

Supplemental Bibliography of Publications by GTL Grantees (2006)

PUBLICATIONS FROM NOTICE 02-13

(NOTICE 02-13)

A. P. ARKIN, LAWRENCE BERKELEY NATIONAL LABORATORY

VIMSS/Genomics:GTL Publications

2006

1. Bender, K., H.-C. Yen, and J. D. Wall. "Analyzing the Metabolic Capabilities of *Desulfovibrio* Species Through Genetic Manipulation," *Biotechnol. Genet. Eng. Rev.* In press.
2. Gentry, T., C. Schadt, and J. Zhou. "Microarrays for Bacterial Detection," in *Advanced Techniques for Diagnostic Microbiology* (invited), ed. Y-W. Tang and C. W. Stratton, Springer-Verlag. In press.
3. Gentry, T., C. Schadt, and J. Zhou. "Microarrays for Environmental Applications," *Microb. Ecol.*, invited. In press.
4. Leaphart, A. B., et al. 2006. "Transcriptome Analysis of *Shewanella oneidensis* Gene Expression in Response to Acidic and Alkaline pH Stress," *J. Bacteriol.* **188**(4), 1633–42.
5. Price, M. N., A. P. Arkin, and E. J. Alm. 2006. "OpWise: Operons Aid the Identification of Differentially Expressed Genes in Bacterial Microarray Experiments," *BMC Bioinformatics* **7**, article 19 (open access, doi:10.1186/1471-2105-7-19).
6. Schadt, C. W., and J.-Z. Zhou. "Advances in Microarrays for Soil Microbial Community Analyses," in *Nucleic Acids and Proteins in Soil (Soil Biology)*, ed. P. Nannipieri and K. Smalla, Springer-Verlag (invited). In press.

2005

1. Alm, E. J., et al. 2005. "The MicrobesOnline Website for Comparative Genomics," *Genome Res.* **15**(7), 1015–22. [[pubmed](#)]
2. DeSantis, T. Z., et al. 2005. "Rapid Quantification and Taxonomic Classification of Environmental DNA from both Prokaryotic and Eukaryotic Origins Using a Microarray," *FEMS Microbiol. Lett.* **245**(2), 271–78. [[download pdf](#)]
3. Fields, M. W., et al. 2005. "Impacts on Microbial Communities and Cultivable Isolates from Groundwater Contaminated with High Levels of Nitric Acid-Uranium Waste," *FEMS Microbiol. Ecol.* **53**(3), 417–28. [[download pdf](#)]

4. Gao, W., et al. 2005. "Effects of a Strong Static Magnetic Field on Bacterium *Shewanella oneidensis*: An Assessment by Using Whole Genome Microarray," *Bioelectromagnetics* **26**(7), 558–63. [[download pdf](#)]
5. Hazen, T. C., and H. H. Tabak. 2005. "Developments in Bioremediation of Soils and Sediments Polluted with Metals and Radionuclides: 2. Field Research on Bioremediation of Metals and Radionuclides," *Rev. Environ. Sci. Biotechnol.* **4**(3), 157–83. [[download pdf](#)]
6. He, Z., et al. 2005. "Empirical Establishment of Oligonucleotide Probe Design Criteria Using Perfect Match and Mismatch Probes and Artificial Targets," *Appl. Environ. Microbiol.* **71**(7), 3753–60. [[download pdf](#)]
7. He, Z., et al. 2005. "Comparison of Microarrays with Different Probe Sizes for Monitoring Gene Expression," *Appl. Environ. Microbiol.* **71**(9), 5154–62. [[download pdf](#)]
8. Koenigsberg, S. S., T. C. Hazen, and A. D. Peacock. 2005. "Environmental Biotechnology: A Bioremediation Perspective," *Remed. J.* **15**(4), 5–25. [[download pdf](#)]
9. Li, X., Z. He, and J.-Z. Zhou. 2005. "Selection of Optimal Oligonucleotide Probes for Microarrays Using Multiple Criteria, Global Alignment, and Parameter Estimation," *Nucleic Acids Res.* **33**(19), 614–23.
10. Liu, Y., et al. 2005. "Transcriptome Analysis of *Shewanella oneidensis* MR-1 in Response to Elevated Salt Conditions," *J. Bacteriol.* **187**(7), 2501–7. [[pubmed](#)]
11. Price, M. N., E. J. Alm, and A. P. Arkin. 2005. "Interruptions in Gene Expression Drive Highly Expressed Operons to the Leading Strand of DNA Replication," *Nucleic Acids Res.* **33**(10), 3224–34. [[download pdf](#)]
12. Price, M. N., et al. 2005. "Operon Formation is Driven by Co-Regulation and Not by Horizontal Gene Transfer," *Genome Res.* **15**(6), 809–19. [[pubmed](#)]
13. Price, M. N., et al. 2005. "A Novel Method for Accurate Operon Predictions in All Sequenced Prokaryotes," *Nucleic Acids Res.* **33**(3), 880–92. [[download pdf](#)]
14. Rodionov, D., et al. 2005. "Dissimilatory Metabolism of Nitrogen Oxides in Bacteria: Comparative Reconstruction of Transcriptional Networks," *PLoS Comput. Biol.* **1**(5), e55.
15. Schadt, C. W., et al. 2005. "Design and Use of Functional Gene Microarrays (FGAs) for the Characterization of Microbial Communities," pp. 331–68 in *Methods in Microbiology V34: Microbial Imaging*, ed. T. Savidge and H. Pothulakis, Academic Press, London (invited).

2004

1. Arkin, A., et al. 2004. "Data Standards for the Genomes to Life Program," Doc. 1 (Overview) in *Technical Reference: Compilation and Review of Data Standards and Application to the Genomes to Life Program*. [[download pdf](#)]

2. Gao, H., et al. 2004. "Global Transcriptome Analysis of the Heat Shock Response of *Shewanella oneidensis*," *J. Bacteriol.* **186**(22), 7796–7803.
3. McAdams, H., B. Srinivasan, and A. Arkin. 2004. "The Evolution of Genetic Regulatory Systems in Bacteria," *Nat. Rev.* **5**, 169–78. [[pubmed](#)]
4. Nielsen, J. L., et al. 2004. "Flow Cytometry-Assisted Cloning of Specific Sequence Motifs from Complex 16S ribosomal RNA Gene Libraries," *Appl. Environ. Microbiol.* **70** (12): 7550–54.
5. Rodionov, D. A., et al. 2004. "Reconstruction of Regulatory and Metabolic Pathways in Metal-Reducing Delta-Proteobacteria," *Genome Biol.* **5**(11), R90. [[pubmed](#)]
6. Tiquia, S. M., et al. 2004. "Oligonucleotide-Based Functional Gene Arrays for Analysis of Microbial Communities in the Environment," in *Molecular Microbial Ecology Manual*, ed. G. A. Kowalchuk et al., Kluwer Academic Press. [[online format](#)]

2003

1. Alm, E., and A. Arkin. 2003. "Biological Networks," *Curr. Opin. Struct. Biol.* **13**, 193–202. [[download pdf](#)]
2. DeSantis, T., et al. 2003. "Comprehensive Aligned Sequence Construction for Automated Design of Effective Probes (CASCADE-P) Using 16S rDNA," *Bioinformatics* **19**, 1461–68. [[download pdf](#)]
3. Wolf, D. M., and A. P. Arkin. 2003. "Motifs, Modules, and Games in Bacteria," *Curr. Opin. Microbiol.* **6**(2), 125–34. [[download pdf](#)]

(NOTICE 02-13)

M. V. BUCHANAN, JOINT OAK RIDGE NATIONAL LABORATORY AND PACIFIC NORTHWEST NATIONAL LABORATORY PROJECT

2006

1. Khalsa-Moyers, G., and W.H. McDonald. 2006. "Developments in Mass Spectrometry for the Analysis of Complex Protein Mixtures," *Brief. Funct. Genomic. Proteomic.*, in press.
2. Strader, M.B., et al. 2006. "Efficient and Specific Trypsin Digestion of Microgram to Nanogram Quantities of Proteins in Organic-Aqueous Solvent Systems," *Anal. Chem.* **78**(1), 125-34.
3. Tabb, D.L., et al. 2006. "Determination of Peptide and Protein Ion Charge States by Fourier Transformation of Isotope-Resolved Mass Spectra," *J. Am. Soc. Mass Spectrom.*, in press.
4. VerBerkmoes, N.C., et al. 2006. "Determination and Comparison of the Baseline Proteomes of the Versatile Microbe *Rhodospseudomonas palustris* under Its Major Metabolic States," *J. Proteome Res.*, ASAP Article 10.1021/pr0503230 S1535-3893(05)00323-4. [[online format](#)]

2005

1. Cannon, W.R., et al. 2005. "Comparison of Probability and Likelihood Models for Peptide Identification from Tandem Mass Spectrometry Data," *J. Proteome Res.* **4**(5), 1687-98. [[download PDF](#)]
2. Foote, R. S., et al. 2005. "Preconcentration of Proteins on Microfluidic Devices Using Porous Silica Membranes," *Anal. Chem.* **77**(1), 57–63. [[download PDF](#)]
3. Lin, C.T., et al. 2005. "An Improved System for Functional Over-Expression of Multi-Heme c-Type Cytochromes," *Biotechniques*, in press.
4. Markillie, L.M., et al. 2005. "Simple Protein Complex Purification and Identification Method for High-Throughput Mapping of Protein Interaction Networks," *J. Proteome Res.*, **4**(2), 268-74. DOI: 10.1021/pr049847a [[download PDF](#)]
5. Pan, C., and R. L. Hettich. 2005. "Multipole-Storage Assisted Dissociation (MSAD) for the Characterization of Large Proteins and Protein Mixtures by ESI-FTICR-MS," *Anal. Chem.* **77**, 3072–82. [[download PDF](#)]
6. Sullivan, C. J., et al. 2005. "Mounting of *Escherichia coli* Spheroplasts for AFM Imaging," *Ultramicroscopy* **105**(1–4), 96–102. [[online format](#)]
7. Tabb, D. L., et al. 2005. "DBDigger: Reorganized Proteomic Database Identification Improves Flexibility and Speed," *Anal. Chem.* **77**, 2464–74. [[download PDF](#)]
8. Weaver-Feldhaus, J.M., et al. 2005. "Directed Evolution for the Development of Conformation-Specific Affinity Reagents Using Yeast Display," *Prot. Eng. Des. Sel.* **18**(11), 527-36. [[download PDF](#)]

2004

1. Anderson, K. K., M. E. Monroe, and D. S. Daly. 2004. "Estimating Probabilities of Peptide Assignment to LC-FTICR-MS Observations," *Proceedings of the 2004 International Conference on Mathematics and Engineering Techniques in Medicine and Biological Sciences (METMBS '04), June 21–24, 2004, Las Vegas, Nevada, USA*, Computer Science Research, Education, and Applications (CSREA) Press. [[download PDF](#)]
2. Holmes, M. R., and M. C. Giddings. 2004. "Prediction of Post-Translational Modifications Using Intact-Protein Mass Spectrometric Data," *Anal. Chem.* **76**(2), 276–82. [[download PDF](#)]
3. Hurst, G. B., T. K. Lankford, and S. J. Kennel. 2004. "Mass Spectrometric Detection of Affinity Purified Crosslinked Peptides," *J. Am. Soc. Mass Spectrom.* **15**, 832–39. [[online format](#)]
4. Micic, M., et al. 2004. "Correlated Atomic Force Microscopy and Fluorescence Lifetime Imaging of Live Bacterial Cells," *Colloids and Surfaces B: Biointerfaces* **34**, 205–12. [[online format](#)]
5. Strader, M. B., et al. 2004. "Characterization of the 70S Ribosome from *Rhodospseudomonas palustris* Using an Integrated 'Top-Down' and 'Bottom-Up' Mass Spectrometric Approach," *J. Proteome Res.* **3**, 965–78. [[online format](#)]

