

Chemistry & Chemical Biology News

PDB Supports Scientific Advances Worldwide

Helen M. Berman, Rutgers Board of Governors Professor of Chemistry and Chemical Biology, has received many honors over the years for her achievements in building what she calls a "scientific collaboratory," the Research Collaboratory for Structural Bioinformatics (RCSB) Protein Data Bank (PDB).

The PDB has been headquartered at Rutgers since 1998, but Berman's training as a scientist and community organizer really started in Brooklyn, N.Y. long before anyone envisioned the worldwide success of the data bank.

"My father, Dr. David Bernstein, was a professor at NYU Medical School and a surgeon who practiced medicine in Brooklyn for over 40 years and my mother, Dorothy, was his office manager and a community organizer on various health initiatives," said Berman. "She was given the Mayor's Volunteer Action Award for her work in health education and preventive medicine. So I like to think I have a little bit of both of them in me."

The American Society for Biochemistry and Molecular Biology recently presented Berman with the DeLano

Award for Computational Biosciences, which acknowledges technological innovation that enhances research in the life sciences at the molecular level and is readily available to the scientific community.

Berman, now a Princeton resident, was raised in Brooklyn and studied Chemistry at Barnard College before earning a Ph.D. at the University of Pittsburgh. Berman worked at Fox Chase Cancer Center for 20 years, researching nucleic acid crystallography and drug nucleic acid interactions. She moved to Rutgers in 1989, expanded her program to include the study of the structures of collagen and protein-nucleic acid complexes, and at the same time developed structural databases and ontologies.

"Structures of proteins began to emerge in the late 1950s and 1960s and there were groups of people who were very interested in seeing if it was possible to understand how proteins form into their final conformation," Berman recalls. "I began to talk to a lot of people in my community about archiving those structures so we could have easy access to them. I was absolutely convinced that archiving and open sharing of these structures



Rutgers Board of Governors Professor of Chemistry and Chemical Biology
Helen M. Berman

would enable scientists to understand the relationships between sequence, structure and function and their importance in health and disease."

In the 1970s Berman began working with colleagues to establish the PDB archive at Brookhaven National Laboratory as a place to store and share data about the 3D structures of proteins and nucleic acids. In 1998, when the RCSB won funding for PDB and moved it to Rutgers, the data bank had 9,000 archived structures. Today, PDB uses the most advanced

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New Home on the Horizon, CCB Continues to Grow

Welcome to the Summer 2013 edition of Chemistry & Chemical Biology (CCB) News!

It has been a particularly exciting year for the department with plans moving forward at a rapid pace for a new home for CCB. Later this year, we will announce all the details on the new building so watch for future announcements on this exciting development.

It would appear the new facilities are coming not a moment too soon, as the number of students enrolled in chemistry courses at Rutgers contin-

ues to grow. In the last five years, the number of students in Rutgers chemistry courses has risen from 4,800 to 6,900 per semester. With that kind of demand for CCB education, we continue to seek out new ways to help our students advance, including development of a novel e-learning system that will make its debut this Fall. Led by Professor Darrin York, this innovative project promises to be a significant resource for faculty and students alike and is featured on page 8.

With the increasing demand for chemistry at Rutgers, I am thankful that we continue to attract and retain some of the finest faculty anywhere. It is noteworthy that Professors KiBum Lee and Joseph Marcotrigiano were recently promoted to Associate Professors with tenure, and Lawrence Williams was promoted to Professor I. These are three rising stars in our department with significant research, teaching, and leadership portfolios. I look forward to their future with CCB. I am sure you will join me in wishing them continued excellence at Rutgers.

Our faculty continues to achieve great success in secur-

ing funding for new and ongoing research on some of the most important issues affecting our society. Richard Ebright, Board of Governors Professor of Chemistry and Laboratory Director at the Waksman Institute of Microbiology, has been selected to receive a National Institutes of Health MERIT Award totaling \$1.5 million to \$3 million for a project titled Bacterial Transcription Complexes. The project is being supported by the National Institute for General Medical Sciences. The MERIT Award will fund years 25 through 29, and provided satisfactory progress, years 30 to 34 of this multi-year project.

Other funding news comes from Professor Alan Goldman, who recently received a \$201,700 one-year grant from Chevron for the development of catalysts for the conversion of methane (natural gas) to liquids; Assistant Professor Deirdre O'Carroll, who received a \$230,764 two-year grant from NSF for the theoretical and experimental design of multifunctional plasmonic electrodes for polymer-based optoelectronics; and Associate Professor Daniel Seidel, who was awarded an NSF grant for \$420,000 over three years to help advance the field of asymmetric catalysis through exploration of conceptually new and underdeveloped methods of substrate activation.

