

Leszczynski receives PAESMEM Award

Jackson State University's (JSU) Dr. Jerzy Leszczynski is a recipient of this year's prestigious award given by the president of the USA, Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring (PAESMEM Program).



Leszczynski is a professor and the founder/director of the CREST Interdisciplinary Center for Nanotoxicity at JSU. Receiving the Presidential Award for Excellence in Science, Mathematics, Engineering Mentoring (PAESMEM) is the highest federal recognition award for mentoring in the country.

The award is made to recognize individuals or organizations that have made significant contributions to the mentoring of students at various educational levels from underrepresented groups in science, technology, engineering and mathematics.

Awards are intended as a symbol of recognition at the highest level and to highlight the achievements of individuals and organizations that serve the

important function of developing our future scientists, engineers, and mathematicians. Awardees receive \$10,000 and are invited to Washington, D.C. for a visit to the White House, photos with the President, presentation of a citation signed by the President and a working session on mentoring at the National Science Foundation.

This award doesn't come as a surprise as Leszczynski uses EPSCoR funding to support his efforts in mentoring graduate students entering the Ph.D. program in chemistry through lectures, workshops, seminar series, editing a book series and international scientific journals in the area of computational chemistry. He also provides summer research programs which includes mentoring of undergraduate and graduate students and postdoctoral fellows.



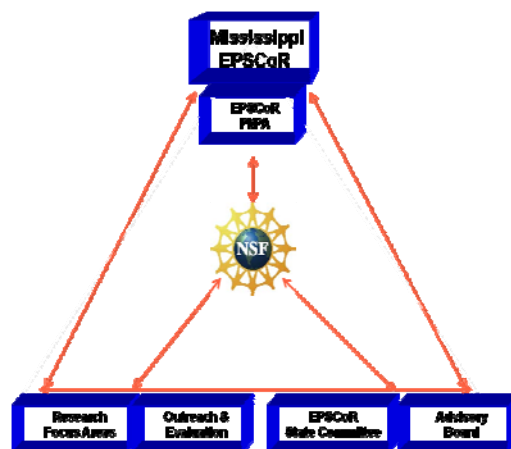
EPSCoR HIGHLIGHT

Doerksen's Summer Research



Dr. Robert J. Doerksen, professor of Chemistry at the University of Mississippi hosted a summer, 2009 research group that included (front, l-r) Charles Rich, Rust College instructor; Dion Keven, UM undergraduate; Dr. Ronak Patel, postdoctoral fellow; Dr. Haining Liu, postdoctoral fellow; Justin Deloach, Rust College undergraduate; Kitae Myoung, UM undergraduate; Gang Fu, PhD student. Back row (l-r) Pankaj Daga, PhD student; Khaled Elokely, PhD student and Dr. Doerksen.

Dr. Doerksen's group was supported by the Mississippi NSF EPSCoR project in the computational chemistry area. Rich, Deloach, and Kevin were all supported by the Education and Outreach funding from the Mississippi EPSCoR project.



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MISSISSIPPI EPSCoR



NEWSLETTER

NSF awards \$20M EPSCoR

The National Science Foundation has rewarded EPSCoR's continuing efforts at growing Mississippi research by granting a seventh round of research funding to the four research institutions in our state—Jackson State University, Mississippi State University, University of Mississippi/University of Mississippi Medical Center, and the University of Southern Mississippi.

Titled "Modeling and Simulation of Complex Systems," the research addresses three critical focus areas—biological systems simulation, computational biology and computational chemistry—and then integrates technologies from these three multidisciplinary areas to address emerging scientific and workforce development challenges.

The integrated research in modeling and simulation of complex systems will make seminal contributions in the areas of multi-scale simulation of biological systems (BioSim), modeling of biological networks (CompBio), and modeling and simulation of nanoscale chemistry (CompChem).

"Building on the strengths of our four research institutions, we'll be able to develop foundational infrastructure and human capital across a broad spectrum of application areas which in turn will yield next-generation science and technology advances in computational simulation and modeling of biological and biologically-relevant systems," said EPSCoR project director Sandra Harpole.

Yu to present in Puerto Rico

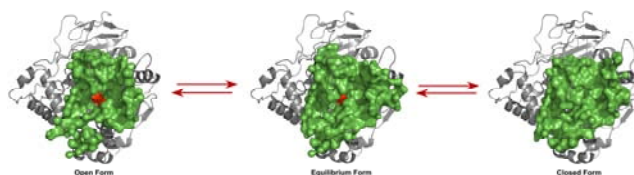
Carboxylesterases (CEs) are ubiquitous enzymes responsible for the detoxification of xenobiotics. They are found in organisms ranging from bacteria to man. In humans, therapeutically useful drugs are metabolized by these proteins, which impacts upon the efficiency of some drug treatments. For example, CEs convert inactive prodrugs to active metabolites, a process that is essential for the biological activity of drugs such as the anticancer agents CPT-11 and capecitabine, the antibiotics Cefitin and Vantin, as well as the illicit street drug heroin. Both CE substrates and inhibitors of CEs show selectivity among enzymes from different species, despite the overall structural homology of the enzymes. Examples are 2 human enzymes (hiCE and hCE1) that have different substrates and are inhibited selectively by different inhibitors.

