DOE Prog Rep '04

Functional Analysis and Discovery of Microbial Genes Transforming Metallic and Organic Pollutants: Database and Experimental Tools

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Summary

The University of Minnesota Biocatalysis/Biodegradation Database (UM-BBD) has been updated and expanded throughout the three years of the project. Moreover, we added to the functionality of the database by adding a pathway prediction system (PPS) with 250 rules governing the prediction system.

We have discovered new metabolism during the current grant period; novel enzymes metabolizing an organobismuth compound, organoboron compounds, azetidine rings, and polyamide substrates. Some of this work has been published in the second year of the project (see publications below). We have conducted enrichment culturing and have been successful in identifying microbes that metabolize other novel compounds. The results from these studies have been published and, further, depicted on the UM-BBD to help disseminate the information.

Publications

Year 1 publications

Lynda B.M. Ellis, Bo Kyeng Hou, Wenjun Kang, Lawrence P. Wackett (2003)
The University of Minnesota Biocatalysis/Biodegradation Database:
Post-Genomic Data Mining. *Nucleic Acids Research* (submitted).

Wackett, L.P. (2002) Expanding the map of microbial metabolism. *Environ. Microbiol.* **4**: 12-13.

Handelsman, J. and L.P. Wackett (2002) Microbial diversity: Sustaining the earth and industry. *Curr. Op. Microbiol.* **5**:237-239.

Wackett, L.P. (2002) Application of genomics to biocatalysis and biodegradation. In (C.M. Fraser, T. Read and K.E. Nelson, eds.) *Microbial Genomes*. The Human Press, Inc., Totowa, New Jersey (in press).

Bo Kyeng Hou, Wenjun Kang, Larry P. Wackett and Lynda B.M. Ellis (2002)
Predicting Microbial Metabolism: A Functional Group Approach (abstract).
10th Annual International Conference on Intelligent Systems in Molecular Biology, August 3-7, 2002, Edmonton, Alberta, Canada
http://ismb02.org/posterlist.htm#_Toc13331946

Year 2 publications

Shapir, N., J.P. Osborne, G. Johnson, M.J. Sadowsky and L.P. Wackett (2002)
Purification, substrate range and metal center of AtzC: The N-isopropylammelide hydrolase involved in bacterial atrazine metabolism. *J. Bacteriol.* **184**:5376-5384.

Parales, R.E., N.C. Bruce, A. Schmid and L.P. Wackett (2002) Biodegradation, biotransformation and biocatalysis. *Appl. Environ. Microbiol.* **68**:4699-4709.

Ellis, L.B.M., B.K. Hou, W. Kang and L.P. Wackett (2003) The University of Minnesota Biocatalysis/Biodegradation Database: Post genomic data mining. *Nucl. Acids Res.* **31**:262-265.

Wackett, L.P. (2003) *Pseudomonas putida* – a versatile biocatalyst. *Nature Biotech.* **21**:136-138.

Fruchey, I., N. Shapir, M.J. Sadowsky and L.P. Wackett (2003) On the origins of cyanuric acid hydrolase: Purification, substrates and prevalence of AtzD from *Pseudomonas* sp. ADP. *Appl. Environ. Microbiol.* **69**:3653-3657.

Negrete-Raymond, A.C., B. Weder, and L.P. Wackett (2003) Catabolism of arylboronic acids by *Arthrobacter nicotinovorans* strain PBA. *Appl. Environ. Microbiol.* **69**:4263-4267.

Hou, B.K., L.P. Wackett, and L.B.M. Ellis (2003) Microbial pathway prediction: A functional group approach. *J. Chem. Inf. Comp. Sci.* **43**:1051-1057.

Hou, B.K., L.P. Wackett, and L.B.M. Ellis (2003) Encoding microbial metabolic logic: Predicting biodegradation. *Appl. Environ. Microbiol.* (under review)

Wackett, L.P., T. Dodge and L.B.M. Ellis. 2003. Microbes and the elements. *Appl. Environ. Microbiol.* (revised manuscript pending editor's decision).
Based on DOE-funded compilations of microbial metabolism of the elements on the University of Minnesota Biocatalysis/Biodegradation Database.

Year 3 publications

Wackett, L.P. A.G. Dodge, and L.B.M. Ellis. (2004) Microbial genomics and the periodic table. *Appl. Environ. Microbiol.* **70**:647-655.

Vetting, M.W., L. P. Wackett, L. Que Jr., J. D. Lipscomb and D. H. Ohlendorf (2004) A crystallographic comparison of a manganese and an iron-dependent extradiol dioxygenase. *J. Bacteriol.* **186**:1945-1958.

Wackett, L.P. (2004) Applications of genomics to biocatalysis and biodegradation. In (C.M. Fraser, T. Read and K.E. Nelson, eds.) *Microbial Genomes*. The Human Press, Inc., Totowa, New Jersey, pp. 443-459.

Wackett, L.P. (2004) Stable isotope probing in biodegradation research. *Trends Biotechnol.* **22**:153-154.

Sajjaphan, K., N. Shapir, L.P. Wackett, M. Palmer, J. Tomkins, B. Blackmon, and M.J. Sadowsky (2004) The *Arthrobacter aurescens* TC1 atrazine catabolic genes *trzN*, *atzB* and *atzC* are linked on a 160 kb region and functional in *E. coli*. *Appl. Environ. Microbiol.* **70**:4402-4407.