6. Razumovskaya, J., et al. 2004. "A Computational Method for Assessing Peptide-Identification Reliability in Tandem Mass Spectrometry Analysis with SEQUEST," *Proteomics*, **4**, 961-69.
7. VerBerkmoes, N., C. Connelly, and R. Hettich. 2004. "Mass Spectrometric Approaches for Characterizing Bacterial Proteomes," *Expert Rev. Proteomics* **1**, 433–47.
8. VerBerkmoes, N., J. Sharp, and R. L. Hettich. 2004. "Mass Spectrometry," pp. 241–82 in *Microbial Functional Genomics*, ed. J. Zhou, D. Thompson, Y. Xu, and J. Tiedje, John Wiley & Sons, N.J.
9. Weaver-Feldhaus, J., et al. 2004. "Yeast Mating for Combinatorial Fab Library Generation and Surface Display," *FEBS Lett.* **564**, 24–34. [[online format](#)]

2003

1. Doktycz, M. J., et al. 2003. "AFM Imaging of Bacteria in Liquid Media Immobilized on Gelatin Coated Mica Surfaces," *Ultramicroscopy* **97**(1–4), 209–16. [[online format](#)]
2. Larimer, F. W., et al. 2003. "Complete Genome Sequence of the Metabolically Versatile Photosynthetic Bacterium *Rhodospseudomonas palustris*," *Nat. Biotechnol.* **22**, 55–61. [[download PDF](#)]

2002

1. Buchanan, M. V., et al. 2002. "Genomes to Life 'Center for Molecular and Cellular Systems': A Research Program for Identification and Characterization of Protein Complexes," *OMICS* **6**(4), 287–303. [[online format](#)]

(NOTICE 02-13)

G.M. CHURCH, HARVARD UNIVERSITY

2006

1. Leptos, K. C., et al. 2006. "MapQuant: Open-Source Software for Large-Scale Protein Quantitation," *Proteomics*. **6**(6), 1770-82. [Data and software supplementary material](#).

2005

1. Ahmad, R., et al. 2005. "Molecular Weight Assessment of Proteins in Total Proteome Profiles Using 1D-PAGE and LC/MS/MS," *Proteome Sci.* **3**(1), 6. [[download PDF](#)]
2. Dudley, A., et al. 2005. "A Global View of Pleiotropy and Phenotypically Derived Gene Function in Yeast," *Mol. Syst. Biol.* **1**, open access (doi: 10.1038/msb4100004). [[online format](#)]
3. Kharchenko, P., G. M. Church, and D. Vitkup. 2005. "Expression Dynamics of a Cellular Metabolic Network," *Mol. Syst. Biol.* **1** (doi:10.1038/msb4100023).

4. Lindell, D., et al. 2005. "Photosynthesis Genes in Marine Viruses Yield Proteins During Host Infection," *Nature* **438**, 86–89.
5. Shendure, J., et al. 2005. "Accurate Multiplex Polony Sequencing of an Evolved Bacterial Genome," *Science* **309**(5741), 1728–32. [[download PDF](#)]
6. Tompa, M., et al. 2005. "An Assessment of Computational Tools for the Discovery of Transcription Factor Binding Sites," *Nat. Biotechnol.* **23**(1), 37–44. [[download PDF](#)]
7. Wade, J. T., et al. 2005. "Genomic Analysis of LexA Binding Reveals the Permissive Nature of the *Escherichia coli* Genome and Identifies Unconventional Target Sites," *Genes Dev.* **19**(21), 2619–30.

2004

1. Aach, J. A., and G. M. Church. 2004. "Mathematical Models of Diffusion-Constrained Polymerase Chain Reactions: Basis of High-Throughput Nucleic Acid Assays and Simple Self-Organizing Systems," *J. Theor. Biol.* **228**(1), 31–46. [[Supplementary material](#)].
2. Bulyk, M. L., et al. 2004. "A Motif Co-Occurrence Approach for Genome-Wide Prediction of Transcription-Factor-Binding Sites in *Escherichia coli*," *Genome Res.* **14**(2), 201–8. [[download PDF](#)]
3. Grainger D. C., et al. 2004. "Genomic Studies with *Escherichia coli* MelR Protein: Applications of Chromatin Immunoprecipitation and Microarrays," *J. Bacteriol.* **186**(20), 6938–43. [[download PDF](#)]
4. Jaffe, J. D., H. C. Berg, and G. M. Church. 2004. "Proteogenomic Mapping Reveals Genomic Structure and Novel Proteins Undetected by Computational Algorithms," *Proteomics* **4**(1), 59–77. [[download PDF](#)] [[Supplementary material](#)]
5. Jaffe, J. D., et al. 2004. "The Complete Genome and Proteome of *Mycoplasma mobile*," *Genome Res.* **14**, 1447–61. [[download PDF](#)] [[Supplementary material](#)]
6. Janse, D. M., et al. 2004. "Localization to the Proteasome is Sufficient for Degradation," *J. Biol. Chem.* **279**(20), 21415–20. [[download PDF](#)]
7. Kharchenko, P., D. Vitkup, and G. M. Church. 2004. "Filling Gaps in a Metabolic Network Using Expression Information," *Bioinformatics* **20** (Supplement 1), i178–i185. [[download PDF](#)]
8. Lelandais, G., et al. 2004. "yMGV: A Cross-Species Expression Data Mining Tool," *Nucleic Acids Res.* **32**(90001), D323–D325. [[online format](#)]
9. Mikkilineni, V., et al. 2004. "Digital Quantitative Measurements of Gene Expression," *Biotechnol. Bioeng.* **86**(2), 117–24. [[download PDF](#)]
10. Segre, D., et al. 2004. "Modular Epistasis in Yeast Metabolism," *Nat. Genet.* **37**, 77–83. [[download PDF](#)]
11. Shendure, J., et al. 2004. "Advanced Sequencing Technologies: Methods and Goals," *Nat. Rev. Genet.* **5**(5), 335–44. [[download PDF](#)]

12. Tian, J., et al. 2004. "Accurate Multiplex Gene Synthesis from Programmable DNA Chips," *Nature* **432**, 1050–54. [[download PDF](#)] [[Supplementary material](#)]

(NOTICE 02-13)

G.S. HEFFELFINGER, SANDIA NATIONAL LABORATORIES

2006

1. Brown, W. M., et al. "Prediction of Beta-Strand Packing Interactions Using the Signature Product," *J. Mol. Model.* In press.
2. Mao, F., et al. 2006. "Mapping of Orthologous Genes in the Context of Biological Pathways: An Application of Integer Programming," *Proc. Nat. Acad. Sci.* **103**(1), 129–34.
3. Park, B.-H., et al. 2006. "In Silico Recognition of Protein-Protein Interactions: Theory and Applications" in *Advanced Data Mining Technologies in Bioinformatics*, Idea Group Publishing.
4. Su, Z., et al. 2006. "Computational Inference and Experimental Validation of Nitrogen Assimilation Regulatory Networks in *Cyanobacterium Synechococcus* sp. WH8102," *Nucleic Acids Res.* **34**(3), 1050–65.

2005

1. Belgrano, A., et al. 2005. *Aquatic Food Webs: An Ecosystem Approach*, Oxford University Press, Oxford, U.K.
2. Chen, X., et al. 2005. "Assignment of Orthologous Genes via Genome Rearrangement," *Proceedings of the Third Asia-Pacific Bioinformatics Conference*, World Scientific Publishing Co., 363–78.
3. Chen, Z., and Y. Xu. 2005. "Multi-Scale Hierarchical Structure Prediction of Helical Transmembrane Proteins," *IEEE Computational Systems Bioinformatics Conference (CSB2005) Proceedings*, 203–7.
4. Huang, J., Z. Su, and Y. Zu. 2005. "The Evolution of the Microbial Phosphonate Degradative Pathways," *J. Mol. Evol.* **61**(5), 682–90.
5. Huang, J., Y. Xu, and J. P. Gogarten. 2005. "Ancient Lateral Gene Transfer Marks the Opisthokont," *Mol. Biol. Evol.* **22**(11), 2142–46.
6. Leung, K., and S. B. Rempe. 2005. "Ab Initio Molecular Dynamics Study of Glycine Intramolecular Proton Transfer in Water," *J. Chem. Phys.* **122**(18), article 184506 (doi: 10.1063/1.1885445).
7. Liu, Z., et al. 2005. "Gene Expression Data Clustering with Kernel Principal Component Analysis," *J. Bioinform. Comput. Biol.* **3**(2), 303–16.
8. Liu, Z., et al. 2005. "Logistic Support Vector Machines and Their Application to Gene Expression Data," *Int. J. Bioinform. Res. Appl.* **1**(2), 169–82.

9. Liu, Z., et al. 2005. "Quantitative Validation of Protein-DNA Interaction Using an Optimized Knowledge-Based Potential," *Nucleic Acids Res.* **33**(2), 546–58.
10. Martin, S., et al. 2005. "Inverse Design of Large Molecules Using Linear Diophantine Equations," *IEEE Computational Systems Bioinformatics Conference (CSB2005) Proceedings*, 4.
11. Martin, S., D. Roe, and J.-L. Faulon. 2005. "Predicting Protein-Protein Interactions Using Signature Products," *Bioinformatics* **21**(2), 218–26.
12. Su, Z., et al. 2005. "Comparative Genomics Analyses of ntcA Regulons in Cyanobacteria: Regulation of Nitrogen Assimilation and its Coupling to Photosynthesis," *Nucleic Acids Res.* **33**(16), 5156–71.
13. Timlin, J., et al. 2005. "Hyperspectral Microarray Scanning: Impact on the Accuracy and Reliability of Genomic Data," *BMC Genomics* **6**, article 72 (open access, doi: 10.1186/1471-2164-6-72).
14. Wu, H., et al. 2005. "Prediction of Functional Modules Through Comparative Genome Analysis and Application of Gene Ontology," *Nucleic Acids Res.* **33**(9), 2822–37.
15. Yan, B., et al. 2005. "A Graph-Theoretic Approach to Separation of b- and y-ions in Tandem Mass Spectra," *Bioinformatics* **21**, 563–74.
16. Yan, B., et al. 2005. "PRIME: A Mass Spectrum Data Mining Tool for De Novo Sequencing and PTMs Identification," *J. Comp. Sci. Technol.* **20**(4), 483–90.

2004

1. Arkin, A., et al. 2004. "Compilation and Review of Data Standards and Application to the Genomes to Life Program," *Technical Reference: Compilation and Review of Data Standards and Application to the Genomes to Life Program*, vol. 1.2.
2. Asthagiri, D., et al. 2004. "Hydration Structure and Free Energy of Biomolecularly Specific Aqueous Dications, Including Zn²⁺ and First Transition Row Metals," *J. Am. Chem. Soc.* **126**, 1285–89.
3. Chen, X., et al. 2004. "Operon Prediction by Comparative Genomics: An Application to the *Synechococcus* sp. WH8102 genome," *Nucleic Acids Res.* **32**(7), 2147–57.
4. Chen, X., et al. 2004. "Computational Prediction of Operons in *Synechococcus* sp. WH8102," *Proceedings of the 14th International Conference on Genome Informatics*, 211–22, best paper award.
5. Churchwell, et al. 2004. "The Signature Molecular Descriptor. 3. Inverse Quantitative Structure-Activity Relationship of ICAM-1 Inhibitory Peptides," *J. Mol. Graph. Model.* **22**, 263–73.
6. Dam, P., et al. 2004. "In Silico Construction of the Carbon Fixation Pathways in *Synechococcus* sp. WH8102," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 614–15.
7. Dam, P., et al. 2004. "In Silico Construction of the Carbon Fixation Pathway in *Synechococcus* sp. WH8102," *J. Biol. Syst.* **12**, 97–125. Invited paper.

