



Mauricio Esguerra

COMPUTATIONAL CHEMIST

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Profile

Experienced computational chemist in industry and academia with an international background in Sweden (Gothenburg, Uppsala, Stockholm), Barcelona (Spain), Denmark, 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 RNA, the Ribosome, tRNA modifications, G-Protein Coupled Receptors (GPCR's), Kinases, AI-QSAR 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'm passionate from top to bottom about science and well trained on learning and appropriating complex scientific topics fast and deeply. Accordingly my career goals are tuned to a will for a constant growth process of such passion, exploring both the broad and detailed aspects of where the fundamental structural principles of chemistry can take us today, whether that is in drug discovery, molecular engineering and/or the coupling of specialized knowledge and the general public.

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, DNA, GPCR and Kinase 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

AstraZeneca

Associate Director | Chemical Toxicology (CPSS)

Möln达尔, Sweden

July 2022 - present



- Project support work across therapeutic areas, Oncology, CVRM, RI. Drug safety using computational biology and computational chemistry in-silico techniques integrating data analytics, bioinformatic and structural knowledge to understand safety risks and influence chemistry to design them out.
- Chemical Toxicology, QSAR AI graph-based models for ADME.
- PFAS, structure properties classification (PBT).
- Personal Ombudsmän (POM).
- High Performance Computing cluster Business Reference Group representative for the CPSS department.
- Computational Biology liaison to early Respiratory and Immunology therapeutic area.



Nostrum Biodescovery

Senior Project Manager

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

Barcelona, Spain

June. 2021 - May 2022



University of Copenhagen

Assistant Professor

- 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.

Copenhagen, Denmark

Jan. 2020 - May 2021

PENSIONS
MYNDIGHETEN



UPPSALA
UNIVERSITET



UPPSALA
UNIVERSITET



Karolinska
Institutet



Alvaro Castellanos y Cia.

Patent Advisor

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

Barcelona, Spain

June. 2021 - May 2022

Swedish Pensions Agency

Agile Webstream Team System Administrator

- 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.

Stockholm, Sweden

August 2019, December 2019

Uppsala University

Researcher

- 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, Sweden

Apr. 2015 - Feb. 2019

Uppsala University

Carl Tryggers Fellow

- 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.

Uppsala, Sweden

Apr. 2013 - Apr. 2015

Karolinska Institute

Post-doctoral Fellow

- 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.

Huddinge, Sweden

Oct. 2010 - Apr. 2013

Rutgers University

Teaching Assistant in various chemistry courses

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

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

2003 - 2009

Universidad de los Andes

Course instructor in physics for pre-freshman students

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

Bogota, Colombia

2002, 2003

Baker & McKenzie

Patent Engineer

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

Bogota, Colombia

2000

Education



Rutgers, The State University of New Jersey

Ph. D.

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

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

Chemistry Bachelor in Science

Bogotá, Colombia

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

Sudarsana Reddy Vanga, PhD carrying industrial internship at AstraZeneca

AstraZeneca AB, Mölndal, Sweden (2025)

Using Quantum Mechanics simulations to understand reaction mechanisms of degradation of nitrosamines coupled to results obtained in enhanced AMES test of genotoxicity.

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

Chem-Bioinfo	AlphaFolds, Maestro, MOE, D360, Gromacs, CHARMM, OpenMM, Q, Gaussian, GAMESS, Pymol, VMD, RNASeq, KNIME, RDKit, jalview, geneious-prime, NF-core, IPA
Programming	Python, R, Fortran, Bash, LaTeX
SysAdmin	Rocks, Docker, TravisCI, CentOS, Fedora, Debian, MacOS, Windows 11
Web	Flask, Streamlit, Dash, 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>