The specificity of CEs for a particular substrate or inhibitor depends on the enzyme's molecular structure, and importantly, on the dynamics of conformational substructures present within an enzyme when a substrate is bound (i.e., "conformational sampling"). Structural dynamics of CEs, therefore, have critical roles in drug detoxification and can be studied by a combination of experimental and theoretical techniques. Once a fundamental understanding of the relationship between enzyme dynamics and substrate selectivity is established, modulation of CE activity by

mutation of known enzymes may allow for improvements in, and potentiation of, substrate conversion. Such mutants might, for example, be used as a therapeutic agent for treatment of heroin overdoses or for exposure to nerve agents such as sarin.

Researchers in the Wadkins Lab at the University of Mississippi are studying the catalytic properties of these enzymes via molecular dynamics (MD). Enzymes are in constant motion at temperatures near 37°C and the understanding of the fluctuation is crucial for understanding of the interactions of the enzyme with its substrate or inhibitors. In the a/b hydrolase family, the active site residues are at the bottom of a ~22 Å gorge, the walls of which are also fluctuating. Xiaozhen Yu, a graduate student in Dr. Randy Wadkins's lab has found that the loops covering the active site of the enzyme fluctuate to allow substrate to enter and exit the active site.

(Figure 1 below). Yu is now using a combination of computational chemistry and conventional molecular biology to study the features of this motion that are responsible for enzyme substrate selectivity. He will be presenting his data at the upcoming Southeastern Regional Meeting of the American Chemical Society, Oct. 21-24, in Puerto Rico.



JSU's Ashley White presents poster at NSF-AAAS Conference

Historically black colleges and universities play a significant—but often unrecognized—role in the science, technology, engineering, and mathematics education of minority students in the United States. They produce scientists and engineers ready to apply their education to the important problems of the day.

These messages were strongly delivered by students and educators at the National Science Foundation's (NSF) 2008 Historically Black Colleges and Universities Undergraduate Program Research Conference, organized by the AAAS. According to Shirley Malcom, director of Education and Human Resources at AAAS: "We must invest in development of talent and potential for science and engineering. HBCUs provide access to many students and introduce them to the possibilities of education and careers in STEM." HBCUs, she said, "contribute disproportionately as the baccalaureate origins institutions in many fields that are crucial to U.S. competitiveness and national security." Much of the research described by HBCU undergraduates at the event directly addresses pressing national needs. For example, a poster headlined "Preparation of Biodiesel from Waste Oil" was presented by Ashley White, a junior chemistry major at JSU. When



White was asked why the work is important, she responded, "Because we need cheaper gas! And we need to stop depending on foreign oil. We can do this ourselves." She went on to describe the chemistry involved in converting discarded vegetable oil used for cooking into diesel fuel. "The quality of the fuel is acceptable," she added, "but the process needs to be improved for greater yield."

(Story can be found at NSF website: http://www.nsf.gov/news/news_summ.jsp?org=EHR&cntn_id=12651&preview=false)

Summer Bioinformatics workshop is successful

Bioinformatics is not a topic that is typically covered as part of the high school curriculum, but that is quickly changing in Mississippi high schools. The *Bioinformatics Workshop for High School Teachers and College Instructors*, a workshop designed to help high school teachers and community college instructors to integrate transdisciplinary science and cyberinfrastructure concepts into their high school and college classroom curricula, was hosted at Mississippi State University, June 15-19, 2009.

Twenty-nine teachers from throughout the state attended the week-long workshop while learning novel techniques in the field of Computational Biology and Bioinformatics. Workshop participants included science, mathematics, and technology teachers from grades 8-12 and college instructors from 2-year institutions. Funded by the National Science Foundation, participants experienced inquiry-based and laboratory instruction and received research-based curriculum materials. Contributors to the workshop included research and education faculty from member institutions of the Mississippi Research Consortium (Jackson State University, Mississippi State University, University of Mississippi/University of Mississippi Medical Center, University of Southern Mississippi) and BioRad Laboratories (CA).

Participants gained biotechnology and bioinformatics skills and developed curriculum around various disciplines of biology, such as microbiology, genetics, cell biology, forensics, evolution and biotechnology. The program emphasized scenario-based curriculum with emphasis on computer-based activities that utilize public databases of scientific information to address real-world biological applications and principles.

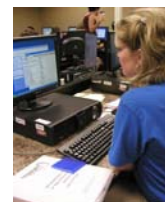
Sessions included topics such as

DNA/ Protein; Intro to Lab, Protocol, Safety; Genes in a Bottle; Phylogenetics Analysis; Bioinformatic Language: Sequence Analysis Software, Sequence Formats and Conversation Programs; Bioinformatics and the Human Genome Project Module; PGlo Transformation/PV92; Mathematical Modeling of Human Physiology; Analysis of Gene Expression; PGlo Extension; Column Chromatography and Protein Gel, and Mining Biological Information for Function, Network Building.