8. Day, R., A. Borziak, and A. Gorin. 2004. "PPM-Chain-De Novo Identification Program Comparable in Performance to Sequest," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 505–8.
9. Faulon, J. L., S. Martin, and R. D. Carr. 2004. "Dynamical Robustness in Gene Regulatory Networks," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings* **3**, 626–27.
10. Gorin, A., et al. 2004. "Probability Profile Method – New Approach to Data Analysis in Tandem Mass Spectrometry," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 499–502.
11. Gorin, A., and H. M. Al-Hashimi. 2004. "Computational Challenges in Rapid Characterization of Protein-Protein Interactions by NMR Based Methods," *Proceedings of Moscow Conference on Computational Molecular Biology (MCCMB '03)*, Moscow State University, 86–87.
12. Leung, K., and S. B. Rempe. 2004. "Ab Initio Molecular Dynamics Study of Formate Ion Hydration," *J. Am. Chem. Soc.* **126**, 344–51.
13. Li, G., et al. 2004. "A Linear-Time Algorithm for Computing Translocation Distance Between Signed Genomes," *Lecture Notes in Computer Science* **3109**, 323–32.
14. Li, Y., V. Protopopescu, and A. Gorin. 2004. "Accelerated Simulated Tempering," *Phys. Lett. A* **328**(4–5), 274–83.
15. Mao, F., et al. 2004. "Pathway Mapping with Operon Information: An Integer-Programming Method," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 642–43.
16. Martin, S., et al. 2004. "Inferring Genetic Networks from Microarray Data," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings* **3**, 566–69.
17. Olman, V., et al. 2004. "Mapping of Microbial Pathways Through Constrained Mapping of Orthologous Genes," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 363–70.
18. Rempe, S. B., D. Asthagiri, and L. R. Pratt. 2004. "Inner Shell Definition and Absolute Hydration Free Energy of K⁺(aq) on the Basis of Quasi-Chemical Theory and Ab Initio Molecular Dynamics," *Phys. Chem. Chem. Phys.* **6**, 1966–69 (doi: 10.1039/b313756b).
19. Rohl, C. A., et al. 2004. "Modeling Structurally Variable Regions in Homologous Proteins with Rosetta," *Proteins* **55**(3), 656–77.
20. Rohl, C. A., et al. 2004. "Protein Structure Prediction Using Rosetta," *Methods Enzymol.* **383**, 60–93.
21. Sinclair, M. B., et al. 2004. "Design, Construction, Characterization, and Application of Hyperspectral Microarray Scanner," *Appl. Optics* **43**(10), 2079–88.

22. Stork, C., M. Keenan, and D. Haaland. 2004. "Multivariate Curve Resolution for the Analysis of Remotely Sensed Thermal Infrared Hyperspectral Images," *Proc. Int. Soc. Opt. Eng.* **5546**, 271–85.
23. Su, Z., et al. 2004. "Computational Construction of Nitrogen Assimilation Pathway in Cyanobacteria *Synechococcus* sp. WH8102," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 640–41.
24. Timlin, J. A., et al. 2004. "Hyperspectral Imaging of Biological Targets: The Difference a High Resolution Spectral Dimension and Multivariate Analysis Can Make," *Biomedical Imaging: Macro to Nano, 2004, IEEE International Symposium* **2**, 1529–32.
25. Wang, P., Z. Su, and Y. Xu. 2004. "A Knowledge Base for Computational Pathway Reconstruction in *Synechococcus* sp. WH8102," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 612–13.
26. Yan, B., et al. 2004. "Separation of Ion Types in Tandem Mass Spectrometry Data Interpretation—A Graph-Theoretic Approach," *IEEE Computational Systems Bioinformatics Conference (CSB2004) Proceedings*, 236–44.
27. Yip, G., and E. Zuiderweg. 2004. "A Phase Cycle Scheme that Significantly Suppresses Offset-Dependent Artifacts in the R(2)-CPMG (15)N Relaxation Experiment," *J. Magn. Reson.* **171**(1), 25–36.

2003

1. Chivian D., et al. 2003. "Automated Prediction of CASP-5 Structures Using the Robetta Server," *Proteins* **53**, Suppl. **6**, 524–33.
2. Fridman, T. D., et al. 2003. "Probability Profiles - Novel Approach in Mass Spectrometry de novo Sequencing," *IEEE Computational Systems Bioinformatics Conference (CSB2003) Proceedings*, 415–18.
3. Gorin, A., and H. M. Al-Hashimi, 2003. "Combinatorial Assignment Procedure for RNA and Proteins," *Frontiers of NMR in Molecular Biology VIII Conference Proceedings*, 166.
4. Haaland, D. M., et al. 2003. "Multivariate Curve Resolution for Hyperspectral Image Analysis: Applications to Microarray Technology," *Proc. Intl. Soc. Opt. Eng.* **4959**, 55–66.
5. Martinez, M. J., et al. 2003. "Identification and Removal of Contaminating Fluorescence from Commercial and In-House Printed DNA Microarrays," *Nucleic Acids Res.* **31**(4), e18.
6. Olken, F. 2003. "Graph Data Management for Molecular Biology," *OMICS* **7**(1), 75–78.
7. Xu, D., et al. 2003. "Characterization of Protein Structure and Function at Genome-Scale Using a Computational Prediction Pipeline," *Genetic Engineering: Methods and Principles*, ed. J. Setlow, Kluwer Academic/Plenum Press, by invitation.

8. Park, H., et al. 2003. "Inference of Protein-Protein Interactions by Unlikely Profile Pair," *Third IEEE International Data Mining Conference Proceedings*, 735–38.
9. Shah, M., et al. 2003. "A Computational Pipeline for Protein Structure Prediction and Analysis at Genome Scale," *Bioinformatics* **19**, 1985–96.
10. Su, Z., et al. 2003. "Computational Inference of Regulatory Pathways in Microbes: An Application to Phosphorus Assimilation Pathways in *Synechococcus* sp. WH8102," *Genome Inform.* **14**, 3–13.
11. Xu, D., et al. 2003. "EXCAVATOR: A Computer Program for Gene Expression Data Analysis," *Nucleic Acids Res.* **31**(19), 5582–89.
12. Yu, G., et al. 2003. "An SVM-Based Algorithm for Identification of Photosynthesis-Specific Genome Features," *IEEE Computational Systems Bioinformatics Conference (CSB2003) Proceedings*, 235–43.

2002

1. Heffelfinger, G. S., et al. 2002. "Carbon Sequestration in *Synechococcus* sp.: From Molecular Machines to Hierarchical Modeling," *OMICS* **6**(4), 305–30.

(NOTICE 02-13)

D. R. LOVLEY, UNIVERSITY OF MASSACHUSETTS, AMHERST

Publications From *Geobacter* Genomics:GTL Project

2006

1. Butler, J. E., et al. 2006. "Genetic Characterization of a Single Bifunctional Enzyme for Fumarate Reduction and Succinate Oxidation in *Geobacter sulfurreducens* and Engineering of Fumarate Reduction in *Geobacter metallireducens*," *J. Bacteriol.* **188**, 450–55.
2. Giometti, C. S. "A Tale of Two Metal Reducers: Comparative Proteome Analysis of *Geobacter sulfurreducens* PCA and *Shewanella oneidensis* MR-1," *Microbial Proteomics: Functional Biology of Whole Organisms*, ed. I. Humphery-Smith and M. Hecker, Wiley & Sons Inc., New York. In press, June 2006.
3. Khare, T. M., et al. "Nondenaturing Two-Dimensional Gel Electrophoresis Reveals Differential Expression of Proteins and Protein Complexes in the Metal-Reducing Bacterium *Geobacter sulfurreducens* Grown with Different Electron Acceptors," *Proteomics*. In press.

2005

1. Afkar, E. A., et al. 2005. "A Novel *Geobacteraceae*-Specific Outer Membrane Protein, OmpJ, is Essential for Electron Transport to Fe (III) and Mn (IV) Oxides in *Geobacter sulfurreducens*," *BMC Microbiol.* **6**, 41.

2. Bond, D. R., and D. R. Lovley. 2005. "Evidence for Involvement of an Electron Shuttle in Electricity Generation by *Geothrix fermentans*," *Appl. Environ. Microbiol.* **71**, 2186–89.
3. Bond, D. R., et al. 2005. "A Eukaryotic-Like Citrate Synthase with Novel Biochemical Properties in the *Geobacteraceae*," *Appl. Environ. Microbiol.* **71**, 3858–65.
4. Coppi, M. V. 2005. "The Hydrogenases of *Geobacter sulfurreducens*: A Genomic Perspective," *Microbiol.* **151**, 1239–54.
5. Esteve-Núñez, A., et al. 2005. "Growth of *Geobacter sulfurreducens* Under Nutrient-Limiting Conditions in Continuous Culture," *Environ. Microbiol.* **7**, 641–48.
6. Holmes, D. E., et al. 2005. "Potential for Quantifying Expression of the *Geobacteraceae* Citrate Synthase Gene to Assess the Activity of *Geobacteraceae* in the Subsurface and on Current-Harvesting Electrodes," *Appl. Environ. Microbiol.* **71**(11), 6870–77.
7. Kim, B.-C., et al. 2005. "OmcF, a Putative c-Type Monoheme Outer Membrane Cytochrome Required for the Expression of Other Outer Membrane Cytochrome Genes in *Geobacter sulfurreducens*," *J. Bacteriol.* **187**, 4505–13.
8. Leang, C., C. Nunez, and D. R. Lovley. 2005. "Differential Transcriptional Regulation and Function of Two Highly Similar Genes, *omcB* and *omcC*, in a 10-kb Chromosomal Duplication in *Geobacter sulfurreducens*," *Microbiol.* **151**, 1761–67.
9. Leang, C., et al. 2005. "Adaption to Disruption of Electron Transfer Pathway for Fe(III) Reduction in *Geobacter sulfurreducens*," *J. Bacteriol.* **187**, 5918–26.
10. Lovley, D. R. 2005. "In Situ Biology Meets in Situ Phenomenology," *Environ. Microbiol.* **7**, 478–79.
11. Methé, B. A., et al. 2005. "DNA Microarray Analysis of Nitrogen Fixation and Fe(III) Reduction in *Geobacter sulfurreducens*," *Appl. Environ. Microbiol.* **71**, 2530–38.
12. Nevin, K. P., et al. 2005. "*Geobacter bemidjiensis* sp. nov. and *Geobacter psychrophilus* sp. nov., Two Novel Fe(III)-Reducing Subsurface Isolates," *Int. J. Syst. Bacteriol.* **55**, 1667–74.
13. Reguera, G., et al. 2005. "Extracellular Electron Transfer Via Microbial Nanowires," *Nature* **435**, 1098–1101.

2004

1. Butler, J. E., et al. 2004. "MacA, a Diheme c-Type Cytochrome Involved in Fe(III) Reduction by *Geobacter sulfurreducens*," *J. Bacteriol.* **186**, 4042–45. 305–30.
2. Chin, K.-J., et al., 2004. "Direct Correlation Between Rates of Anaerobic Respiration and Levels of mRNA for Key Respiratory Genes in *Geobacter sulfurreducens*," *Appl. Environ. Microbiol.* **70**, 5183–89.

