

## Costas D. Maranas

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Google Scholar: <https://scholar.google.com/citations?hl=en&user=l3M1PW0AAAAJ>

### EDUCATION

*1990-1995*      **Princeton University**, Princeton, New Jersey  
Ph.D. in Chemical Engineering, May 1995  
M.A. in Chemical Engineering, June 1992

*1985-1990*      **Aristotle University**, Thessaloniki, Greece  
Diploma in Chemical Engineering, June 1990

### PROFESSIONAL HISTORY

*Jun. 2004-present*      **The Pennsylvania State University,  
Department of Chemical Engineering**  
Professor

*June 2005-present*      Donald B. Broughton Professor in Chemical Engineering

*May 2005-2015*      Director of Graduate Student Recruiting for the Bioinformatics & Genomics  
Option

*Jan. 2012-present*      Member of the Bioengineering Intercollege Graduate Program

*Jan. 2004-present*      Faculty Affiliate of the Center for Supply Chain Research

*Sep. 2001-present*      Member of Faculty of the Intercollege Graduate Degree in Integrative  
Biosciences (Bioinformatics and Genomics & Cell and Developmental Biology  
Options)

*Jun. 2001-June 2004*      **The Pennsylvania State University,  
Department of Chemical Engineering**  
Associate Professor

*Sep. 1997-present*      Member of Faculty of the Operations Research Program

*Sep. 1995-Jun. 2001*      **The Pennsylvania State University,  
Department of Chemical Engineering**  
Assistant Professor

*Sep. 1994-Aug. 1995*      **Princeton University, Dept. of Chemical Engineering**  
Pre-doctoral Research Assistant

*Feb.-Jun. 1992*      **Princeton University, Dept. of Chemical Engineering**

Assistant in Instruction

*Feb.-Jul. 1990*

**Chemical Process Research Institute (CPERI), Greece**  
Research Assistant

*Jul.-Sep. 1989*

**Koninklijke Shell/Laboratorium in Amsterdam, NL,  
Mathematics and Systems Engineering Department**  
Research Assistant

*Jul.-Oct. 1988*

**Greek Fuels and Lubricants (EKO), Thessaloniki, Greece**  
Process Engineer Assistant in Refinery Operations

## **RESEARCH INTERESTS**

Reconstruction and analysis of metabolic networks, computational strain design, metabolism of cyanobacteria and plants, metabolism of obligatory anaerobes, systems and synthetic biology, computational design of proteins, enzymes and antibodies, protein pore design for separations and DNA sequencing, optimization theory and applications.

## **PROFESSIONAL SOCIETY MEMBERSHIPS**

Fellow of the American Institute of Chemical Engineers (Nov. 2020-present)

Fellow of the American Institute for Medical and Biological Engineering (Nov. 2007-present)

Member, American Chemical Society (ACS) (2004-present)

Member, Biological Systems Engineering (2004-2008)

Member, Society for Biological Engineering (SBE) (2003-present)

Member, International Metabolic Engineering Society (IMES) (2015-present)

Member, Biophysical Society (2000-present)

Member, Computer-Aided Systems Technology (CAST) (1992- present)

Member, American Institute of Chemical Engineers (1992-present)

## **PROFESSIONAL SOCIETY ACTIVITIES**

Organizing Committee Member & Participant of inter-BRC workshop on Artificial Intelligence and Machine Learning for Biosystems Design, Washington, DC, Feb. 26, 2020.

Conference Organizing Committee, International Conference on Microbiome Engineering, Nov. 4-6, 2018.

Conference co-Chair, Biochemical and Molecular Engineering, June 26-30, 2011 (over 200 participants)

Conference Advisory Board member for Metabolic Engineering Meeting (2008-present)

Conference Advisory Board member for Biochemical Engineering Meeting (2009-present)

Conference Committee member for FOCAPO (2008)

Advisory Board Member, Society for Biological Engineering SBE (2008-present)

Steering Committee member for EcoCyc database (2006-present)

PNNL Advisory Committee member for “Microbiomes in Transition” (2015-2020)

PNNL/EMSL Advisory Committee member for “Earth & Biological Sciences Directorate (EBSD)” (2015-2021)

### **JOURNAL EDITORIAL ACTIVITIES**

Editorial Board, Journal of Industrial Microbiology & Biotechnology (May 2017-present)

Editorial Board, IEEE Life Sciences Letters (July 2014-June 2017)

Associate Editor, BMC Systems Biology (Apr. 2011-present)

Associate Editor, PLoS Computational Biology (Feb. 2010-present)

Advisory Board of Biotechnology Journal (Nov. 2009-present)

Associate Editor, Bioprocess and Biosystems Engineering (Aug. 2007-Dec. 2007)

Editorial Board, Biophysical Journal (2005-2011)

Editorial Board, Journal of Global Optimization (2005-2007)

Editorial Board, Computers & Chemical Engineering (2004-2009)

Editorial Board, Metabolic Engineering (2001-present)

Editorial Board, Metabolic Engineering Communications (2018-present)

### **PROPOSAL REVIEWING ACTIVITIES**

Proposal Reviewer for NSF, DOE, NIH, EPA, Novo Nordisk Foundation, Weizmann Inst. of Science, Qatar National Research Fund, European Commission, Swiss National Science Foundation, ARISTEIA Research Program Greece, Technical University of Denmark, Research Foundation Flanders (FWO), and FNR Luxembourg.

### **INTERNAL ADMINISTRATIVE SERVICES**

Member, Dept., of Chemical Engineering Graduate Admissions Committee (2020-present)

Member of Advising Committee of Center of Excellence for Industrial Biotechnology (2017-present)

Member, Dept. of Chemical Engineering Faculty Search Committee (2019-20)

Member, Dept. of Chemical Engineering Undergraduate Curriculum Committee (2019-20)

Chair of Dept. of Chemical Engineering Awards Committee (2017-present)

Associate Member, Institute for CyberScience at Penn State (2017-present)

Member, Dept. of Chemical Engineering P&T Committee (2016-present)

Member, Dept. of Chemical Engineering Faculty Search Committee (2017-18)

Member, Dept. of Chemical Engineering Seminars Committee (2015-2016)

Chair of Associate Dean of Research and Innovation Search Committee (2016)

Chair of Chemical Engineering Faculty Search Committee (2016)

Member, COE P&T Committee (2013-2015)

Member, COE Dean Search Committee (2013)

Member, Bioengineering Intercollege Graduate Program (2011-present)

Chair of Committee on Faculty Recruiting (2010)

Chair of Departmental P&T Committee (2010-2011)

Member of AD-14 CSE Chair Review Committee (2010-2011)

Member, COE P&T Committee (2008-2010)

Chair, Committee on Bio-Chair Faculty Recruiting (2009)

Member, Network Science Committee (2008-present)

Director of Graduate Student Recruiting for Bioinformatics & Genomics Option (2005-Present)

Member, Homeland Security Initiative (2005)

Faculty Affiliate, Center for Supply Chain Research (2004-Present)

Chair, Sabbatical Review Committee (2004)

Member, Department Head Search Committee (2003)

Chair, Space Committee (2002)

Member, Departmental Awards Committee (2002-2003)

Member, Faculty of the Intercollege Graduate Degree in Integrative Biosciences: CDB and B&G Options. (2001-Present)

Member, Junior Faculty Search Committee (2000)

Member, Undergraduate Curriculum Committee (1999-2001)

Member, ABET Committee (1999)

Member, Department Head Search Committee (1999-2000)

Omega Chi Epsilon Academic Advisor (1998-2002)

Member, Faculty of the Operations Research Program (1997-present)

Member, Graduate Student Admissions Committee (1996-1998)

## **AWARDS AND HONORS**

### **Internal Recognitions**

Penn State Engineering Alumni Society (PSEAS) Premier Research Award, (2016)

Penn State Engineering Alumni Society (PSEAS) Outstanding Research Award, (2012)

### **External Recognitions**

2020 Biotechnology Progress Award for Excellence in Biological Engineering Publication

2021 International Metabolic Engineering Award, July 12-16, Honolulu, HI

Special Award for your Outstanding Contribution to Tsinghua Forum on Chemical Engineering (No. 12), October 24, 2014.