Bioinformatics is defined as research, development, and/or application of computational tools and approaches for expanding the use of biological, medical, behavioral or health data, including those to acquire, store, organize, archive, analyze, and/or visualize such data. Hands-on experiences in computational sciences and biotechnologies increased participants' awareness of and excitement in the field and better prepared them to implement activities in the classroom and share the excitement of hands-on science with their students.

Teachers face the challenge of taking this new idea and translating it into something interesting for a sophomore, a junior, or a senior. Therefore teachers must find a way to integrate the bioinformatics smoothly into biology and programming courses commonly taught at the secondary level. Bioinformatics is the application of mathematical, computing and statistical techniques to the understanding of the information of molecular biology. It was used by scientists in decoding the human genome and is an important tool in the treatment of genetic diseases.

High-tech jobs require a highly educated workforce familiarized at an early age with advancements in math and science. So to guarantee the continued growth of bioinformatics in the



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Digital Human project gains domain name

The University of Mississippi Medical Center will be hosting the EPSCoR work with Mississippi State University and Jackson State University on a new web site that will be implemented in early 2010. UMMC has purchased the domain name DigitalHuman.org and this will be the site for dissemination of the simulation work done by researchers at UMMC, JSU and MSU. This site will support the development of the DigitalHuman and all projects associated with the DigitalHuman, including the DigitalLung and DigitalAstronaut. DigitalAstronaut will be supported through work with NASA.

Bioinformatics

(continued from page 2)

region, educators must introduce students to biological and computational sciences in high school, as well as teach them some of the basic skills used in bioinformatics. High school bioinformatics curriculum increases the chances that local students will enter the field and remain in our state. The workshop was coordinated by MSU undergraduate student, Hailey O'Neal, under the direction of Dr. Giselle Thibaudau, MS-EPSCoR Education and Outreach Coordinator, Director of MSU's Electron Microscope Center, and Associate Professor of Biological Sciences. Contributors to the workshop included Dr. Susan Bridges, Professor of Computer Science (MSU), Dr. Sherry Herron, Director, Center for Science & Mathematics (USM), Dr. Robert Hester, Professor of Physiology (UMMC), Dr. Andy Perkins, Assistant Professor, Computer Science and Engineering (MSU), Ms. Essy Levy, Curriculum and



Jackson State Univ. hosts Microbial Bioinformatics summer program

The Microbial Bioinformatics Summer Program organized by the Center for Bioinformatics & Computational Biology at Jackson State University was held from June 1 - 26, 2009. A total of 16 participants from middle school, high school, and college categories participated in the pilot enrichment program with an aim to: (i) Expose students to New Computational and Biological Sciences; (ii) Excite students to consider careers in Science, Technology, Mathematics and Engineering; and (iii) Encourage students to work in teams. Participants received lectures on bioinformatics and microbiology topics and were taught how to make oral presentations. Students also participated in group research projects on genome analysis of microbial food-borne and zoonotic pathogens. The program also allowed graduate students in the Center for Bioinformatics & Computational Biology to build mentoring and instruction skills. A guest speaker from the National Biodefense Analysis and Countermeasure Center, a federally funded research and development center, also gave a talk on Bioforensics to participants. The summer program in-

cluded a field trip to the Mississippi Veterinary Research and Diagnostic Laboratory (MVRDL) located in Pearl, MS. The MVRDL is part of the Department of Pathobiology & Population Medicine, College of Veterinary Medicine, Mississippi State University. The summer program serves a purpose of building the interest of students in careers in which bioinformatics knowledge and skill sets are crucial. The summer program was completed with a closing ceremony where students presented results of their projects. Three students trained in the program won awards for poster presentations at the Sixth Annual International Symposium on Recent Advances in Environmental Health Research held in Jackson MS from September 13 - 16, 2009. The program was supported by Mississippi's National Science Foundation EPSCoR project which helps to fund research infrastructure for bioinformatics and computational biology at Jackson State University. Additional information on the Center for Bioinformatics & Computational Biology is available at <http://compbio.jsu.edu>.



Three students from this group who attended the summer Microbial Bioinformatics Program at JSU won awards for poster presentations at a September conference held in Jackson. The sum-

mer program was held at the Center for Bioinformatics and Computational Biology at Jackson State University from June 1 - 26, 2009. This effort was led by Dr. Raphael Isokpehi, JSU.

Training Specialist (Bio-Rad Laboratories), Dr. Fiona McCarthy, Assistant Professor, College of Veterinary Medicine, Basic Science Department (MSU), and Dr. Bindu Nanduri, Assistant Research Professor, College of Veterinary

Medicine, Basic Science Department (MSU).

Ten teachers who attend the previous summer bioinformatics workshop returned to review lesson plans and develop new curriculum.