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EDUCATION

2005-2009 Ph.D. in Biology, Rensselaer Polytechnic Institute

Dissertation topic:

“Study of protein conformational and interaction dynamics by molecular dynamics simulations and nuclear magnetic resonance experiments”

Adviser: Professor Angel E. Garcia

2004-2005 M.Sc. in Bioinformatics (first in class), National University of Athens

Thesis subject:

“Prediction of the coupling specificity of GPCRs to four families of G-proteins”

Adviser: Professor Stavros J. Hamodrakas

2000-2004 B.Sc. in Biology (top 10% of class), National University of Athens

Thesis in Bioinformatics:

“Prediction of the coupling specificity of GPCRs to G-proteins”

RESEARCH EXPERTISE

Doctoral Research in Molecular Biophysics

2005-present

Functional dynamics of proteins using a variety of MD simulation methods and NMR experiments

I have implemented replica-exchange MD simulations combined with NMR experiments to characterize the conformations accessible to the Amyloid- β peptides which are involved in Alzheimer's disease^{4,5}. In a more NMR-intensive project, I focused on solving the solution structure and characterizing recognition dynamics of a complex between ubiquitin and a ubiquitin interacting motif (UIM) involved in endosomal sorting, in collaboration with George Makhatadze and Scott McCallum (RPI)². Another aspect of my research involves the modeling and simulation of the membrane protein complex between the G-protein coupled receptor rhodopsin and its heterotrimeric G-protein partner transducin¹. The aim of this project is to characterize the interface formed by the different subunits and its plasticity due to protein dynamics.

Undergraduate/Master's Research in Bioinformatics

2003-2005

Development of sequence analysis tools for G-protein coupled receptors (GPCRs)

I focused on the development of tools for the prediction of the coupling specificity of GPCRs to G-proteins (PRED-COUPLE series of programs). As an undergraduate student I worked on the discovery and optimization of profile Hidden Markov Models (pHMMs) to perform this task⁷. During my Master's Thesis I became familiar with Neural Networks and combined them with pHMMs to create the first computational method that predicts the coupling specificity of GPCRs to all four families of G-proteins⁸. The resulting algorithm, PRED-COUPLE2 has been used in genome annotation projects with high efficiency. Later, this work was given the international NRW undergraduate science award in bioinformatics and genome research.

ACADEMIC HONORS

2005 Merck PhD Fellowship from Carnegie Mellon University (declined)

2005 European Program Scholarship award to the top student for the M.Sc. degree in bioinformatics

2007 NRW Undergraduate Science Award in Bioinformatics and Genome research (1st place in international competition for my work on GPCRs^{7,8} from the German State of North-Rhine Westphalia)

2009 National Institute of General Medical Sciences (NIGMS) Scholarship (awarded for my participation and contributed talk in the Keystone Symposium in protein dynamics, allostery and function)

PROFESSIONAL SKILLS

Computational biology modeling and simulation tools:

Pattern discovery, pattern recognition and data mining techniques, targeted at computational biology applications: profile hidden Markov models (and optimization of their discovery), neural networks, support vector machines. Thorough knowledge of clustering algorithms

Molecular modeling and simulation tools: AMBER, GROMACS (developers list), NAMD, CHARMM

Molecular Visualization tools: pymol, VMD, VMD-xplor

Programming in C++, C, Java and FORTRAN

Scripting environments: perl, python, awk, shells

Research analysis environments: Mathematica, Matlab

NMR spectroscopy (theory and practice):

NMR pulse sequences for the investigation of protein structure and dynamics as implemented in common commercial platforms (Bruker TopSpin)

NMR structure determination suites (Sparky, CYANA, X-plor-NIH)

Basic Molecular biology skills/techniques aiming at cloning, expressing and purifying labeled proteins for NMR.

PROFESSIONAL AFFILIATIONS

Reviewer for *Nucleic Acid Research* Database issue

Reviewer for *Proteins*

Reviewer for *Biophysical Journal*

Member, The Protein Society

Member, The Biophysical Society

Member, Federation of European Biochemical Societies (FEBS)

TALKS AND LECTURES

9/2009 Los Alamos National Lab, Center for Non-linear Studies, q-Bio Conference series: "*Protein conformational and interaction dynamics by MD simulations and NMR experiments*" (invited talk)

8/2009 Center for Theoretical Biological Physics, San Diego: "*Protein conformational and interaction dynamics*" (invited talk)

7/2009 Telluride Science Research Center: "*Biological membranes and membrane complexes: Challenges for theory and experiment*"

