

## Mauricio Esguerra

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## PERSONAL INFORMATION

Nationality: Swedish, Colombian  
Marital Status: Single  
Languages: Spanish (advanced), English (advanced), Swedish (conversational), French (beginner)

## RESEARCH

Researcher - Uppsala Universitet (current)  
Carl-Tryggers Fellow - Uppsala Universitet (2015)  
Post-Doctoral Fellow - Karolinska Institutet (2013)

## EDUCATION

Ph.D. in Chemistry - Rutgers, The State University of New Jersey (2010)  
Chemist - Universidad Nacional de Colombia (2000)  
9th Grade – 11th Grade Gimnasio Moderno - Bogotá, Colombia  
9th Grade Sevier County High School - Sevierville, TN, USA  
Elementary School:  
8th Grade Pi Beta Phi Elementary School - Gatlinburg, TN, USA  
Montessori (Kindergarden) – 7th Grade Gimnasio Moderno - Bogotá, Colombia

## AWARDS

Chemistry 171 Teaching Excellence Award. Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey. 2003-3004.

## PROFESSIONAL EXPERIENCE

- Academic Monitor for the course, Synthesis of Heterocyclic Compounds, for Pharmaceutical Chemistry Students at Universidad Nacional de Colombia.(1998).
- Academic Monitor for the course, Organic Synthesis, for Chemistry Students at Universidad Nacional de Colombia.(1998)
- Patent Engineer for the law firm Baker & Mackenzie (i.e. patent preparation for filling and submitting to the Colombian Superintendence of Industry and Commerce). (May – August 2000)
- Lab and recitation Teaching Assistant at Universidad de los Andes. (August 2000 – February 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)
- Course instructor for “Prelude to the Sciences”, Physics module, Faculty of Sciences at Universidad de los Andes. (June26 – July19 2001)
- Patent advisor for the law firm Alvaro Castellanos y Cia. (September 2001 – July 2002)
- Course instructor for “Prelude to the Sciences”, Physics module, Faculty of Sciences at Universidad de los Andes. (Summer 2002, Summer2003)
- Teaching assistant for Introduction to Chemical Experimentation lab at Rutgers, The State University of New Jersey. (Fall 2003, Fall 2004, Fall 2006, Fall 2008)
- Teaching assistant for General Chemistry at Rutgers, The State University of New Jersey. (Spring 2004, Spring 2005, Fall 2005)
- Teaching assistant for Physical Chemistry of Biochemical Systems, Rutgers, The State University of New Jersey. (Spring 2009)
- Teaching assistant for Principles of Quantitative Biology, Rutgers, The State University of New Jersey. (Fall 2009)
- Co-lecturer, Principles of Nucleic Acid Structure, Karolinska Institute Doctoral Course 2430 (Spring 2011, Spring 2012, Spring 2014)
- Post-Doctoral Fellow - Karolinska Institutet (2010 - 2013)
- Carl-Tryggers Fellow - Uppsala Universitet (2013 - 2015)
- Researcher - Uppsala Universitet (2015 - current)

## MEMBERSHIPS

American Chemical Society member. 2006-Present.  
Svenska Kemisamfundet. 2018-Present.

## CONFERENCES / SCHOOLS

- Second Latin-American Course on Parallelism and High Performance Computing, Merida, Venezuela (December 3-7 2001).
- A.C.S. Mid-Atlantic Regional Meeting, Piscataway, NJ. (May 22-25, 2005).
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. (May 6, 2005).
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. (May 5, 2006).
- NSBP and NSHP Annual Conference, Boston, MA. (2007).
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. (May 4, 2007).
- IMA Workshop: RNA in Biology, Bioengineering and Nanotechnology, Minneapolis, MN. (October 29 - November 2, 2007).
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. (May 6, 2008).
- 5th Annual ROC (RNA Ontology Consortium) Meeting, Madison, WI. (May 25-26, 2009).
- The 16th Conversation in Biomolecular Dynamics and Structure, Albany, NY. (June 16-20, 2009).
- Molecular Simulation and Structure Prediction using CHARMM and the MMTSB Tool Set, San Diego, CA. (August 4-7, 2009).
- The 17th Conversation in Biomolecular Dynamics and Structure, Albany, NY. (June 14-18, 2011).
- Biennial ISQBP President's Meeting. Challenges in Biomolecular Modeling – From QM to Coarse-Graining, Stockholm, Sweden (17-20 June, 2012).
- 244th American Chemical Society National Meeting and Exposition, Philadelphia, PA. (2012).
- 6th International Theoretical Biophysics Symposium, Gothenburg, Sweden (June 24-27, 2013).
- Selected talk. Glisten Budapest 2014 Conference, New features for GPCR modeling implemented on GPCR-MODSYM and PYMEMDYN, Budapest, Hungary (October 3, 2014).
- Glisten Meeting on GPCR's at Actelion Pharmaceuticals, Allschwill, Switzerland (April 1-2, 2015).
- Ribosome Structure and Function 2016, Strasbourg, France (July 6-10, 2016)
- RNAseq course, National Bioinformatics Infrastructure Sweden (NBIS), Uppsala, Sweden (November 6-8, 2017)

