David Jimenez-Morales PhD, MSc, BSc

Tel: (+1) 773.983.9381 | biodavidjm@gmail.com | Chicago, Illinois 60622 (USA)

Education

2006 - 2013 PhD Bioinformatics

Department of Bioengineering. University of Illinois at Chicago.

Chicago, Illinois (USA)

2003–2004 MSc Computational Biology

Universidad Complutense de Madrid. Madrid (Spain)

Organized by Complutense University, the National Center for Biotechnology (CSIC),

Alma Bioinformatics S.L. and Bioforum

1999 Teaching Certificate

Postgraduate Certificate in Education.

Instituto de Ciencias de la Educación. Universidad Complutense de Madrid.

Madrid (Spain)

1998 - 2000 Microbiology PhD Program and Research Certificate

Department of Microbiology, Universidad Complusense de Madrid.

Madrid (Spain)

1993 - 1998 BSc Biology (specialty in Fundamental Biology)

Facultad de Ciencias. Universidad de Granada.

Granada (Spain)\

Research Experience

2006 - PhD Graduate Student. Liang's Molecular and Systems Computational lab.

Department of Bioengineering. University of Illinois-Chicago. Chicago

Research Work: Evolutionary biology. Protein design. Structural bioinformatics. Bioinformatics Models and Prediction Tools.

Under the guidance of Prof. Jie Liang, I have been studying physicochemical and functional constraints acting on proteins and their evolutionary patterns.

> Characterization of the <u>pattern of amino acid substitutions</u> at the transmembrane segments of outer (beta-barrel) membrane proteins, which allows a better detection of these membrane proteins and it can be useful as part of a toolkit for protein engineering design. Mutants of OmpF were designed based on this pattern of substitutions and <u>experimental results validated our predictions</u> (Collaborator: Prof. Linda Kenney).

Computational tool: bbTM-ST (beta-barrel Transmembrane Search Tool)

- > Identification of a physicochemical property of the site where the catalytic action takes place at protein enzymes: we found that the catalytic active site is an unusual electrostatic and steric environment in which side chains and reactants are crowded together in a mixture more like an ionic liquid than an ideal infinitely dilute solution (Collaborator: Prof. Bob Eisenberg).
- > Characterization of the signature microenvironment of lysine carboxylation sites and its defining features. Development of a computational method and implemented a tool for the detection of lysine carboxylation (PreLysCar) in proteins with available 3D structure. We have unveiled a larger prevalence of this modification, with important biological consequences. Paper accepted in the journal <u>Acta D</u> (Collaborator: Dr. Daniel Shi).

Computational Tool: PreLysCar (Predictor of Lysine Carboxylation)

> Evolutionary analysis of the catalytic active site of proteins and their relationship with metabolic fluxes. We explore the relationship between enzyme structures, enzyme functions, metabolite concentrations and fluxes in the glycolysis and pentose-phosphate pathways, which form the central carbon metabolism of *E.coli* (Collaborator: Dr. Lei Liu)

2003 - 2005 Research Assistant. Proteomics Unit & Department of Microbiology II. Universidad Complutense de Madrid – Parque Científico de Madrid. Madrid

MSc. Bioinformatics Project: Bioinformatics Study of glycolytic proteins presence on the cell surface of Saccharomyces cerevisiae.

I worked on the hypothesis that a classical and well-known group of citoplasmatic proteins could exist outside the cell. With this proposal, we used predicting methods for localization and multifunctional evaluation, in addition to three-dimensional protein structure studies.

Bioinformatics Research Work: *Ecm33 protein family characterization as previous step in structure and function prediction*.

New protein family characterization at protein sequence level and prediction the secondary and tertiary protein structure (using homology modeling, fold recognition and *ab initio* methods)

1998 - 2000 Research Assistant. Department of Microbiology I. Faculty of Medicine. Universidad Complutense de Madrid. Madrid.

Identification of bacterial species isolated from oral human flora. Determined the effects of sublethal doses of some antimicrobial agents. Isolation, characterization and identification of bacteria species with nosocomial interest isolated from the guts of farm animals and measured the resistance levels through antimicrobial agents.

