UNDERGRADUATE RESEARCH Highlights

Recent Peer-Reviewed Publications by CUR Members with Undergraduate Coauthors

Fox N, Jagodzinski F, Li Y, Streinu I. KINARI-Web: a server for protein rigidity analysis. *Nucleic Acids Res*. 2011;39. (Smith College and University of Massachusetts Amherst)

This paper presents KINARI-Web, an interactive web server for analyzing and visualizing rigidity properties of proteins. It also provides tools for preprocessing input data, such as selecting relevant chains from PDB files, adding hydrogen atoms and identifying stabilizing interactions. Rigidity analysis in KINARI-Web relies on a novel, customizable modeling of protein mechanics and an efficient rigidity analysis engine. The enhanced Jmol-based visualization tool allows the user to view calculated rigidity properties of a molecular structure at different levels of detail. Ileana Streinu is the Charles N. Clark professor of computer science and mathematics at Smith College, and a Five Colleges 40th Anniversary Professor and adjunct at University of Massachusetts Amherst. Yang Li was an undergraduate at Smith College when she undertook the work, first as a summer REU (2008), then as part of a Mellon Mays Undergraduate Fellowship research project (2009-2011). She graduated in May 2011 and will start her doctoral studies in computer science at Stanford University in September 2011. This work was supported by the National Science Foundation [DMS-0714934] and the Defense Advanced Research Projects Agency [HR0011-09-1-0003] grants of Ileana Streinu.

Mohrig JR, Reiter NJ, Kirk R, Zawadski MR, Lamarre-Vincent N. Effect of buffer general acid-base catalysis on the stereoselectivity of ester and thioester H/D exchange in D_2O. *J Am Chem Soc*. 2011;133:5124-5128. (Carleton College)

We have found that the stereoselectivity of the H/D exchange of simple esters and thioesters in D2O is strongly influenced by the presence of buffers. The results are put into the context of what is known about the mechanism of H/D exchange as well as the relevance of this buffer effect to the mechanism of enzymatic catalysis. It is likely that hydrogen bonding in the enolate-buffer acid encounter complex is an important stereochemical determinant. Jerry Mohrig is professor of chemistry, emeritus. The research of the four undergraduate co-authors was carried out during the summers of 1998-2003, following their sophomore and junior years and often continued as independent studies during the academic year. Nicholas Reiter and Nathan Lamarre-Vincent are post-doctoral fellows at Northwestern and Harvard, respectively. Randy Kirk and Michelle Zawadski are employed in private industry. The research was funded through NSF-RUI, Howard Hughes, and ACS-PRF grants.

Thompson M, McLaughlin TF, Derby KM. The use of differential reinforcement to decrease the inappropriate verbalizations of a nine-year-old girl with autism. *Elec J Ed Res. In Psych*. 2011;9:183-196. (Gonzaga University)

The present case study examined the use of differential reinforcement to reduce the number of inappropriate verbalizations for a single elementary student with autism. The overall outcomes indicated large decreases in inappropriate verbalizations when differential reinforcement was applied across three academic settings. The procedures were seen as highly positive and effective by classroom staff T. F. McLaughlin and K. Mark Derby are full professors in the Department of Special Education. K. Johnson is a middle school special education teacher in the Spokane Public Schools. K. Ruwe completed this data based project as part of her student teaching in special education. This project was used as documentation of mission of the Department of Special Education to develop preservice special education teachers who serve students with care, competence, and commitment. K Ruwe is currently a special education teacher in the State of Washington.

Lippert MJ, Kim N, Cho J-E, Larson RP, Schoenly NE, O'Shea SH, Jinks-Robertson S. Role for topoisomerase 1 in transcription-associated mutagenesis in yeast. *Proc Natl Acad Sci USA*. 2011;108:2:698-703. (Saint Michael's College and Duke University Medical Center)

Previously we showed that high levels of transcription through a yeast gene stimulated 2-nucleotide deletions, thereby identifying a unique signature for transcription-associated mutation (TAM) in yeast. The present study demonstrated that TAM deletions occur at hotspots and require topoisomerase 1 (Top1), the main enzyme responsible for dealing with transcription-related supercoiling. These data implicate Top1 in spontaneous mutagenesis at highly transcribed genes. Malcolm Lippert is an associate professor of biology at Saint Michael's College. Nayun Kim, Jang-Eun Cho, Shannon O'Shea, and Sue Jinks-Robertson are collaborators at Duke University. Ryan Larson and Nathan Schoenly, both biology majors, performed summer research projects at Saint Michael's College. Ryan and Nate received Undergraduate Summer Research Fellowships from the Vermont Genetics Network and the American Society for Microbiology, respectively. Ryan is currently a pre-doctoral student in the Department of Immunology at the University of Washington, Seattle. Nate attends the University of Buffalo School of Dental Medicine. Work in the Lippert and Jinks-Robertson laboratories was supported by NIH Grants R15 GM079778 and RO1 GM038464, respectively.