Our students also continue to achieve great success. The recent Jean Wilson Day Undergraduate Research Symposium poster display of undergraduate research reinforced the tremendous contributions our students make every day. These contributions were further underscored during the year-end awards ceremony also highlighted in this issue.

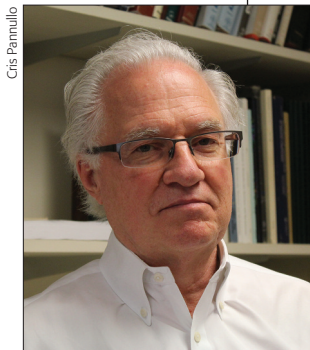
Board of Governors Professor of Chemistry and Chemical

Biology Helen M. Berman was recently honored by the American Society for Biochemistry and Molecular Biology for her many contributions to the field of computational biosciences as noted on page 1. And the research team headed by Chemistry Professor Kathryn Uhrich has developed an exciting controlled delivery system called PolyMorphine that has the potential to improve patient care and save healthcare costs at the same time. You will want to read about the exciting details of this research on page 7.

Finally, the integration of Rutgers with the University of Medicine and Dentistry of New Jersey will be formalized on July 1, a historic milestone marking the largest reorganization of New Jersey's university system in decades. For Rutgers, the integration results in the addition of two medical schools, a osteopathic medical school, dental school, nursing school, comprehensive cancer institute, graduate school of biomedical sciences, school of health related professions, and university behavioral health care. These added components, along with existing health related entities at Rutgers, will constitute a powerful academic health center, resulting in enhanced prestige, greater access to federal research funding, and coordination between CCB researchers and life science translational and clinical efforts.

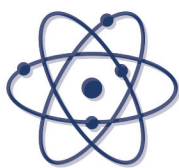
The future is indeed quite bright for Rutgers and CCB. We thank all of you for your support and look forward to the great opportunities for growth and partnership that lie on the horizon.

Sincerely,
Roger A. Jones
Professor and Chair



Cris Pannullo

"Our faculty continues to achieve great success in securing funding for new and ongoing research."



CCB IS GETTING A NEW HOME!

RUTGERS

School of Arts and Sciences



LOOKING EAST TOWARDS THE FRONT ENTRANCE

LEARN ALL ABOUT PLANS FOR THE NEW, STATE-OF-THE-ART FACILITIES IN THE *NEXT* ISSUE OF CHEMISTRY AND CHEMICAL BIOLOGY NEWS!

As we approach the official groundbreaking, learn more about how you can become a key supporter of this exciting initiative.

Contact **Emily Miller** at emiller@sas.rutgers.edu or 848-932-6455 for more information.

**OUR
RUTGERS
OUR
FUTURE**

A CAMPAIGN FOR EXCELLENCE

IGERT Promotes Education Exchange with Africa

A joint Rutgers-Princeton Nanotechnology for Clean Energy graduate training program is providing students with the opportunity to develop relationships with noted institutions and researchers in Africa. Funded by the National Science Foundation, this Integrative Graduate Education Research Traineeship (IGERT) program is a five-year, \$3 million venture focusing on nanoscale energy technology development with a special emphasis on educational exchange between U.S. and African universities. Recently, some students have taken advantage of this program by visiting and collaborating with their African counterparts as they pursue their research.

This December, Chemistry and Chemical Biology student Aleksandra Biedron spent time in the Ethiopian capital of Addis Ababa. Biedron was selected to participate in the first Materials Research School of the Joint U.S.-Africa Materials Institute (JUAMI) held at Addis Ababa University. The program brought together

approximately 50 graduate students and early-career materials researchers from across the United States and East Africa, as well as 15 internationally recognized instructors, for two weeks of lectures, problem solving, and cultural exchange.

"I was interested in meeting young African scientists to discuss energy materials, a universal concern which is relevant to my research in ionic liquids. I was also excited to see Addis Ababa, Ethiopia, and experience the culture and historical attractions," said Biedron.

A cornerstone of the Nanotechnology for Clean Energy IGERT program is having the students apply their training in a dynamic educational exchange program with African institutions, promoting development of the students' global awareness and understanding of the challenges involved in global scientific and economic development. In Addis Ababa, Biedron quickly noticed how different the scope of

research was between the African scientists and their international counterparts.

"The African scientists' research was really solution-based," said Biedron. "They were looking at how they could use their natural resources to solve some of their region's most pressing issues, not only for energy, but also health, clean water, and housing. You don't really see that as much in the U.S. because we are already thinking about the future,

10 or 20 years from now."