3. Coppi, M. V., R. A. O'Neil, and D. R. Lovley. 2004. "Identification of an Uptake Hydrogenase Required for Hydrogen-Dependent Reduction of Fe(III) and Other Electron Acceptors by *Geobacter sulfurreducens*," *J. Bacteriol.* **186**, 3022–28.
4. Esteve-Núñez, A., C. Núñez, and D. R. Lovley. 2004. "Preferential Reduction of Fe(III) Over Fumarate by *Geobacter sulfurreducens*," *J. Bacteriol.* **186**, 2897–99.
5. Holmes, D. E., D. R. Bond, and D. R. Lovley. 2004. "Electron Transfer to Fe(III) and Graphite Electrodes by *Desulfobulbus propionicus*," *Appl. Environ. Microbiol.* **70**, 1234–37.
6. Holmes, D. E., K. P. Nevin, and D. R. Lovley. 2004. "Comparison of 16S rRNA, *nifD*, *recA*, *rpoB*, and *fusA* Genes Within the Family *Geobacteraceae*," *Int. J. Syst. Evol. Microbiol.* **54**, 1591–99.
7. Holmes, D. E., K. P. Nevin, and D. R. Lovley. 2004. "In Situ Expression of *Geobacteraceae nifD* in Subsurface Sediments," *Appl. Environ. Microbiol.* **70**, 7251–59.
8. Holmes, D. E., et al. 2004. "Microbial Communities Associated with Electrodes Harvesting Electricity from a Variety of Aquatic Sediments," *Microb. Ecol.* **48**, 178–90.
9. Holmes, D. E., et al. 2004. "Potential Role of a Novel Psychrotolerant *Geobacteraceae*, *Geopsychrobacter electrodiphilus* gen. nov., sp. nov., in Electricity Production by the Marine Sediment Fuel Cell," *Appl. Environ. Microbiol.* **70**, 6023–30.
10. Lin, W. C., M. V. Coppi, and D. R. Lovley. 2004. "*Geobacter sulfurreducens* can Grow with Oxygen as a Terminal Acceptor," *Appl. Environ. Microbiol.* **70**, 2525–28.
11. Lovley, D. R., D. E. Holmes, and K. P. Nevin. 2004. "Dissimilatory Fe(III) and Mn(IV) Reduction," *Adv. Microb. Physiol.* **49**, 219–86.
12. Mehta, T. A., et al. 2004. "Outer Membrane c-Type Cytochromes Required for Fe(III) and Mn(IV) Oxide Reduction in *Geobacter sulfurreducens*," *Appl. Environ. Microbiol.* **71**(12), 8634–41
13. Núñez, C., et al. 2004. "The RpoS Sigma Factor in the Dissimilatory Fe(III)-Reducing Bacterium *Geobacter sulfurreducens*," *J. Bacteriol.* **186**, 5543–46.
14. Yan, B., et al. 2004. "Computational Prediction of Conserved Operons and Phylogenetic Footprinting of Transcription Regulatory Elements in the Metal-Reducing Bacterial Family *Geobacteraceae*," *J. Theor. Biol.* **230**, 3–144.

2003

1. Jara, M., et al. 2003. "*Geobacter sulfurreducens* has Two Autoregulated *lexA* Genes Whose Products Do Not Bind the *recA* Promoter: Differing Responses of *lexA* and *recA* to DNA Damage," *J. Bacteriol.* **185**, 2493–502.
2. Leang, C., M. V. Coppi, and D. R. Lovley. 2003. "OmcB, a c-Type Polyheme Cytochrome, Involved in Fe(III) Reduction in *Geobacter sulfurreducens*," *J. Bacteriol.* **185**, 2096–2103.

3. Lovley, D. R. 2003. "Cleaning Up with Genomics: Applying Molecular Biology to Bioremediation," *Nat. Rev. Microbiol.* **1**, 35–44.
4. Methé, B. A., et al. 2003. "The Genome of *Geobacter sulfurreducens*: Insights Into Metal Reduction in Subsurface Environments," *Science* **302**, 1967–69.

2002

1. Lovley, D. R. 2002. "Analysis of the Genetic Potential and Gene Expression of Microbial Communities Involved in the In Situ Bioremediation of Uranium and Harvesting Electrical Energy from Organic Matter," *OMICS* **6**, 331–39.

(NOTICE 02-13)

J. C. VENTER, VENTER INSTITUTE

2004

1. Venter, J. C., et al. 2004. "Environmental Genome Shotgun Sequencing of the Sargasso Sea," *Science* **304**, 266–74.

2003

1. Smith, H. O., et al. 2003. "Generating a Synthetic Genome by Whole Genome Assembly: phiX174 Bacteriophage from Synthetic Oligonucleotides," *Proc. Natl. Acad. Sci. USA* **100**, 15440–45.
2. Venter, J. C., et al. 2003. "Massive Parallelism, Randomness, and Genomic Advances," *Nat. Genet.* **33** (supplement), 219–27.

2002

1. Hutchison, C. A., III, and M. G. Montague. 2002. "Mycoplasmas and the Minimal Genome Concept," pp. 221–53 in *Molecular Biology and Pathogenicity of Mycoplasmas*, ed. S. Razin and R. Herrmann, Kluwer Academic/Plenum Publishers.

PUBLICATIONS FROM NOTICE 03-05

(NOTICE 03-05)

G. L. JENSEN, CALIFORNIA INSTITUTE OF TECHNOLOGY

2006

1. Iancu, C. V., et al. "A Comparison of Liquid Nitrogen and Liquid Helium as Potential Cryogens for Electron Cryotomography," *J. Struct. Biol.* In press.
2. Komeili, A., et al. 2006. "Magnetosomes are Cell Membrane Invaginations Organized by the Actin-Like Protein MamK," *Science* **311**(5758), 242–45.

3. Wright, E. R., et al. "Observations on the Behavior of Vitreous Ice at ~82 and ~12° K," *J. Struct. Biol.* In press.

2005

1. Iancu, C. V., et al. 2005. "A 'Flip-Flop' Rotation Stage for Routine Dual-Axis Electron Cryotomography," *J. Struct. Biol.* **151**, 288–97.
2. Leong, P. A., J. B. Heymann, and G. J. Jensen. 2005. "Peach: A Simple Perl-Based System for Distributed Computation and its Application to cryoEM Data Processing," *Structure* **13**, 1–7.
3. Murphy, G. E., and G. L. Jensen. 2005. "Electron Cryotomography of the *E. coli* Pyruvate and 2-Oxoglutarate Dehydrogenase Complexes," *Structure* **13**(12), 1765–73.

(NOTICE 03-05)

G. BAO, GEORGIA TECH

2006

1. Agrawal, A., et al. 2006. "Counting Single Native Biomolecules and Intact Viruses with Color-Coded Nanoparticles," *Anal. Chem.* **78**, 1061–70.
2. LeDuc, P., and R. Bellin. "Nanoscale Intracellular Organization and Functional Architecture Mediating Cellular Behavior," *Ann. Biomed. Eng.* In press.
3. Puskar, K., et al. "Spatial Constraints in Polymer Assembly Systems Through Coarse-Grained Modeling," *Cell Biochem. Biophys.* In press.
4. Santangelo, P., N. Nitin, and G. Bao. "Nanostructured Probes for RNA Detection in Living Cells," *Ann. Biomed. Eng.* In press.
5. Smith, A. M., et al. "Engineering Luminescent Quantum Dots for In-Vivo Molecular and Cellular Imaging," *Ann. Biomed. Eng.* In press.

2005

1. Cheng, C-M, B. Li, and P. R. LeDuc. 2005. "Optical Fabrication of Three-Dimensional Polymeric Microstructures," *Appl. Phys. Lett.* **87**, article 164104 (online, doi: 10.1063/1.2108114).
2. Gao, X. H., et al. 2005. "In-Vivo Molecular and Cellular Imaging with Quantum Dots," *Curr. Opin. Biotechnol.* **16**, 63–72.

2004

1. Kubicek, J., et al. 2004. "Integrated Lithographic Membranes and Surface Adhesion Chemistry for Three-Dimensional Cellular Stimulation," *Langmuir* **20**(26), 11552–56.

(NOTICE 03-05)

A. BRADBURY, LOS ALAMOS NATIONAL LABORATORY

2005

1. Di Niro, R., et al. 2005. "Characterizing Monoclonal Antibody Epitopes by Filtered Gene Fragment Phage Display," *Biochem. J.* **12**, 99–112.

2004

1. Bradbury, A., and J. D. Marks. 2004. "Antibodies from Phage Antibody Libraries," *J. Immunol. Methods* **290**, 29–49.
2. Bradbury, A., and J. D. Marks. 2004. "PCR Cloning of Human Immunoglobulin Genes," pp. 117–34 in *Antibody Engineering: Methods and Protocols*, ed. B. K. C. Lo, vol. 248 of *Methods in Molecular Medicine* series, Humana Press, Totowa, N.J.
3. Bradbury, A., and J. D. Marks. 2004. "Selection of Human Antibodies from Phage Display Libraries," pp. 161–76 in *Antibody Engineering: Methods and Protocols*, ed. B. K. C. Lo, vol. 248 of *Methods in Molecular Medicine* series, Humana Press, Totowa, N.J.
4. Bradbury, A., et al. 2004. "Antibodies in Proteomics," pp. 519–40 in *Antibody Engineering: Methods and Protocols*, ed. B. K. C. Lo, vol. 248 of *Methods in Molecular Medicine* series, Humana Press, Totowa, N. J.
5. Mawuenyega1, K. G., et al. 2004. "Mycobacterium tuberculosis Functional Network Analysis by Global Subcellular Protein Profiling," *Mol. Biol. Cell* **16**, 396–404.
6. Siegel, R. W., et al. 2004. "Recombinatorial Cloning Using Heterologous Lox Sites," *Genome Res.* **14**, 1119–29.

2003

1. Bradbury, A., et al. 2003. "Antibodies in Proteomics I: Selecting Antibodies," *Trends Biotechnol.* **21**, 275–81.
2. Bradbury, A., et al. 2003. "Antibodies in Proteomics II: Screening and Using Antibodies," *Trends Biotechnol.* **21**, 312–17.
3. Pavlik, P., et al. 2003. "Predicting Antigenic Peptides Suitable for the Selection of Phage Antibodies," *Hum. Antibodies* **12**, 99–112.
4. Sepúlveda, J., et al. 2003. "Binders Based on Dimerisation of Immunoglobulin VH Domains," *J. Mol. Biol.* **333**, 355–65.
5. Zacchi, P., et al. 2003. "Filtering DNA for Open Reading Frames," *Genome Res.* **13**, 980–90.
6. Zeytun, A., et al. 2003. "Fluorobodies Combine GFP Fluorescence with the Binding Characteristics of Antibodies," *Nat. Biotechnol.* **21**, 1473–79, retracted.

2001

1. Siegel, R. W., R. Jain, and A. Bradbury. 2001. "Using an In Vivo Phagemid System to Identify Noncompatible loxP Sequences," *FEBS Lett.* **505**, 467–73.

(NOTICE 03-05)

C. BUSTAMANTE, LAWRENCE BERKELEY NATIONAL LABORATORY

2005

1. Cecconi, C., et al. 2005. "Direct Observation of the Three-State of a Single Protein Molecule," *Science* **309**, 2057–60.
2. Chemla, Y. R., et al. 2005. "Mechanism of Force Generation of a Viral DNA Packaging Motor," *Cell* **122**, 683–92.
3. Collin, D., et al. 2005. "Verification of the Crooks Fluctuation Theorem and Recovery of RNA Folding Free Energies," *Nature* **437**, 231–34.
4. Pease, P. J., et al. 2005. "Sequence-Directed DNA Translocation by Purified FtsK," *Science* 307(5709), 586–90.