The Korean Society for Biotechnology and Bioeng. Lectureship at the KSBB Fall Meeting, (2007)

Stratis V. Sotirchos Lectureship at 6<sup>th</sup> Panhellenic Chemical Engineering Conference (2007)

Outstanding Young Investigator Award, AIChE Computing and Systems Technology Division Award (2006)

Allan P. Colburn Award for Excellence in Publications by a Young Member of the Institute, AIChE Institute Award (2002)

NSF CAREER Award (1997)

Du Pont Educational Aid Grant (1996-98)

Wallace Memorial Fellowship in Engineering, Princeton University (1993-94)

Technical Chamber of Greece Award (1988-1990)

National Scholarship Foundation of Greece Award (1987-1990)

## **INVITED LECTURES AND SEMINARS (2000-present)**

### *Universities & Institutes*

The University of Tennessee, Knoxville, Department of Chemical and Biomolecular Engineering seminar, March 30, (2021)

UMass-Amherst Chemical Engineering Seminar, March 23, (2021)

Operations Research (OR 590) Colloquium, Penn State University, January 26, (2021)

Future of Bioenergy and Biorenewables workshop, Penn State University, Dec. 15, (2020)

Alper Lab Online Seminar Series, University of Texas, Austin, Oct. 23, (2020)

MCIBS & Pathobiology Annual Research Retreat, Penn State University, Aug. 18, (2020)

Oden Institute for Computational Engineering & Sciences, University of Texas Austin, January 22, (2020)

Department of Chemical Engineering, Carnegie-Mellon University, September 26, (2019)

Department of Biomedical Engineering, Penn State University, September 7, (2019)

Department of Chemical Engineering, Monash University, December 3, (2018)

Department of Chemical Engineering, Colorado State University, May 18, (2018)

Department of Chemical Engineering, Monash University, Apr. 10, (2018)

Department of Chemical and Biomolecular Engineering, Princeton University, Feb. 12, (2018)

Applied Mathematics Group, Argonne National Lab (ANL), Sept. 1, (2017)

Department of Biochemical Engineering, Centre for Process Systems Engineering Seminar Series, University College London, June 7, (2017)

Department of Chemical, Biochemical and Environmental Engineering, University of Maryland Bucks County (UMBC), May 1, (2017)

Department of Chemical and Biomolecular Engineering, Tulane University, March 24, (2017)

MolES seminar at the University of Washington, Jan. 15, (2017)

Distinguished Lecture Series at the Monk Family Dept. of Chemical Engineering & Materials Science, University of Southern California, Dec. 1, (2016)

Department of Chemical Engineering, Massachusetts Institute of Technology (MIT), Oct. 21, (2016)

The Children's Hospital of Philadelphia (CHOP), Microbiome Program, University of Pennsylvania, May 25, (2016)

Department of Chemical Engineering, University of California Santa Barbara (UCSB), Jan. 14, (2016)

Department of Chemical and Biomolecular Engineering, Rutgers University, Nov. 19, (2015)

Department of Chemical and Biomolecular Engineering, University of Delaware, Oct. 2, (2015)

Institute of Systems Biology, Seattle WA, Sept. 25, (2015)

Bioengineering Department, UC San Diego, May 11, (2015)

School of Chemical and Biomolecular Engineering, Georgia Tech., Feb. 18, (2015)

Department of Chemical and Biomolecular Engineering, University of Colorado Boulder, Dec. 9, (2014)

Biological Engineering Department, Utah State University, Dec. 6, (2014)

Department of Chemical Engineering, Tsinghua University, Beijing, China, Oct. 24, (2014)

J. D. Lindsay Lecture Series, Department of Chemical Engineering, Texas A&M University, Sept. 3, (2014)

Department of Chemistry and Chemical Engineering, CalTech, Apr. 17, (2014)

Department of Chemical and Biomolecular Engineering, John Hopkins University, Apr. 10, (2014)

CEIT Centro de Estudios e Investigaciones Técnicas, Guipuzkoa, Spain, Dec. 18, (2013)

Department of Industrial Engineering, Penn State, Oct. 10, (2013)

School for Engineering of Matter, Transport and Energy, Arizona State University, Jan. 28, (2013)

Department of Chemical and Biomolecular Engineering, Univ. of Illinois at Urbana-Champaign, Oct. 2, (2012)

Ecole polytechnique fédérale de Lausanne, Institut des sciences et ingénierie chimiques, Lausanne, Switzerland, Apr. 25, (2012)

A. L. Bortree/Molecular Toxicology Seminar Series, Dept. of Veterinary and Biomedical Sciences, Penn State, Jan. 25, (2012)

Dept. of Chemical and Biological Engineering, University of Wisconsin, Nov. 8, (2011)

Dept. of Microbiology and Biochemistry, Michigan State University, Apr. 26, (2011)

NSF Engineering Research Center for Biorenewable Chemicals (CBiRC), Feb. 3, (2011)

Dept. of Chemical and Biological Engineering, Rice University, Oct. 28, (2010)

Dept. of Microbiology and Cell Science, Florida Univ., Feb. 22, (2010)

Joint BioEnergy Institute (JBEI), Jan. 29, (2010)

Operations Research Colloquium Seminar, Penn State, Dec. 8, (2009)

Dept. of Chemical, Biological and Environmental Engineering, Washington Univ., Dec. 4, (2009)

Dept. of Chemical Engineering Lindsey Lecture, Texas A&M, Oct. 28, (2009)

Dept. of Chemical and Biomolecular Engineering, Tufts Univ., Mar. 30, (2009)

Ecole polytechnique fédérale de Lausanne, Institut des sciences et ingénierie chimiques, Lausanne, Switzerland, Mar. 8, (2009)

Dept. of Chemical and Biological Engineering, Buffalo University, Feb. 25, (2009)

Dept. of Veterinary & Biomedical Sciences (Center for Molecular Immunology & Infectious Disease), Penn State Univ., Oct. 16, (2008)

Dept. of Industrial Engineering, Penn State Univ., Oct. 9, (2008)

Dept. of Chemical Engineering, Univ. of Maryland, Sept. 30, (2008)

Dept. of Chemical and Biomolecular Engineering, U. Penn, Sept. 24, (2008)

TIGEM Telephon Institute of Genetics and Medicine, Italy, May 23, (2008)

Dept. of Biological Sciences, Korea Advanced Institute of Science and Technology (KAIST), Korea, October 18, (2007).

Dept. of Chemical Engineering, RPI, Sept. 12, (2007).

Department of Biochemistry & Molecular Biology, College of Medicine, Hershey, PA, March 21, (2006).

Depts. of BME/ChemE and ICES, University of Texas, Austin, TX, October 13, (2005).

Sandia National Laboratories, Biological and Energy Science Center, Albuquerque, NM, May 12, (2005).



Dept. of Electrical Engineering, ETH, Switzerland, November 22, (2004).

Center for Process Biotechnology, Department of Biotechnology, Dept. of Biological Engineering, DTU, Denmark, November 19, (2004).

Dept. of Chemical Engineering, University of Connecticut, October 5, (2004).

Dept. of Chemical Engineering, University of Houston, September 3, (2004).

Division of Engineering and Applied Sciences, Harvard University, March 3, (2004).

Dept. of Bioengineering, University of California at San Diego, October 22, (2003).

Dept. of Chemical Engineering, Massachusetts Institute of Technology, October 17, (2003).

Dept. of Chemical Engineering, University of Massachusetts at Amherst, October 16, (2003).

Chemical Process Engineering Research Institute, Thessaloniki Greece, June 13, (2003).

Dept. of Chemical Engineering, Brooklyn Polytechnic University, April 11, (2003).

School of Chemical Engineering, Georgia Institute of Technology, March 19, (2003).

Dept. of Chemical and Biochemical Engineering, Rutgers University, February 27, (2003).

Dept. of Chemical Engineering, Princeton University, February 26, (2003).

Dept. of Chemical Engineering, University of California at Santa Barbara, November 21, (2002).

Dept. of Chemical Engineering, Northwestern University, September 26, (2002).