This is the fourth consecutive academic year that IGERT trainees have been given the opportunity to travel to Africa. In December 2011, Biedron and six other IGERT trainees traveled to Victoria Falls, Zimbabwe to attend the 6th International Conference of the Africa Materials Research Society along with Chemistry Professors Jing Li and Eric Garfunkel. Garfunkel served as Chair of the International Advisory Committee for the conference and is currently leading Rutgers' materials-related exchange efforts with Africa. At the conference, the IGERT trainees presented their research to a diverse group of over 300 scientists from around the world.

In the future, Rutgers students will have even more opportunities to collaborate with African scientists. Having seen the positive effects of the IGERT program's African component, Garfunkel and colleagues founded the Rutgers Institute for Science and Technology Leadership in Africa (RISTLA) earlier this year. Established to foster science and technology research collaboration and scholarly exchange between Rutgers and African institutions, Garfunkel envisions RISTLA as a boon for both Rutgers students and their African counterparts. "The overall goal of evolving RISTLA programs is twofold: We are looking to focus on capacity building in Africa through education of their workforce, while also teaching U.S. students how to address global problems outside the United States," Garfunkel said.

Exposure to African cultures and scientific institutions is already helping to give Rutgers students a broader worldview: "Collaboration is always a good thing. You have more perspectives, resources, and solutions to the same problem,"

IGERT trainees at Victoria Falls in Africa (clockwise from left) Gautam Jain, Mojgan Roushan, Kim Scott, Eric Gauthier, Bright Kusema, Aleksandra Biedron, Tiffany Tong, Ryan Thorpe and Jesse Kohl.



said Biedron, adding that after two trips to Africa, she is interested in future collaborations.

"Going to Africa was great," Biedron said. "I had a chance to see what it's like over there and

to interact with the people. Now I'd feel comfortable going for a long-term internship in Africa."

For additional information on the Nanotechnology for Clean Energy IGERT, please visit

www.energyigert.rutgers.edu/ or contact Program Coordinator Johanna Bernstein at (848) 445-1557 or jrbernst@rci.rutgers.edu.

Moss Earns NSF Support for a Record 51 Years

When he's not busy writing about baseball, stamp collecting or Sherlock Holmes, Rutgers Chemistry Research Professor Robert A. Moss searches for innovations in reactive organic intermediates—something the National Science Foundation (NSF) has funded for over half a century.

"By the time my NSF funding expires in 2016, I will have received the foundation's support for 51 years," said Moss, 72, who retired from teaching in 2006 so he could focus on his research. "I believe that's a record for Rutgers Chemistry. I have received support from many agencies and organizations over the years, but NSF has been with me the longest. They recently extended my funding without my requesting an extension so I guess they like what I am doing."

Moss grew up in Brooklyn and graduated from Brooklyn College in June of 1960 with a degree in Chemistry before earning his doctorate at the University of Chicago. After a postdoctoral fellowship at Columbia University, he came to Rutgers as an Assistant Chemistry Professor in 1964.

Moss taught for over 40 years before exclusively pursuing his first love—a class of unusual molecules known as reactive intermediates, which are fundamental to organic chemistry. These ephemeral

molecules, appearing ever so briefly during certain chemical reactions, may live for as little as one trillionth of a second.

"These intermediates are crucial to pathways through which scientists can create new and different materials, things we need and use like new drugs for human health or coatings to protect our buildings and bridges," Moss said. "To make such things, we need a full understanding of the reactions that produce them—and all the players involved."

He supervised a team of up to 12 students during the height of his career, including 61 Ph.D. candidates and 50 postdoctoral associates. Moss and his associates have authored more than 430 scientific publications, including eight co-edited books, the latest of which, *Contemporary Carbene Chemistry*, is expected to be published by Wiley later this year. Published contributions over the years have included reactive intermediates (carbenes, carbocations, carbanions), reactions in organic aggregates (micelles and liposomes), and the decontamination of toxic organic phosphorous compounds.

Moss has received many honors, including the Distinguished Alumnus Medal of Brooklyn College; Fellow of the American Association for the Advancement of Science; Arthur C. Cope Scholar Award from the American Chemical

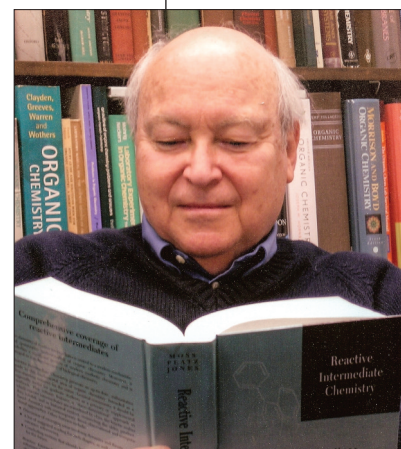
Society; and Fellow of the American Chemical Society.