Publications

Peer-reviewed Journals

- 2013 <u>Jimenez-Morales D</u>, Adamian L, Shi D, and Liang J. Lysine Carboxylation: Unveiling a spontaneous posttranslational modification. Acta Crystallographica Section D. Vol 69. doi:10.1107/S0907444913023640
- **2012 -** <u>Jimenez-Morales D</u>, Liang J, and Eisenberg B *Ionizable Side Chains at Catalytic Active Sites of Enzymes*. <u>Eur Biophys J</u>. Vol 41, Issue 5 (2012), P 449-460 <u>PubMed</u>.
- 2012 Naveed H, <u>Jimenez-Morales D</u>, Tian J, Pasupuleti V, Kenney L, Liang L (2012) Engineered oligomerization state of OmpF protein through computational design decouples oligomer dissociation from unfolding J Mol Biol. 2012 May 25;419(1-2):89-101. Epub 2012 Mar 3. PubMed
- 2011 Liang J, Naveed H, <u>Jimenez-Morales D</u>, Adamian L, Lin M Computational studies of membrane proteins: Models and predictions for biological understanding. <u>Biochim Biophys Acta</u>. 2011 Oct 12. <u>PubMed</u>.
- 2011 <u>Jimenez-Morales D</u> and Liang J

Pattern of Amino Acid Substitutions in Transmembrane Domains of β-Barrel Membrane Proteins for Detecting Remote Homologs in Bacteria and Mitochondria.

PLoS ONE. 2011;6(11):e26400. Epub 2011 Nov 1. PubMed.

Supplementary information and bbTM-ST.

- 2008 <u>Jimenez-Morales D</u>, Adamian L, and Liang J Detecting Remote Homologues Using Scoring Matrices Calculated from the Estimation of Amino Acid Substitution Rates of Beta-Barrel Membrane Proteins. Conf Proc IEEE Eng Med Biol Soc. 2008, 30:1347-1350. <u>PubMed</u>.
- 2008 <u>Jimenez-Morales D</u>
 Substitution Rates of Amino Acid residues in Transmembrane Regions of Beta-Barrel Membrane Proteins.
 BioE Student Journal. N1, 2008. Front Cover.

Books

- **2001** Coauthor. *Propiedades adicionales no antibióticas de los macrólidos*. Scientific Communication Management Editors.
- 2001 Coauthor. Guía Setas Autóctonas. Editorial Doyma. Madrid.

Popular Science Articles

- 2000 <u>Jimenez-Morales D</u>

 Problematic in the use of antiobiotics in animal farms.

 N°41. Ganaderos Magazine. sp
- **2000 -** <u>Jimenez-Morales D</u> *Bovine spongiform encephalopathy.*N°37. Ganaderos Magazine. sp

Abstracts & Communications

- 2011 <u>Jimenez-Morales D</u>, Liang J, and Eisenberg B. Active Sites of Enzymes are Crowded with Charge. <u>Biophysical Journal</u>. 100(3): p. 218a. Abstract 1191-Pos and Poster Board B101
- 2011 <u>Jimenez-Morales D</u>, Liang J, and Eisenberg B.
 Active Sites of Enzymes are Crowded with Charge.
 6th Annual Midwest Conference on Protein Folding, Assembly, and Molecular Motions.
 University of Notre Dame.
- 2010 <u>Jimenez-Morales D</u>, Li R, Wang Z, Li Y, Liu L, Liang J. Evolutionary Speed of Enzymes Functional Surfaces and their Relationship with Metabolic Fluxes in Networks of Central Carbon Metabolism of Bacteria. <u>Biophysical Journal 98(3) pp. 741a</u>
- 2008 <u>Jimenez-Morales D</u>, Adamian L, Liang J. Substitution Rates Of Amino Acid Residues In Transmembrane - Extracellular And Periplasmic- Regions Of Beta-Barrel Membrane Proteins. Biophysical Journal 94(2) pp. 1959
- **2002 -** <u>Jimenez-Morales D.</u> *Tools for the Apored Virtual.*V-Aporeunión. Tordesillas (Valladolid)
- 1999 <u>Jimenez-Morales D</u>, Heredia S, Calvo A, Gomez-Luz ML, Prieto J. Sensibilidad a antimicrobianos de Enterococcus faecalis de procedencia animal. Spanish Chemotherapy Society Congress. May 1999
- **1999 -** <u>Jimenez-Morales D</u>, Heredia S, Calvo A, Gomez-Luz ML, Prieto J. Sensibilidad a antimicrobianos de Enterococcus faecalis de procedencia animal. Spanish Chemotherapy Society Congress. May 1999

Invited talks

- 3/28/2013 Department of Microbiology and Immunology.
 Loyola University Chicago (2160 South First Avenue. Maywood, IL)
- **10/4/2012** Midwest Center for Structural Genomics & Biosciences Division. Argonne National Laboratory (9700 S. Cass Av. Argonne, IL)

Teaching

Instructor

Department of Bioengineering. University of Illinois at Chicago. Fall 2010 - BIOE480: Introduction to Bioinformatics

Fall 2012 - BIOE481: Bioinformatics Laboratory

Teaching Assistant

Department of Bioengineering. University of Illinois at Chicago.