Dept. of Chemistry, Penn State University, September 19, (2002).

Dept. of Chemical Engineering, Delaware University, February 13, (2002).

Dept. of Chemical Engineering, Carnegie-Mellon University, December 17, (2001).

Dept. of Chemical Engineering, Wisconsin University, November 27, (2001).

Dept. of Chemical Engineering, John Hopkins University, October 25, (2001).

Dept. of Chemical Engineering, University of Virginia, October 18, (2001).

Dept. of Chemical Engineering, University of Pennsylvania, October 15, (2001).

Dept. of Chemical Engineering, Cornell University, September 10, (2001).

Dept. of Chemical Engineering, Imperial College, UK, September 3, (2001).

Dept. of Chemical Engineering, Rice University, February 22, (2001).

Centre for Process Systems Engineering, Imperial College, UK, June 30, (2000).

*Corporations*

GreenLight Technologies, Medford, MA, Aug. 31, (2016)

DuPont CR&D, Wilmington, DE, March 13, (2015).

Genomatica, Inc., San Diego CA, Apr. 18, (2014).

MedImmune, Gaithersburg MD, October 25, (2013).

BASF Corporation, Tarrytown NY, March 13, (2013).

Synthetic Genomics, April 30, (2007).

CACHE Corporation, WebCast, May 12, (2006).

Sigma-Aldrich, December 3, (2004).

Bristol Myers Squibb, April 27, (2004).

Xencor, Inc., Sept. 17, (2003).

Cargill, Inc., Industrial Bioproducts Business, Wayzata, MN, August 22, (2003).

Diversa Corporation, San Diego, CA, August 14, (2003).

DuPont Experimental Station, Wilmington DE, July 25, (2003).

Genencor International, Inc., Palo Alto, CA, July 11, (2002).

Xencor, Inc., April 10, (2002).

IBM Watson Center, Computational Biology Group, February 6, (2002).

Diversa Corporation, San Diego, CA, July 18, (2001).

Genomatica, Inc., March 15, (2001).

Enchira Biotechnology Corporation, January 5, (2001).

Maxygen Corporation, December 20, (2000).

Rutgers Organics, July 12, (2000).

Air Products & Chemicals, March 14, (2000).

*Conferences, Workshops & Symposia*

Metabolic Pathway Analysis (MPA), Aug. 12-16, 2019, Riga, Latvia, “Identifying Functional Roles of SNPs Using Metabolic Networks”

Biochemical and Molecular Engineering XXI. July 14-18, 2019, Mont Tremblant, Canada, “K-FIT: Parameterizing kinetic models of metabolism using multiple fluxomic datasets”

5<sup>th</sup> Conference on Constraint-Based Reconstruction Methods and Analysis (COBRA 2018). Oct. 14-16, 2018, Seattle, WA, “From 13C labeling data to parameterized kinetic models with a genome-wide coverage”

2018 Bioinformatics & Genomics Retreat. Oct. 5 & 6, 2018, Penn State, “Metabolic pathway design through uncharted biochemical spaces”

ISGSB 2018 (International Study Group for Systems Biology). Sept. 24-28, 2018, Tromsø, Norway, “From 13C labeling data to parameterized kinetic models with a genome-wide coverage”

YSGSB 2018 (Young Study Group for Systems Biology). Sept. 23, 2018, Tromsø, Norway, “Shaping production hosts by design”

Metabolic Engineering XII conference. Systems metabolic engineering for superior bio-production. June 24-28, 2018, Munich, Germany, “Shaping metabolism and production hosts by design”

MilliporeSigma Synthetic Biology and Metabolic Engineering Symposium, April 27, 2018, St. Louis, MO, “Shaping metabolism and production hosts by design”

Biocon China 2018, 4th International Symposium on Biopharmaceutical Innovation and Development, Computational antibody design session, Shanghai, China, April 20-21, 2018, “OptMAVEN: Computational antibody design”

Topical A conference on "Microbiomes and Microbial Communities" as part of the Annual Meeting of Chemical Engineers 2017, Minneapolis, MN, Nov. 1, 2017, “Metabolic modeling of microbial communities”

Metabolic Engineering Summit, Oct. 22-24, 2017, Beijing, China, “Atom mapping information in novel pathway design and metabolic flux elucidation”

CBiRC 9th Annual Site Visit, Oct. 9-10, 2017 Ames, IA, “Pathway synthesis using de novo steps through uncharted biochemical spaces”

Metabolic Pathway Analysis 2017. In silico & in vitro metabolism conference: From pathways to cells to communities and tissues, Bozeman, MT, July 24-28, 2017, “Exploring the combinatorial space of complete pathways to chemicals”

Biochemical and Molecular Engineering XX. The Next Generation of Biochemical Engineering: From Nanoscale to Industrial Scale, Newport Beach, CA July 16-20, 2017, “Computational redesign of acyl-ACP thioesterase with improved selectivity towards medium-chain fatty acids at high production levels”

Christodoulos A. Floudas Memorial Symposium, Princeton University, May 6, 2017, “Computational biology and bioinformatics”

EcoFAB summit. Developing a community strategy to advance standardized model ecosystems, Washington DC, April 27-28, 2017, “Challenges and Opportunities in Modeling Metabolism in Communities”

Fifth Annual Winter Q-Bio Meeting, Kauai, HI, Feb. 21-24, 2017, “Constructing predictive kinetic models of metabolism for guiding strain design”

DOE/BER Annual Grantees Meeting. Computing in Biology session, Crystal City, VA, Feb. 5-8, 2017, “Computational bottlenecks in metabolic networks and protein design”

Microbial Communities: Modelling Meets Experiments, EMBL, Germany, Dec. 8-11, 2016, “Modeling of metabolism in microbial communities”

Hellenic Bioinformatics (HBIO), Thessaloniki, Greece, Nov. 18-21, 2016, “Reconstruction, analysis and redesign of metabolic networks”

Gas Fermentation Workshop, Heron island, Australia, July 2-6, 2016, “Assessing methanotrophic capabilities of Methanosarcina acetivorans for bioproduction”

Metabolic Engineering XI: Metabolic Engineering Meeting, Kobe, Japan, June 26-30, 2016, “Computational Tools and Methods for Metabolic Engineering”

CBiRC 8<sup>th</sup> Annual Site Visit, May 9-12, 2016 Ames, IA, “Medium and short-chain fatty acid overproduction in E. coli through integrated fluxomics and computational strain design approach”

Indo-US Workshop on Cell Factories, Mar. 18-20, 2016, Mumbai, India, “Reconstruction, analysis and redesign of metabolism”

Genomics Science Contractors-Grantees Annual Meeting XIV, Mar. 6-9, 2016 Vienna VA, “Constructing predictive kinetic models of metabolism for guiding strain design”

Arpa-E REMOTE Annual Review Meeting, Jan. 20-21, 2016, LaJolla, CA, “Engineering A Methane-to-acetate Pathway For Producing Liquid Biofuels”

NSF Workshop on Designing Principles for Engineering Biology, Tysons Corner, VA, Nov. 10-11, 2015, “Engineering of biomolecular Networks”

CBiRC 7<sup>th</sup> Annual Meeting, Oct. 11-13, 2015 Ames, IA, “Progress in the integrated flux platform design”

4th Conference on Constraint-Based Reconstruction & Analysis (COBRA), Heidelberg, Germany, Sept. 18, 2015, “OptStoic: Designing overall stoichiometric conversions and intervening reactions”

IDEAS Lab Midterm Workshop, London, UK, Sept. 16, 2015, “Designing Nitrogen Fixation in Oxygenic Photosynthetic Cells”

Biochemical and Biomolecular Engineering XIX, Puerto Vallarta, Mexico, July 12-16, 2015, “Computational Tools for Enzyme and Antibody Design”

BioEnergy Science Center (BESC) Annual Retreat, Keynote Speaker, June 16, 2015, “Reconstruction, Analysis and Redesign of Metabolism”

COBRA Workshop on Modelling Microbial Communities, 5<sup>th</sup> International Human Microbiome Congress, Luxembourg, March 30, 2015, “Modeling microbial communities using bilevel programming”

