

Daniel E. Almonacid Coronado, Ph.D.

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SUMMARY

- **Education:** clinical biochemist; Ph.D. in molecular informatics; postdoctoral training in bioengineering
- **Research:** study of enzyme catalysis using computational biology approaches. Special interest in annotation of genomes and metagenomes; selection of targets for structure and function determination; development of algorithms for comparison of chemical reactions; study of convergent and divergent function evolution
- **Teaching:** supervisor of rotation projects of Ph.D. students; demonstrator of theoretical practicals for undergraduate students; monitor at summer camp for elementary school kids
- **Leadership:** founding member of the students and young researchers council of SoIBio; program chair for ISCB Latin America; editor of the Journal of Postdoctoral Affairs; vice-president, treasurer and acting president of the postdoctoral scholars association at UCSF; president and financial advisor of the Encuentros conferences of Chileans abroad
- **Entrepreneurship:** international adjunct director for RedCiencia; co-author EvolveMol business plan

EDUCATION

Ph.D. Molecular Informatics – Dept. Chemistry & St John’s College, U. of Cambridge, UK Oct ’04 – Nov ’07

Thesis title: *The chemistry and evolution of protein catalysis*, supervised by Dr John Mitchell. The work helped develop the MACiE database of enzyme reaction mechanisms, facilitated the creation of novel algorithms for quantifying similarity of enzyme reactions, analyzed the dominant strategies of evolution of enzyme function, and studied the chemical repertoire of enzyme catalysis and the function of catalytic residues.

BSc Biochemistry – Universidad de Concepción, Chile. First-Class degree Mar ’99 – Sep ’04

Thesis title: *Intra-phycoyanin and inter-phycoyanin preferential light transfer pathways in phycobilisomes*, supervised by Dr Marta Bunster and Dr Adelio Matamala. Elucidation of the structure-function relationship in the light-harvesting protein phycocyanin from *Gracilaria chilensis* and *Fremyella diplosiphon* using semi-empirical calculations and protein-protein docking.

Courses included: inorganic, organic, physical, analytical and radiochemistry. Calculus, statistics, anatomy, histology, biophysics, physiology, physiopathology, biochemistry, immunology, pharmacology, clinical biochemistry, nutrition, microbiology, parasitology, haematology, and toxicology.

High School Education – Kingston College, Concepción, Chile Mar ’95 – Dec ’98

Graduated as the best student of the year of 1998.

LICENSES, CERTIFICATIONS

Biochemist – Chile

Sep ’04

PRINCIPAL POSITIONS HELD

Postdoctoral Scholar – Dept. Bioeng. & Therapeutic Sciences, U. California San Francisco, USA Dec '07 – Present
Supervised by Prof. Patricia Babbitt, I develop and use quantitative metrics of reaction and substrate similarity to compare enzymes from both mechanistically diverse superfamilies and convergently evolved groups. Our aim is to create new classifications for enzyme functions based on these quantitative measures. For the past two years I have been part of the Enzyme Function Initiative (EFI), a multidisciplinary collaboration aiming at developing a large-scale sequence/structure-based strategy for assigning the *in vitro* functions and *in vivo* contexts of unknown enzymes, involving more than 80 researchers from 14 academic groups across the USA. Here, I use the quantitative metrics described above, in conjunction with sequence similarity networks, to define structure-function relationships to inform function annotation of sequences and structures recently discovered in the genome and metagenome projects, and to select the most informative targets for structure and function determination. Recently, we have also been using metrics of reaction and substrate similarities to identify putative metabolic pathways from metabolomics data. Additionally, my work in the EFI has involved extensive examination of the isoprenoid synthase superfamily of enzymes.

Research Assistant – Dept. Chemistry, Universidad de Concepción, Chile Mar '03 – Feb '04
Part-time work alongside undergraduate studies in a project entitled *SPF oscillator: An anharmonic model to rotation-vibration molecular dynamics*, involving quantum mechanical calculations of small molecules.

OTHER POSITIONS HELD CONCURRENTLY

External Thesis Supervisor – Master Program in Bioch. and Bioinformatics, U. de Concepción Apr '12 – Present
I am an accredited external thesis supervisor for graduate students in the Master program in biochemistry and bioinformatics of the Universidad de Concepción.

