

Daniel W. Udvary
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Education

Postdoctoral research, University of California San Diego, Scripps Institution of Oceanography, 2005-2007.

Postdoctoral research, University of Arizona, College of Pharmacy, 2003-2005.

Ph.D. in Bioorganic Chemistry, The Johns Hopkins University, 2003.

M.A. in Chemistry, The Johns Hopkins University, 1999.

B.S. in Chemistry, University at Albany, 1996.

Work Experience

Secondary Metabolism Computational Biologist, Department of Energy Joint Genome Institute, Secondary Metabolites Science Program (Oct 2018 – Present)

Responsibilities include:

- Creation, development, and maintenance of a pipeline for secondary metabolism analysis
- Leading revisions and updates to Atlas of Biosynthetic Clusters (ABC), JGI's web portal and database of secondary metabolism
- Seek and carry out research collaborations with JGI users in the area of secondary metabolism
- Outreach to the scientific community and the general public

Bioinformatics Computing Consultant, National Energy Research Supercomputing Center, Data Science Engagement Group (Apr 2015-Oct 2018)

Responsibilities Include:

- Adaptation of bioinformatics pipelines to HPC environments
- Conducting research efforts in secondary metabolism analysis in collaboration with the JGI's Synthetic Biology and Metabolomics groups.
- Data analysis using Perl, Python, R and Bash
- Advising and training NERSC users on best practices for use of the Genepool, Denovo, and Cori supercomputing clusters
- Preparing and leading training sessions and workshops in continuous integration, containerization of bioinformatics software, programming, software management, and common bioinformatics tools.
- Elucidation of performance and efficiency metrics to identify wasteful users and pipelines
- Installation and maintenance of >1000 bioinformatics software packages in a complex, user-focused HPC environment

Senior Scientist, Warp Drive Bio, Cambridge MA. (Jun 2013-April 2015)

Responsibilities included:

- Elucidation and prediction of chemical products of bacterial biosynthetic gene clusters and metabolic pathways.
- Bioinformatics software development to support molecular and synthetic biology efforts company-wide.

- Development and deployment of specialized genome sequence analysis pipeline.
- Database and web site development to deliver sequence information to molecular biology and chemistry groups to aid drug discovery, strain engineering, and generation of expression constructs.
- Sequencing and analysis of >150,000 bacterial genomes, with closure and complete annotation of >150 actinomycete bacterial genomes.
- Direct communication, both written and verbal, of genomic information and findings to senior leadership and business partners.

Assistant Professor, University of Rhode Island, College of Pharmacy, Department of Biomedical and Pharmaceutical Sciences. (Jan 2008-May 2013).

Activities included:

- Utilization of genetic or genomic data to discover and/or manipulate biosynthetic pathways of drug-like molecules.
- Creation of the SMOR database (Secondary Metabolism Online Repository)
- Functional annotation (and re-annotation) of genes from genomic data.
- Synthesis, manipulation, and expression of biosynthetic operons.
- Genomic sequencing and analysis of unique microbial species.
- Enzymology of natural product biosynthetic enzymes.
- Database design and administration.
- Director of the IDeA Network for Biological Research Excellence (INBRE) Bioinformatics Core (2007-2009, 2011-2012).
- Classroom instruction in courses covering bioinformatics, molecular biology, sequence analysis, natural products chemistry, medicinal chemistry, and infectious diseases.
- Preparation and submission of grant proposals and manuscripts.
- Supervised and mentored 5 graduate students, 7 undergraduates, 1 post-doctoral researcher in bioinformatics, natural products, and molecular biology research.
- Service on College Curriculum and Professionalism committees.

Postdoctoral Researcher, UCSD, Scripps Institute of Oceanography (Nov 2005-Dec 2007)

Prof. Bradley S. Moore, advisor.