6/2009 JBSD Albany 2009 Conversation

6/2009 Keystone Symposium: "*Protein Dynamics, Allostery and Function*"

3/2009 The Biophysical Society: "*51st Annual Meeting Platform Session: Membrane receptors & signal transduction*"

5/2008 Rensselaer Biology Program Symposium: "*At the Interface*"

1/2008 Proteins under pressure meeting (sponsored by the NSF, RPI and Los Alamos Ntl. Lab)

10/2007 9th Upstate New York NMR Symposium

9/1007 National Science Foundation Symposium: "*Cyber-Enabled Discovery and Innovation*"

5/2007 NRW award ceremony (invited talk)

3/2007 The Biophysical Society: "*51st Annual Meeting Platform Session: Structure of Unfolded Peptides & Proteins*"

11/2006 8th Upstate New York NMR Symposium

POSTER PRESENTATIONS IN CONFERENCES

7/2009 22nd Symposium of the Protein Society: "*Proteins in motion*"

3/2008 50th Experimental NMR Conference (ENC) (Student Travel Award)

5/2008 Gordon Research Conference: "*Biopolymers*"

2/2008 The Biophysical Society: "*52nd Annual Meeting*"

1/2008 Gordon Research Conference: "*Protein folding dynamics*"

6/2008 20th Symposium of the Protein Society: “*Proteins: from birth to death*”
7/2007 32nd Federation of European Biochemical Societies Congress: “*Molecular Machines*”
(Young Scientist Fellowship)
4/2007 48th Experimental NMR Conference (ENC) (Student Travel Award)

PUBLICATIONS

- [1] “*Atomic-detail characterization of the interaction interface dynamics between rhodopsin and transducin using μ sec-timescale molecular dynamics simulations*” Sgourakis N.G. and Garcia A.E. *under review in PNAS*;
- [2] “*Helix docking dynamics: Molecular recognition within a Ubiquitin/UIM fusion protein*” Sgourakis N.G., Patel M., Garcia, A.E., Makhatadze G.I. and McCallum S.A. *under review in JMB*;
- [3] “*Pressure effects on the ensemble dynamics of Ubiquitin inspected with molecular dynamics simulations and isotropic reorientational Eigenmode dynamics*” Sgourakis N.G., Day R., McCallum S.A. and Garcia A.E. *Biophysical Journal* 2008;
- [4] “*Computational Methods for the Prediction of GPCRs Coupling Selectivity*” Sgourakis N.G., Bagos P.G. and Hamodrakas S.J. *Handbook of Research for Systems Biology Applications in Medicine (Max Plank institute for Molecular Genetics, Berlin 2008)*;
- [5] “*Global versus local features of an unfolded peptide system – A β 42 modeled by molecular dynamics simulations and NMR experiments*” Sgourakis N.G. and Garcia A.E. *Unfolded proteins: From denatured to intrinsically disordered (Nova Science, 2007)*;
- [6] “*The Alzheimer’s Peptides A β 40 and 42 Adopt Distinct Conformations in Water: A Combined MD/NMR Study*” Sgourakis N.G., Yan Y., McCallum S.A., Wang C. and Garcia A.E. *Journal of Molecular Biology* 2007 368(5):1448-1457;
- [7] “*A method for the prediction of GPCRs coupling specificity to G-proteins using refined profile Hidden Markov Models*” Sgourakis N.G., Bagos P.G., Papasaikas P.G. and Hamodrakas S.J. *BMC Bioinformatics* 2005 6:104;
- [8] “*Prediction of the coupling specificity of GPCRs to four families of G-proteins using Hidden Markov Models and Artificial Neural Networks*” Sgourakis N.G., Bagos P.G. and Hamodrakas S.J. *Bioinformatics* 2005 21(22):4101-4106;

NEWS ARTICLES

1. NRW Ministry of Science and Research: “*Verleihung der Undergraduate Science Awards der sieben NRW Graduate Schools / Minister Professor Andreas Pinkwart: Diese studentischen Preisträger sind Zukunftsträger*”
(<http://www.nrw.de/presse/preise-an-nachwuchsforscher-verliehen-2933>)
2. RPI Alumni magazine, October 2009, featured article

LANGUAGES/ACTIVITIES

French (fluent), Greek (native)
Classical flautist. Athens conservatory finalist. Principal Player of the RPI symphony orchestra
Start-up player of the RPI water polo team for seasons 2007-2009

References available upon request.