HONORS AND AWARDS

Travel fellowships from the International Society for Computational Biology to attend their annual international meeting in Vienna, Toronto and Long Beach, respectively	2012, 2008, 2007
Scholarship from the Cambridge Overseas Society for graduate studies at U. of Cambridge, UK	2005
Republic's President Scholarship for graduate studies abroad, Chile	2004
Graduation from the BSc in biochemistry with the highest grade in clinical biochemistry, Universidad de Concepción, Chile	2004
Highest entry grade to the degree in biochemistry at Universidad de Concepción, Chile	1999
Highest national score in the chemistry aptitude test for entry into Chilean universities	1998

KEYWORDS/AREAS OF INTEREST

enzymes, catalytic residues, reaction similarity, mechanism similarity, sequence similarity, networks, enzyme superfamilies, convergently evolved enzymes, isoprenoid synthases, function annotation, target selection, metabolic reconstruction, binding specificity, catalytic specificity, biological and chemical databases, sequence alignment, phycobilisomes, phycocyanin, fluorescence resonance energy transfer, *Gracilaria chilensis*, *Fremyella diplosiphon*, computational biology, cheminformatics, bioinformatics, computational chemistry, scientific networking, diasporas, brain circulation, entrepreneurship

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Page 2 of 7

RESEARCH AND CREATIVE ACTIVITIES

RESEARCH AWARDS AND GRANTS

NIH R01 GM60595 – Laying the Foundations for Genomic Enzymology

Jul '11 – Mar '15

Involvement: Scientific and Writing Contribution; Role: Project Scientist; PI: Patricia Babbitt.

PUBLICATIONS

PEER REVIEWED PUBLICATIONS

According to Google Scholar, as of August 28th 2012, my publications have 162 citations and an h-index of 6. My Google Scholar public profile can be accessed at: <http://scholar.google.com/citations?user=NhQRF08AAAAJ>

Holliday GL, Andreini C, Fischer JD, Rahman SA, Almonacid DE, Williams ST, Pearson WR: **MACiE: exploring the diversity of biochemical reactions**. *Nucleic Acids Research* 2012, 40:D783-D789.

Almonacid DE, Babbitt PC: **Toward Mechanistic Classification of Enzyme Functions**. *Current Opinion in Chemical Biology* 2011, 15:435-442.

Almonacid DE, Yera ER, Mitchell JBO, Babbitt PC: **Quantitative Comparison of Catalytic Mechanisms and Overall Reactions in Convergently Evolved Enzymes: Implications for Classification of Enzyme Function**. *PLoS Computational Biology* 2010, 6:e1000700.

Holliday GL*, Almonacid DE*, Mitchell JBO, Thornton JM: **The Chemistry of Protein Catalysis**. *Journal of Molecular Biology* 2007, 372:1261-1277. *Joint first authors.

O'Boyle NM, Holliday GL, Almonacid DE, Mitchell JBO: **Using Reaction Mechanism to Measure Enzyme Similarity**. *Journal of Molecular Biology* 2007, 368:1484-1499.

Matamala AR, Almonacid DE, Figueroa MF, Martinez-Oyanedel J, Bunster MC: **A Semiempirical Approach to the Intra-Phycocyanin and Inter-Phycocyanin Fluorescence Resonance Energy-Transfer Pathways in Phycobilisomes**. *Journal of Computational Chemistry* 2007, 28:1200-1207.

Contreras-Martel C, Matamala A, Bruna C, Poo-Caamaño G, Almonacid D, Figueroa M, Martinez-Oyanedel J, Bunster MC: **The Structure at 2Å Resolution of Phycocyanin from *Gracilaria chilensis* and the Energy Transfer Network in a PC-PC Complex**. *Biophysical Chemistry* 2007, 125:388-396.

Holliday GL, Almonacid DE, Bartlett GJ, O'Boyle NM, Torrance JW, Murray-Rust P, Mitchell JBO, Thornton JM: **MACiE (Mechanism, Annotation and Classification in Enzymes): Novel Tools for Searching Catalytic Mechanisms**. *Nucleic Acids Research* 2007, 35:D515-D520.

Holliday GL, Bartlett GJ, Almonacid DE, O'Boyle NM, Murray-Rust P, Thornton JM, Mitchell JBO: **MACiE: A Database of Enzyme Reaction Mechanisms**. *Bioinformatics* 2005, 21:4315-4316.

OTHER CREATIVE ACTIVITIES

Almonacid DE: **Conferencia Encuentros 2011**. (In Spanish) El Mercurio, 2011, November 10, pp. A2.

Almonacid DE: **Conferencia Encuentros 2011**. (In Spanish) El Mercurio, 2011, June 13, pp. A2.