Gillen-Christandl K, Copsey B. Polarization-dependent atomic dipole traps behind a circular aperture for neutral-atom quantum computing. *Phys. Rev. A*. 2011;83:023408. (California Polytechnic State University, San Luis Obispo)

The future of data security and simulation of complex systems resides in quantum computing, which uses quantum mechanical particles, such as atoms, ions, or photons as the basis for computation, rather than the traditional transistor based bit. Our research focuses on quantum computing using laser-cooled neutral atoms. We explored the atom traps formed in the diffraction pattern behind a pinhole illuminated by a laser in order to solve the remaining scalability problem of neutral atom quantum computing. We found that the light polarization dependence of the traps can be used to create a large addressable array of atoms that can be brought together and apart controllably for the implementation of quantum gates. Katharina Gillen-Christandl is an assistant professor of physics. Bert Copsey participated in this research since his sophomore year initially as part of the Cal Poly Honors Program and continued the work on grant support. Bert is currently completing a Master's degree in Mechanical Engineering at Cal Poly, and plans to enter a doctoral program in physics in the near future. This work was supported by the National Science Foundation and the Office of Naval Research.

Manning C, Brooks W, Crotteau V, Diedrich A, Moser J, Zwiefelhofer A. Tech tools for teachers, by teachers: Bridging teachers and students. *Wisconsin English Journal*. 2011;53:1:24-28. (University of Wisconsin-Eau Claire)

It is easy to characterize the incorporation of 21st century literacy skills and technology into the classroom as a clash between the old and new. A more constructive approach, however, is to acknowledge the value of both old and new ways used together in order to meet students where they are, helping bring them forward in the technologies they are already using. As we contemplate what it means for students to be literate in the 21st century, we must pay particular attention to how literacy has evolved and continues to evolve. In using innovative tools to approach learning, students and teachers can work together to re-envision how school will function for the century to come. Dr. Carmen Manning is an associate professor of English. William Brooks, Vanessa Crotteau, Annelise Diedrich, Jessie Moser, and Amanda Zwiefelhofer are all pre-service students in Education.

Close DM, Hahn RE, Patterson SS, Baek SJ, Ripp SA, Sayler GS. Comparison of human optimized bacterial luciferase, firefly luciferase, and green fluorescent protein for continuous imaging of cell culture and animal models. *J. Biomed*. Opt. 2011;16:4. (University of Tennessee, Knoxville)

In this study, the recently described human-optimized bacterial bioluminescence cassette (holux) was compared and contrasted with the popular firefly luciferase (Luc) bioluminescent and green fluorescent protein (GFP) fluorescent reporter systems in both cell culture and small animal imaging conditions. Experimentally relevant acquisition times, injection volumes, and minimum detectable cellular population sizes were determined, as well as differences in the dynamics of light production kinetics for each system. It was determined that at and above average cell populations sizes, the holux system compared favorably with both the Luc and GFP imaging systems under cell culture and near surface (subcutaneous) small animal imaging conditions. Dr. Dan Close is a postdoctoral research associate with the Joint Institute for Biological Sciences, Dr. Stacey Patterson and Dr. Steven Ripp are both senior level researchers in the laboratory of Dr. Gary Sayler. Dr. Seung Baek is an associate professor in the department of pathobiology in the college of veterinary medicine. Ruth Hahn, a sophomore undergraduate, participated in this research during a summer internship in the laboratory. Ruth is currently attending Trinity University in Texas and majoring in Engineering Sciences. This work was supported by the National Institutes of Health, National Cancer Institute, the National Science Foundation, and the Army Defense University Research Instrumentation Program.

Schneider KD, Ortega CJ, Renck NA, Bonomo RA, Powers RA, Leonard DA. Structures of the class D carbapenemase OXA-24 from Acinetobacter baumannii in complex with doripenem. *J Mol Biol*. 2011;406:4:583-94. (Grand Valley State University)

The emergence of class D beta-lactamases with carbapenemase activity presents an enormous challenge to health practitioners. To better understand the details of the how these enzymes bind and hydrolyze carbapenems, the X-ray crystal structures of two deacylation-deficient variants (K84D and V130D) of the class D carbapenemase OXA-24 with doripenem were determined. These findings represent a snapshot of a key step in the catalytic mechanism of an important class D enzyme, and might be useful for the design of novel inhibitors. David Leonard and Rachel Powers are associate professors of chemistry. Kyle Schneider is currently a doctoral student at Northwestern University. Caleb Ortega is a medical student at Michigan State University. Nicholas Renck is employed. This work was funded by the National Institutes of Health (to DAL) and an internal Student Summer Scholar grant (to KDS).