2004

1. Bustamante, C., et al. 2004. "Mechanical Process in Biochemistry," *Ann. Rev. Biochem.* **73**, 705–48.
2. Goedken, E. R., et al. 2004. "Fluorescence Measurements on the *E. coli* DNA Polymerase Clamp Loader: Implications for Conformational Changes During ATP and Clamp Binding," *J. Mol. Biol.* **5**, 1047–59.
3. Trepagnier, E. H., et al. 2004. "Experimental Test of Hatano and Sasa's Nonequilibrium Steady-State Equality," *Proc. Natl. Acad. Sci. USA* **101**, 15038–41.

2003

1. Bryant, Z., et al. 2003. "Structural Transitions and Elasticity from Torque Measurements on DNA," *Nature* **424**, 338–41.
2. Bustamante, C., Z. Bryant, and S. B. Smith. 2003. "Ten Years of Tension; Single-Molecule DNA Mechanics," *Nature* **421**, 423–27.
3. Gore, J., F. Ritort, and C. Bustamante. 2003. "Bias and Error in Estimates of Equilibrium Free-Energy Differences from Nonequilibrium Measurements," *Proc. Natl. Acad. Sci. USA* **100**, 12564–69.
4. Keller, D., D. Swigon, and C. Bustamante. 2003. "Relating Single-Molecule Measurements to Thermodynamics," *Biophys. J.* **84**, 733–38.
5. Matouschek, A., and C. Bustamante. 2003. "Finding a Protein's Achilles Heel," *Nat. Struct. Biol.* **10**(9), 674–76.

6. Onoa, B., et al. 2003. "Identifying the Kinetic Barriers to Mechanical Unfolding of the *T. thermophila* Ribozyme," *Science* **299**, 1892–95.
7. Rivetti, C., et al. 2003. "Visualizing RNA Extrusion and DNA Wrapping in Transcription Elongation Complexes of Bacterial and Eukaryotic RNA Polymerases," *J. Mol. Biol.* **326**, 1413–26.
8. Smith, S. B., Y. Cui, and C. Bustamante. 2003. "Optical-Trap Force Transducer that Operates by Direct Measurement of Light Momentum," *Methods Enzymol.* **361**, 134–62.
9. Stone, M. D., et al. 2003. "Chirality Sensing by *Escherichia coli* Topoisomerase IV and the Mechanism of Type II Topoisomerases," *Proc. Natl. Acad. Sci. USA* **100**, 8654–59.

2002

1. Forde, N., et al. 2002. "Using Mechanical Force to Probe the Mechanism of Pausing and Arrest During Continuous Elongation by *Escherichia coli* RNA Polymerase," *Proc. Natl. Acad. Sci.* **99**, 11682–87.
2. Liphardt, J., et al. 2002. "Equilibrium Information from Nonequilibrium Measurements in an Experimental Test of Jarzynski's Equality," *Science* **296**, 1832–35.
3. Ritort, F., C. Bustamante, and I. Tinoco, Jr. 2002. "A Two-State Kinetic Model for the Unfolding of Single Molecules by Mechanical Force," *Proc. Natl. Acad. Sci.* **99**, 13544–48.
4. Tinoco, I., Jr., and C. Bustamante. 2002. "The Effect of Force on Thermodynamics and Kinetics of Single Molecule Reactions," *Biophys. Chem.* **101–102**, 513–33.

(NOTICE 03-05)

B. CHURCH, GENE NETWORK SCIENCES

2005

1. Shuler, M. L. 2005. "Computer Models of Bacterial Cells to Integrate Genomic Detail with Cell Physiology," pp. 54–62 of *Proceedings of the KBM International Symposium on Microorganisms and Human Well-Being, June 30–July 1, 2005, Seoul, Korea.*

(NOTICE 03-05)

F. COLLART, ARGONNE NATIONAL LABORATORY

2005

1. Bond, D. R., et al. 2005. "Characterization of Citrate Synthase from *Geobacter sulfurreducens*, and Evidence for a Family of Eukaryotic-Like Citrate Synthases Throughout the *Geobacteraceae*," *Appl. Environ. Microbiol.* **71**(7), 3858–65.
2. Dieckman, L. J., W. C. Hanly, and F. R. Collart. 2005. "Strategies for High-Throughput Gene Cloning and Expression," *Genet. Eng.* **27**, 171–82.
3. Kolker, E., et al. 2005. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of Hypothetical Genes and Improved Functional Annotations," *Proc. Natl. Acad. Sci. USA* **102**(6), 2099–2104.
4. Stevens, F. J., et al. 2005. "Efficient Recognition of Protein Fold at Low Sequence Identity by Conservative Application of Psi-BLAST: Application," *J. Mol. Recognit.* **18**, 150–57.

2004

1. Scholle, M. D., F. R. Collart, and B. K. Kay. 2004. "In Vivo Biotinylated Proteins as Targets for Phage Display Selection Experiments," *Protein Expr. Purif.* **37**, 243–52.

(NOTICE 03-05)

J. COLLINS, BOSTON UNIVERSITY

2006

1. Driscoll, M. E., and T. S. Gardner. 2006. "Identification and Control of Gene Networks in Living Organisms via Supervised and Unsupervised Learning," *J. Process Control* **16**, 303–11.

2005

1. di Bernardo, D., et al. 2005. "Chemogenomic Profiling on a Genome-Wide Scale Using Reverse-Engineered Gene Networks," *Nat. Biotechnol.* **23**, 377–83.
2. Gardner, T. S., and J. Faith. 2005. "Reverse-Engineering Transcription Control Networks," *Phys. Life Rev.* **2**, 65–88.

(NOTICE 03-05)

T. R. HUSER, LAWRENCE LIVERMORE NATIONAL LABORATORY

2006

1. Chan, J. W., et al. "Raman Spectroscopy: Chemical Analysis of Biological Samples" in *Biophotonics from Fundamental Principles to Health, Environment, Security, and Defense Applications*, ed. B. Wilson, IOS Press, Amsterdam. In press.
2. Talley, C. E., et al. "Nanoparticle-Based Surface-Enhanced Raman Spectroscopy" in *Biophotonics from Fundamental Principles to Health, Environment, Security, and Defense Applications*, ed. B. Wilson, IOS Press, Amsterdam. In press.

2004

1. Laurence, T., et al. 2004. "Application of SERS Nanoparticles for Intracellular pH Measurements," *Proc. SPIE Int. Soc. Opt. Eng.* **5512**, 80–86.
2. Talley, C. E., et al. 2004. "Intracellular pH Sensors Based on Surface-Enhanced Raman Scattering," *Anal. Chem.* **76**, 7064–68.

(NOTICE 03-05)

J. KEASLING, LAWRENCE BERKELEY NATIONAL LABORATORY

2006

1. Carroll, K. S., et al. 2005. "Investigation of the Iron-Sulfur Cluster in *Mycobacterium tuberculosis* APS Reductase: Implications for Substrate Binding and Catalysis," *Biochemistry* **44** (44), 14647–57.

2005

1. Carroll, K. S., and H. Gao. 2005. "A Conserved Mechanism for Sulfonucleotide Reduction," *PloS Biology* **3**(8), e250.

(NOTICE 03-05)

M. KELLER, DIVERSA

2005

1. Zengler, K., et al. 2005. "High-Throughput Cultivation of Microorganisms Using Microcapsules," *Meth. Enzymol.* **397**, 124–30.

(NOTICE 03-05)

S. B. H. KENT, UNIVERSITY OF CHICAGO

2005

1. Bang, D., and S. B. H. Kent. 2005. "His6 Tag-Assisted Chemical Protein Synthesis," *Proc. Natl. Acad. Sci. USA* **102**, 5014–19.
2. Bang, D., et al. 2005. "Total Chemical Synthesis and X-Ray Crystal Structure of a Protein Diastereomer: [D-Gln35] Ubiquitin," *Angew. Chem. Int. Ed. Engl.* **44**, 3852–56.
3. Newberg, L. A., L. A. McCue, and C. E. Lawrence. 2005. "The Relative Inefficiency of Sequence Weights Approaches in Determining a Nucleotide Position Weight Matrix," *Stat. Appl. Genet. Mol. Biol.* **4**(1), Article 13. [[online format](#)]

2004

1. Bang, D., N. Chopra, and S. B. H. Kent. 2004. "Total Chemical Synthesis of Crambin," *J. Am. Chem. Soc.* **126**, 1377–83.
2. Bang, D., and S. B. H. Kent. 2004. "A One-Pot Chemical Synthesis of Crambin," *Angew. Chem. Int. Ed. Engl.* **116**, 2588–92.

(NOTICE 03-05)

C. E. LAWRENCE, BROWN UNIVERSITY

2005

1. Conlan, S., C. E. Lawrence, and L. A. McCue. 2005. "Rhodospseudomonas palustris Regulons Detected by a Cross-Species Analysis of Alpha-Proteobacterial Genomes," *Appl. Envir. Microbiol.* **71**, 7442–52.
2. Kolker, E., et al. 2005. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of Hypothetical Genes and Improved Functional Annotations," *Proc. Natl. Acad. Sci. USA* **102**(6), 2099–2104.
3. Tan, K., L. A. McCue, and G. D. Stormo. 2005. "Making Connections Between Novel Transcription Factors and Their DNA Motifs," *Genome Res.* **15**(2), 312–20.
4. Thompson, W., L. A. McCue, and C. E. Lawrence. 2005. "Using the Gibbs Motif Sampler to Find Conserved Domains in DNA and Protein Sequences," pp. 2.8.1–2.8.38 in *Current Protocols in Bioinformatics*, ed. A. D. Baxevanis et al., John Wiley & Sons, New York.

2004

1. Auger, I., and C. E. Lawrence. 2004. "Discussions on a Bayesian Approach to DNA Sequence Segmentation," *Biometrics* **60**(3), 581.

2. Newberg, L. A., and C. E. Lawrence. 2004. "Mammalian Genomes Ease Location of Human DNA Functional Segments but Not Their Description," *Stat. Appl. Genet. Mol. Biol.* **3**, 1–12.
3. Wan, X. F., et al. 2004. "Transcriptomic and Proteomic Characterization of the Fur Modulon in the Metal-Reducing Bacterium *Shewanella oneidensis*," *J. Bacteriol.* **186**(24), 8385–8400.

2003

1. Qin, Z. S., et al. 2003. "Identification of Co-Regulated Genes Through Bayesian Clustering of Predicted Regulatory Binding Sites," *Nat. Biotechnol.* **21**, 435–39.
2. Thompson, W., E. C. Rouchka, and C. E. Lawrence. 2003. "Gibbs Recursive Sampler: Finding Transcription Factor Binding Sites," *Nucleic Acids Res.* **31**, 3580–85.

2002

1. Ecker, J. G., et al. 2002. "An Application of Nonlinear Optimization in Molecular Biology," *Eur. J. Oper. Res.* **138**, 452–58.
2. McCue, L. A., et al. 2002. "Factors Influencing the Identification of Transcription Factor Binding Sites by Cross-Species Comparison," *Genome Res.* **12**, 1523–32.

2001

1. Liu, J. S., et al. 2001. "Bayesian Methodology in Genomics Research," *Case Studies in Bayesian Statistics*, Carnegie Mellon University. [\[online format\]](#)

(NOTICE 03-05)

H. M. SAURO, KECK GRADUATE INSTITUTE

2006

1. Vallabhajosyula, R., V. Chickarmane, and H. M. Sauro. 2006. "Conservation Analysis of Large Biochemical Networks," *Bioinformatics* **22**(3), 346–53.