EPFL/Nestle workshop: From single genome to metagenomic metabolic modelling, Lausanne, Switzerland, Jan. 26, 2015, “Reconstruction, Analysis, & Redesign of Metabolic Pathways”

Indo-US NSF Workshop on Synthetic and Systems Biology, JNU New Delhi, India, November 9-12, 2014, “Using computations to reconstruct, analyze and redesign metabolism”

Bioengineering Workshop: Cell factory design from enzyme to metabolic network, Tsinghua University, Beijing, China, October 27, 2014, “Using Computations for Enzyme and Antibody Design”

Metabolic Engineering X, Vancouver BC, June 15-19, 2014, “Integrating Kinetic Models of Metabolism with k-OptForce for Strain Design”

COBRA Conference, Wintergreen VA, May 20-23, 2014, “Using MetRxn for metabolic model reconstruction, flux elucidation and redesign”

DOE BER Contractor-Grantee Annual Meeting, Washington DC, Feb. 9-12, 2014, “Using MetRxn to reconstruct and redesign metabolism”

CBiRC NSF Engineering Research Center for Biorenewable Chemicals Fifth Annual Meeting, Oct. 6-8, Ames, IA, “Progress in the integrated flux platform design”

Biochemical and Molecular Engineering XVIII: Frontiers in Biological Design, Synthetic Biology and Processing East Meets West, Beijing China, June 16-20, 2013, “Computational methods for the rational de novo design of human antibodies”

American Society of Microbiology Annual Meeting, Denver, CO, May 18-22, 2013, “Kinetic modeling of metabolism and computational strain design”

3<sup>rd</sup> Conference on Cell Factories and Biosustainability, Copenhagen Bioscience Conferences, Novo Nordisk Foundation, Denmark, May 5-8, 2013, “Using Computations to Simulate and Assemble Cell Factories”

Cobra 2012 - 2nd International conference on constraint-based reconstruction and analysis, Elsinore, Denmark, Oct. 7-9, 2012, “OptCom: A Multi-Level Optimization Framework for the Metabolic Modeling and Analysis of Microbial Communities”

MARM 2102, Session: Bioenergy/Biofuels for Clean Energy, Baltimore, MD, June 1, 2012, “Integrating Computations with Experiments to Drive Biofuel Overproduction”

ICiS Genomics Driving Modeling in Biology Workshop, Park City, UT, July 24-29, 2011, “Challenges and Opportunities in Reconstructing and Analyzing Genome Scale Models”

1st Conference on Constraint-Based Reconstruction and Analysis, Reykjavik, Iceland, June 24-26, 2011, "Reconstruction of Genome-Scale Metabolic and Isotope Mapping Models"

2011 GTL Contractor-Grantee Workshop: Modeling in a Systems Biology Environment, USDA-DOE Plant Feedstock Genomics for Bioenergy Awardee Workshop, Bethesda, MD, Apr. 10-13, 2011, "Using Computations to Facilitate Metabolic Reconstructions and Guide Strain Optimization"

International Conference on Biomolecular Engineering, San Francisco, CA, January 16-19, 2011, "MetRxn: Reaction/Metabolite Standardization and Congruency across Databases and Genome-Scale Metabolic Models"

Bioinformatics & Genomics Retreat, Penn State University, Sept. 11, 2010, "Using Computations to Reconstruct, Quantify and Redirect Metabolism"

Society of Industrial Microbiology (SIM) Annual Meeting, San Francisco, CA, August 1-5, 2010, "Using computations to reconstruct and redirect metabolism"

Society of Industrial Microbiology (SIM) Annual Meeting, San Francisco, CA, August 1-5, 2010, "Using computations to drive novel enzyme and antibody design"

Metabolic Engineering VIII: Metabolic Engineering for Green Growth, Jeju Island, South Korea, June 13-18, 2010, "Using Computations to Reconstruct, Analyze and Redesign Metabolism"

Mini-Workshop on challenges in experimental data integration within genome-scale metabolic models, Institut Henri Poincare, Paris, France, October 10-11, 2009, "Genome-scale metabolic model reconstruction, curation and redesign"

3<sup>rd</sup> Annual Advances in Biomolecular Engineering: Protein Design Symposium, The New York Academy of Sciences, New York, NY, June 12, 2009, "Using Computations to Redesign Enzymes, Binding Sites and Antibodies"

GTL Contractor-Grantee Workshop VII: Modeling in a Systems Biology Environment, USDA-DOE Plant Feedstock Genomics for Bioenergy Awardee Workshop, Bethesda, MD, Feb. 8-11, 2009, "Using Computations to Reconstruct, Analyze and Redesign Metabolism"

Metabolic Engineering VII: Health and Sustainability, Puerto Vallarta, Mexico, Sept. 14-19, 2008, "Using Computations to Make Sense out of 'Omics Data'"

EMCC5, 5<sup>th</sup> Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries, Cetraro, Italy, May 25-29, 2008, "Systems Engineering Challenges and Opportunities in Biological Networks"

The Korean Society for Biotechnology and Bioengineering Fall Meeting, Daegu, Korea, October 19, 2007, "Computational Protein Engineering"

15th Annual International Conference on Microbial Genomics, University of Maryland College Park Campus, September 16-20, 2007, "Optimization-based Refinement of Metabolic Models"

Biochemical Engineering XV: Engineering Biology from Biomolecules to Complex Systems, Quebec City, July 15-16, 2007, "Metabolic Model Generation and Automated Curation: *Mycoplasma genitalium*"

Stratis V. Sotirchos Lectureship 2007, 6<sup>th</sup> Panhellenic Chemical Engineering Conference, Athens Greece, May 31- June 3, “Systems Engineering Challenges and Opportunities in Biological Networks”

Microbial Genomes 2007, Hinxton Hall, Cambridge, UK, April 11-14, 2007, “Analysis and Redesign of Microbial Metabolic Pathways”

Institute of Biological Engineering (IBE) 2007 annual meeting, St. Louis, Missouri, March 30-April 1, 2007, Session: Biology Inspired Modeling, “Computational Design of Biological Circuits”

IECA 2006: The International E. Coli Alliance Conference on Systems Biology, Jeju Island, Republic of Korea, October 31-Novemembr 4, 2006, “Computational Analysis and Redesign of Biological Pathways”

Metabolic Engineering VI: From recDNA towards Engineering Biological Systems, Noordwijkerhout, The Netherlands, October 1-5, 2006, “Optimal design of recombination and degenerate oligo based protein combinatorial libraries using pairwise residue scoring matrices”

ICCSB – First International Conference on Computational Systems Biology, Shanghai, China, July 20-23, 2006, “Analysis and Redesign of Biological Networks: Metabolic & Signaling Pathways”

ASM2006 - 106<sup>th</sup> General Meeting of the American Society for Microbiology, Orlando, FL, May 21-25, 2006, “Analysis and Redesign of Metabolic Networks”

DIMACS Workshop on Clustering Problems in Biological Networks, Rutgers University, Piscataway, NJ, May 9-11, 2006, “Analysis and Redesign of Biological Networks”

GTL2006 Contractor-Grantee Workshop IV and Metabolic Engineering Working Group Interagency Conference on Metabolic Engineering, Bethesda, MD, Feb. 12-15, 2006, “Development of Experimental and Computational Tools to Evaluate Metabolic Flux”

ICSB 2005 – Sixth International Conference on Systems Biology, Workshop on gene network models and their application: from gene function to drug discovery, Cambridge, MA, October 23, 2005, “Signaling network analysis and redesign”

13<sup>th</sup> Annual International Conference on Microbial Genomes, Madison, WI, September 11-15, 2005, “Computational Tools for the Analysis and Redesign of the E. coli Metabolic Network”

Phage Display for Engineering Protein Therapeutics Conference, Cambridge, MA, May 16-17 2005, “Computational Protein Library Design”

National Science Foundation workshop on Control and Systems Integration of Micro-and Nano-Scale Systems, March 29-30 2004, “Challenges and Opportunities in the Design and Analysis of Biological Systems”

Pacific Symposium on Biocomputing (PSB2004), Big Island HI, January 2004, “A Mixed Integer Linear Programming Framework (MILP) for Inferring Time Delay in Gene Regulatory Networks”

Ninth Annual Symposium on Frontiers of Engineering, National Academy of Engineering (NAE), September 18-20, 2003.

