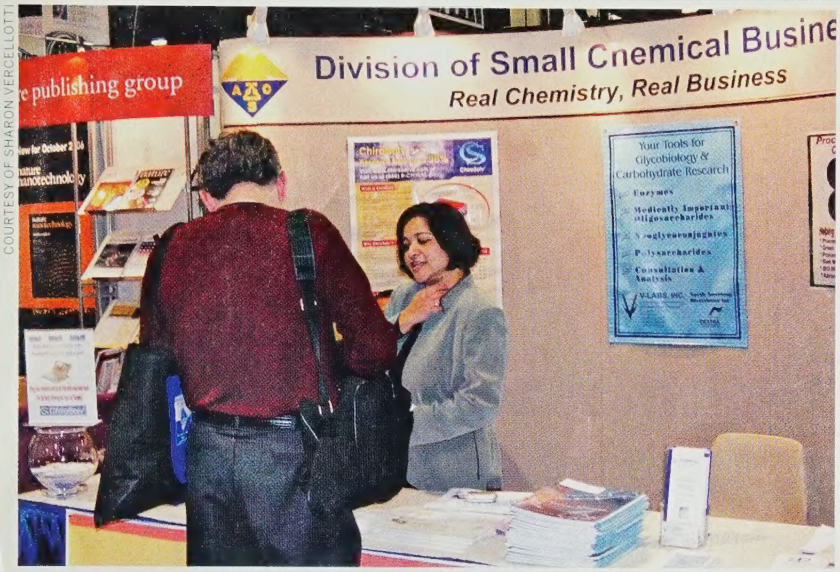
Alfred Bader

Articles

[Articles about Alfred Bader]



COURTESY OF SHARON VERCELLOTTI

EXPO Vaidya answers questions about ChiroSolv products in the Division of Small Chemical Businesses booth at the ACS national meeting in Atlanta last March.

ENTREPRENEURIAL SPIRIT

Combine science and hard work with creativity, then **GET DOWN TO BUSINESS**

RACHEL PETKEWICH, C&EN WASHINGTON

"I'VE OFTEN BEEN ASKED, 'Bader, when you started out, did you plan to build a large fine chemicals company?' said Alfred Bader last month at the National Institutes of Health about cofounding Aldrich Chemical and giving advice to young scientists who want to start their own businesses. "No, I didn't," he said. But Bader said he realized that he could have a place in the business while he was a Ph.D. student at Harvard University in the late 1940s.

He recalled ordering some 2-isopropylphenol from Kodak's catalog. When it didn't arrive in six weeks, Bader wrote to the company. Kodak replied via postcard: "We have your order. We will ship it when we have the material. In the meantime, do not add to the paperwork. Do not write to us again."

Bader never forgot his poor customer service experience in graduate school. Several years later, while working at PPG in Milwaukee, he proposed starting a fine chemicals division. When the research director rejected the idea, citing that no one could compete with Kodak, Bader and a lawyer friend gathered $500, usurped the lawyer's wife's maiden name for their fledgling firm, made chemicals in a rented garage at night and on the weekends, and sold them under the Aldrich label.

Businesses that start small are a big component of the U.S. economy. According to 2004 statistics from the U.S. Census Bureau, 99.7% of companies have fewer than 500 employees. Of the 5.75 million firms in the U.S. that year, 5.15 million employed fewer than 20 people.

In their first year, Bader and his partner offered a single chemical and made a $20 profit. A few years later, Bader left PPG to work full-time for Aldrich. The research director at PPG kindly offered to take Bader back if Aldrich failed.

Bader never took him up on that offer because his company prospered. Now called Sigma-Aldrich, it is the world's largest supplier of research chemicals, with annual sales of more than $1.6 billion.

Bader is just one example of hundreds of entrepreneurial successes in the chemical sciences. The entrepreneurs C&EN interviewed for this story agree that time and money are vital for success, but so are good bookkeeping, flexibility for dealing with inconsistent income, doing whatever needs to be done (from technical sales to cleaning the bathroom), networking, and asking for help from more experienced people. But clearly, people use many different formulas to start their own businesses.

"Being an entrepreneur is a different way of taking responsibility for your own life. It's scary, but I wouldn't trade it."

SMALL COMPANIES can spin off from large companies. Take the case of George Y. Li, who enjoys taking results from the lab to the marketplace. Personal funding and a licensing agreement with DuPont allowed him to start his business in 2001. His company, CombiPhos, based in Princeton, N.J., commercialized a novel catalyst technology that Li invented while working at DuPont Central R&D in Wilmington, Del.

The beauty of these highly active and air-stable cross-coupling catalysts is that they work for many coupling reactions for which traditional palladium catalysts do not work or are less efficient to use, says Li, a Ph.D. chemist.

CombiPhos now has seven employees in the U.S. and two joint ventures in China. More than 240 pharmaceutical companies use CombiPhos catalysts, Li says. The company is also manufacturing a line of novel boronic acids and esters for pharmaceutical applications. He adds that more than 30 large pharmaceutical companies have already used these intermediates for drug discovery and process chemistry projects.

"So far, the major hurdle appears to be keeping up with the growing demand," he says. For example, this year, a large pharmaceutical company applied 30 kg of a CombiPhos product to its pipeline, he says.

Technologies created at universities can help launch companies, too, as Earl

H. Wagener experienced. He got a call from Dennis W. Smith Jr., currently on the chemistry faculty at Clemson University in South Carolina. Smith and two other Clemson chemistry colleagues (John Ballato and Stephen H. Foulger) were thinking about starting a company by licensing polymer technologies from Clemson. They wanted Wagener to help them and act as chief executive officer. Wagener said, "Why not?" They called their company Tetramer Technologies to play up the fact that they had four founders working on polymer products.