When not writing about chemistry, Moss authors articles on baseball, stamp collecting and Sherlock Holmes for various media outlets, including *NINE*, *The American Philatelist* and *The Baker Street Journal*.

A stamp collector as well, Moss owns an extensive collection of stamps of the Faroe Islands, which lie halfway between Iceland and Scotland and west of Norway.

He has lived in Metuchen for the last 40 years with his wife, Sandra Wolman Moss, a retired physician who now writes and lectures on medical history. They have two sons, Kenneth, who is Associate Professor of History at Johns Hopkins University, and Daniel, who is Assistant Professor of English at Southern Methodist University. They also have two grandsons.

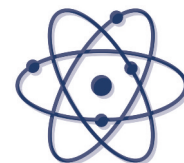
"I love research, but when the new NSF grant expires it probably will be time to do something else," said Moss. "I think I can find something to keep me busy."



Lionel Goodman

Chemistry Research Professor Robert A. Moss

When not writing about chemistry, Moss authors articles on baseball, stamp collecting and Sherlock Holmes.



Arnold's HIV Research Secures \$10.1 Million

The groundbreaking, 25 years of anti-HIV research of Eddy Arnold, Rutgers Board of Governors Professor of Chemistry and Chemical Biology and Center for Advanced Biotechnology and Medicine faculty, recently achieved another significant milestone, securing an expected \$10.1 million in new federal funding. Already a partner in enabling the discovery and development of two FDA-approved drugs, Arnold's team of researchers continues to pursue the growing medical problem presented by resistant strains of HIV.

"The virus is constantly mutating and the changes can diminish or completely prevent

the effectiveness of existing AIDS drugs," said Arnold. "In the 30 years since the virus appeared on the scene, we have gone from having no medication to having 26 drugs on the market. Our challenge remains to provide the most effective therapy and to get it to people in need in a cost-effective way."

Arnold spearheaded an effort with Rutgers Chemistry Professors Roger A. Jones, Ronald M. Levy and Joseph Marcotrigiano, that has gained a projected five-year \$6.3 million grant from the National Institute of General Medical Sciences, under the National Institutes of Health (NIH). "HIV Macromolecular Interactions and Impact on Viral Evolution of Drug Resistance" aims to fill in missing pieces of the HIV/AIDS structural puzzle, and to study the viral enzymes reverse transcriptase, integrase, and protease in different parts of the viral life cycle.

"The research will focus on aspects of HIV structure/function that relate to viral assembly and maturation, drug design, and drug resistance," said Arnold. The overall grant is directed by Professor Arthur Olson of The Scripps Research Institute in La Jolla, Calif., and also includes investigators at Harvard University, Ohio State University and the University of Pittsburgh.

Arnold has also been notified that his NIH Method to Extend Research in Time (MERIT) Award has been extended for a second five-year period (2014-2019), with total expected funding of \$3.8 million, for the project, "HIV-1 reverse transcriptase structure: function, inhibition, and resistance." The National Institute of Allergy and Infectious Diseases grant, which originated in 1988, supports Arnold's structure-function stud-

ies of HIV reverse transcriptase, a central component of the virus and the target of the most widely used anti-AIDS drugs.

The grant represents the second consecutive NIH MERIT award for Arnold, an honor bestowed on fewer than 5% of investigators. His team's basic research results are used worldwide to interpret new scientific and clinical research findings in AIDS research.

"We hope to better understand the evolution of drug resistance and to improve drug design methodologies in the treatment of HIV-infected individuals," said Arnold. "Enhanced understanding of HIV assembly, maturation, reverse transcription, and integration will help us create better therapies."

Arnold and his group began working with the late Dr. Paul Janssen over two decades ago to create drugs to fight AIDS. Janssen was a legendary drug developer and founder of Johnson & Johnson subsidiary, Janssen Pharmaceutica. Arnold's research was essential in bringing two anti-HIV drugs to market—Intelence (etravirine) in 2008 and Edurant (rilpivirine) in 2011.

Arnold's team developed innovative models that not only explain why Edurant and Intelence are particularly effective against drug-resistant viruses, but that can also be used in the development of treatments for a wide variety of other diseases. The gist of the model is that flexibility of a drug can allow it to adapt to changes in HIV or other disease-causing agents, thereby evading resistance.