Biochemical Engineering XIII, Boulder CO, July 19-23, 2003, “In Silico Prescreening of Protein Hybrids in Directed Evolution Experiments”

Foundations of Computer-Aided Process Operations (FOCAPO2003), Coral Springs FL, January 2003, “Challenges and Opportunities for Systems Engineering in Computational Biology”

Metabolic Engineering IV, Barga Italy, October 2002, “Inference of Gene Regulatory Networks from DNA microarray experiments”

Metabolic Engineering IV, Barga Italy, October 2002, “In Silico Design of Metabolic Pathways”

Biochemical Engineering XII, Sonoma CA, July 2001, “Probing the Performance Limits of Metabolic Networks and Identifying Regulatory Barriers through Boolean Constraints”

European Symposium of Computer-Aided Process Engineering (ESCAPE11), Denmark, June 2001, “Optimization in Molecular Design and Bioinformatics”

Metabolic Engineering III, Colorado Springs CO, October 2000, “Modeling and Optimization of Directed Evolution Protocols”

## **PUBLICATIONS**

### ***Textbooks***

Costas D. Maranas and Ali R. Zomorodi (2016), “Optimization Methods in Metabolic Networks,” John Wiley & Sons.

### ***Journal Publications***

1. Wang, L. and C.D. Maranas (2021), “Computationally Prospecting Potential Pathways from Lignin Monomers and Dimers toward Aromatic Compounds,” *ACS Synth. Biol.*, <https://doi.org/10.1021/acssynbio.0c00598>.
2. Hendry, J.I., H.V. Dinh, D. Sarkar, L. Wang, A. Bandyopadhyay, H.B. Pakrasi and C.D. Maranas (2021), “A genome-scale metabolic model of *Anabaena* 33047 to guide genetic modifications to overproduce nylon monomers,” *Metabolites*, Vol. 11, issue 3, 166.
3. Foster, C., K. Charubin, E.T. Papoutsakis and C.D. Maranas (2021), “Modeling Growth Kinetics, Interspecies Cell Fusion, and Metabolism of a *Clostridium acetobutylicum*/*Clostridium ljungdahlii* Syntrophic Coculture,” *mSystems*, DOI: 10.1128/mSystems.01325-20.
4. Liu, D., M. Liberton, J.I. Hendry, J. Aminian-Dehkordi, C.D. Maranas and H.B. Pakrasi (2021), “Engineering biology approaches for food and nutrient production by cyanobacteria,” *Current opinion in biotechnology*, Vol. 67, 1-6.
5. Foster, C.J. L. Wang, H.V. Dinh, P.F. Suthers and C.D. Maranas (2021), “Building kinetic models for metabolic engineering,” *Current opinion in biotechnology*, Vol. 67, 35-41.
6. Suthers, P.F., C.J. Foster, D. Sarkar, L. Wang and C.D. Maranas (2021), “Recent advances in constraint and machine learning-based metabolic modeling by leveraging stoichiometric



balances, thermodynamic feasibility and kinetic law formalisms,” *Metabolic Engineering*, Vol. 63, 13-33.

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9. Hendry, J.I., A. Bandyopadhyay, S. Srinivasan, H.B. Pakrasi and C.D. Maranas (2020), “Metabolic model guided strain design of cyanobacteria,” *Current Opinion in Biotechnology*, Vol. 64, 17-23.
10. Suthers, P.F., H.V. Dinh, Z. Fatma, Y. Shen, S.H.J. Chan, J.D. Rabinowitz, H. Zhao and C.D. Maranas (2020), “Genome-scale metabolic reconstruction of the non-model yeast *Issatchenkia orientalis* SD108 and its application to organic acids production,” *Metabolic Engineering Communications*, Vol. 11, <https://doi.org/10.1016/j.mec.2020.e00148>.
11. Chowdhury, R., V. S. Boorla, C.D. Maranas (2020), “Computational biophysical characterization of the SARS-CoV-2 spike protein binding with the ACE2 receptor and implications for infectivity,” *Computational and Structural Biotechnology Journal*, <https://doi.org/10.1016/j.csbj.2020.09.019>.
12. Hendry, J.I., H.V. Dinh, C. Foster, S. Gopalakrishnan, L. Wang and C.D. Maranas (2020), “Metabolic flux analysis reaching genome wide coverage: lessons learned and future perspectives,” *Current Opinion in Biotechnology*, Vol. 30, 17-25.
13. Chowdhury, R., M.J. Grisewood, V.S. Boorla, Q. Yan, B.F. Pflieger and C.D. Maranas (2020), “IPRO+/-: Computational Protein Design Tool Allowing for Insertions and Deletions,” *Structure*, <https://doi.org/10.1016/j.str.2020.08.003>.
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### ***Refereed Conference Proceedings***

1. Vital-Lopez, F.-G., A. Armaou and C. Maranas (2008), "Hybrid multi-scale modeling of brain tumor progression," *Proceedings of the 18th International symposium on Mathematical Theory of Networks & Systems*, RSBioSystems.2, Blacksburg, VA.
2. Vital-Lopez, F.G., C.D. Maranas and A. Armaou (2006), "Bifurcation analysis of the metabolism of *E. coli* at optimal enzyme levels," *Proceedings of the 2006 American Control Conference*, Minneapolis, MN.
3. Nikolaev, E.V., P. Pharkya, C. D. Maranas, and A. Armaou (2005), "Optimal selection of enzyme levels using large-scale kinetic models," *Proceedings of 16th International Federation of Automatic Control World Congress*, Prague, Czech Republic, 6 pages.



4. Pharkya, P. and C.D. Maranas (2005), "A hierarchical framework for metabolic pathway discovery and strain design," *FOSBE 2005 Proceedings*, 141-144.
5. Rogers, M. J., M. Ding, and C. D. Maranas (2004), "A Case Study on the Design of Pharmaceutical R&D Licensing Deals," *FOCAPD Conference Proceedings*, 475-479.
6. Dasika, M.S., Gupta, A., and C.D. Maranas (2004), "A Mixed Integer Linear Programming Framework (MILP) for Inferring Time Delay in Gene Regulatory Networks," *Pacific Symposium on Biocomputing, Vol. 9*, 474-485.
7. Maranas, C.D., G.L. Moore, A.P. Burgard and A. Gupta (2003), "Systems Engineering Challenges and Opportunities in Computational Biology," *Proceedings of Foundations of Computer-Aided Process Operations IV*, Coral Springs, FL, January 12-15, 2003, CACHE, 13-26.
8. Rogers, M.J., A. Gupta and C.D. Maranas (2003), "Risk Management in Real Options Based Pharmaceutical Portfolio Planning," *Proceedings of Foundations of Computer-Aided Process Operations IV*, Coral Springs, FL, January 12-15, 2003, CACHE, 241-244.
9. Gupta, A. and C.D. Maranas (2001), "Multiperiod Planning of Multisite Supply Chains Under Demand Uncertainty," *European Symposium on Computer-Aided Process Engineering, Vol. 11*, 871-882.
10. C.D. Maranas (2001), "Optimization in Molecular Design and Bioinformatics," *European Symposium on Computer-Aided Process Engineering, Vol. 11*, 1157-1164.
11. Vaidyaraman, S. and C.D. Maranas (1999b), "Simultaneous Refrigeration Cycle Synthesis and Refrigerant Selection," In proceedings of PRES'99, 2nd Conference on Process Integration, Modeling and Optimisation for Energy Saving and Pollution Reduction, May 31-June 2, Budapest, Hungary.
12. Maranas, C.D., I.P. Androulakis and C.A. Floudas (1995), "A Deterministic Global Optimization Approach for the Protein Folding Problem," *Proc. of DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Vol. 23*, 133-150.
13. Maranas, C.D. and C.A. Floudas, (1993b), "A Global Optimization Method For Weber's Problem With Attraction And Repulsion," *Proc. of Large Scale Optimization: State of the Art Conference*, (February 15-17, 1993, Florida University), Kluwer Academic Publishers B.V., 259-293.
14. Pistikopoulos, E.N., T.A. Mazzuchi, C.D. Maranas and T.V Thomaidis (1991), "Simultaneous Assessment of Flexibility, Reliability and Availability for In-Line Blending Systems: A Unified Framework for Analysis and Retrofit Design," *Proc. of Fourth International Symposium on Process Systems Engineering (PSE 91)*, 1.4.1-1.4.16.