Wagener, a Ph.D. chemist, gained his business savvy working in R&D leadership positions for decades at Dow and Stepan. He had even worked for an internal venture capital, entrepreneur-type enterprise inside Dow and admired the ideas and drive of the entrepreneurs who came seeking funding. But he never thought he would be an entrepreneur himself.

Wagener likes the challenges, but has found that being an entrepreneur is not always glamorous. For example, Tetramer Technologies began proudly but humbly in a dilapidated building between a car wash and a veterinarian's office in Pendleton, S.C. Five years later, it has renovated its space and now employs 11 people. The four founders prefer funding from three different National Science Foundation-funded Small Business Innovation Research grants to venture capital.

Wagener emphasizes the importance of having business partners who can work well together and recommends making sure that the goals of the university align with the goals of the company to avoid conflict. He also teaches a business-infused course in the chemistry department at Clemson. He hired four people from the first class, and of the 18 people who have worked for Tetramer, he says, only one was not educated at Clemson.

RENOVATION Tetramer Technologies transformed a run-down building into modern lab space for its polymer business.

Partners often start businesses with their own resources. In 1979, chemists Sharon V. Vercellotti and her husband, John, started V-Labs Inc., a carbohydrate-manufacturing and analytical services company. They used a combination of their own money and a guaranteed Small Business Administration loan to start up in their hometown of Covington, La. "We found that we didn't need to be located anywhere special. We just needed a good phone, FedEx, and an airport nearby," Sharon says.

Sharon ran the business by herself from 1985 to 1995, while John took a job at with the Department of Agriculture. Over the years, she says, the technical work has been stimulating. She cites some "anxious moments" but says, "We're still here." V-Labs has four employees. Sharon is also active in the American Chemical Society Division of Small Chemical Businesses (SCHB) and says, "Membership in the division has been very valuable to me."

In addition to ACS, professional societies such as the American Institute of Chemical Engineers and the American Association for the Advancement of Science hold sessions at their annual meetings for people with entrepreneurial aspirations. In meeting technical sessions, speakers discuss how they became entrepreneurs and what services are available. During panel discussions, social hours, or receptions, entrepreneurs get valuable networking time with potential clients, investors, scientific advisers, business mentors, and other entrepreneurs.

ACS meetings can also be a chance to showcase new products, and SCHB provides free booth space in the exposition hall to division members.

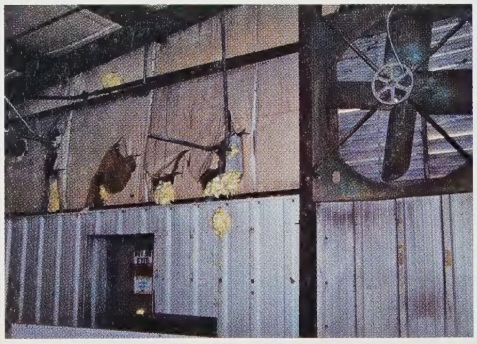
ChiroSolv Inc., based in San Francisco, is one of the companies that has appeared at the SCHB booth in the past year. Four years ago, Niteen A. Vaidya, a Ph.D. organic chemist, began developing prepackaged, 96-vial research tool kits that can speed up R&D screening of chirally pure compounds. In 2006, when he had sold more than 200 kits, he and his wife, Neelam, who is a software engineer, formed ChiroSolv Inc. with equal ownership. Neelam is the CEO, and Niteen is the chief technology officer. Their clients include biotechnology companies.

RACHEL PETKEWICH/C&EN

SPIRITED Jones (left) and Vercellotti take a break at a session for women entrepreneurs at the ACS national meeting in San Francisco in September.

Conferences and expositions are good places to meet new clients and practice giving a brief description of a product. Neelam says she's seen a lot of people with good products who didn't have a short explanation to convince buyers or investors.

Lynda J. Jones, who also showed off her product at the recent national meeting in San Francisco, met her new business partner, Jerry DeMenna, at an ACS meeting last year. Over the past six years, Jones has been developing Holy Mol-ee!, a strategy for teaching chemistry through song, dance, visual aids, and skits. The teaching materials are geared primarily toward middle and high school students, but they can be used for earlier grades and even community colleges. Jones is based in California and has



COURTESY OF EARL WAGENER

INNOVATION

Educating Entrepreneurs

All over the world, whether in Tokyo or Strasbourg or California, kids coming out of school have a rough time adjusting to the culture and practices of industry, even if they had the highest possible grade-point average in school, says Earl H. Wagener, chief executive officer of Tetramer Technologies. So he designed a class to teach students a little bit about industry before they leave academia.

Several university chemistry departments offer a class like Wagener's, a whole program, or even a graduate degree, but some academics debate whether these kinds of classes even have a place on the university campus.

Wagener, who has decades of experience in industrial R&D, got a Discovery Corps Senior Fellowship from the National Science Foundation in 2003 to teach his course at Clemson University in South Carolina. In the course, students evaluate four technologies using project analysis tools similar to those that companies use to evaluate the economic value of a research project. The students rate, for example, competitive advantage, market attractiveness, value to the customer, and technical feasibility. According to Wagener's design, the class should not be taught by an academic; limited to 24 students, it must be taught by someone with extensive industrial experience.

Finding someone with that experience to commit to prepare and attend the class for 14 consecutive weeks is a challenge, Wagener says. Both graduate and undergraduate students sign up for the class. And three years after the pilot course at Clemson, Auburn University in Alabama and Virginia Polytechnic Institute & State University have adopted the class model, and the University of Tennessee, the College of Charleston in South Carolina, and the University of South Carolina are considering it. Even better, Wagener says, his students who went on to jobs in industry are writing to thank him.