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Page 3 of 7

INVITED PRESENTATIONS

NATIONAL & INTERNATIONAL

Annual International Conference on Intelligent Systems for Molecular Biology; Long Beach, USA, 2012 (poster and talk); Stockholm, Sweden, 2009 (poster); Toronto, Canada, 2008 (poster & talk); Vienna, Austria, 2007 (poster & talk); Detroit, USA, 2005 (poster & talk)

Encuentros Conferences of Chilean Students and Professionals Abroad; Paris, France, 2012 (session chair); Cambridge, UK, 2010 (poster); Gottingen, Germany, 2009 (talk)

International Society for Computational Biology Latin America Meeting; Santiago, Chile, 2012 (talk); Montevideo, Uruguay, 2010 (program chair, poster & talk)

Nexos Chile-USA; Washington D.C., USA, 2010 (talk)

American Chemical Society; San Francisco, USA, 2010 (talk)

UK QSAR Society; Cambridge, UK, 2006 (talk)

Meeting of the Chilean Chemical Society; Concepción, Chile, 2006 (poster)

Meeting of the Chilean Society of Biochemistry and Molecular Biology; Villa Alemana, Chile, 2003 (poster); Puyehue, Chile, 2002 (poster)

Meeting of Chilean Biochemistry Students; Concepción, Chile, 2002 (talk)

OTHER INVITED PRESENTATIONS

University of California Berkeley, USA	2011
European Bioinformatics Institute, UK	2009
University of California San Francisco, USA	2009
Unilever, Colworth, UK	2007
University of Cambridge, UK	2005

TEACHING AND MENTORING

PREDOCTORAL STUDENTS SUPERVISED OR MENTORED

Supervisor of Ph.D. Student's Rotations – Dept. Bioeng. & Th. Sci., U. Calif. San Francisco, USA Jun '08 - Present

I have directly supervised the research performed by students while performing their rotations at the Babbitt lab at UCSF. Graduate students supervised have been: Marc Yago, 2010, pharmaceutical sciences and pharmacogenomics graduate student; Jaline Gerardin, 2009, biophysics graduate student; Emmanuel Yera, 2008, biomedical informatics graduate student.

FORMAL SCHEDULED CLASSES

Demonstrator for Theoretical Practicals – Dept. Chemistry, University of Cambridge, UK Oct '04 – Sep '07

Teaching groups of up to 14 students how to carry out experiments and helping with the theory behind them. Courses taught included: chemical informatics (3rd year chemistry students; michaelmas term '06-'07, lent term '05-'06); part 2 chemistry (3rd year chemistry students; michaelmas term '05-'06, lent term '04-'05); part 1B chemistry (2nd year chemistry students; lent term '04-'05).

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Page 4 of 7

INFORMAL TEACHING

Biology Monitor – Chilean National Commission of Science and Technology, Cañete, Chile Jan '02
Biology monitor at the summer camp “Holidays with the Sciences”. It involved organizing a full week of activities for 10-13 year old students to teach them about the molecular constituents of cells which they learned by creating models of DNA and visualizing protein structures using computer software.

PROFESSIONAL ACTIVITIES AND LEADERSHIP

PROFESSIONAL ORGANIZATIONS

Memberships

Iberoamerican Society for Bioinformatics	Mar '12 – Present
American Chemical Society	Oct '09 – Oct '10
National Postdoctoral Association, USA	Apr '08 – Present
International Society for Computational Biology	May '07 – Present

Service to Professional Organizations

Founding Member Students & Young Researchers Council – Iberoamerican Soc. for Bioinf. Mar '12 – Present
The students and young researchers council of the Iberoamerican Society for Bioinformatics aims at connecting young members of the community to exchange ideas and collaborate on projects, and to promote the development of new talents in bioinformatics in the Iberoamerican region.

Program Chair – Int. Society for Computational Biology Latin America Meeting, Uruguay Aug '08 – Mar '10
Program chair for the first International Society for Computational Biology (ISCB) Latin America meeting held in Montevideo, Uruguay in March 2010 with 170 attendees. Work involved coordinating speakers and poster presenters from all over the world.

SERVICE TO PROFESSIONAL PUBLICATIONS

Founding Member and Editor – Journal of Postdoctoral Affairs, USA Aug '10 – Present
Founding member and editor of the first journal addressing issues that pertain exclusively to the postdoctoral community. Areas of editorial expertise are compensation and networking.