Duties included:

- Discovery, analysis, annotation and prediction of chemical products of biosynthetic gene clusters deriving from the genomic sequencing of the obligate marine bacteria *Salinispora tropica* CNB-440 and *Salinispora arenicola* CNS-205.
- Leading and implementing a large, 24-person group project to analyze biosynthetic gene clusters and predict chemical products from the complete genomes of three bacterial plant-associated *Frankia* species.
- Communication of newly discovered genomic information to group members, collaborators, and the news media.
- Design and oversight of novel projects resulting from genomic analyses.
- Working in a leadership role mentoring and training graduate and undergraduate students as part of Prof. Moore's Type III PKS, *Salinispora* and *Frankia* project teams.
- Preparing, publishing and reviewing manuscripts and grant applications.

- Structure-based evaluation of reactivity and enzymology of Type III polyketide synthases from numerous microorganisms.
- Identification of novel reactivity in tetrahydroxynaphthalene synthase and germicidin synthase, *Streptomyces coelicolor* Type III polyketide synthase enzymes.

Research Associate, University of Arizona, College of Pharmacy (February 2003 – October 2005)

Prof. Bradley S. Moore, advisor.

Participated in interdisciplinary, collaborative research projects investigating the enzymology of numerous microbial natural product enzyme systems. Achievements include:

- Examining enzyme structure and function of numerous type III polyketide synthases to elucidate a global mechanism of polyketide biosynthesis in collaboration with the laboratory of Prof. Joseph P. Noel at the Salk Institute.
- Initiation of a project to functionally alter/engineer type III polyketide synthases using site-directed mutagenesis and directed evolution techniques.

Graduate Researcher, The Johns Hopkins University (September 1996 - February 2003)

Prof. Craig A. Townsend, advisor.

Employed an interdisciplinary approach to understanding aspects of the biosynthesis of the fungal mycotoxin aflatoxin B1 in *Aspergillus parasiticus*. Achievements include:

- Examining norsolorinic acid synthase, a multienzyme complex consisting of a type I polyketide synthase and fatty acid synthase.
- Developing UMA, a computerized tool for determining the locations of linker regions in multi-domain proteins, and applying it to norsolorinic acid synthase.
- Expression, purification, and kinetic characterization of the thioesterase domain and a previously unidentified acyl transferase domain of norsolorinic acid synthase.
- DNA sequencing, cloning, expression, and evaluation of the unusual catalytic abilities of the cytochrome P450 oxidoreductase, *ordA*.
- Natural product isolation and identification, as well as minor chemical modifications to evaluate enzyme substrate specificity.
- Acted as a teaching assistant for two semesters of general chemistry, and three semesters of organic chemistry, which included extensive classroom teaching.

Teaching Experience

Bioinformatics I (BPS542), URI (Spring 2008, 2009, 2010, 2013). A graduate-level project-based course taken by computer science- and biologically-oriented students, instructing in the use and theory behind current bioinformatics algorithms and software.

Practical Tools for Molecular Sequence Analysis (BPS450X/550X), URI (Fall 2009, 2011). Designed and implemented a course instructing Biology researchers in the use of common bioinformatics software. Includes didactic and laboratory instruction.

Natural Products and Biological Drugs (BPS445), URI (Spring 2013). Undergraduate didactic course for Biomedical and Pharmaceutical Sciences majors.

Molecular Biology and Medicinal Chemistry Laboratory (BPS451), URI (Fall 2011-2012). An advanced undergraduate laboratory course for Pharmaceutical Sciences students training on techniques in gene synthesis, PCR, cloning, protein expression and purification, bioassay design, and drug discovery.

Advanced Medicinal Chemistry (BPS691), URI (Fall 2010-2012). An entry-level graduate course instructing students with varied chemical and biological backgrounds in the principles of medicinal chemistry.

Chemistry of Natural Products (BPS551), URI (Fall 2010). Course instructing graduate students in principles of modern natural products chemistry, including design of isolation protocols, structure determination using spectroscopy, and biosynthesis.

Interactive Learning (IAL) – Infectious and Pulmonary Diseases, URI (Fall 2008-Spring 2012). Led students in presentation and discussion of topics related to PharmD program core course content.

Topics in Marine Natural Products (SIO264), UCSD, Scripps Institution of Oceanography (April-June 2007). A graduate-level project course in which students were taught methods to analyze DNA encoding biosynthetic gene clusters to predict chemical structures. Students worked as teams, applying these lessons to three previously-unanalyzed actinomycete genomes, and manuscripts describing their findings are in preparation for submission to a peer-reviewed journal.