Other schools address entrepreneurial aspirations. For example, Cornell University has an alumni-funded, cross-disciplinary, and active program called Entrepreneurship@Cornell. It's not a major or a separate department; rather, it is a series of courses taught by faculty in the science, engineering, business, humanities, and social science departments, says Bruce Ganem, an organic chemistry professor who teaches an entrepreneurship class in the department of chemistry and chemical biology.

Ganem acknowledges the reservations that some academics have regarding teaching entrepreneurship on campus. However, he says, the pedagogical values are student empowerment and problem-solving skills. "It's not all about making money or really even about starting businesses. It's about setting goals and figuring out how to achieve them," Ganem adds. "I enjoy teaching these entrepreneurship courses because you put science students in situations where they have to decide what they would do if they were faced with a business decision, a marketing decision, or a regulatory decision. That's a useful life skill."

Meanwhile, at Case Western Reserve University, students in the Science & Technology Entrepreneur Program (STEP) can undertake commercialization assistantships as part of a master's degree program. Students can specialize in disciplines such as chemistry. At roughly 20 hours per week for 12–18 months working on an actual commercialization project, it's less like a traditional internship and more like a laboratory research assistant position, says STEP Director Cyrus Taylor.

Many of the students in the STEP program already have graduate degrees in science. "We've had a steady stream of interesting students come through the chemistry program in STEP." Due to changes at the university, including Taylor being appointed as the university's interim dean of the College of Arts & Sciences, STEP admissions were suspended this year, but they should be open next year, Taylor says.

Despite the various methods already being used, educational institutions around the world continue to polish their methods of teaching future entrepreneurs. Taylor says a great venue for sharing success stories and brainstorming new techniques is the Roundtable on Entrepreneur Education for Scientists & Engineers, an invitation-only event coordinated by Stanford University, which has a prominent and lively entrepreneurship center. Roundtables will be held this year in the U.S., Ecuador, Germany, and Thailand. Previous participants have included private and state universities, businesses, colleges, and research institutes.

Other resources for educators and entrepreneurs include the National Network for Technology Entrepreneurship & Commercialization (N2TEC) and the National Collegiate Inventors & Innovators Alliance.

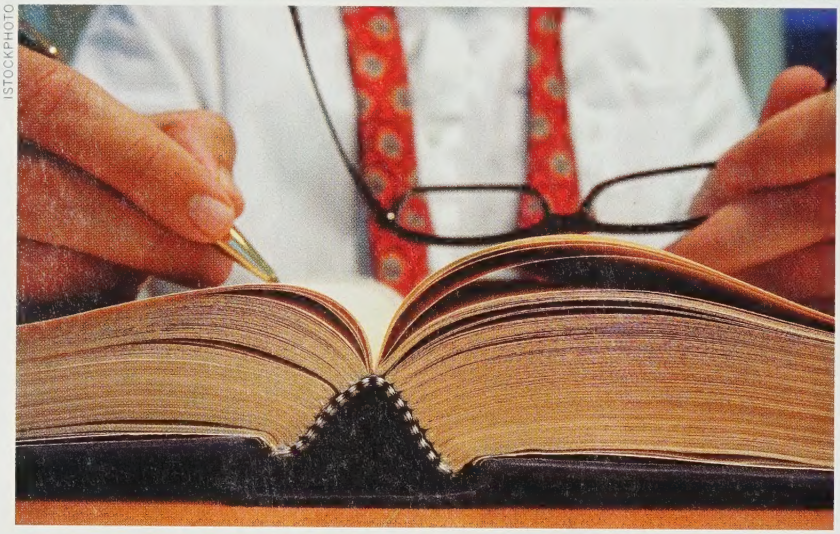
a master's degree in chemistry and experience as a high school and college teacher.

"Teachers are buying it, using it, and giving me feedback," she remarks. Approximately 600 customers, including public, private, and home-school teachers, have bought the product at different stages of its development.

The road has been rocky for Jones, from hiring recommended singers who couldn't carry a tune to contracting with a video editor who lost the footage. Financing initial product development on a credit card wasn't the best monetary strategy, but she has a good product, a vision for the future, and numerous opportunities, she says. For example, she has a television and podcast show in the works and an offer to franchise an after-school learning program based on her material. Jones and DeMenna have also combined their talents to produce a line of technology-teaching kits, which were introduced at the San Francisco meeting.

"Being an entrepreneur is a different way of taking responsibility for your own life. It's scary, but I wouldn't trade it," Jones says.

Entrepreneurs offer a wide range of advice for budding small-business owners. What advice does Aldrich cofounder Alfred Bader give to scientific entrepreneurs? Find a niche market, get good people to work with you, and be sure to answer every customer's query. "Don't be like Kodak," he said. "They are no longer in the fine chemicals business." ■



ISTOCKPHOTO

A PATENTLY SATISFYING CAREER

Scientists-turned-lawyers offer tips on navigating a career in INTELLECTUAL PROPERTY LAW

LINDA WANG, C&EN WASHINGTON

IN 1995, PAUL E. DIETZE, then an associate professor of chemistry at the University of Maryland, Baltimore County, made a life-changing decision: He left academics and went to law school.

Today, Dietze is a patent attorney with the intellectual property firm Kenyon & Kenyon LLP in Washington, D.C. "In retrospect, not being tenured was the best thing that probably could have happened to me. I really enjoy what I do now."

Most people don't arrive at the decision to practice patent law the way Dietze did, but most people also don't intend early on to become patent lawyers. "I can't think of too many people who started out as undergraduates thinking that what they wanted to do was patent law," Dietze says.