2005

1. Chickarmane, V., et al. 2005. "Bifurcation Discovery Tool," *Bioinformatics* **21**(18), 3688–90.

(NOTICE 03-05)

T. C. SQUIER, PACIFIC NORTHWEST NATIONAL LABORATORY

2005

1. Chen, B., M. U. Mayer, and T. C. Squier. 2005. "Structural Uncoupling Between Opposing Domains of Oxidized Calmodulin Underlies the Enhanced Binding Affinity and Inhibition of the Plasma Membrane Ca-ATPase," *Biochemistry* **44**(12), 4737–47 (doi:10.1021/bi0474113).
2. Chen, B., et al. 2005. "Dynamic Motion of Helix A in the Amino-Terminal Domain of Calmodulin is Stabilized Upon Calcium Activation," *Biochemistry* **44**, 905–14. [[download PDF](#)]
3. Mayer, M. U., L. Shi, and T. C. Squier. 2005. "One-Step, Nondenaturing Isolation of an RNA Polymerase Enzyme Complex Using an Improved Multiuse Affinity Probe Resin," *Mol. Biosyst.* **1**(1), 53–56 (doi:10.1039/b500950b).

(NOTICE 03-05)

F. W. STUDIER, BROOKHAVEN NATIONAL LABORATORY

2005

1. Studier, F. W. 2005. "Protein Production by Auto-Induction in High-Density Shaking Cultures," *Protein Expr. Purif.* **41**, 207–34.

PUBLICATIONS FROM SHEWANELLA

SHEWANELLA FEDERATION

J. K. FREDRICKSON, SHEWANELLA FEDERATION (PNNL)

2006

1. Giometti, C. S. "A Tale of Two Metal Reducers: Comparative Proteome Analysis of *Geobacter sulfurreducens* PCA and *Shewanella oneidensis* MR-1," *Microbial Proteomics: Functional Biology of Whole Organisms*, ed. I. Humphery-Smith and M. Hecker, Wiley & Sons, New York. In press: June 2006.
2. Gorby, Y. A., et al. "c-Type Cytochromes Facilitate Extracellular Electron Transfer via Nanowires in *Shewanella oneidensis* MR-1," *Proc. Natl. Acad. Sci.* In press.
3. Khare, T., et al. 2006. "Differential Protein Expression in the Metal-Reducing Bacterium *Geobacter sulfurreducens* PCA Grown with Fumarate or Ferric Citrate," *Proteomics* **6**(2), 632–40.

2005

1. Abboud, R., et al. 2005. "Low-Temperature Growth of *Shewanella oneidensis* MR-1," *Appl. Environ. Microbiol.* **71**, 811–16.
2. Beliaev, A. S., et al. 2005. "Global Transcriptome Analysis of *Shewanella oneidensis* MR-1 Exposed to Different Terminal Electron Acceptors," *J. Bacteriol.* **187**(20), 7138–45.

3. Elias, D. A., et al. 2005. "Global Detection and Characterization of Hypothetical Proteins in *Shewanella oneidensis* MR-1 Using LC-MS Based Proteomics," *Proteomics* **5**, 3120–30.
4. Fredrickson, J. K., and M. F. Romine. 2005. "Genome-Assisted Analysis of Dissimilatory Metal-Reducing Bacteria," *Curr. Opin. Microbiol.* **16**(3), 269–74.
5. Gao, W., et al. 2005. "Effects of a Strong Static Magnetic Field on Bacterium *Shewanella oneidensis*: An Assessment by Using Whole Genome Microarray," *Bioelectromagnetics* **26**, 1–6.
6. Inagaki, F., et al. 2005. "The Paleome: A Sedimentary Genetic Record of Past Microbial Communities," *Astrobiology* **5**, 141–53.
7. Kolker, E., et al. 2005. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of 'Hypothetical' Genes and Improved Functional Annotations," *Proc. Natl. Acad. Sci. USA* **102**, 2099–2104.
8. Kus, E., et al. 2005. "The Concept of the Bacterial Battery," *Corrosion Sci.* **47**, 1063–69.
9. Masselon, C., et al. 2005. "Targeted Comparative Proteomics by Liquid Chromatography–Tandem Fourier Ion Cyclotron Resonance Mass Spectrometry," *Anal. Chem.* **77**(2), 400–406.
10. Nealson, K. H., and R. Popa. 2005. "Metabolic Diversity in the Microbial World: Relevance to Exobiology," pp. 1151–71 in *SGM Symposium 65: Microorganisms and Earth Systems—Advances in Geomicrobiology*, ed. G. M. Gadd, K. T. Semple, and H. M. Lappin-Scott, Cambridge Univ. Press, Oxford, U.K.
11. Nealson, K. 2005. "Hydrogen and Energy Flow as 'Sensed' by Molecular Genetics," *Proc. Nat. Acad. Sci. USA* **102**, 3889–90.
12. Qiu, X., J. M. Tiedje, and G. W. Sundin. 2005. "Genome-Wide Examination of the Natural Solar Radiation Response in *Shewanella oneidensis* MR-1," *Photochem. Photobiol.* **81**(6), 1559–68.
13. Qiu, X., et al. 2005. "Comparative Analysis of Differentially Expressed Genes in *Shewanella oneidensis* MR-1 Following Exposure to UVC, UVB, and UVA Radiation," *J. Bacteriol.* **187**(10), 3556–64.
14. Yang, F., et al. 2005. "Characterization of Purified Heme-Containing Peptides and Identification of Heme-Attachment Sites in c-Type *Shewanella oneidensis* Cytochromes Using Mass Spectrometry," *Proteome Res.* **4**(3), 846–54.

2004

1. Bakermans, C., and K. H. Nealson. 2004. "Relationship of Critical Temperature to Macromolecular Synthesis and Growth Yield in *Psychrobacter cryopegella*," *J. Bacteriol.* **186**, 2340–45.
2. Gao, H., et al. 2004. "Global Transcriptome Analysis of the Heat Shock Response of *Shewanella oneidensis*," *J. Bacteriol.* **186**(22), 7796–7803.

3. Micic, M., et al. 2004. "Correlated Atomic Force Microscopy and Fluorescence Lifetime Imaging of Live Bacterial Cells," *Colloids Surf. B Biointerfaces* **34**(4), 205–12.
4. Johnson, C. M., et al. 2004. "Isotopic Constraints on Biogeochemical Cycling of Fe," *Rev. Mineral. Geochem.* **55**, 359–408.
5. Kemner, K. M., et al. 2004. "Elemental and Redox Analysis of Single Bacterial Cells by X-Ray Microbeam Analysis," *Science* **306**, 686–87.
6. Meyer, T. E., et al. 2004. "Identification of 42 Possible Cytochrome C Genes in the *Shewanella oneidensis* Genome and Characterization of Six Soluble Cytochromes," *OMICS* **8**, 57–87.
7. Romine, M. F., et al. 2004. "Validation of *Shewanella oneidensis* MR-1 Small Proteins by AMT Tag-Based Proteome Analysis," *OMICS* **8**(3), 239–54.
8. Qiu, X., et al. 2004. "Survival of *Shewanella oneidensis* MR-1 after UV Radiation Exposure," *Appl. Environ. Microbiol.* **70**(11), 6435–43.
9. Venter, J. C., et al. 2004. "Environmental Genomic Shotgun Sequencing of the Sargasso Sea," *Science* **304**, 66–74.
10. Wan, X. F., et al. 2004. "Transcriptomic and Proteomic Characterization of the Fur Modulon in the Metal-Reducing Bacterium *Shewanella oneidensis*," *J. Bacteriol.* **186**(24), 8385–8400.

2003

1. Yost, C., et al. 2003. "A Computational Study of *Shewanella oneidensis* MR-1: Structural Prediction and Functional Inference of Hypothetical Proteins," *OMICS* **7**(2), 177–91.

2002

1. Beliaev, A. S., et al. 2002. "Microarray Transcription Profiling of a *Shewanella oneidensis* *etrA* Mutant," *J. Bacteriol.* **184**, 4612–16.

PUBLICATIONS FROM OTHERS

E. H. DAVIDSON CALIFORNIA INSTITUTE OF TECHNOLOGY

GTL PROJECT PUBLICATIONS (since inception of Project 11/03)

2005

1. Istrail, S., and E. H. Davidson. 2005. "Logic Functions of the Genomic *cis*-Regulatory Code," *Proc. Natl. Acad. Sci. USA* **102**, 4954–59.

2. Minokawa, T., A. H. Wikramanayake, and E. H. Davidson. 2005. “*cis*-Regulatory Inputs of the *wnt8* Gene in the Sea Urchin Endomesoderm Network,” *Dev. Biol.* **288**, 545–58.
3. Yuh, C.-H., E. R. Dorman, and E. H. Davidson. 2005. “Brn1/2/4, the Predicted Midgut Regulator of the *endo16* Gene of the Sea Urchin Embryo,” *Dev. Biol.* **281**, 286–98.

2004

1. Cameron, R. A., et al. 2004. “*cis*-Regulatory Activity of Randomly Chosen Genomic Fragments from the Sea Urchin,” *Gene Expr. Patterns* **4**, 205–13.
2. Howard, M. L., and E. H. Davidson. 2004. “*cis*-Regulatory Control Circuits in Development,” *Dev. Biol.* **271**, 109–18.
3. Lee, P. Y., and E. H. Davidson. 2004. “Expression of *Spgatae*, the *Strongylocentrotus purpuratus* Ortholog of Vertebrate GATA4/5 Factors,” *Gene Expr. Patterns* **5**, 161–65.
4. Oliveri, P., and E. H. Davidson. 2004. “Gene Regulatory Network Analysis in Sea Urchin Embryos,” *Meth. Cell Biol.* **74**, 775–93.
5. Oliveri, P., and E. H. Davidson. 2004. “Gene Regulatory Network Controlling Embryonic Specification in the Sea Urchin,” *Curr. Opin. Genet. Dev.* **14**, 351–60.
6. Revilla-i-Domingo, R., T. Minokawa, and E. H. Davidson. 2004. “R11: A *cis*-Regulatory Node of Sea Urchin Embryo Gene Network that Controls Early Expression of *SpDelta* in Micromeres,” *Dev. Biol.* **274**, 438–51.
7. Yuh, C.-H., et al. 2004. “An *otx cis*-Regulatory Module: A Key Node in the Sea Urchin Endomesoderm Gene Regulatory Network,” *Dev. Biol.* **269**, 536–51.

2003

1. Bolouri, H., and E. H. Davidson. 2003. “Transcriptional Regulatory Cascades in Development: Initial Rates, Not Steady State, Determine Network Kinetics,” *Proc. Natl. Acad. Sci. USA* **100**, 9371–76.
2. Revilla-i-Domingo, R., and E. H. Davidson. 2003. “Developmental Gene Network Analysis,” *Int. J. Dev. Biol.* **47**, 695–703.

D. EISENBERG, UNIVERSITY OF CALIFORNIA, LOS ANGELES

Selected Publications 2004–2005 Supported in Part or Whole by BER-DOE

UCLA-DOE Institute for Genomics and Proteomics

2005

1. Beeby, M., et al. 2005. “The Genomics of Disulfide Bonding and Protein Stabilization in Thermophiles,” *PLoS Biol.* **3**, 1549–58.
2. Bowie, J. U. 2005. “Border Crossing,” *Nature* **433**, 367–69.