The Johns Hopkins University. Teaching assistant (1997-2002). Three semesters classroom teaching experience grading exams, holding office hours, and lecturing weekly in Organic Chemistry. Two semesters grading exams, holding office hours, and lecturing weekly in General Chemistry.

Publications

Erbilgin, Onur; Rübél, Oliver; Louie, Katherine; Trinh, Matthew; Raad, Markus; Wildish, Tony; **Udwary, Daniel**; Hoover, Cindi; Deutsch, Samuel; Northen, Trent; Bowen, Benjamin. "MAGI: A method for metabolite, annotation, and gene integration". *ACS Chem Biol*. 2019 Apr 19;14(4):704-714. doi: 10.1021/acscchembio.8b01107. Epub 2019 Apr 4.

Mouncey NJ, Otani H, **Udwary D**, Yoshikuni Y. "New voyages to explore the natural product galaxy". *J Ind Microbiol Biotechnol* 2019 Mar;46(3-4):273-279. doi: 10.1007/s10295-018-02122-w. Epub 2019 Jan 4.

Uddhav K. Shigdel, Seung-Joo Lee, Mat E. Sowa, Keith Robison, Khian Hong Pua, Dylan T. Stiles, Joshua A. V. Blodgett, Brian R. Bowman, **Daniel W. Udwary**, Andrew T. Rajczeszki, Alan S. Mann, Siavash Mostafavi, Sukrat Arya, Tara Hardy, Zhigang Weng, Kyle Kenyon, Jay P. Morgenstern, Ende Pan, Daniel Gray, Roy M. Pollock, Andrew M. Fry, Sharon A. Townson, Gregory L. Verdine. "A Novel Natural Small Molecule Harnesses FKBP12 to Target a Flat Protein Surface". Submitted for review.

Wang Q, Arighi CN, King BL, Polson SW, Vincent J, Chen C, Huang H, Kingham BF, Page ST, Farnum Rendino M, Thomas WK, **Udwary DW**, Wu CH; the North East

Bioinformatics Collaborative Curation Team. "Community annotation and bioinformatics workforce development in concert--Little Skate Genome Annotation Workshops and Jamborees." *Database* (Oxford). 2012 Mar 20. Available online.

Udwary DW, Gontang EA, Jones AC, Jones CS, Schultz AW, Winter JM, Yang JY, Beauchemin N, Capson TL, Clark BR, Esquenazi E, Eustáquio AS, Freel K, Gerwick L, Gerwick WH, Gonzalez D, Liu WT, Malloy KL, Maloney KN, Nett M, Nunnery JK, Penn K, Prieto-Davo A, Simmons TL, Weitz S, Wilson MC, Tisa LS, Dorrestein PC, Moore BS. "Significant natural product biosynthetic potential of actinorhizal symbionts of the genus *Frankia*, as revealed by comparative genomic and proteomic analyses." *Appl Environ Microbiol*. 2011 Jun;**77**(11):3617-25.

Udwary DW. "Natural Product Combinatorial Biosynthesis: Promises and Realities", *Natural Product Chemistry for Drug Discovery*, Buss AD, Butler MS, Eds., Royal Society of Chemistry RSC Press (2010)

Penn K, Jenkins C, Nett M, **Udwary DW**, Gontang EA, McGlinchey RP, Foster B, Lapidus A, Podell S, Allen EE, Moore BS, Jensen PR. "Genomic islands link secondary metabolism to functional adaptation in marine Actinobacteria." *ISME J*. 2009 Oct;**3**(10):1193-203.

DW Udwary, JA Kalaitzis, and BS Moore, "Emerging marine biotechnologies – Cloning of marine biosynthetic gene clusters", *Oceans and Human Health: Risks and Remedies from the Seas*, P. J. Walsh, S. L. Smith, L. E. Flemming, H. Solo-Gabriele, and W. H. Gerwick, Eds., Elsevier, 507-524 (2008).

Jason M. Crawford, Anna L. Vagstad, Kenneth C. Ehrlich, **Daniel W. Udwary**, and Craig A. Townsend. "Acyl-Carrier Protein–Phosphopantetheinyltransferase Partnerships in Fungal Fatty Acid Synthases." *ChemBioChem*. 2008 Jul 2;**9**(10):1559-63.

