent Engineer *2000*

- Translate patents
- Prepare submission to local patent office.
- Prepare replies to local patent office.
- Hold phone conferences with patent clients, both companies and inventors.

Education

Rutgers, The State University of New Jersey *New Brunswick, New Jersey, U.S.A.*

Ph. D. *2010*

- The work focused on the basic principles of RNA structure. We constructed and explored databases of RNA structures to find patterns unique to RNA in conformational space. We also connected our knowledge based databases to Flory-like polymer models, to estimate fundamental polymer properties such as persistence length. The goal was to understand the connection between such properties and RNA sequence, with the ultimate lofty aim of understanding RNA folding.

Universidad Nacional de Colombia *Bogotá, Colombia*

Chemistry Bachelor in Science *2000*

- Final work focused on exploring the PES of two reactions ocurring over naive interstellar ice analogs using traditional Hartree-Fock quantum chemistry calculations.

Supervision and Teaching

SUPERVISION

Laura Timonet, M.Sc. Student from Spain
Uppsala University, Uppsala, Sweden (2016)
Worked on setting up and creating homology models of a class C GPCR's dimer for the UMAMI receptor using our in-house *pymemdyn* recipe for Gromacs membrane embedding and equilibration.

Prerana Pradhan, Bachelor's final project
Rutgers, The State University of New Jersey, New Brunswick, New Jersey (2010)
Directed her work on our project for automated recognition of GNRA motifs on RNA structures. Poster presented at the regional ACS meeting in Wilmington, Delaware.

TEACHING

Free Energy Perturbation Lab, Molecular and Statistical Mechanics Course 1mb412, Uppsala University, (Fall 2016, Fall 2017)
Co-lecturer, Principles of Nucleic Acid Structure, Karolinska Institute Doctoral Course 2430 (Spring 2011, Spring 2012, Spring 2014)
Teaching assistant for Principles of Quantitative Biology, Rutgers, The State University of New Jersey. (Fall 2009)
Teaching assistant for Physical Chemistry of Biochemical Systems, Rutgers, The State University of New Jersey. (Spring 2009)
Teaching assistant for General Chemistry at Rutgers, The State University of New Jersey. (Spring 2004, Spring 2005, Fall 2005)
Teaching assistant for Introduction to Chemical Experimentation lab at Rutgers, The State University of New Jersey. (Fall 2003, Fall 2004, Fall 2006, Fall 2008)
Course instructor for "Prelude to the Sciences", Physics module, Faculty of Sciences at Universidad de los Andes. (Summer 2002, Summer2003)
Course instructor for "Prelude to the Sciences", Physics module, Faculty of Sciences at Universidad de los Andes. (June26 – July19 2001)
Guide elaboration for the course "Prelude to the Sciences", Physics module, prepared for the Faculty of Sciences at Universidad de los Andes. (June – July 2001)
Lab. and recitation Teaching Assistant at Universidad de los Andes. (August 2000 – February 2001)

Skills

Programming	Python, Fortran, R, Bash, LaTeX
SysAdmin	Rocks, Docker, TravisCI, CentOS, Fedora, Debian, MacOS, Windows 10
Web	Django, HTML5, CSS3, HUGO, Jekyll, nginx, apache, gunicorn, postgresql, mysql
Chemistry	Maestro, Gromacs, CHARMM, Q, Gaussian, GAMESS, Pymol, Knime
Languages	English, Swedish, Spanish

Publications

A complete list of publications can be found at ORCID online:
`https://orcid.org/0000-0002-1775-586X`