



Mauricio Esguerra

COMPUTATIONAL CHEMIST

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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, and project management of research projects. 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.

“...he managed the project and revealed himself as an excellent team-worker and project coordinator. He showed independence, creativity, critical thinking and a particularly methodical work-style, which I can say was key for the success of the project. ”

Hugo Gutiérrez de Terán
Associate Professor, UU

Career Goal

I am passionate from top to bottom about science and well trained on learning and appropriating complex scientific topics fast and deeply. One of my main goals is to continue my ongoing passion for science whether in new technical areas such as Machine Learning (Deep learning or A.I.) or Data Science, and/or areas of biological relevance, such as the development of new medicines with the aid of computational methods.

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 have a continued interest in pharmaceutical sciences coming from the principles of my GPCR and RNA research which can be linked to understanding better and better how to treat cancer with small molecules, for example. I would like to apply my basic knowledge in reaching out to general healthcare professionals and decision makers so that they can make a difference where it really matters. I also consider myself an avid english reader and enjoy writing and editing. I also enjoy being involved with people and intellectual 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

Researcher

Uppsala, Sweden

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 maintenance.
- Constant interaction, project management and collaboration with graduate students.

Uppsala University

Carl Tryggers Fellow

Uppsala, Sweden

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

Post-doctoral Fellow

Huddinge, Sweden

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 Nussinov algorithm for secondary structure folding predictions of RNA.

Rutgers University

Teaching Assistant in various chemistry courses

N. B., New Jersey, U.S.A

2003 - 2009

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

Universidad de los Andes

Course instructor in physics for pre-freshman students

Bogotá, Colombia

2002, 2003

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

Alvaro Castellanos y Cia.

Patent Advisor

Bogotá, Colombia

2001-2002

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

Baker & Mackenzie

Patent Engineer

Bogotá, Colombia

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

N. B., 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 occurring 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>