But people who are trained as scientists are perhaps best equipped for this type of work. Patents in the life sciences can involve highly sophisticated inventions, and people with scientific backgrounds have an advantage when it comes to understanding the material. In fact, to qualify for the patent bar exam, candidates either need to have a bachelor's degree in natural sciences, technology, or engineering or must have completed a certain number of semester hours in science or engineering.

At Summa, Allan & Additon P.A., an intellectual property firm in Charlotte, N.C., all but one of the 11 patent attorneys have science degrees. At Myers, Bigel, Sibley & Sajovec P.A., an intellectual property firm in Raleigh, N.C., all 30 patent attorneys have science degrees.

Kenneth D. Sibley, a founding partner of Myers Bigel, says his firm is particularly interested in hiring people with advanced degrees in biology or life sciences. Sibley has a B.A. in biology and psychology and an M.A. in neurobiology.

The demand for such specialized talent is growing. "We're seeing an explosion of innovation and activity in the life sciences area, and I think the demand is continuing quite strongly for the services of people who can provide intellectual property protection," says Lee Carl Bromberg, a partner at Bromberg & Sunstein LLP, a Boston law firm specializing in intellectual property and business litigation.

Patent law is divided into prosecution and litigation. Prosecutors write and process patent applications to be submitted to the Patent & Trademark Office (PTO); litigators go to court to defend or attack the validity of an existing patent.

Edmund J. Sease, who has a bachelor's degree in chemistry and is a partner at McKee, Voorhees & Sease PLC, an intellectual property firm in Des Moines, describes the two types of lawyers this way: "There are patent lawyers who are more fascinated with the science. They tend to be more interested in prosecution. And then there are patent lawyers who are more interested in the legal side of patent law. They tend more often to be litigators. You have to look within yourself to figure out which discipline suits you best."

DEMANDS Patent law involves a lot of research.

Regardless of which type of law one practices, a patent lawyer first needs to be a good lawyer, says Philip Summa, who has a B.A. and an M.S. in chemistry and is a shareholder and founding partner of Summa, Allan & Additon. He offers this practical advice: "Go to the best college you can get accepted into, and get the best grades you can get. Then go to the best law school you can get accepted into, and get the best grades you can get. Those are the two things we really look for."

Having a Ph.D. helps, says Dietze, who has a Ph.D. in organic chemistry. "It's another feather in your hat when you apply for jobs." Bromberg says his firm frequently hires top-notch Ph.D.s and sends them to law school.

But both Bromberg and Dietze are quick to point out that a Ph.D. is not a requirement for practicing law. In fact, they say, many patent lawyers do not have advanced science degrees. Bromberg does predict, however, that 10 or 20 years from now the people in the most senior positions will likely have Ph.D.s, particularly in the biotech and pharma areas.

FOR PEOPLE without advanced degrees, in particular those who want to go into litigation, one way to get a leg up is to clerk for the Court of Appeals for the Federal Circuit. "For us, the opportunity to hire a young lawyer who has worked as a clerk for a federal judge is probably every bit as valuable as hiring someone who has a Ph.D.," says Summa, noting that two of their lawyers are former federal court clerks. "Young people who train there come out with an outstanding level of experience in the law."

Summa says his ideal candidate would be a Ph.D. biochemist who has spent two years as a clerk for the Court of Appeals for the Federal Circuit. "That person could probably name their price," he says.

Meanwhile, people interested in the

GOETHE HOUSE
OF WISCONSIN

PERSPEKTIVEN

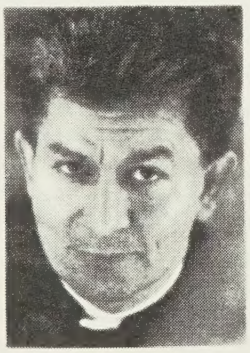
PERSPEKTIVEN Volume 5, No. 2 Spring 2006

The adventures of Alfred Bader

A life of innovation, achievement, cultivation and generosity

A standing ovation from Americans for German-born Delfs

Milwaukee Symphony music director also enthralls audiences worldwide



Andreas Delfs

By Kathleen Geraghty

Since his arrival in Milwaukee almost 10 years ago, Andreas Delfs has earned standing ovations as the music director of the Milwaukee Symphony Orchestra. But this native of Germany is a fan of all things American – including music from rock legend Sting, the TV show "The Brady Bunch," and contemporary American composers such as Corigliano, Glass, and Gershwin.

[Please turn to Delfs, Page 10]

Alfred Bader

For more than a half century, Austrian-born Alfred Bader has made a home in the Milwaukee area, but his reach has been without boundaries.

That was best summed up in a ceremony October 6, 2005, when Simon Fraser University in British Columbia, Canada, presented him with the honorary degree of Doctor of Science:

"A chemist, art collector and philanthropist, Alfred Bader has fashioned a life of innovation, achievement, cultivation and generosity from beginnings fraught with hardship, danger and injustice."

That award is among dozens of honorary degrees and other honors, including the Commander of the British Empire, that have been conferred on Bader through the years. He is a graduate of Queen's University, Kingston, Ontario, and from Harvard University.