3. Chaudhuri, B. N., and T. O. Yeates. 2005. "A Computational Method to Predict Genetically Encoded Rare Amino Acids in Proteins," *Genome Biol.* **6**, R79.
4. Edwards, M. D., et al. 2005. "Gating the MscS Mechanosensitive Channel: Pivotal Role of the Glycine Rich TM3 Helix," *Nat. Struct. Mol. Biol.* **12**, 113–19.
5. Faham, S., et al. 2005. "Crystallization of Bacteriorhodopsin from Bicelle Formulations at Room Temperature," *Protein Sci.* **14**, 836–40.
6. Fung, E., et al. 2005. "A Synthetic Gene-Metabolic Oscillator," *Nature* **435**, 118–22.
7. Kerfeld, C. A., et al. 2005. "Protein Structures Forming the Shell of Primitive Bacterial Organelles," *Science* **309**, 936–38.
8. Lee, C., A. Alekseyenko, and D. S. Parker. 2005. "Pygr: A Python Graph Database Framework for Bioinformatics," in *Intelligent Systems in Molecular Biology*, International Society for Computational Biology, Detroit.
9. Li, H., M. Pellegrini, and D. Eisenberg. 2005. "Detection of Parallel Functional Modules by Comparative Analysis of Genome Sequences," *Nat. Biotechnol.* **23**, 253–60.
10. Li, H., et al. 2005. "Crystal Structure of a RuBisCO-Like Protein from the Green Sulfur Bacterium *Chlorobium tepidum*," *Structure* **13**, 779–89.
11. Loo, O., et al. 2005. "Top-Down, Bottom-Up, and Side-to-Side Proteomics with Virtual 2-D Gels," *Int. J. Mass Spectrom.* **240**, 317–25.
12. Pal, D., and D. Eisenberg. 2005. "Inference of Protein Function from Protein Structure," *Structure* **13**, 121–30.
13. Riley, R., et al. 2005. "Inferring Protein Domain Interactions from Databases of Interacting Proteins," *Genome Biol.* **6**, R89.
14. Rohlin, L., et al. 2005. "The Heat-Shock Response of *Archaeoglobus fulgidus*," *J. Bacteriol.* **187**, 6046–57.
15. Tran, L. M., et al. 2005. "gNCA: A Framework for Determining Transcription Factor Activity Based on Transcriptome: Identifiability and Numerical Implementation," *Metab. Eng.* **7**, 128–41.

2004

1. Bowers, P. M., et al. 2004. "PROLINKS: A Database of Protein Functional Linkages Derived from Coevolution," *Genome Biol.* **5**, R35.1–R35.13.
2. Bowers, P., et al. 2004. "Use of Logic Relationships to Decipher Protein Network Organization," *Science* **306**, 2246–49.
3. Faham, S., et al. 2004. "Side Chain Contributions to Membrane Protein Structure and Stability," *J. Mol. Biol.* **335**, 237–305.
4. Hermjakob, H., et al. 2004. "The HUPO PSIs Molecular Interaction Format—A Community Standard for the Representation of Protein Interaction Data," *Nat. Biotechnol.* **22**, 177–83.

5. Melnyk, R. A., et al. 2004. "The Affinity of GXXXG Motifs in Transmembrane Helix-Helix Interactions is Modulated by Long-Range Communication," *J. Biol. Chem.* **279**, 16591–97.
6. O'Connor, B. D., and T. O. Yeates. 2004. "GDAP: A Web Tool for Genome-Wide Protein Disulfide Bond Prediction," *Nucleic Acids Res.* **32**, W360–64.
7. Salwinski, L., and D. Eisenberg. 2004. "In Silico Simulation of Biological Network Dynamics," *Nat. Biotechnol.* **22**, 1017–19.
8. Salwinski, L., et al. 2004. "The Database of Interacting Proteins: 2004 Update," *Nucleic Acids Res.* **32**, D449–D451.
9. Yohannan, S., et al. 2004. "A C_α-H···O Hydrogen Bond in a Membrane Protein is Not Stabilizing," *J. Am. Chem. Soc.* **126**, 2284–85.
10. Yohannan S., et al. 2004. "Evolution of Transmembrane Helix Kinks and the Structural Diversity of G-Protein Coupled Receptors," *Proc. Natl. Acad. Sci. USA* **101**(4), 959–63.
11. Yohannan, S., et al. 2004. "Proline Substitutions are Not Easily Accommodated in a Membrane Protein," *J. Mol. Biol.* **341**(1), 1–6.

PROTEOMICS APPLICATIONS

J. K. FREDRICKSON, PACIFIC NORTHWEST NATIONAL LABORATORY

2006

1. Callister, S. J., et al. 2006. "Normalization Approaches for Removing Systematic Biases Associated with Mass Spectrometry and Label-Free Proteomics," *J. Proteome Res.* **5**(2), 277–86.
2. Lipton, M. S., et al. "The AMT Tag Approach to Proteomic Characterization of *Deinococcus radiodurans* and *Shewanella oneidensis*," *Microbial Proteomics: Functional Biology of Whole Organisms*, ed. I. Humphery-Smith and M. Hecker, John Wiley & Sons, New York. In press: June 2006.

2005

1. Elias, D. A., et al. 2005. "Global Detection and Characterization of Hypothetical Proteins in *Shewanella oneidensis* MR-1 Using LC-MS-Based Proteomics," *Proteomics* **5**, 3120–30.
2. Havre, S. L., et al. 2005. "Enabling Proteomics Discovery Through Visual Analysis," *IEEE Eng. Med. Biol. Mag.* **24**, 50–57.
3. Schmid, A. K., et al. 2005. "Global Whole-Cell FTICR Mass Spectrometric Proteomics Analysis of the Heat Shock Response in the Radioresistant Bacterium *Deinococcus radiodurans*," *J. Proteome Res.* **4**, 709–18.

4. Yang, F., et al. 2005. "Characterization of Purified Heme-Containing Peptides and Identification of Heme-Attachment Sites in *c*-Type *Shewanella oneidensis* Cytochromes Using Mass Spectrometry," *Proteome Res.* **4**, 846–54.

2004

1. Kolker, E., et al. 2004. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of 'Hypothetical' Genes and Improved Functional Annotations," *Proc. Natl. Acad. Sci. USA* **102**, 2099–2104.
2. Romine, M. F., et al. 2004. "Validation of *Shewanella oneidensis* MR-1 Small Proteins by AMT Tag-Based Proteome Analysis," *OMICS* **8**, 239–54.

2002

1. Lipton, M. S., et al. 2002. "Global Analysis of *Deinococcus radiodurans* Proteome by Using Accurate Mass Tags," *Proc. Nat. Acad. Sci.* **99**, 11049–54.

2001

1. Conrads, T. P., et al. 2001. "Quantitative Analysis of Bacterial and Mammalian Proteomes Using a Combination of Cysteine Affinity Tags and ¹⁵N-Metabolic Labeling," *Anal. Chem.* **73**, 2132–39.

GENOME ANNOTATION

M. LAND, OAK RIDGE NATIONAL LABORATORY

2005

1. Feil, H., et al. 2005. "Comparison of the Complete Genome Sequences of *Pseudomonas syringae* pv. *syringae* B728a and pv. *tomato* DC3000," *Proc. Natl. Acad. Sci. USA* **102**(31), 11064–69.
2. Kolker, E., et al. 2005. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of Hypothetical Genes and Improved Functional Annotations," *Proc. Natl. Acad. Sci. USA* **102**(6), 2099–2104.
3. Oren, A., et al. 2005. "How to be Moderately Halophilic with Broad Salt Tolerance: Clues from the Genome of *Chromohalobacter salexigens*," *Extremophiles* **9**(4), 275–79.
4. VerBerkmoes, N. C., et al. 2005. "Evaluation of 'Shotgun' Proteomics for Identification of Biological Threat Agents in Complex Environmental Matrixes: Experimental Simulations," *Anal. Chem.* **77**(3), 923–32.

2004

1. Armbrust, E. V., et al. 2004. "The Genome of the Diatom *Thalassiosira pseudonana*: Ecology, Evolution, and Metabolism," *Science* **306**(5693), 79–86.

- Hendrickson, E. L., et al. 2004. "Complete Genome Sequence of the Genetically Tractable Hydrogenotrophic Methanogen *Methanococcus maripaludis*," *J. Bacteriol.* **186**(20), 6956–69.
- Strader, M. B., et al. 2004. "Characterization of the 70S Ribosome from *Rhodospseudomonas palustris* Using an Integrated 'Top-Down' and 'Bottom-Up' Mass Spectrometric Approach," *J. Proteome Res.* **3**(5), 965–78.
- Wan, X. F., et al. 2004. "Transcriptomic and Proteomic Characterization of the Fur Modulon in the Metal-Reducing Bacterium *Shewanella oneidensis*," *J. Bacteriol.* **186**(24), 8385–8400.

PROTEOMICS

R. D. SMITH, PACIFIC NORTHWEST NATIONAL LABORATORY

2006

- Jacobs, J. M., and R. D. Smith. "Proteomic Analyses Using High-Efficiency Separations and Accurate Mass Measurements," *Separation Methods in Proteomics*, ed. G. B. Smejkal, Apex Publishing, Madison, Wis. In press.
- Kiebel, G. R., et al. "PRISM: A Data Management System for High-Throughput Proteomics," *Proteomics*. In press.

2005

- Bogdanov, B., and R. D. Smith. 2005. "Proteomics by FTICR Mass Spectrometry: Top Down and Bottom Up," *Mass Spectrom. Rev.* **24**, 168–200.
- Huang, Y., et al. 2005. "Statistical Characterization of the Charge State and Residue Dependence of Low-Energy CID Peptide Dissociation Patterns," *Anal. Chem.* **77**, 5800–5813.
- Luo, Q., et al. 2005. "Preparation of 20- μ m-i.d. Silica-Based Monolithic Columns and Their Performance for Proteomics Analyses," *Anal. Chem.* **77**, 5028–35.
- Masselon, C., et al. 2005. "Targeted Comparative Proteomics by Liquid Chromatography–Tandem Fourier Transform Mass Spectrometry," *Anal. Chem.* **77**, 400–406.
- Norbeck, A. D., et al. 2005. "The Utility of Accurate Mass and LC Elution Time Information in the Analysis of Complex Proteomes," *J. Am. Soc. Mass Spectrom.* **16**, 1239–49.
- Page, J. S., et al. 2005. "Automatic Gain Control in Mass Spectrometry Using a Jet Disrupter Electrode in an Electrodynamic Ion Funnel," *J. Am. Soc. Mass Spectrom.* **16**, 244–53.
- Page, J. S., et al. 2005. "Variable Low-Mass Filtering Using an Electrodynamic Ion Funnel," *J. Mass Spectrom.* **40**, 1215–22.

8. Shen, Y., and R. D. Smith. 2005. "Advanced Nanoscale Separations and Mass Spectrometry for Sensitive High-Throughput Proteomics," *Expert Rev. Proteomics* **3**, 431–47.
9. Shen, Y., et al. 2005. "Automated 20 Kpsi RPLC-MS and MS/MS with Chromatographic Peak Capacities of 1000–1500 and Capabilities in Proteomics and Metabolomics," *Anal. Chem.* **77**, 3090–3100.
10. Shen, Y., et al. 2005. "Ultrahigh-Throughput Proteomics Using Fast RPLC Separations with ESI-MS/MS," *Anal. Chem.* **77**(20), 6692–6701.
11. Simpson, D. C., and R. D. Smith. 2005. "Combining Capillary Electrophoresis with Mass Spectrometry for Applications in Proteomics," *Electrophoresis* **26**, 1291–1305.
12. Tang, K., et al. 2005. "High-Sensitivity Ion Mobility Spectrometry/Mass Spectrometry Using Electrodynamic Ion Funnel Interfaces," *Anal. Chem.* **77**, 3330–39.