Arnold's current research program focuses on developing fundamental knowledge about new therapeutics for diseases including AIDS and influenza. With colleagues in his group and at Rutgers, he has co-founded

John Emerson



Rutgers Board of Governors Professor of Chemistry and Chemical Biology Eddy Arnold

Prodaptics Pharmaceuticals, a company that has established a structure-based drug design platform for discovery of new therapeutics for treatment of

infectious diseases.

According to the Joint United Nations Programme on HIV/AIDS, more than 34 million people are living with HIV world-

wide. The Centers for Disease Control and Prevention estimates that 1.1 million U.S. residents are living with the disease.

Research Targets Pain Management, Health Costs

Patent-pending technology developed by Rutgers Chemistry Professor Kathryn Uhrich and her colleagues has the potential to greatly diminish morphine abuse while significantly improving pain management for patients coping with acute and chronic illness or injury. PolyMorphine (PM), an extended delivery system for morphine, an opioid drug commonly prescribed for pain management, could significantly reduce the billions of dollars in annual healthcare costs that result from improper medication dosing and abuse.

An internationally renowned polymer scientist, Uhrich and colleagues previously developed a polymerization technology that enables a drug to be its own biodegradable delivery vehicle, which was first utilized in PolyAspirin. PolyMorphine is part of this family of "extended-delivering drugs" that are utilized more efficiently and can be administered at higher concentrations to specific sites in the body utilizing biodegradable poly(anhydride-esters) that turn into therapeutically active molecules.

"Our research has shown that PolyMorphine (PM) extends the duration of the analgesic effect of morphine from less than four hours to three days, almost ten times longer the pain-relieving effect," said Uhrich, Rutgers Dean of Mathematical & Physical Sciences. "The use of PM has

the potential to improve patient comfort and quality of life by decreasing dosing frequency and controlling treatment compliance."

Uhrich's team conducted in vivo studies using mice to determine the analgesic effect from PolyMorphine, and demonstrated extended analgesia of PM due to its multi-day slow release, when compared to free morphine. In addition, preliminary results demonstrate no signs of morphine tolerance development in the animals.

The novel invention has the potential to increase specificity through localized drug release, eliminate requirements for frequent dosing, prevent accidental overdose, and reduce the occurrence of undesired side effects. The study was published in the *Journal of Controlled Release* this past September.

"The genius of Dr. Uhrich's invention lies in the simplicity of the design: take a well-known drug—morphine—and chemically tatter it together, sort of like a string of beads," said Profes-



Rutgers Chemistry Professor Kathryn Uhrich holds PolyMorphine in her CCB lab.

sor Lei Yu of the Department of Genetics and Center of Alcohol Studies at Rutgers, who collaborated on the study. "This 'morphine-on-a-string' now is a pro-drug. Once administered into the body, the hydrolysis processed by the body's water content gradually releases individual morphine 'beads' to achieve long-lasting pain relief. The concept is just brilliant."

Opioid analgesics such as morphine are among the strongest pain relievers and are

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Novel CCB e-Learning System Set for the Fall

CB is quickly moving forward with a novel e-learning system that could transform the way students learn chemistry at universities and grade schools nationwide, while helping educators fill the void for better trained personnel in the science industries.

"Any student that has taken a general chemistry class at a large university understands the challenge of learning the complex subject in a lecture hall with 350 to 400 students," said Chemistry Professor and General Chemistry Coordinator Darrin York, who directs the technical software design and implementation of the General Chemistry eLearning System (GCeLS). "Even for the strongest students, general chemistry is a struggle because they need to develop problem solving skills that reach far beyond what they have learned in high school. We believe GCeLS is vital to managing this challenge and preparing students for coursework and careers in the sciences."

GCeLS will provide a cyber-infrastructure with an interactive website and relational chemical databases that are integrated with a hierarchical network of critical skills required to solve chemistry problems. Students will do homework problems on the GCeLS website, <http://elearning.rutgers.edu/>, which will go live in the Fall. GCeLS is an intuitive technology that never creates the same problem twice and is geared toward the unique skills of each student. The system will store each student's progress and allow faculty to



Chemistry Professor Darrin York (far right) demonstrates the General Chemistry eLearning System with (from left) Ph.D. candidates Thakshila Dissanayake and Maria Panteva.

determine where students have problems. Online tools will also be available to allow students to self-diagnose their learning challenges, leading to better utilization of lecture and recitation time as well as faculty office hours.