### **Book chapters**

1. Simons-Senfle, M.N., D. Sarkar and C.D. Maranas (2018), "Modeling Plant Metabolism: Advancements and Future Capabilities. In: Shrawat A., Zayed A., Lightfoot D. (eds) *Engineering Nitrogen Utilization in Crop Plants*. Springer, Cham. DOI [https://doi.org/10.1007/978-3-319-92958-3\\_4](https://doi.org/10.1007/978-3-319-92958-3_4).

2. Nazem-Bokaei H., Y.Z., Maranas C.D., Ferry J.G. (2018), "The Biochemistry and Physiology of Respiratory-Driven Reversed Methanogenesis," In: Kalyuzhnaya M., Xing XH. (eds) *Methane Biocatalysis: Paving the Way to Sustainability*. Springer, Cham. DOI [https://doi.org/10.1007/978-3-319-74866-5\\_12](https://doi.org/10.1007/978-3-319-74866-5_12).
3. Chan, S.H.J., M. Simons and C.D. Maranas (2017), "Computational Modeling of Microbial Communities," *Systems Biology*, chapter 6.
4. Moore, G.L. and C.D. Maranas (2003), "Modeling and Optimization of Directed Evolution Protocols." *Enzyme Functionality: Design, Engineering, and Screening*, edited by A. Svendsen (pp. 185-212). New York, NY: Marcel Dekker, Inc.

## **PATENTS**

Maranas, C.D., M. Kumar, R. Chowdhury and T. Ren, "Angstrom-scale separations by design using precision biomimetic membrane," US Patent App. 16/397,416, 2019

Pfleger B.F., N.J. Hernandez-lozada, C.D. Maranas and M. Grisewood, "Gene construct encoding mutant thioesterase, mutant thioesterase encoded thereby, transformed host cell containing the gene construct, and method of using them to produce medium-chain fatty acids," US 10,421,951 B2, filed June 22 and issued Sept. 24, 2019 issued Dec. 28, 2017.

Ferry, J.G., C.D. Maranas and T.K. Wood, "Methane-to-acetate pathway for producing liquid biofuels and biorenewables," Publication number: 20150147791. Filed: Nov. 21, 2014. Publication date: May 28, 2015.

Maranas C.D., A.P. Burgard and P. Pharkya, "Method for determining gene knockouts," US 8,457,941, filed Aug. 16, 2011, and issued Apr. 16, 2013.

Maranas C.D., A.P. Burgard and P. Pharkya, "Method for redesign of microbial production systems," US 8,108,152, filed Oct. 21, 2010, and issued Jan. 1, 2012.

Maranas C.D. and A.P. Burgard, "Method and system for modeling cellular metabolism," US 8,086,414, filed Mar. 15, 2010, and issued Dec. 27, 2011.

Maranas C.D., A.P. Burgard and P. Pharkya, "Method for determining gene knockouts," US 8,027,821, filed Jul. 9, 2003, and issued Sept. 27, 2011.

Maranas C.D., A.P. Burgard and P. Pharkya, "Method for redesign of microbial production systems," US 7,826,975, filed Aug. 26, 2004, and issued Nov. 2, 2010.

Maranas C.D. and A.P. Burgard, "Method and system for modeling cellular metabolism," US 7,711,490, filed Jan. 10, 2002, and issued May 4, 2010.

Maranas C.D. and G. Moore "Modeling framework for predicting the number, type and distribution of crossovers in directed evolution experiments," US 2003/0073092, filed Nov. 9, 2001.

## **Post-Doctoral Research Associates**

1. Dr. Wheaton Schroeder, 2021-present. PhD: University of Nebraska
2. Dr. Chen Chen, 2020-present. PhD: Wuhan University
3. Dr. Shyam Srinivasan, 2019-2020. PhD: U. of Toronto
4. Dr. Patrick Suthers, 2018-present. PhD: U. of Wisconsin
5. Dr. John Hendry Rajeswaran, 2018-present. PhD: IIT Bombay
6. Dr. Siu Hung (Joshua) Chan, 2015-2018. PhD: DTU. Current position: Assistant Professor, Colorado State University.
7. Dr. Hadi Nazem-Bokaei, 2014-2017. PhD: Virginia Tech. Current position: CSIRO Research scientist, Australia.
8. Dr. Tong Li, 2013-2016. PhD: University of Leuven, Belgium. Current position: BASF, San Diego, CA.
9. Dr. Ali Zomorodi, 2012-2013. PhD: Pennsylvania State University. Current position: Instructor in Pediatrics, faculty of Harvard Medical School (HMS) and Mass General Hospital (MGH).
10. Dr. Patrick Suthers, 2005-2013. PhD: University of Wisconsin-Madison.
11. Dr. Yang Chang, 2007-2008. PhD: University of Illinois at Urbana-Champaign. Current position: Research Associate, Merck Sharp & Dohme Corp.
12. Dr. Evgeni Nikolaev, 2002-2005. PhD: Lobachevsky Nizhegorod State University, Russia. Current position: Instructor of Mathematics, New Jersey State University (Rutgers).
13. Dr. Anshuman Gupta, 2002-2005. PhD: Pennsylvania State University. Current position: Vice President-Analytics, Indicus Analytics, India.
14. Kyle Camarda, 1998-2000. PhD: University of Illinois at Urbana-Champaign. Current position: Associate Professor, Department of Chemical and Petroleum Engineering, University of Kansas.

## **PH.D. THESES SUPERVISED**

1. "Genome reduction of cyanobacterial production systems," Mahmudul Rifat, ongoing.
2. "Kinetic models of yeast production platforms," Jack Hu, ongoing.
3. "Modeling the interplay of circadian rhythm and metabolic changes in cyanobacteria," Deepro Banerjee, ongoing.
4. "Development of protein design tools for enzyme and antibody design," Veda Sheesh Boorla, ongoing.

5. "Retrosynthetic algorithms for pathway design," Vikas Upadhyay, ongoing
6. "Computational protein design," Soodabeh Gaffari, ongoing.
7. "Metabolic modeling of microbiome," Bipin Rimal, ongoing.
8. "Reconstruction of yeast metabolic models", Hoang Dinh, ongoing
9. "Metabolic models of cyanobacteria and plants," Debolina Sarkar, ongoing.
10. "ME metabolic models and lignin pathway analysis," Lin Wang, ongoing.
11. "Kinetic modeling of clostridia", Charles Foster, ongoing.
12. "Computational redesign of protein channels, enzyme and antibodies," Ratul Chowdhury, December 2019. Current position: Postdoctoral Researcher, Harvard Medical School.
13. "Metabolic modeling of clostridia for biofuel production," Satyakam Dash, April 2019. Current position: Zymergen.
14. "Nonlinear optimization techniques for genome-scale flux elucidation and kinetic model parameterization," Sarat Gopalakrishnan, April 2019. Current position: post-doc UCSD.
15. "Computational Methods for Enzyme Redesign," Matthew Grisewood, January 2018. Current position: Schodinger, Inc.
16. "Development of synthetic biology tools for microbial metabolic engineering," Chiam Yu Ng, July 2017. Current position: Amyris.
17. "Application of multi-tissue and multi-organism genome-scale models for analyzing plant metabolism", Maggie Simons, June 2017. Current position: Instructor, dept. of Chemical Engineering, Rice University.
18. "Elucidation and Synthetic Design of Biochemical Pathways," Akhil Kumar, February 2017: Current position: Amazon, Inc.
19. "Construction of dynamic metabolic models for metabolic engineering applications," Ali Khodayari, January 2017. Current position: Genomatica, Inc.
20. "Development of genome-scale and dynamic models to analyze metabolism in Cyanobacteria," Thomas Mueller, September 2016. Current position: Axtria.
21. "Development of computational tools to redirect metabolism," Anupam Chowdhury, August 2016. Current position: Zymergen.
22. "Reconstruction and analysis of genome-scale metabolic models of photosynthetic organisms," Rajib Saha, June 2014. Current position: Assistant Prof., University of Nebraska.
23. "Computational methods for the de novo design of antibodies", Robert Pantazes, January 2014. Current position: Assistant Professor, Auburn University.