2004

1. Belov, M. E., et al. 2004. "An Automated High-Performance Capillary Liquid Chromatography-Fourier Transform Ion Cyclotron Resonance Mass Spectrometer for High-Throughput Proteomics," *J. Am. Soc. Mass Spectrom.* **15**, 212–32.
2. Camp, D. G., and R. D. Smith. 2004. "The Use of Accurate Mass and Time Tags Based upon High-Throughput Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Global Proteomic Characterization," pp. 183–224 in *Proteome Analysis: Interpreting the Genome* (ed. D. W. Speicher), Elsevier, Amsterdam.
3. Kim, J.-K., D. G. Camp II, and R. D. Smith. 2004. "Improved Detection of Multi-Phosphorylated Peptides in the Presence of Phosphoric Acid in Liquid Chromatography/Mass Spectrometry," *J. Mass Spectrom.* **39**, 206–15.
4. Martinovic, S., L. Paša-Tolić, and R. D. Smith. 2004. "Capillary Isoelectric Focusing–Mass Spectrometry of Proteins and Protein Complexes," pp. 291–304 in *Capillary Electrophoresis of Proteins and Peptides* (ed. M. A. Strege and A. L. Lagu), Vol. 276 of *Methods in Molecular Biology* series, Humana Press, Totowa, N.J.
5. Page, J. S., C. D. Masselon, and R. D. Smith. 2004. "FTICR Mass Spectrometry for Qualitative and Quantitative Bioanalyses," *Curr. Opin. Biotechnol.* **15**, 3–11.
6. Paša-Tolić, L., et al. 2004. "Proteomic Analyses Using an Accurate Mass and Time Tag Strategy," *Biotechniques* **37**, 621–36.
7. Qian, W., D. G. Camp, and R. D. Smith. 2004. "High Throughput Proteomics Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry," *Expert Rev. Proteomics* **1**, 87–95.
8. Shen, Y., et al. 2004. "Nanoscale Proteomics," *Anal. Bioanal. Chem.* **378**, 1037–45.
9. Shen, Y., et al. 2004. "Ultrasensitive Proteomics Using High-Efficiency On-Line Micro-SPE-NanoLC-NanoESI MS and MS/MS," *Anal. Chem.* **76**, 144–54.

10. Smith, R. D., Y. Shen, and K. Tang. 2004. "Ultrasensitive and Quantitative Analyses from Combined Separations-Mass Spectrometry for the Characterization of Proteomes," *Acc. Chem. Res.* **37**, 269–78.
11. Strittmatter, E. F., et al. 2004. "Application of Peptide Retention Time Information in a Discriminant Function for Peptide Identification by Tandem Mass Spectrometry," *J. Proteome Res.* **3**(4), 760–69.
12. Tang, K., J. S. Page, and R. D. Smith. 2004. "Charge Competition and the Linear Dynamic Range of Detection in Electrospray Ionization Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* **15**, 1416–23.
13. Vilkov, A. N., et al. 2004. "Tailored Noise Waveform—Collision-Induced Dissociation of Ions Stored in a Linear Ion Trap Combined with Liquid Chromatography—Fourier Transform Ion Cyclotron Resonance Mass Spectrometry," *Rapid Commun. Mass Spectrom.* **18**, 2682–90.

2003

1. Belov, M. E., et al. 2003. "Automated Gain Control and Internal Calibration with External Ion Accumulation Capillary Liquid Chromatography-Electrospray Ionization—Fourier Transform Ion Cyclotron Resonance," *Anal. Chem.* **75**, 4195–4205.
2. Belov, M. E., et al. 2003. "Initial Implementation of External Accumulation Liquid Chromatography/Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry with Automated Gain Control," *Rapid Commun. Mass Spectrom.* **17**, 627–36.
3. Ferguson, F. L., and R. D. Smith. 2003. "Proteome Analysis by Mass Spectrometry," *Annu. Rev. Biophys. Biomol. Struct.* **32**, 399–424.
4. Goshe, M. B., and R. D. Smith. 2003. "Stable Isotope-Coded Proteomic Mass Spectrometry," *Curr. Opin. Biotechnol.* **14**, 101–109.
5. Masselon, C., et al. 2003. "Identification of Tryptic Peptides from Large Databases Using Multiplexed-MS/MS: Simulations and Experimental Results," *Proteomics* **3**, 1279–86.
6. Mohan, D., et al. 2003. "Integration of Electrokinetic-Based Multidimensional Separation/Concentration Platform with ESI-FTICR-MS for Proteome Analysis of *Shewanella oneidensis*," *Anal. Chem.* **75**, 4432–40.
7. Petritis, K., et al. 2003. "Use of Artificial Neural Networks for the Prediction of Peptide Liquid Chromatography Elution Times in Proteome Analyses," *Anal. Chem.* **75**, 1039–48.
8. Shen, Y., et al. 2003. "High-Efficiency On-Line SPE Coupling to 15–150 μm I.D. Column LC for Proteomic Analysis," *Anal. Chem.* **75**, 3596–3605.
9. Smith, R. D., et al. 2003. "High-Performance Separations and Mass Spectrometric Methods for High-Throughput Proteomics Using Accurate Mass Tags," pp. 85–131 in

Advances in Protein Chemistry **65**, ed. R. D. Smith and T. D. Veenstra, Elsevier Science, San Diego.

10. Strittmatter, E. F., N. Rodriguez, and R. D. Smith. 2003. "High Mass Measurement Accuracy Determination for Proteomics Using Multivariate Regression Fitting: Application to Electrospray Ionization Time-of-Flight Mass Spectrometry," *Anal. Chem.* **75**, 460–68.
11. Strittmatter, E. F., et al. 2003. "Proteome Analyses Using Accurate Mass and Elution Time Peptide Tags with Capillary LC Time-of-Flight Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* **14**, 980–91.
12. Tolmachev, A. V., H. R. Udseth, and R. D. Smith. 2003. "Modeling the Ion Density Distribution in Collisional Cooling RF Multipole Ion Guides," *Int. J. Mass Spectrom.* **222**, 155–74.
13. Tolmachev, A. V., et al. 2003. "Suppression of the Lower Charge State Ions in the External Accumulation RF Multipole with a Reduced Trapping DC Potential," *J. Am. Soc. Mass Spectrom.* **14**, 1229–35.

2002

1. Belov, M. E., G. A. Anderson, and R. D. Smith. 2002. "Higher-Resolution Data-Dependent Selective External Ion Accumulation for Capillary LC-FTICR," *Int. J. Mass Spectrom.* **218**, 265–79.
2. Berger, S. J., et al., 2002. "High-Throughput Global Peptide Proteomic Analysis by Combining Stable Isotope Amino Acid Labeling and Data-Dependent Multiplexed-MS/MS," *Anal. Chem.* **74**, 4994–5000.
3. Blonder, J., et al. 2002. "Enrichment of Integral Membrane Proteins for Proteomic Analysis Using Liquid Chromatography–Tandem Mass Spectrometry," *J. Proteome Res.* **1**, 351–60.
4. Buchanan, M. V., et al. 2002. "Genomes to Life 'Center for Molecular and Cellular Systems': A Research Program for Identification and Characterization of Protein Complexes," *OMICS* **6**, 287–303.
5. Chen, Y., et al. 2002. "Integration of Capillary Isoelectric Focusing with Capillary Reversed-Phase Liquid Chromatography for Two-Dimensional Proteomics Separation," *Electrophoresis* **23**, 3143–48.
6. Conrads, T. P., et al. 2002. "High-Throughput, Quantitative Proteomics of Intact and Proteolytically Digested Proteins," *Recent Res. Devel. Anal. Chem.* **2**, 97–122.
7. Paša-Tolić, L. et al. 2002. "Gene Expression Profiling Using Advanced Mass Spectrometric Approaches," *J. Mass Spectrom.* **37**, 1185–98.
8. Paša-Tolić, L., et al. 2002. "Increased Proteome Coverage Based upon High-Performance Separations and DREAMS FTICR Mass Spectrometry," *J. Am. Soc. Mass Spectrom.* **13**, 954–63.
9. Shen, Y., and R. D. Smith. 2002. "Proteomics Based on High-Efficiency Capillary Separations," *Electrophoresis* **23**, 3106–24.

10. Shen, Y., et al. 2002. "High-Efficiency Nanoscale Liquid Chromatography Coupled Online with Mass Spectrometry Using Nanoelectrospray Ionization for Proteomics," *Anal. Chem.* **74**, 4235–49.
11. Smith, R. D. 2002. "Advanced Mass Spectrometric Methods for the Rapid and Quantitative Characterization of Proteomes," *Comp. Funct. Genomics* **3**, 143–50.
12. Smith, R. D. 2002. "Trends in Mass Spectrometry Instrumentation for Proteomics," *Trends Biotechnol.* **20S**, S3–S7.
13. Smith, R. D., et al. 2002. "Advanced Mass Spectrometric Approaches for Rapid and Quantitative Proteomics," Chap. 8, pp. 307–60 in *Applied Electrospray Mass Spectrometry*, ed. B. N. Pramanik, A. K. Ganguly, and M. L. Gross.
14. Smith, R. D., et al. 2002. "An Accurate Mass Tag Strategy for Quantitative and High-Throughput Proteome Measurements," *Proteomics* **2**, 513–23.
15. Tang, K., et al. 2002. "Independent Control of Ion Transmission in a Jet Disrupter Dual Channel Ion Funnel Electrospray Ionization-MS Interface," *Anal. Chem.* **74**, 5431–37.

PUBLICATIONS FROM NOTICE 04-15

(NOTICE 04-15)

M. E. COLVIN, UNIVERSITY OF CALIFORNIA, MERCED

2006

1. Kim, A. D., and J. C. Schotland. "Self-Consistent Scattering Theory for the Radiative Transport Equation," *J. Opt. Soc. Am. A*. In press.

2005

1. Kim, A. D. 2005. "A Boundary Integral Method to Compute Green's Functions for the Radiative Transport Equation," *Waves in Random and Complex Media* **15**, 17–42.
2. Kim, A. D., and M. Moscoso. 2005. "Light Transport in Two-Layer Tissues," *J. Biomed. Opt.* **10**, 1–10.
3. Lau, E. Y., F. C. Lightstone, and M. E. Colvin. 2005. "Dynamics of DNA Encapsulated in a Hydrophobic Nanotube," *Chem. Phys. Lett.* **412**, 82–87.
4. Sulchek, T. A., et al. 2005. "Dynamic Force Spectroscopy of Parallel Individual Mucin1-Antibody Bonds," *Proc. Natl. Acad. Sci.* **102**(46), 16638–643.

(NOTICE 04-15)

M. E. PAULAITIS, JOHNS HOPKINS UNIVERSITY

Institute in Multiscale Modeling of Biology Interactions (IMMBI)

IMMBI Publications in Year 1

The following publications resulted from IMMBI-sponsored research conducted by the postdoctoral fellows in the institute.

2006

1. Atilgan, E., D. Wirtz, and S. X. Sun. 2006. "Mechanics and Dynamics of Actin-Driven Thin Membrane Protrusions," *Biophys. J.* **90**(1), 65–76.
2. Jeong, J. I., Y. Jang, and M. K. Kim. 2006. "A Connection Rule for Alpha-Carbon Coarse-Grained Elastic Network Models Using Chemical Bond Information," *J. Mol. Graph. Model* **24**(4), 296–306.
3. Jeong, J. I., E. E. Lattman, and G. S. Chirikjian. "A Method for Finding Candidate Conformations for Molecular Replacement Using Relative Rotation Between Domains of a Known Structure," *Acta Crystallogr. D Biol. Crystallogr.* (Accepted)
4. Jeong, J. I., E. E. Lattman, and G. S. Chirikjian. "A Method for Finding Candidate Conformations for Molecular Replacement Using Relative Rotation Between Domains of a Known Structure," *Acta Crystallogr. D Biol. Crystallogr.* (Accepted)

2005

1. Atilgan, E., D. Wirtz, and S. X. Sun. 2005. "Morphology of the Lamellipodium and Organization of Actin Filaments at the Leading Edge of Crawling Cells," *Biophys. J.* **89**, 3589–3602.
2. Panasik, N., P. K. Fleming, and G. D. Rose. 2005. "Hydrogen-Bonded Turns in Proteins: The Case for a Recount," *Protein Sci.* **14**, 2910–14.