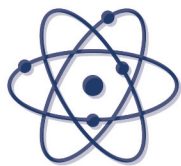
"We have tried every e-learning technology on the marketplace today and none of them did what we wanted, so we decided to create our own artificial intelligence system," said York, a computation scientist who came to Rutgers from the University of Minnesota in 2010. "GCeLS is not meant to replace classroom interaction, but to enhance it. Our goal is to have lectures focus on the key chemistry concepts and their inter-relationships, and illustrate real life examples where they are important. After class, students digest the material by using our e-learning tool to work through numerical exercises that place the concepts into a practical context. What we want to

avoid is number crunching through problems in lecture to the point students don't see the chemistry—that's how you lose the interest of a lecture hall with 400 students."

John Brennan, Rutgers Chemistry Professor and Vice Chair of the Undergraduate Program, notes that there is an ever-increasing demand for undergraduate students majoring in science, technology, engineering and mathematics—the STEM fields. The demand is driven by the needs of high tech industries, academia, medical professions, and basic and applied science research labs.

"General chemistry is really the cultural gateway to the sciences, but there is a very high failure rate for students because the subject material is challenging and students frequently jump into the class too early in their collegiate careers," said Brennan. "Faculty members are faced with the challenge of dumbing down the class or finding innovative

"We believe our model for e-learning cyber infrastructure can be extended to other STEM courses."



ways to educate students. Nowhere is this need more evident than in chemistry, which is considered the central science that connects the physical and life basic sciences. Chemistry forms a bridge with applied sciences such as material science, engineering and medicine. As a result, universities nationwide have had to face great challenges to provide quality entry-level training for students in gateway STEM classes."

York said the Rutgers team, which includes lead content developer Francesca Guerra and lead technical developer Karlun (James) Chun, hopes to create a powerful GCELS tool that can be utilized by higher education institutions and grade schools nationwide. "We believe our model for e-learning cyber infrastructure can be extended to other STEM courses," said York, who serves on the Rutgers Online Educational Steering Committee and the Committee for Undergraduate Education.

Also in the Fall, the Chemistry department plans to offer general chemistry recitation classes online every day and at least one section of the chemistry lecture online. The department also established a Chemistry Lecture Demonstration Facility, directed by York, which brings demonstrations into the classroom.

"We are trying to address student frustrations, such as not being able to get the recitation class times they want," York said. "At the same time, we are looking for every opportunity to help faculty keep students engaged and develop the science leaders of tomorrow."

STUDENT AWARDS - SPRING 2013

Undergraduate Awards

CRODA AWARDS:

Titania Chin, Karim Elmorshedy, Nicholas Raffa, and Jenny Shah received the General Chemistry 161-162 & 162 Solid Gems Award for Excellence in General Chemistry.

Mark Quilon was recognized as an Outstanding Student in Sophomore Chemistry Classes for Excellence in Organic Chemistry.

Tianyi Liu was recognized as an Outstanding Student in Junior Organic Chemistry Laboratory for Excellence in Organic Chemistry Laboratory.

COURSEWORK AWARDS:

Cassandra Burdziak received The Rufus Kleinhans Award for Excellence in Honors General Chemistry.

Julia Xia received The Roger Sweet Award for Excellence in Organic Chemistry.

Deepak Gupta and Manank Patel received The Phyllis Dunbar Award for Excellence in Physical Chemistry.

Christopher Kaplan received the ACS Inorganic Division Award for Excellence in Inorganic Chemistry.

Tamr Atieh received the ACS Analytical Division Award for Excellence in Instrumental Analysis.

Jessalyn Devine received The Hypercube Award for Excellence in Chemical Physics.

Reem Asraf, Efua Bolouvi, Neeta Chakraverthy, Kevin Hejnas, Sarah Indano, and

Richa Rana received the Chemistry and Chemical Biology Service Award, presented to Chemistry majors with a strong record of participation, outreach, and departmental service.

JUNIOR AWARD:

Sarah Goodman received The Ning Moeller Award for Outstanding Academic Achievement by a Chemistry Major in the Junior Year.

SENIOR AWARDS:

Jimmy Patel received The Merck Award for General Academic Excellence & Research.

Aaron Sun received The Bruce Garth Award for General Academic Excellence & Research.

Michael Olson received The Van Dyke Award for Academic Excellence & Research in Chemistry.

CHEMICAL RESOURCES AWARDS DONATED BY PAUL KEIMIG:

Alicja Cygan, Sarah Goodman, Christopher Kaplan, Diana Sun, and Peter Waddell received the Chemical Resources Award for Distinction in Research.

Justin Corbo, Michael Olson, Jimmy Patel, and Aaron Sun received the Chemical Resources Award for Highest Distinction in Research.

PHI BETA KAPPA INITIATES:

Zhaozhi Jiang, Tianyi Liu, and Gram M. Townsend were elected to the Phi Beta Kappa Society.