24. "Computational tools for genome-scale synthetic lethality analysis and metabolic modeling of microbial communities", Ali Zomorodi, August 2012. Current position: Instructor in Pediatrics, faculty of Harvard Medical School (HMS) and Mass General Hospital (MGH).
25. "Using computations to analyze and redesign metabolism", Sridhar Ranganathan, December 2011. Current position: Staff Scientist, Synthetic Biology, Life Technologies.
26. "Development of hybrid intracellular/extracellular models of brain tumor progression and medication strategies", Francisco Vital-Lopez, 2011. Current position: Research scientist, Biotechnology High Performance Computing Software Applications Institute (BHS AI).
27. "Systems based optimization approaches to analyze and improve metabolic networks", Vinay-Satish Kumar, 2010. Current position: Data Scientist, Facebook.
28. "Engineering and analysis of cofactor partitioning for NADPH-dependent xylitol production in Escherichia coli", Jonathan Chin, 2010. Current position: Scientist, Algenol Biofuels.
29. "Computational design and experimental characterization of proteins with novel functions", Hossein Fazelinia, 2009. Current position: Postdoctoral research fellow, Fox Chase Cancer Center.
30. "Systems engineering based approaches for biological network, inference, analysis and redesign", Madhukar Dasika, August 2007. Current position: Scientist, DuPont.
31. "Development of computational tools for the design and optimization of combinatorial protein libraries", Manish Saraf, May 2006. Current position: Vice President, Citigroup.
32. "Modeling and optimization in directed evolution protocols and protein engineering", Gregory Moore, May 2005. Current position: Senior Scientist, Protein Engineering, Xencor.
33. "Optimization based redesign of microbial production systems", Priti Pharkya, December 2005. Current position: Senior Research Scientist II, Genomatica.
34. "Molecular design in chemical and biological systems", Andreas Lehmann, December 2004. Current position: Postdoctoral Associate, Fox Chase Cancer Center.
35. "Optimization-based frameworks for the analysis and redesign of metabolic networks", Anthony Burgard, 2004. Current position: Associate Director, Computational Technologies, Genomatica.
36. "Supply chain management under uncertainty", Anshuman Gupta, August 2002. Current position: Vice President-Analytics, Indicus Analytics, India.
37. "Optimization based methodology for refrigeration system synthesis and molecular design", Shankar Vaidyaraman, August 2001. Current position: Research scientist, Eli Lilly and Company.

## **M.S. STUDENT THESES/PROJECTS SUPERVISED**

1. "Computational design of thioesterases", N. Gifford, Oct. 2014.

2. "OptZyme: A Computational Tool for Altering Enzymatic Specificity", M. Grisewood, May 2013. Current position: Doctoral Student, Department of Chemical Engineering, Pennsylvania State University.
3. "MetRxn: a knowledgebase of metabolites and reactions spanning metabolic models and databases", A. Kumar, 2013. Current position: Doctoral student, Department of Bioinformatics and Genomics, Pennsylvania State University.
4. "Optimization-driven design of synthetic genetic circuits using biobricks", A. R. Zomorodi, 2011. Current position: Postdoctoral Research Associate, Bioinformatics Program & Biomedical Engineering Department, Boston University.
5. "Reconstruction of a genome-scale metabolic model of maize metabolism", R. Saha, January 2011. Current position: Doctoral Student, Department of Chemical Engineering, Pennsylvania State University.
6. "Construction of a genome-scale atom mapping model of E.coli for metabolic flux analysis", P. Ravikirthi, 2010. Current position: Bioinformatician, Positive Bioscience, India.
7. "Computational design to switch protein cofactor specificity and create enzymatic activity", G. Khoury, 2010. Current position: Doctoral Student, Department of Chemical and Biological Engineering, Princeton University.
8. "Optimization methods to compare strain design strategies in metabolic networks using different cellular objectives", V. S. Kumar, December 2008. Current position: Data Scientist, Facebook.
9. "Metabolic Engineering and Strain Design procedures for valuable chemical synthesis", S. Ranganathan, 2008. Current position: Staff Scientist, Synthetic Biology, Life Technologies.
10. "Real options based planning of pharmaceutical product pipelines", M. Rogers, May 2004. Current position: Business Development Manager, DuPont.
11. "Development of process design case studies for the capstone design course", M. Kalp, 1999. Current position: Project Engineer, Croda.
12. "Analysis and optimization of chemical process systems under uncertainty", S. Petkov, August 1997. Current position: Director Business Development, Huvepharma, Bulgaria.

## **FUNDED RESEARCH PROJECTS**

### ***Ongoing Research Projects***

Apr. 1, 2020-Mar. 31, 2025, "Integrative Analysis of Metabolic Phenotypes (IAMP) Predoctoral Training Program," National Institutes of Health, \$1,051,273 (total), Pled by A. Patterson, PSU.

Sept. 1, 2020-Aug. 31, 2023, "Ruggedized solvent stable engineered beta-barrel membrane protein based biomimetic membranes for CWA protective fabrics," DTRA,

subcontract to U. of Texas at Austin, \$400,000 (to C. Maranas, PSU), PIed by M. Kumar, UT.

Sept. 1, 2020-Aug. 31, 2025, “AI Institute: Molecule Maker Lab Institute (MMLI), an Artificial Intelligence Driven Ecosystem for NextGen Molecule Discovery and Manufacturing,” subcontract to University of Illinois at Urbana-Champaign, \$593,945 (to C. Maranas), PIed by H. Zhao UIUC.

Jul. 1, 2020-Jun. 30, 2022, “Susceptibility and the potential adaptation of SARS-CoV-2 in livestock,” USDA, \$978,101 (total), PIed by S. Kuchipudi, PSU.

Dec. 1, 2019-Nov. 30 2022, “Integration of regulatory and resource balance constraints onto metabolic models of *R. toruloides*,” subcontract to CABBI DOE Bioenergy Center, \$372,923 (to C. Maranas), PIed by E. deLucia UIUC.

Oct. 2017-Oct. 2022, “The Center for Bioenergy Innovation,” DOE DE-AC05-000R22725, \$1,580,000 (to C. Maranas), PIed by J. Tuskan, ORNL.

Sept. 2017-Aug. 2022, “Genome-scale Design and Engineering of Non-model Yeast Organisms for Production of Biofuels and Bioproducts,” DOE DE-SC0018260, \$1,153,635 (to C. Maranas), PIed by H. Zhao, UIUC.

June 2017-May 2020, “Collaborative Research: SusChEM: Unlocking the fundamental mechanisms that underlie selectivity in oleochemical producing enzymes,” NSF, \$300,000 (to C. Maranas), coPIed by B. Pflieger, U. Wisc. (under NCE)

March 2016-Feb. 2020, “Collaborative Research: Developing a comprehensive kinetic model of *Escherichia coli* metabolism,” NSF/MCB-1615646, \$270,000 (to C. Maranas), coPIed by M. Antoniewicz, U. Del. (under NCE)

Sept. 2018-Aug. 2021, “Development of a diazotrophic platform cyanobacterial strain for the production of advanced biofuels and nitrogen containing petrochemical replacement compounds,” DOE DESC0019386, \$483,039 (to C. Maranas), PIed by H. Himadri, Wash. U.

Sept. 2018-Aug. 2021, “Syntrophic Co-Cultures of *Clostridium* Organisms to Produce Higher Alcohols & Other C6-C8 Metabolites,” DOE DE-SC0019155, \$310,000, (to C. Maranas), PIed by T. Papoutsakis, U. Del.