[Please turn to Bader, Page 7]

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From the President

Fruehling ist da! It is time to think about and organize activities that are on the GOETHE HAUS agenda. Before we get to that task, we bring you some news with pride and delight. First, we are happy to announce the elevation of two of our board of directors, Lorraine Hoffmann and Wolfgang Schmidt to the corporate Board of Directors of Milwaukee School of Engineering. Second, we are pleased to announce the addition of Dan Sweeney to our board of directors. Dan comes to us after a very successful management career with Midwest Airlines (that's in chocolate chip cookies). His experience will give us a tremendous boost in GOETHE HAUS' marketing activities. You will read more about him in our summer Germanfest issue. Now for upcoming activities. In this issue there is an announcement about a Biedermeier exhibit that will be held from September-January at the Milwaukee Art Museum. GOETHE HAUS will be participating in this exhibit thanks to the efforts of two of our board members, Drs. Sy Kreilein and Ronald Ross. GOETHE HAUS will also join with Milwaukee School of Engineering in presenting a program examining furniture produced in the Biedermeier tradition. With spring comes planning for Germanfest. The Kultur Allee has been moved to the south end of the Summerfest grounds to what is called the Pepsi pavilion. All of the cultural groups will housed under one roof. This change presents new challenges and opportunities. Jill Haas will again chair this activity. Volunteers will be needed. The dates are July 27-30. To sign up call the GOETHE HAUS office, 414-276-7435.

Alles gute Alles Goethe

Ted E. Wedemeyer Jr.

Summer fun at Goethe House Kinder Kamps

Es fruehlingt! In this edition I have given my corner over to the Kinder Summer Day Camps, which have some exciting new changes. I am especially excited about the soccer camps, having experienced some of the World Cup fervor on a recent trip to Berlin this year. Children learn more when they are moving and the context is something relevant to their world, and soccer is such a vehicle. This is the ninth year of the Goethe House of Wisconsin summer Kinder Kamps program. As many as nine camps with a variety programs are planned. The Kinder summer day camps present opportunities of German for kids. Singing, dancing, games and soccer themes are on the agenda.

Katharina Hren, executive director

The Kinder Kamps schedule:

1. World Cup Celebration Camp, June 26-30
   Location: Milwaukee Kickers Soccer Club, N. 76th & W. Good Hope, ages 4-11.
2. German Soccer Camp, July 10-15
   Location: Milwaukee Kickers Soccer Club, N. 76th & W. Good Hope, ages 4-7.
3. German Soccer Camp, July 17-21
   Location: Milwaukee Kickers Soccer Camp, N. 76th & W. Good Hope, ages 8-11.
4. The World of Song, July 24-28 (tentative)
   Location: Ridgewood Baptist Church, Brookfield, ages 4-7.
5. The World of Grimm, July 24-28
   Location: Tamarack Community School, East Side of Milwaukee, ages 8-11.
6. The World of Grimm, July 31- August 4
   Location: Tamarack Community School, East Side of Milwaukee, ages 4-7.
7. The World of Song, July 31- August 4 (tentative)
   Location: Ridgewood Baptist Church, Brookfield, ages 8-11.
8. The Flavors of Germany, August 7- 11
   Location: First Congregational Church, Wauwatosa, ages 4-7.
9. The Flavors of Germany, August 14-18
   Location: First Congregational Church, Wauwatosa, ages 8-11.

Professor Umlaut and fans

All camps are Monday - Friday (9 a.m. to noon) - Registration April 1- June 15
Cost is $115 for one week – Limited scholarships (based on financial need) are available
Sponsored by Goethe House of Wisconsin
Email address: goethe@execpc.com Telephone: (414.276.7435)

REGISTRATION

To register:
Send us this form with payment to:
Goethe House Wisconsin, 814 W. Wisconsin Ave, Milwaukee, WI 53233

Name(s) of child(ren):_____ age(s): _____
Telephone: _____ e-mail: _____
Mailing address:_____
Name(s) of parent(s): _____
Site and date preferred: _____
(Psst.....Hey parents! Did you know that adult German classes are available also!)

Gooooaaaaallll for Germany

World Cup 2006 matches set for 12 of nations's cities

Germany will be the host for the FIFA World Cup 2006 from June 9 through July 9. Seventeen years after the fall of the Berlin Wall and 32 years after the first World Cup held in a divided nation, the country will welcome soccer fans from around the world.

The opening match will be held in Munich and the championship match in Berlin.

While Brazil may have won the World Cup more times and in more flamboyant style, the Germans are second only to the samba stars in the list of all-time greats and are renowned as one of the legendary sides in the history of the competition. Finalists in seven of the 17 World Cups since the inaugural tournament in Uruguay all the way back in 1930, Germany has been champion three times and has graced the final, although unsuccessfully, a further four times.

All around great achievements

Germany's record in World Cup finals speaks for itself but many of the team's greatest achievements have come in other games within the tournament. While in some cases Germany's route to the World Cup has been little more than effective, the team has always risen to the challenge of the big stage once qualification has been achieved.

Germany became World Cup champion for the first time in Switzerland in 1954 in a fairytale final against Hungary that started the German World Cup legend.

Almost 15,000 journalists from around the world will be present to directly report from the World Cup 2006 in Germany. The international media center will be located in Munich. There the reporters will be provided with sophisticated technology and the working area of 40,000 square meters. In addition, helpers in press centers in each of the 12 stadiums will ensure that information will quickly be distributed and players statements will be translated without delay.

The dozen venues for the matches across Germany are:

■ Berlin - The nation's capital, largest city and most lively tourist destination. The Berlin matches will be played in the Olympiastadium, capacity 74,500. Originally designed by architect Werner March and built between 1934-36 for around 42 million Reichsmark, American sprinter Jesse Owens won four gold medals here at the Olympic Games in 1936. Today, one of the avenues leading to the ground bears the great runner's name. Since 1985, the German Cup Final has been played in the stadium, which received a facelift prior to hosting three games in the 1974 FIFA World Cup.