Schultz AW, Oh DC, Carney JR, Williamson RT, **Udwary DW**, Jensen PR, Gould SJ, Fenical W, Moore BS. "Biosynthesis and structures of cyclomarins and cyclomarazines, prenylated cyclic peptides of marine actinobacterial origin." *J Am Chem Soc*. 2008 Apr 2;**130**(13):4507-16.

Daniel W. Udwary, Lisa Zeigler, Ratnakar N. Asolkar, Vasanth Singan, Alla Lapidus, William Fenical, Paul Jensen, Bradley S. Moore. "Genome sequencing reveals complex secondary metabolome in the marine actinomycete *Salinispora tropica*." *Proc Natl Acad Sci U S A*. 2007 Jun 19;**104**(25):10376-81.

Lijiang Song, Francisco Barona-Gomez, Christophe Corre, Longkuan Xiang, **Daniel W. Udwary**, Michael B. Austin, Joseph P. Noel, Bradley S. Moore and Gregory L. Challis. "Type III Polyketide Synthase *b*-Ketoacyl-ACP Starter Unit and Ethylmalonyl-CoA Extender Unit Selectivity Discovered by *Streptomyces coelicolor* Genome Mining." *J Am Chem Soc*. 2006 Nov 22;**128**(46):14754-14755

Crawford JM, Dancy BCR, Hill EA, **Udwary DW**, Townsend CA. "Identification of a starter unit acyl-carrier protein transacylase domain in an iterative type I polyketide synthase." *Proc Natl Acad Sci U S A*. 2006 Nov 7;**103**(45):16728-33.

Austin MB, Izumikawa M, Bowman ME, **Udwary DW**, Ferrer JL, Moore B, Noel JP. "Crystal structure of a bacterial type III polyketide synthase and enzymatic control of reactive polyketide intermediates." *J. Biol Chem.* 2004 Oct 22;**279**(43):45162-74

Udwary DW, Merski M, Townsend CA. "A method for prediction of linker regions within large multi-functional proteins, and its application to a type I polyketide synthase." *J. Mol. Biol.*, 2002, **323**, 585-598.

Udwary DW, Casillas LK, Townsend CA. "Synthesis of 11-Hydroxyl O-Methylsterigmatocystin and the role of a cytochrome P-450 in the final step of aflatoxin biosynthesis", *J. Am. Chem. Soc.* 2002, **124**, 5294-5303.

Invited Talks

"Secondary Metabolism in Metagenome-Associated Microbial Genomes". Helmholtz Institute for Pharmaceutical Research Saarland. Universitat des Saarlandes, Germany. Jan 21, 2020.

"Sequencing and in silico analysis of the Warp Drive Genome Databank". Joint Genome Institute GSC-17 Satellite Workshop: Genomes to Secondary Metabolites: From Big Data to Small Molecules. Walnut Creek, CA. May 7-8, 2015.

"Sequencing and *in silico* analysis of the Warp Drive Genome Databank" SIMB Natural Product Discovery and Development in the Post-Genomic Era. San Diego, CA. Jan 11-14, 2015.

"Cataloging Gene Clusters of Bacterial Secondary Metabolism to Enable Drug Discovery." BioIT-World Conference and Expo '13. Boston, MA. April 9-11, 2013.

"Cataloging Gene Clusters of Bacterial Secondary Metabolism to Enable Drug Discovery and Explore Microbial Adaptation." NSF EPSCoR Workshop in Bioinformatics to Foster Collaborative Research, Little Rock AR. March 3-5, 2013.

"SMOR: A database and web analysis tool to identify bacterial secondary metabolism and enable drug discovery." Brown University, Center Computational and Molecular Biology. Sept 26, 2012.

"A crash course in analyzing and comparing sequence information." Bryant University. February 28, 2012.

"Drug discovery in a new age of biology: Progress toward a platform for comprehensive microbial natural products chemoinformatics." University of Rhode Island, Department of Chemistry Seminar series. February 7, 2011.