Sept. 2019-Sept. 2023, “COLLABORATIVE RESEARCH: Systems analysis of the interplay between oxygenic photosynthesis and nitrogen fixation in a unicellular cyanobacterium,” NSF/MCB, \$400,000 (to C. Maranas), PIed by H. Himadri, Wash. U.

### ***Completed Research Projects***

Jan. 2016-Dec. 2019, “INSPIRE: Factors that determine growth rate and yield of a photosynthetic microbe,” NSF/MCB-1546840, \$430,000 (to C. Maranas), coPIed by H. Pakrasi, Wash. U. (under NCE)

Sept. 2018-March 2019, “Software implementation of OptStoic algorithm for designing overall stoichiometries towards targeted products,” BP Biotechnology, \$20,000 (to C. Maranas).

Sept. 2017-Aug. 2018, “Computationally Assessing the Effect of Fatty Acid Chain Length on Engineering Escherichia coli,” NSF BRC EEC-0813570, \$52,000 (to C. Maranas), PIed by Shanks, Iowa St.

Aug. 2011-July 2015, “Use of Systems Biology Approaches to Develop Biofuels-Synthesizing Cyanobacterial Strains,” DOE DE-SC0006870, \$476,053 (100% pf subcontract) co-PI with H. Pakrashi, Wash. U. & L. Sherman, Purdue U.

Aug 2011-July 2015, “Dynamic Metabolic Model Building Based on Ensemble Modeling Approach,” DOE DE-FOA-0000368, \$444,600 (100% of subcontract) co-PI with J. Liao, UCLA & G. Stephanopoulos, MIT

Sept. 2015-Aug. 2016, “Computationally Assessing the Effect of Fatty Acid Chain Length on Engineering Escherichia coli,” NSF, \$67,000, (100%) annual subcontract from CBiRC Iowa State

Aug. 2014-July 2017, “Systems Level Study of a Novel Fast Growing Cyanobacterial Strain for Next Generation Biofuel Production,” DOE \$1,500,000 (25%) coPI with H. Pakrasi and Y. Tang, Wash. U.

Aug. 2014-July 2017, “Ensemble cell-wide kinetic modeling of anaerobic organisms to support fuels and chemicals production,” DOE \$1,500,000 (33%) PI with G. Stephanopoulos, MIT and J. Liao, UCLA.

Jan 2014-Dec. 2016, “Engineering a Methane-to-Acetate Pathway for Producing Liquid Biofuels,” DOE Arpa-E, \$3,000,000, (~33%) co-PI with T. Wood and G. Ferry, PSU

Aug. 2013-July 2016, “Designing Nitrogen Fixation Ability in Oxygenic Photosynthetic Cells,” NSF-MCB, \$506,932, (100% of subcontract) co-PI with H. Pakrasi, T.S. Moon and F. Zhang, Wash. U.

July 2012-June 2015, “Development of a Knowledgebase (MetRxn) of Metabolites, Reactions and Atom Mappings to Accelerate Discovery and Redesign” DOE DE-SC10822882, \$1,076,608 (100%)

Aug. 2011 – July 2015, “An Integrated Approach for Computationally Designing and Experimentally Characterizing Fully-Human Antibodies,” NSF, \$600,000, (50%) co-PI with T. Wood, PSU

Sept. 2014-Aug. 2015, “Computationally Assessing the Effect of Fatty Acid Chain Length on Engineering Escherichia coli,” NSF, \$65,000, (100%) annual subcontract from CBiRC Iowa State

Sept. 2013-Aug. 2014, “Computationally Assessing the Effect of Fatty Acid Chain Length on Engineering Escherichia coli,” NSF, \$65,000, (100%) annual subcontract from CBiRC Iowa State



Aug 2011-July 2014, "Experimental Systems Biology Approaches for Clostridia-Based Bioenergy Production," DOE DE-SC0007092, \$282,620 (100% of subcontract) co-PI with T. Papoutsakis, U. of Delaware

July 2010-June 2014, "Computational Design of Cytochrome P450 Reactivity and Substrate Specificity," NSF, \$394,905 (33%), co-PI with M. Janik and P. Cirino, PSU

Apr. 2009-Mar. 2014, "Artificial Metabolons: Models for proximity-driven control over multienzyme pathways, NIH, \$461,872 (50% of subcontract) co-PI with S. Benkovic, C. Keating and A. Armaou, PSU

Sept. 2011-Aug. 2013, "Computationally Assessing the Effect of Fatty Acid Chain Length on Engineering Escherichia coli," NSF, \$132,000 (100%), subcontract from CBiRC Iowa State

Sept. 2008-Aug. 2011, "Development of Computational Tools for Metabolic Model Curation, Flux Elucidation and Strain Design," DOE, \$1,089,671 (100%)

July 2007-June 2010, "Development of Computational Tools and Experimental Verifications for Protein Design," NSF, \$375,000.00 (75%), co-PI with P. Cirino, PSU

Jan. 2009-Dec. 2009, "Elucidation and modeling of signaling pathways implicated in metastasis due to the disruption of the endothelium barrier," ICS-PSU, \$10,000 (50%), co-PI with A. Armaou and C. Dong, PSU

Sept. 2003-July 2006, "Engineering E. coli to Maximize the Flux of Reducing Equivalents Available for NAD(P)H-Dependent Transformations," NSF, \$845,665 (25%), co-PI with P. Cirino, PSU and F. Arnold, CalTech

Aug. 2003-July 2006, "An Integrated Computational Framework for Optimally Allocating Diversity in Directed Evolution Studies," NSF/QSB, \$499,743 (100%)

Sept. 2005-Aug. 2008, "Development of computational tools for analyzing and redesigning metabolic networks," DOE Mathematical, Information and Computational Sciences Division, \$1,249,619.00 (75%), co-PI with A. Burgard, Genomatica, Inc.

Aug. 1999-July 2004, "Supply Chain Optimization Under Uncertainty for the Chemical Process Industries," NSF-GOALI, \$262,336 (100%), co-PI with C.M. McDonald, Du Pont

Aug. 2001-July 2004, "Discrete Optimization Techniques for Probing the Performance Limits of Metabolic Networks," NSF Quantitative Systems Biotechnology, \$327,247 (100%)

Oct. 2001-Sept. 2004, "Development of the Next Generation of Genome-scale Flux Balance Models," DOE, \$600,000 (100%), subcontract to Genomatica, Inc.

Jan. 2000-Dec. 2000, "Planning under Uncertainty," SCA Technologies, \$8,000 (100%)

Aug. 1999-July 2000, "Modeling and Optimization of in vitro Evolution Experiments for Molecular Design," LSC, Innovative Biotechnology Research Fund, \$21,619 (100%)

July 1999-June 2000, "Supply Chain Optimization," Du Pont Educational Aid Grant, \$11,000 (100%)

May 1999-Aug. 1999, "Optimization in Molecular Design," NSF-REU, \$5,400 (100%)

Sept. 1997-Aug. 1998, "Polymer Design," Du Pont Educational Aid Grant, \$15,000 (100%)

May 1997-April 2002, "Optimization Under Property Prediction Uncertainty in Molecular Design," NSF CAREER Award in Engineering, \$285,000 (100%)

Sept. 1996-Aug. 1997, "Process Synthesis," Du Pont Educational Aid Grant, \$20,000 (100%)

Sept. 1995-Aug. 1996, "Process Synthesis," Du Pont Educational Aid Grant, \$20,000 (100%)

### **EDUCATIONAL GRANTS**

May 2011-Apr. 2012, "International Conference on Biochemical and Molecular Engineering," NSF, \$25,000

### **COURSES TAUGHT**

**Graduate level:** Nonlinear Optimization: Theory and Applications, Optimization in Biological Networks, Optimization Methods in Metabolic Networks

**Undergraduate level:** Design of Chemical Plants, Design Projects in Chemical Engineering, Process Dynamics, Process Heat Transfer, Mathematical Modeling in Chemical Engineering

### **SHORTCOURSE AND WORKSHOP LECTURE/INSTRUCTOR**

Pan American Program on Process Systems Engineering, Iguazu Falls, Argentina, October 15-25, 2005, "Biological Pathways Analysis and Engineering"