The new capital is booming. The place, where modern architecture is redefining the skyline, has a magical appeal. Berlin is the current high light for tourists not only as a place for hip events like the Love Parade, but also as a first-grade cultural metropolis like the Philharmonics, the Berlin Film Festival "Berlinale" or the musical "Cats." The number of sights is unrivaled and the offers for tourists are chameleonic as the city's mentality.

■ Kaiserslautern - A provincial city noted for its

[Please turn to Soccer, Page 5]

Members of the 2004 German national team in Yokohama

Gooooaaaaallll for Germany

World Cup 2006 matches set for 12 of nations's cities

[Soccer, from Page 4]

U.S. Army presence and football tradition. This charming region in western Germany is home to picturesque villages, romantic castles and famous wine-growing areas. From June 9 to July 9 Soccer World Cup fever hits Rhineland-Palatinate – a date for the diary is June 17 when the U.S. Team will play Italy in Kaiserslautern.

- Cologne - The historical city in the Rhine-Ruhr area, famed for its massive cathedral.
- Dortmund - The beer capital of Germany.
- Frankfurt - Cosmopolitan modern city and Germany's financial center.
- Gelsenkirchen - Post-industrial city in the northern Ruhr built on coal, iron and steel.
- Hamburg - Prosperous, liberal Baltic port city famed for its nightlife.
- Hanover - Historical city famous for the exquisite gardens at Herrenhausen.
- Leipzig - Transformed dramatically since reunification, the city of Bach, Mendelssohn and Wagner.
- Munich - Bavaria's high-tech, cosmopolitan capital, famed for its palaces, museums and the annual Oktoberfest.
- Nuremberg - Historical and charming Bavarian city of commerce and culture.
- Stuttgart - Capital of Baden-Wurttemberg: modern, dynamic home to Daimler Benz and Porsche.

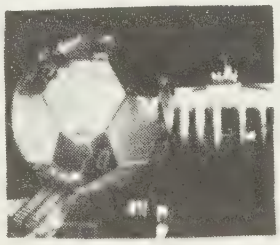
Live broadcasts at numerous public squares will make the World Cup 2006 a major group experience. FIFA is organizing "public viewing events" in the 12 World Cup cities. For example, at the Brandenburg Gate in Berlin, the Olympic Park in Munich, and the artificial Main Island in Frankfurt. Many other towns will also install big screens. The entire German nation will be a big World Cup arena.

"Shoot goals! Shoot movies!" This is the slogan of the official short film competition accompanying the World Cup 2006. It had been organized on behalf of the DFB Kulturstiftung by the Berlinale Talent Campus and the 622 young film makers from around the world who submitted their entries showing the soccer enthusiasm in their home countries. Forty-five films about soccer from 29 nations were presented during the 55th Berlin International Film Festival. The films will be shown in various German cities during the World Cup.

Credit: Federal Foreign Office, Berlin, Germany

For more information check these internet sites:
FIFAworldcup.com
www.cometogermany.com

Goleo - the mascot of the FIFA world Cup - joins all of Germany in looking forward to a soccer championship with exciting matches and visitors from around the world.



On its tour through German cities, the Soccer Globe by Andre Heller fuels an appetite for soccer and culture. Many regions converyt their public squares to large stages for the World Cup.

Goethe House board members at MSOE

Lorraine Lynn Hoffmann, a director of Goethe House of Wisconsin, and Wolfgang A. Schmidt, also a Goethe House director and a member of the Goethe House Academic Advisory Board, have been voted as corporation members of the Milwaukee School of Engineering board.

Hoffmann, the daughter of German immigrants, is the chief executive officer and president of Harri Hoffmann Co., Milwaukee, which manufactures and sells shoe and leather care products nationally. A retired assistant vice president of Merrill Lynch, Chicago, Hoffmann is extremely active in the non-profit communities in Milwaukee and Chicago. She is the president of Lake Park Synagogue, Milwaukee, and a board member of the Wisconsin Institute for Torah Study, Hillel Academy and the Museum of Beer and Brewing..

Schmidt, a native of Freiburg, Germany, was the owner and chief executive officer of Schmidt Engineering & Equipment, Inc., a manufacturing company specializing in the design , manufacture and distribution of heavy-duty snow removal equipment located in New Berlin, WI. Before coming to the United States in 1992, he was joint managing director of an international group of manufacturing companies overseeing operations in Denmark, France, Germany, Italy, the Netherlands, the United Kingdom and the United States. He is chairman of the advisory board of the Institute of World Affairs at the University of Wisconsin-Milwaukee, and a member of the advisory board of the UWM Center for Jewish Studies.

The Milwaukee School of Engineering, an independent university with about 2,400 students, offers 17 bachelor's degrees and seven master's degrees in the engineering, engineering technology, architectural engineering and building construction, computer, business and health-related fields.

Obituary Gerhard Rauscher

Gerhard Rauscher, an authority on German cultural history who served on the board of directors of Goethe House of Wisconsin, has died. He was 76.

Rauscher was born November 1, 1929 in Stuttgart, Germany, the son of Hermann and Apollonia Rauscher. He died January 14, 2006.

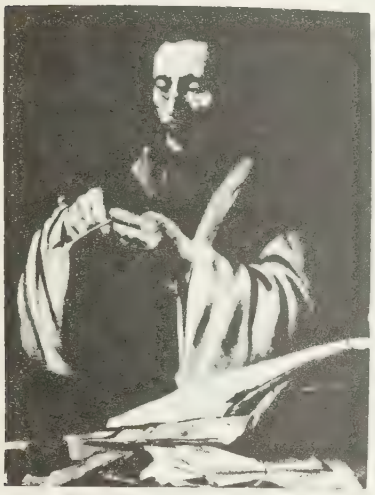
He came to the United States in 1962 and joined the faculty of the University of Wisconsin-Milwaukee. He retired from UWM in 1996 as a professor of German, having served as chairman of the German Department for 14 years.

