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.

MEMBERSHIPS

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

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)

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 Jespers, 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, MauricioEsguerra, Philippe Barrie Wilson, Dan Thomas Major, Johan Åqvist Shina Caroline Lynn Kamerlin.

•Computer Simulations of the Catalytic Mechanism of Wild–Type and Mutant β-Phosphoglucomutase, *Org. and Biom. Chem.*, In Press, (2018), Alexandre Barrozo, Qinghua Liao, Mauricio Esguerra, Gaël 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, postgreSQL, 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).