## POSTERS

- Clustering RNA non-A-type dinucleotide conformations using the base-step parameter space, NSBP & NSHP, Boston, MA. 2007.
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. 2007.
- RNA Dinucleotide Step Parameters, IMA Workshop, Minneapolis, MN. 2007.
- Rutgers-UMDNJ Molecular Biophysics Minisymposium, Piscataway, NJ. 2008.
- Sequence-dependent Deformability of RNA Helical Regions. What We Have Learned So Far, The 16th Conversation in Biomolecular Structure and Dynamics, Albany, NY. 2009.
- Automated Detection of GNRA Tetraloop Prevalance Using 3DNA and Python, MARMACS, Wilmington, Delaware. 2010.
- RNASTEPS, and online database of sequence-dependent deformability of RNA helical regions, The 17th Conversation in Biomolecular Structure and Dynamics, Albany, NY. 2011.
- The DNA Triplex and the bis-LNA construct, 244th American Chemical Society National Meeting and Exposition, Philadelphia, PA. 2012.
- gpcr-modsim.org: A one-stop shop for sequence homology and molecular dynamics modeling, Glisten GPCR Meeting, Basel, Switzerland, 2015.

## PUBLICATIONS

- New information content in RNA base pairing deduced from quantitative analysis of high-resolution structures, *Methods*, 47, 177-186, (2009), Wilma K. Olson, Mauricio Esguerra, Yurong Xin, Xiang-Jun Lu.
- Sequence-dependent deformability of RNA helical regions. What we have learned so far, *Journal of Biomolecular Structure and Dynamics*, 26, 832, (2009), Mauricio Esguerra N., Wilma K. Olson.
- Triple helical DNA in a duplex context and base pair opening, *Nucleic Acids Research*, 42, 11329, (2014), Mauricio Esguerra N., Lennart Nilsson, and Alessandra Villa.
- GPCR-ModSim: A comprehensive web based solution for modeling G-protein coupled receptors, *Nucleic Acids Research*, 44 W455-W462, (2016), Mauricio Esguerra N., Alexey Siretskiy, Xabier Bello, Jessica Sallander, Hugo Gutiérrez de Terán.
- The bis-LNA construct: A promising path in antigene technology, In preparation, Mauricio Esguerra N., Lennart Nilsson.
- A close-up view of codon selection in eukaryotic initiation, *RNA Biology*, 14, 815, (2017), Christoffer Lind, Mauricio Esguerra, Johan Åqvist.
- Characterization of Ligand Binding to GPCRs Through Computational Methods, Chapter II of *Computational Methods for GPCR Drug Discovery*, 23-44, (2017), Silvana Vasile, Mauricio Esguerra, Willem Jaspers, Ana Oliveira, Jessica Sallander, Johan Åqvist, Hugo Gutiérrez-de-Terán.
- Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations, *Software X*, In Press, (2018), Paul Bauer, Alexandre Barrozo, Miha Purga, Beat Anton Amrein, Mauricio Esguerra, Philippe Barrie Wilson, Dan Thomas Major, Johan Åqvist Shina Caroline Lynn Kamerlin.
- Computer Simulations of the Catalytic Mechanism of Wild-Type and Mutant  $\beta$ -Phosphoglucomutase, *Org. and Biom. Chem.*, In Press, (2018), Alexandre Barrozo, Qinghua Liao, Mauricio Esguerra, Gaél Marloie, Jan Florian, Nicholas H. Williams and Shina C. L. Kamerlin.

## SKILLS

Linux/UNIX (Fedora, CentOS, Debian, Ubuntu), macOS, Windows X, ROCKS cluster operating system, zsh, bash, postgresSQL, html5, css3, fortran, c++, python, R, emacs, django web framework, nginx, docker, github, travis-ci, multiple computational chemistry packages (gaussian, gamess-US, Q, CHARMM, gromacs), molecular visualization packages (pymol, VMD, Schrödinger Maestro).