Wackett, L.P. (2004) Novel biocatalysis by database mining. *Curr. Op. Biotech.* **15**: 280-284.

Hou, B.K., L.B.M. Ellis, and L.P. Wackett (2004) Encoding microbial metabolic logic: Predicting biodegradation. *J. Ind. Microbiol. Biotechnol.* **31**:261-272.

Wackett, L.P. (2004) Evolution of enzymes for the metabolism of new chemical inputs in the environment. *J. Biol.Chem.* **279**:41259-41262 (mini-review).

Strong, L.C. and L.P. Wackett (2004) Engineering of bioremediation processes: A critical review. In (M. Fingerman, Ed) *Bioremediation for Aquatic and Terrestrial Ecosystems* (in press).

Dodge, A.G. and L.P. Wackett (2004) Metabolism of bismuth subsalicylate and intracellular accumulation of bismuth by *Fusarium* sp. BI. *Appl. Environ. Microbiol.* (in press).

Public presentations in year 2

L.P. Wackett:

US-EU Workshop on Environmental Biotechnology, Madrid, February 7, 2003
“The Breadth of Biocatalysis and Biodegradation: Computational and Experimental Approaches”

DOE Microbial Genomes Meeting, Arlington, VA, February 10-12, 2003 (poster)
“Functional Analysis and Discovery of Microbial Genes Transforming Metallic and Organic Pollutants: Database and Experimental Tools”

University of Minnesota, Bioinformatics Symposium, March 28, 2003
“Encoding Metabolic Logic: Predicting Biodegradation”

Biotechnology Industry Organization, BIO, Washington, DC, June 24, 2003
“Natural Evolution of Catabolic Enzymes: New Tools for Biotechnology”

L.B.M. Ellis:

Chemical Biology Seminar Series, Department of Chemistry, University of Minnesota. Predicting Microbial Catabolism: A Functional Group Approach May 14, 2003.

LHASA Ltd 9th International Collaborative Group Meeting, Hopewell NJ. Predicting Microbial Catabolism: A Functional Group Approach June 20, 2003.

Undergraduate Bioinformatics Summer Institute, University of Minnesota. "Encoding Metabolic Logic: A Cheminformatics Case Study" July 1, 2003

Public presentations in year 3

Swiss Federal Institute of Technology seminar series,
Zurich, Switzerland, January 9, 2004
"Encoding Metabolic Logic: Predicting Biodegradation"

Univ. of Minnesota, Cargill Microbial & Plant Genomics Seminar Series, Feb. 11, 2004
"Microbial Genomics of Atrazine Biodegradation: A Global Perspective"

University of Minnesota Molecular Evolution Working Group, March 30, 2004
"Evolution and Genome Organization of Microbes Biodegrading New Chemical Inputs in the Environment"

University of Vermont, Department of Microbiology, April 23, 2004
"Evolution of Enzymes and Pathways for *s*-Triazine Herbicide Biodegradation"

University of Uppsalla, Sweden, June 1, 2004
"Microbes and Triazine Herbicides: Biodegradation, Evolution and Genomics"

Swiss Federal Institute of Technology Workshop on Predicting Biodegradation,
Zurich, Switzerland, January 9, 2004
"Determining Biodegradability"

Symposium for Christopher Walsh on his 60th birthday, MIT, April 3, 2004
"The Breadth of Biocatalysis"

American Society for Microbiology Annual Meeting, New Orleans, May, 2004
"Biodegradation and Biotransformation: Roots in Microbial Metabolic Diversity"

Federation of Analytical Chemistry and Spectroscopy Societies Annual Meetng, Portland
Special Symposium on Metallomics, October 7, 2004
"Microorganisms and the Chemical Elements"

University of Iowa Biocatalysis Conference, October 26-28, 2004

“Biocatalytic Release of Nitrogen from Nature’s Heterocycles”

Web publication

We updated all the element pages on the Biochemical Periodic Table beginning on November 15, 2002.

Additionally pages for the following elements were added:

Uranium (U), Cadmium (Cd) and Polonium (Po), May 28, 2003

Plutonium (Pu), July 23, 2003

Cerium (Ce) and Thorium (Th) August 20, 2003

Europium, praseodymium, protactinium, neodymium, promethium, neptunium, samarium, americium, terbium, dysprosium, erbium, ytterbium, September, 2003

Pathways added or updated:

Sept 2002 anaerobic tetrachloroethene updated

Oct 2002 quercetin added

Nov 2002 isoproturon

Feb 2003 iprodione and trichloroethylene updated

Mar 2003 2-chloro-N-isopropylacetanilide and limonene updated

April 2003 hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and nitroglycerin updated

May 2003 anaerobic trichloroethane, nicotine, and alpha-pinene updated

June 2003 pyrrole-2-carboxylate added

July 2003 pyrene added

August 2003 1,1,1-trichloroethane (an/aerobic) added;
phthalate family, beta-1,2,3,4,5,6-hexachlorocyclohexane (an/aerobic), benzoate, and
the phenanthrene (fungal 9S,10S) and (fungal 9R,10R) updated

Pathway Prediction System Expanded:

Pathway Prediction System was first announced on September 18, 2002, with 40 rules. It now has over 230 rules.

Other Additions to UM-BBD database:

April 2003 - Sixth Annual User Survey sent to 608 members of the UM-BBD e-mail list.

June 2003 - The List of All Microorganisms has a new URL and can now accept Boolean operators (AND, OR, NOT) in the microorganism name search.