Rauscher twice received teaching excellence awards at UWM and was a leader in the German American community. He was an active member of a number of professional associations including The Modern Language Association, The Modern Association of Teachers of German and the Wisconsin Association of Foreign Language Teachers. Rauscher was the husband of the former Dolores Krehl and father of Ingrid Gudlin, Karin Burleson and Karl Rauscher.

Katharina Hren, executive director of Goethe House, was a student of Gerhard Rauscher

"I wish to say goodbye to a dear mentor of mine. Dr. Rauscher was one of my professors at UWM, who encouraged me to stay in the German department and to apply for a year's scholarship to study in Berlin at the Freie Universitaet. He is one of the reasons I applied to graduate school. He would ask me how my studies were going, and then with a gentle smile, he would always ask if I was writing any poetry, for he enjoyed the poems I would sometimes share with him. He paid attention to the little human details, beyond the classroom, and I will always remember him as a true Mensch with a bottomless heart. When I would come to work (as a teaching assistant), he was always in this office already, door open. When I think of my time in academia, I always think of Dr. Rauscher's open door. Now when I am in that corridor, something is missing. And yet the memory of that open door is always with me, and I believe that Dr. Rauscher is one of the reasons one of my feet is always planted in the teaching world. There are teachers whom we never forget, and Dr. Rauscher is one of mine. May he rest in peace, always with his open door policy, in a better place." Schoene Gruesse, Katharina

The adventures of Alfred Bader



Paulus de Lesire, *The Quillcutter*
First painting on an Aldrich catalog cover, 1967
[Bader, from Page 1]

When Bader, himself, writes about his adventures he does justice to a definition of that word: remarkable and exciting experiences.

Bader reveals many of his remarkable and exciting experiences in an autobiography, "Adventures of a Chemist Collector," first published in 1995 in Great Britain. This modern day adventurer, now an octogenarian whose activities belie his age, still is on the cutting edge with his fascinating story.

Bader first arrived in Milwaukee in January 1950 at the age of 25, already having experienced enough upheavals and excitement in war-torn Europe and Canada to satisfy most mortals for the rest of their years. Not so with Bader.

"I have liked Milwaukee since the day I arrived," Bader writes. "It is a clean city with many beautiful parks and a shoreline, sandy in parts, along Lake Michigan. You can go swimming if you like cold water, which I do not.

"From my first days in Milwaukee, chemistry, the Bible and art have been the interconnected motifs of my life."

Some 18 months after arriving in Milwaukee, Bader was a co-founder, with Milwaukee attorney Jack Eisendrath, of Aldrich Chemical Company, now Sigma-Aldrich, one of the world's largest suppliers of research chemicals. Eisendrath who won a coin toss and the right to name the new company.

"Jack was engaged to a charming girl, Betty Aldrich, and the company was named Aldrich Chemical Company," Bader recalled.

Bader spent 40 years building Aldrich's distinctive reputation, becoming a multi-millionaire. He tells the extraordinary story of how he eventually was thrown off the board of Sigma-Aldrich only to enhance his fruitful career as an art collector and dealer, operating Alfred Bader Fine Arts, now at 924 East Juneau Avenue, for more than 40 years.

Helen Bader Foundation

Bader's first wife, Helen Ann Daniels, was an equal shareholder and worked with her husband at getting Aldrich up and running. She died in 1989, six years after their divorce, and left almost all of her estate to the Helen Bader Foundation, largely to help causes of special interest to her, including the disadvantaged, the homeless and abused. She had worked at the Milwaukee Jewish Home, mainly to help Alzheimer;s patients, a major area supported by the foundation. She was deeply interested in education, particularly Jewish education in Milwaukee and Israel.

[Please turn to Bader, Page 8]

Man Surprised
Believed to be a portrait of Adriaen Brouwer

The adventures of Alfred Bader

[Bader, from Page 7]

Milwaukee remains Bader's base for his continuing career as an art collector and dealer, and his legacy will run deep as a benefactor in the fields of chemistry, education and Jewish interests.

"I have derived real pleasure in my life from being able to establish prizes, scholarships and awards for students in Canada, the United States, Britain and the Czech Republic," Bader wrote "This is surely rooted in the enormous benefit such awards provided me when I was a student at Queen's University and later at Harvard. Without them, I could not have continued my studies."

ABCs - Art, Bible and Chemistry

"I am an inveterate collector," Bader says. "It may be a sickness and it began with stamps at 8, drawings at 10, paintings at 20 and rare chemicals at 30."

Bader recalls that Walter Rathenau, the statesman of the German Weimar Republic, is reported to have said that any Jew who claims to enjoy hunting is a liar. "Well, I could not bring myself to hunt animals, yet I have been a hunter all my life, in my ABCs - in Art, Bible and Chemistry," Bader says.

Bader has devoted years of study to art, immersing himself in the history of 17th century Dutch and Flemish paintings, and later expanding his interests to include French, Italian and German artists.

Alfred Bader Fine Arts has earned an international reputation, selling to such esteemed museums as the Rijksmuseum in Amsterdam, the National Gallery of Scotland and the Getty. Bader has curated special exhibits, become a renowned lecturer, and was named a fellow of the Royal Society of Arts in London.

Guest curator at Milwaukee Art Museum

He has been a guest curator at the Milwaukee Art Museum.

Bader was born in Vienna on April 28, 1924, the son of Alfred and Elisabeth Bader. He was Jewish on his paternal side and was brought up with a love of Judaism.