"Genomics in 2030." University of Rhode Island, Graduate School of Oceanography faculty retreat. January 2011.

"Using bioinformatics to elucidate microbial natural product biosynthetic pathways." University of Massachusetts Dartmouth. February 19, 2010.

"Bioinformatic and synthetic biology approaches to natural products biosynthesis."
BioNES meeting. December 4, 2009.

"Natural Products Research at the Chemistry/Biology/Information Technology Interface."
University of Rhode Island, Department of Biology Seminar Series. February 9, 2009

"Accessing genomic data for the prediction and elucidation of actinomycete natural
product chemical structures." Brown University, Department of Chemistry. April 8, 2008.

"Elucidating the biosynthetic potential of the *Frankia*, three plant-root symbiont
actinomycete species." University of Rhode Island, College of Pharmacy. Kingston, RI.
October 2, 2007.

"Genome sequencing and bioinformatic analysis of the secondary metabolomes of
Salinispora tropica and *Salinispora arenicola*." Natural Products Affinity Group Meeting,
University of California San Diego. San Diego, CA. May 18, 2007.

"Biosynthesis of salinosporamide A, a potent 20S proteasome inhibitor." Moores Cancer
Center, UCSD Medical Center. San Diego, CA. March 9, 2007.

Other Conference Presentations

Daniel Udwarý, Emiley Eloe-Fadrosch, Nigel Mouncey. Poster – Mining of metagenome-
associated microbial genomes for secondary metabolism 3rd International Conference
on Natural Products Discovery and Development in the Genomic Era. San Diego, CA.
Jan 12-16, 2020.

Daniel Udwarý, Keith Robison, Marc Chevrette, Greg Verdine. Poster – Lessons from
Long Read Assembly of 100+ Actinomycete Genomes. Gordon Conference for Marine
Natural Products, Ventura, CA. March 2014.

Keith Robison, **Daniel Udwarý**, Marc Chevrette, Greg Verdine. Poster - Lessons from
Long Read Assembly of >100 Actinomycete Genomes. Advances in Genome Biology
and Technology (AGBT), Marco Island, FL. February, 2014

Marian Gaviola, Caroline Killian, Ben Roberts, Stephanie Guertin, **Daniel W. Udwarý**.
Poster - Toward a comprehensive database of natural product biosynthetic pathways.
Gordon Research Conference for Marine Natural Products, Ventura, CA. February 2010.

Caroline Killian, Marian Gaviola, **Daniel Udwarý**. Poster - Investigations of biosynthetic
pathways in *Bacillus pumilus* RI06-95 by genome sequencing and comparative analysis.
Gordon Research Conference for Marine Natural Products, Ventura, CA. February 2010.

Udwarý DW, Jensen P, Moore BS. Poster – Secondary metabolic gene clusters from
the marine actinomycete, *Salinispora arenicola* CNS-205. Gordon Research Conference
for Marine Natural Products, Ventura, CA. February 2008.

Schultz A, **Udwarý DW**, Moore BS. Poster – Biosynthesis of cyclomarin, an anti-
inflammatory cyclic heptapeptide produced by *Salinispora arenicola*. Gordon Research
Conference for Marine Natural Products, Ventura, CA. February 2008.

Udworthy DW, Izumikawa M, Austin MB, Noel JP, Moore BS. Poster - Current Investigations of the Biochemical Properties of Type III Polyketide Synthases. Genetics and Molecular Biology of Industrial Microorganisms/Biotechnology of Microbial Products (GMBIM/BMP) Conference, San Diego, CA. November 2004.

Udworthy DW, Austin M, Izumikawa M, Noel JP, Moore BS. Poster – Directed Evolution of Type III Polyketide Synthases, Gordon Conference for Marine Natural Products, Ventura CA. February 2004.

Udworthy DW, Merski M, Galpin JD, Crawford JM, Townsend CA. Poster – A method for prediction of linker regions within large multifunctional proteins, and application to a type I polyketide synthase, SIM 2002 annual meeting, Philadelphia PA, August 2002.

Udworthy DW, Merski M, Townsend CA. A Simple Algorithm for Locating Structural Subdomains in Large Multifunctional Proteins, Polyketides III conference, University of Bristol, September 2001.