Mauricio **Esguerra**

COMPUTATIONAL CHEMIST

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Profile

Experienced researcher with an international background in Barcelona (Spain), Denmark, Sweden, the United States and Colombia. Highly skilled in Structural Molecular Biology, Scientific Programming, 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, 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

"I can recommend Mauricio for his excellent attitude towards science, his constant and contagious interest for cutting edge developments in computational chemistry, biology, and science in general, his ability to work both independently and with colleagues, and his fast learning skills"

David van der Spoel
Head of ICM Department, 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 and medical relevance, such as the development, understanding and promotion of new medicines.

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 RNA and GPCR research which can be linked to understanding better and better how to treat disease with engineered small molecules, nucleotides or peptides. I'm an avid English reader and enjoy writing and editing. I like being involved with people and intellectual discussion, solving problems and discussing them thoroughly, and learning from colleagues, which is one of the ingredients I've been lucky to have throughout my career and want to keep and reinforce.

Professional Experience

Nostrum Biodiscovery — *Barcelona, Spain*

Senior Project Manager — *June. 2021 - present*

- Project management for various pharmaceutical industry clients mainly related to small molecules targeting proteins. Extensive use of the in-house software solution PELE and PELE-platform.
- Joint industry-academy proposals development.
- Integration of new software to the current company pipelines such as R and Community Network Analysis using Bio3D, bioBB for accelerating MD workflows.

University of Copenhagen — *Copenhagen, Denmark*

Assistant Professor — *Jan. 2020 - May 2021*

- Research in David Gloriam's lab. on a project funded by the Novo Nordisk Fonden on GPCR Biased Signaling. Looking at the details of coupling between G-proteins and their cell membrane receptors and what structurally determines downstream signaling.
- DevOps of the GPCRdb platform.

Swedish Pensions Agency *Stockholm, Sweden*

Agile Webstream Team System Administrator *August 2019, December 2019*

- System administrator in team Atlas. Part of the larger webstream infrastructure of the Swedish Pensions Agency.
- Taking care of various tasks needed by the team such as, handling Docker containers, BigIP security, GoCD, ELK among others.

Uppsala University *Uppsala, Sweden*

Researcher *Apr. 2015 - Feb. 2019*

- Main focus has been research on the effect of tRNA modifications on initial selection in protein translation.
- ROCKS cluster deployment and maintenance for the department.
- Constant interaction, project management and collaboration with PhD and Master 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 *N. B., 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*

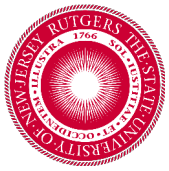
- Translate patents.
- Prepare submission to local patent office.
- Prepare replies to local patent office.

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

Ph. D. *2010*

- Explored 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)
- T.A. in various course at Rutgers, The State University of New Jersey (2003-2009)
- T.A. for first year physics at Universidad de los Andes, Colombia (2001-2003)

Skills

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

Publications

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