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COMPUTATIONAL AWARD

DONATED BY KEVIN J. THEISEN:

Mohammad Malik received the Chemdoodle Award for Excellence in Computational Chemistry & Informatics.

CHEM. 499 – INTRODUCTION TO TEACHING CHEMISTRY LAB:

The following students were recognized for their contribution to the department in the teaching of a freshman chemistry lab: **Tamr Atieh, Emily Buginsky, Milos Cejkov, Alicja Cygan, Neyra Jemal, Clarence Li, Steven Nichol, Michael Olson, Kevin Schaefer, Aaron Sun, and Lan Wei.**

Graduate Awards

THOMAS DUFF TRAVEL AWARD:

Voshadhi Amarasinghe, Mu Chen, Wenchun Feng, Kathleen Field, Lisa Hurd, Fuguo Jiang, Gina Moriarty, Maria Panteva, Shreyas Shah, Boning Wu, and Lu Yang received the **Thomas Duff Travel Award** for students presenting their research at national or international conferences.

DEGREES CONFERRED

JANUARY 2013

M.S.

John Fiske

PH.D.

Bonan Cao

Roselin Rosario-

Melendez

David Wang

MAY 2013

B.A.

Nishat T. Ahmed

Michael D. Amin

Rustam Aminjanov

Absari Z. Arpa

Tamr B. Atieh

Samreen Bano

German Brodskiy

Emily L. Buginsky

Christopher Chan

Steven W. Chin

Byung Mi Choi

Ximena Collado

Justin M. Corbo

Tyler Davenport

Viktor Dubovoy

Allison M. Dyevoich

Joseph A. Esposito

Travis A. Hill

Zhaozhi Jiang

Brian J. Johnson

Moaz S. Kaleem

Chuan Kao

Yesha Kathrani

Sunah Kim

Justin C. Lee

Clarence Li

Tianyi Liu

Enayet Malique

Jack R. Maranhao

Deeb M. Mashni

Fahad Mohammad

Laura Motta

Michael P. Olson

Arpit A. Patel

Jimmy Patel

Manank G. Patel

Neel D. Patel

Priyal L. Patel

Brandon J. Pater

Sanjeev Rai

Kristen M. Reale

Kevin C. Schaefer

Minli Shi

Tyler J. Smith

Aaron X. Sun

Gram M.

Townsend

Lan Wei

Thomas P. Wright

M.S.

Deodialsingh

Guiadeen

Alexandra V.

Zatorski

PH.D.

Fuguo Jiang

David Laviska

Brian Moore

Aniruddh Solanki

Tian Sun

Haohan Wu

Xiao Zhang



CCB on Facebook, YouTube and LinkedIn

Stay in touch with friends and on top of the latest CCB news and events. Like, join or follow our pages on Facebook, YouTube and LinkedIn through the following links or just search Rutgers Chemistry.

- Facebook: www.facebook.com/RutgersChemistry
- LinkedIn: www.linkedin.com/groups?gid=3937350&trk=myg_ugrp_ovr
- YouTube: www.youtube.com/rutgerschem

Among the many useful things you will find on the social media pages are three new Chemistry videos. The videos feature Professors Eddy Arnold and Darrin York discussing their areas of specialty as well as graduate students Wenchun Feng, Katie Field, Michele Ouimet, Paul Smith, and Andrew Steffens discussing their experience in the chemistry program.

PDB

continued from page 1

technology available to share over 88,000 structures with 250,000 unique users.

"I don't think people envisioned how large and complex the PDB would turn out to be," Berman said. "Many of the structure determination methods used today didn't exist. The archive's audience has also changed from being mainly structural biologists to many and various types of users."

The PDB archive is the single worldwide repository of information about the 3D structures of large biological molecules, including proteins and nucleic acids, providing an essential resource of information about biomolecular structures. These molecules of life are found in all organisms, from bacteria and plants to animals and humans.

"Understanding the shape of a molecule helps to understand how it works," Berman said.

"This knowledge can be used to help deduce a structure's role in human health and disease, and in drug development. The structures in the archive range from tiny proteins and bits of DNA to complex molecular machines like the ribosome."

Today, the RCSB PDB member institutions are Rutgers and University of California, San Diego. The majority of the RCSB PDB staff and infrastructure are headquartered at the Rutgers Center for Integrative Proteomics Research, a four-story, 75,000-square-foot facility on the Busch Campus.

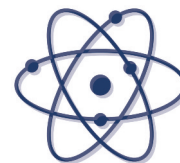
In recognition of the international nature of PDB depositors and data users, Berman helped launch a worldwide collaboration in 2003 to manage the Protein Data Bank. Called the Worldwide Protein Data Bank (wwPDB), the organization joins the RCSB PDB together with wwPDB institutions in the U.S., United Kingdom and Japan. Berman hopes more

international partners will be added in the future.