Rashad S, Bradley J. Smartmobimine: smart mobile data mining techniques to support 4G mobile networks. *Proceeding of the 8th IEEE Consumer Communications and Networking Conference (CCNC 2011)*. 2011;1:703-704. (Morehead State University)

The main objective of this research is to design, implement, and evaluate a new generation of smart mobile data mining techniques called SmartMobiMine that will be used in the integrated structure of the 4G mobile networks to support and develop the essential services in mobile networks. The proposed techniques

will integrate different types of information to support mobile users. Initial results show that SmartMobiMine techniques are promising. Dr. Sherif Rashad is an assistant professor of computer science. Joshua Bradley is a senior Computer Science major. He participated in this research as an undergraduate research fellow at Morehead State University. He was selected to receive the 2010 Barry M. Goldwater Scholarship. He was also selected to participate in the Internship Program held at the National Security Agency (NSA) in 2010 and 2011. Mr. Bradley is currently enrolled in the Computer Science program at Morehead State University. This research is supported by an Undergraduate Research Fellowship from Morehead State University, which was awarded to Mr. Joshua Bradley.

Allen JH, Schoch ET, Stubbs JM. Effect of surface binding on heterogeneous DNA melting equilibria: A Monte Carlo simulation study. *J Phys Chem B*. 2011;115:1720-1726. (The University of New England)

This study examined the changes in double-stranded deoxyribonucleic acid (DNA) stability when one strand is immobilized on a surface. The results indicate that the end of the duplex nearest to the surface binding site is destabilized, while the end furthest from the binding site has enhanced stability. The enhanced stability is due to reduced end fraying in conformations where the duplex is lying flat on the surface, and has implications for the design of DNA microarrays. John Stubbs is an assistant professor of chemistry. Emily Schoch worked during the summer and academic year as both a junior and senior, and John Allen worked during the summer and academic year as a senior. The work was partially supported by a UNE college of arts and sciences student summer research stipend.

Wei-Haas ML, Glumac B, Curran HA. *Sphenothallus-like* fossils from the Martinsburg Formation (Upper Ordovician), Tennessee, USA. *J Paleontol*. 2011;85:2:353–359. (Smith College)

This study documented the occurrence and characteristics of rare and enigmatic Late Ordovician carbonaceous tubular fossils utilizing petrographic, palynologic, and geochemical analyses. The fossils are morphologically similar to many of the previously identified forms of *Sphenothallus*, a tube-dwelling marine invertebrate with uncertain phylogenetic affinity. The results provide new information about these organisms and their early Paleozoic ecosystems. Bosiljka Glumac is an associate professor of geosciences and H. Allen Curran is a professor emeritus of geosciences. Maya Wei-Haas conducted this research as an independent study project during her sophomore year. As a sophomore at Smith College Maya was awarded a Barry M. Goldwater Scholarship, as a junior and senior she was a Mellon-Mays Fellow, and she completed an honors thesis project related to her REU Summer field research in Svalbard. Maya is currently a graduate student at the Ohio State University. She was awarded a NSF Graduate Research Fellowship for her research in the influence of dissolved organic matter on the photodegradation of brominated flame-retardants. This year she also spent a field season in Antarctica on an NSF funded project focused on microbial carbon transformations and structural characterization of organic matter in supraglacial environments. This research was funded by small research grants administered through Smith College.

DeLuna MM, Behan KJ. ABO discrepancy and hemolytic anemia post liver transplant due to Passenger Lymphocyte Syndrome. *LabMedicine*. 2011;42:1:137-139. (University of West Florida)

This paper presents an unusual case of a patient who received a liver transplant to cure a chronic liver disease, and experienced a severe graft versus host condition leading to life threatening anemia. The case is intended for professionals in transplant and transfusion medicine, as it discusses subtleties in organ compatibility between a donor and a recipient. Kristina Behan is an Associate Professor and Director of the Clinical Laboratory Sciences Program. Mark De Luna is a Clinical Laboratory Sciences (Department of Biology) graduate who presented the case as his senior capstone case study in 2010. Not applicable.