Ad hoc Referee – Various Journals Oct '08 – Present
PLoS Computational Biology (1 paper in the past 4 years), Bioinformatics (1 paper in the past 2 years), Journal of Postdoctoral Affairs (1 paper in the past 1 year).

UNIVERSITY SERVICE

Various Positions – Postdoctoral Scholars Association, U. of California San Francisco, USA Feb '08 – Jun '12
I served as acting president, vice president, treasurer, and chair of the practice of science seminar series of the PSA at UCSF, one of the largest (1200 postdocs) and most vibrant postdoctoral communities in the world. Work has focused on industrial outreach, networking events, and fundraising.

Officer – Samuel Butler Room Society, St. John's College, University of Cambridge, UK Oct '06 – Sep '07
I served as website manager and publicity officer for the Samuel Butler (graduate combination) room while a member of St. John's College.

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Page 5 of 7

GOVERNMENT AND OTHER PROFESSIONAL SERVICE

Ad Hoc Reviewer – Portuguese Foundation for Sciences and Technology

Jul '12 – Present

I have served as ad hoc reviewer for one scientific proposal submitted to the Portuguese foundation for science and technology.

President and Financial Advisor – Encuentros 2013 Harvard/MIT (USA), 2012 U. Pierre et Marie Curie (France), 2011 UC Berkeley (USA), 2010 U. Cambridge (UK)

Oct '09 – Present

The 'Encuentros' conferences aim at connecting Chilean students and professionals abroad, with their counterpart in Chile, and with foreigners interested in collaborating with Chile. I was president for Encuentros 2011 (245 attendees) and financial advisor for Encuentros 2013 (280 anticipated attendees), Encuentros 2012 (260 attendees) and Encuentros 2010 (225 attendees). Work has involved networking with opinion leaders from Chile, UK, USA and France, including Nobel prize laureates, former and current Chilean presidents, government officials, Chilean national prize awardees, angel investors, and renown academics and artists. Important effort has been put fundraising \$60,000 - \$100,000 each year, which we have obtained from public and private sponsors and more recently through a crowdfunding platform. The meetings have attracted the attention from the Chilean media, and it has been featured in more than 30 newspaper articles and in 2 full-length TV documentaries. More information can be found at: www.encuentros2013.org

ENTREPRENEURSHIP

Co-author of Business Plan – EvolveMol

Jan '11 – Mar '11

As part of the 'Idea to IPO' class at UCSF, I co-authored a business plan for EvolveMol, a company that generates micro-fluidic devices for the selection of engineered yeast producing high-value chemicals. EvolveMol was selected to participate in the Start-up Chile program, and is currently funded by a Department of Energy SBIR award.

International Adjunct Director for the USA (West Coast) – RedCiencia

Apr '08 – Mar '12

RedCiencia, formerly Bionexa, was the largest web-based scientific collaboration platform in Spanish with more than 7000 users. I joined Bionexa as one of the first users and quickly after became an adjunct director for the USA. Work focused on advertising, expanding the user-base, and generating content (blogs, columns, job postings). It was owned by the Chilean National Commission of Science and Technology, but managed by the Bionexa team.

ADDITIONAL SKILLS

Languages

Spanish (first language); fluent spoken and written English

Computer Skills

Systems (Windows, UNIX, Linux); Software (ChemOffice, ISIS Base, Cytoscape, Waterloo Maple, Gaussian, R, HyperChem, molecular visualization tools, bioinformatics software and databases); Languages (Bash, Python, SQL); Web (HTML, PHP, CSS, JavaScript)

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Page 6 of 7

REFEREES

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Dr John Mitchell, Chemistry Reader, School of Chemistry, University of St Andrews, Biomolecular Sciences Building, North Haugh, St Andrews, KY16 9ST, U.K. Tel: +44 (0)1334 467259; email: jbom@st-andrews.ac.uk

Dr Dame Janet Thornton, DBE, FRS, Director, European Bioinformatics Institute, EMBL Outstation - Hinxton, Wellcome Trust Genome Campus, Hinxton, CB10 1SD, U.K. Tel: +44 (0)1223 494648; email: thornton@ebi.ac.uk

Dr Marta Bunster, Professor, Laboratorio de Biofísica Molecular, Departamento de Biología Molecular, Facultad de Ciencias Biológicas, Universidad de Concepción, Barrio Universitario s/n, Casilla 160-C, Concepción, Chile. Tel: +56 (0)41 2203822; email: mbunster@udec.cl

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