Locally and around the world, RCSB PDB continues to work to enable scientists to achieve medical advances and help everyone from grade school students on up understand the structural view of biology through outreach programs and innovative online tools such as PDB-101.

"In the future, there is no doubt that the number, size, and complexity of the structures in the PDB will continue to grow," Berman said. "The same is true for the armament of hybrid methods utilized to determine structures—a variety of biophysical, biochemical and modeling techniques to represent the shapes of complex molecular machines. Forty years later, our challenge remains to support scientific discovery and to promote public understanding of how the shapes of proteins and nucleic acids are vital to the study of medicine."

The PDB archive is the single worldwide repository of information about the 3D structures.

**PAIN MANAGEMENT**

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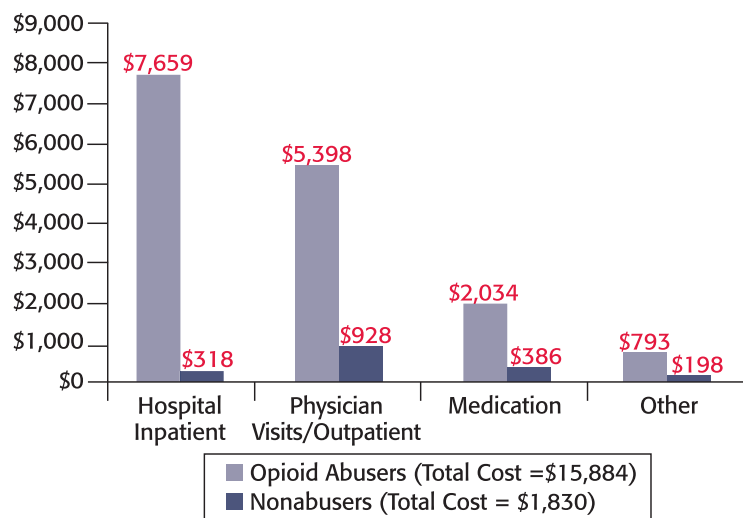
widely used for the treatment and management of acute and chronic pain. Currently available commercial extended-release morphine tablets are successful at maintaining long-term benefits only up to 24 hours.

"PolyMorphine may offer a desirable option as a long-acting, low abuse liability alternative to conventional opioid analgesics because morphine cannot be physically separated from PM," said Roselin Rosario-Meléndez, a project researcher who recently completed her doctorate at Rutgers. "Other controlled release formulations contain a large dose that can be readily separated by crushing or

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FIGURE 2

Direct All-Cause Health Care Costs Per Person (2003 U.S. Dollars) Associated with Opioid Abuse



Adapted from White et al. Direct costs of opioid abuse in an insured population in the United States (2005).

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PAIN MANAGEMENT continued from page 11

breaking the tablet or capsule, which results in increased potential for recreational use."

As a pain management option for abdominal, orthopedic and thoracic surgery patients, the Rutgers Office of Technology Commercialization (OTC) has estimated that Poly-Morphine could potentially save approximately \$1,000 or more per patient, or \$6 billion dollars, based on projections from the more than 6.3 million annual surgeries that fell into these categories in 2010.

"The financial impact of PM could actually be far greater considering that we have an aging population," said Uhrich. "By 2030, it is expected that first-time total knee replace-

ments will increase 700 percent and first-time total hip replacements will increase more than 150 percent. Just as important, but more difficult to calculate are the benefits provided to patients by an improved quality of life, reduced patient concerns about pain relief, reduced physical therapy, lowered immune system stress and the relieved societal costs of drug abuse."

Another benefit of PM is a likely reduction in morphine abuse. Based on published reports, it is known that opioid drug abuse costs in the U.S. alone tallied approximately \$55.7 billion in 2007, including \$25.6 billion (46%) in the workplace, \$25 billion (45%) in healthcare services, and \$5.1 billion (9%) in criminal justice

costs. Workplace costs were driven by lost earnings from premature death (\$11.2 billion) and reduced compensation or lost employment (\$7.9 billion). Health care costs consisted primarily of excess medical and prescription costs (\$23.7 billion). Criminal justice costs were largely comprised of correctional facility (\$2.3 billion) and police costs (\$1.5 billion).

"Our studies have used PM via injection into the body cavity and we also envision that Poly-Morphine can be administered as an implant during surgery or via localized injection," said Nicholas D. Stebbins, the project's current primary graduate student researcher. "We plan to continue our research and hope to extend the analgesic effect of PM up to one week."