Craney C, McKay T, Mazzeo A, Morris J, Prigodich C, deGroot R. Cross-discipline perceptions of the undergraduate research experience. *Journal of Higher Education*. 2011;82:92-113. (Occidental College)

This 6-year-long pre-post assessment of 465 summer undergraduate researchers, ~50% female, ~40% students of color, included first-year and graduated seniors. Researchers (~40% arts, humanities, and social science) ranked many broad benefits and specific outcomes in common. However, science students perceived a greater impact of research participation on their subsequent academic and career paths than social science and humanities students. The mentor-protégé relationship is crucial for all researchers (especially underrepresented) and shows pronounced disciplinary trends. Nearly all researchers graduate in five years; are ~3x more likely to receive a competitive national award; and showed common learning goals that also reflect their discipline's traditions. Chris Craney is a professor of chemistry, April Mazzeo is an administrator, Janet Morris is a research analyst, Robert de Groot is a research analyst. Tara McKay began her research as an undergraduate and is enrolled in the doctoral program at UCLA. Cheryl Prigodich began her work as an undergraduate, subsequently earned her MPH from Dartmouth, and works at the CDC in Atlanta. All were supported by grants from NSF (98738121 and 9988059) and HHMI (52002651 and 52005135).

Dunkin CM, Pokorny A, Almeida PF, Lee HS. Molecular dynamics studies of transportan 10 (Tp10) interacting with a POPC lipid bilayer. *J. Phys. Chem. B* 2011;115:1188-1198. (University of North Carolina at Wilmington)

Transportan 10 (Tp10) is an example of cell-penetrating peptides (CPP), which has an ability to transport cargo across cell membrane. The precise mechanisms of activity of CPP are, however, largely unknown. We performed molecular dynamics simulations in an attempt to better understand the nature of interaction between Tp10 and a zwitterionc membrane. In particular, we assess the plausibility of so-called sinking raft model. The simulations revealed that the Lys-phosphate salt bridge is a key factor in determining the orientation of the peptide in the interfacial region as well as in stabilizing the peptide-membrane interaction. The electrostatic attraction between Lys and phosphate groups is also believed to be the main bottleneck for the translocation of tp10 across the membrane. Hee-Seung Lee and Antje Pokorny are assistant professors and Paulo F. Almeida is an associate professor of department of chemistry and biochemistry Christina Dunkin carried out these calculations as her honors project for an academic year (2009-2010) and a summer at UNC-Wilmington. She is currently in dental school at Virginia Commonwealth University. The research was supported through Cahill Award from UNCW to HSL.

Ruwe K, McLaughlin TF, Derby KM, Johnson K. The multiple effects of direct instruction flashcards on sight word acquisition, passage reading, and errors for three middle school students with intellectual disabilities *J Dev and Phys Dis*. 2011;21:241-255. (Gonzaga University)

Three middle school students with intellectual disabilities were taught sight words using DI flashcards. Changes in student performance were shown to be a function of the intervention. In addition, the passage reading data indicated a decreased likelihood that participants would inaccurately read their individual sight words in passage context. T. F. McLaughlin and K. Mark Derby are full professors in the Department of Special Education. K. Johnson is a middle school special education teacher in the Spokane Public Schools. K. Ruwe completed this data based project as part of her student teaching in special education. This project was used as documentation of mission of the Department of Special Education to develop preservice special education teachers who serve students with care, competence, and commitment. K Ruwe is currently a special education teacher.

Clark AJ, Calvillo JL, Roosa MS, Green DB, Ganske JA. Degradation product emission from historic and modern books by headspace SPME/GC-MS: evaluation of lipid oxidation and cellulose hydrolysis. *Anal Bioanal Chem*. 2011;399:10:3589-3600. (Pepperdine University)

This study is the first utilizing headspace solid phase microextraction/gas chromatography-mass spectrometry to non-intrusively probe the emissions of aging books over a 400 year publication range. Volatile organic compounds were used to distinguish aging mechanisms of paper and the importance of acid hydrolysis of cellulose in paper versus oxidative pathways was examined. The results suggest that oxidative mechanisms are more important in older historic books, while acid hydrolysis dominates the aging of modern papers. Jane Ganske and David Green are professors of chemistry and Mark Roosa is dean of libraries at Pepperdine University. Two undergraduate students participated in the research over summers of 2008, 2009 and 2010. Andrew Clark is currently in a MD/PhD program at University of Southern California and Jesse Calvillo is employed as an analytical chemist. The authors acknowledge financial support from the Dean's Research Fund of Pepperdine University and the Tooma Undergraduate Research Fellowship.