Spring 2013 - BIOE250, Clinical Problems in Bioengineering

Fall 2010, 2012 - BIOE480, Introduction to Bioinformatic

Spring 2007 - BIOE455, Intro to Cell and Tissue Engineering Fall 2006 - BIOE240, Modeling Physiological Data & Systems

Computing

Computer Skills

Bioinformatics Packages: Sequence analysis software (Blast, MEME-MAST, ClustalW, T-Coffee, HMMER, HHsearch,...); molecular structures visualization software (PyMOL, VMD, Rasmol, Dino, SPDBV); molecular dynamics (NAMD); molecular interactions (Mint, Osprey); etc.

Languages: Perl, R, Unix shell scripts, Matlab, C/C++, Java, Html, PHP.

Other applications: Design and internet (Photoshop, Illustrator, Freehand, Flash, Dreamweaver,...); databases (MySql, Access); statistician (SAS, SPSS); etc.

Operating Systems: Unix/Linux and Mac OS X (advance)

Computer Tools

I have developed the following computational tools:

- **PreLysCar** (Predictor of Lysine Carboxylation) http://tanto.bioengr.uic.edu/prelyscar/
- bbTM-ST (beta-barrel TransMembrane Search Tool) http://tanto.bioengr.uic.edu/bbtmst/bbtmstool.php

Web Design and Development

2003 - Proteomic Unit

http://www.ucm.es/info/gyp/proteomica/en/

Proteomics Unit. Facultad de Farmacia. UCM-PCM (Madrid, Spain)

2004 - Genomic Unit

http://www.ucm.es/genomica

Genomic Unit. Facultad de Farmacia. UCM-PCM (Madrid, Spain)

2002, 2005 - Spanish Network of Apoptosis (APORED)

http://apored.bq.uam.es/

Department of Cell and Developmental Biology.

Centro de Investigaciones Biológicas (CIB-CSIC)

Software Administration

2002 - 2005 - Spanish Network of Apoptosis (APORED)

Department of Cell and Developmental Biology. CIB-CSIC

- Administrator of workspace BSCW (Basic Support for Cooperative Work) of the APORED.
- List co-administrator of APORED email distribution list, and list administrator of Apobecarios email distribution list.
- Website updates

Awards

2008 - 2010 Beca Talentia Excellence Grant

Regional Ministry for Innovation, Science and Enterprise. Junta de Andalucía. Spain.

References

Jie Liang, Professor

Bioengineering Department – University of Illinois at Chicago. 820 South Wood St. Room W103. Chicago, IL 60612 USA

Linda J Kenney, Professor

Professor of Microbiology & Immunology, UIC PI, Mechanobiology Institute, Singapore (MBI) National University of Singapore

Robert S. Eisenberg, Professor

Dept of Molecular Biophysics & Physiology - Rush University 1653 West Congress Parkway. Chicago IL 60612 USA

Dashuang (Daniel) Shi, PhD

Children's National Medical Center Center for Genetic Medicine Research (CGMR) 111 Michigan Avenue, NW, Washington, DC 20010-2970

Concha Gil García, PhD.

Microbiology II Department – <u>Proteomics Core Facility</u> - Faculty of Pharmacy. Universidad Complutense de Madrid Avda. Ramón y Cajal, s/n. Madrid, 28040 Spain

Enrique J. de la Rosa, PhD.

Centro de Investigaciones Biológicas Calle Ramiro de Maeztu, 9. Madrid, 28040 Spain

Flora de Pablo, PhD.

Centro de Investigaciones Biológicas Calle Ramiro de Maeztu, 9. Madrid, 28040 Spain

Maria Luisa Gómez-Lus, PhD.

Microbiology I Department – Faculty of Medicine. Universidad Complutense de Madrid Pza. Ramón y Cajal, s/n. Madrid, 28040 Spain