After the Kristallnacht, the Nazi attack on synagogues throughout greater German y in November 1938, the British government allocated 10,000 visas to allow Jewish children between the ages of 12 and 16 to enter Britain. Bader's mother applied for him to go, and he was included in the first Kindertransport.

Alfred Bader, painted in the internment camp

In May 1940, two weeks after his 16th birthday, Bader was attending Hebrew school at a synagogue in Brighton, England, when he was picked up by two detectives, driven to his home to collect clothes and a toothbrush and taken then to a detention center at the Brighton racecourse.

As Bader remembers: "Churchill had become alarmed about the activities of Fifth Columnists during the invasion of Holland, Belgium and France. How many were there among the thousands of refugees in Britain? Churchill said, 'Collar the lot' - all between the ages of 16 and 65. I had just turned 16, and my childhood was over."

Bader was sent to Canada. He was considered an "enemy alien" and interned at a prisoner of war camp on an island in Lake Champlain, near Montreal.

After passing all of his junior and senior matriculation exams with excellent results, he applied to McGill University. However, he was told he wasn't going to be accepted. "McGill's Jewish quota was full and they told me to reapply next year," he said. "But you know, when you are 17, a year seems like a long time."

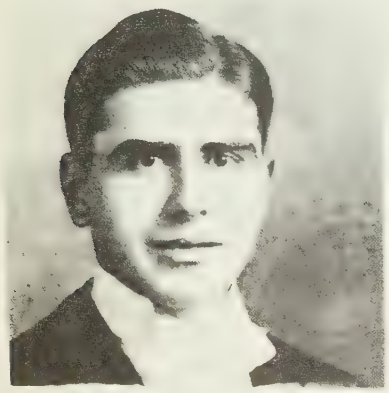
Bader's application to Queen's was accepted, so he enrolled there instead.

He said his experiences at the Queen's changed his attitude towards Canadians.

"My opinion of Canadians when I arrived to the prisoner of war camp was that they were dishonest," he said, explaining that he watched soldiers cut open his

[Please turn to Bader, Page 9]

The adventures of Alfred Bader

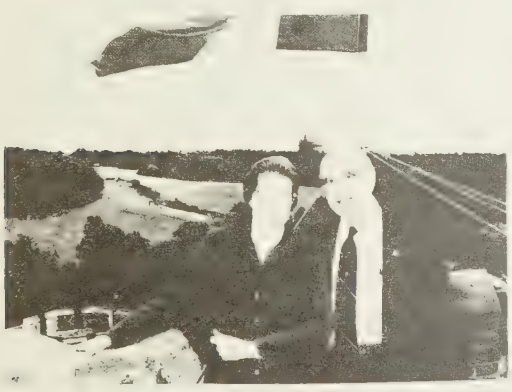


Alfred Bader, Queen's University graduation, 1945

[Bader, from Page 8]

luggage at the camp. "Queen's treated me wonderfully well."

After graduating, Bader moved to Montreal for work. His Montreal employer saw great potential in him, Bader said, and funded the continuation of his education. Bader earned his PhD in chemistry at Harvard and subsequently made his fortune in Milwaukee in the chemical industry.



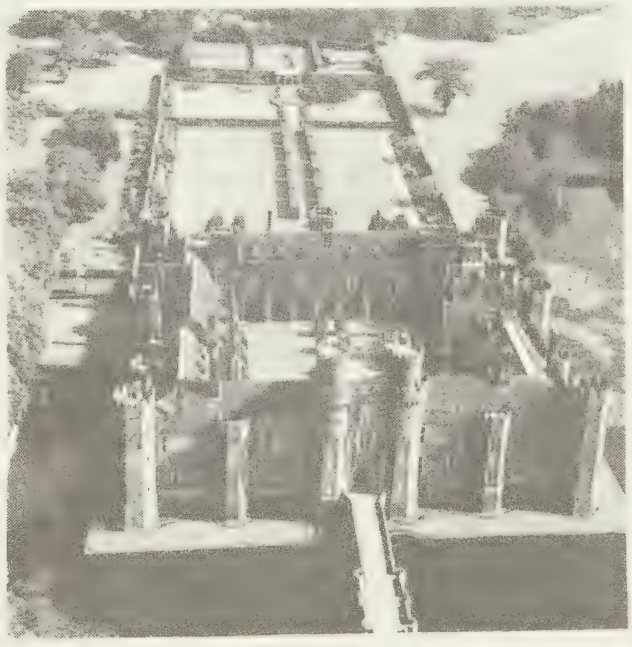
Isabel and Alfred Bader at Herstmonceux Castle

Love for his alma mater, and for his wife, Isabel, inspired Bader to offer to help Queen's University build a performing arts center. Bader is offering Queen's more than $10 million to develop the center.

"I am very fond of Queen's," Bader told the Queen's *Journal*. "[The new facility] would be a good thing to have—there is no great theatre [at Queen's], there is no performing arts centre, there is no musical hall and one could marry all these together."

Another gift of love from Bader to his wife is the 500-seat Isabel Bader Theatre at Victoria University at the University of Toronto, Isabel's alma mater. Bader donated $6 million for the theater.

He gave £6,000,000 to Queen's University to purchase and renovate Herstmonceux Castle in Sussex for use as an international study center - one more thank you to the Canadian institution that had enabled him to take the first steps on the road to success.



Herstmonceux Castle

Herstmonceux is a moated castle, some parts of it dating back to the 15th century, but it was largely rebuilt between 1911 and 1935, with 140 rooms on three floors, and a beautiful walled garden. The 530 acre estate had been the home of the Astronomer Royal and of the Royal Greenwich Observatory from about 1955 until 1988 when the operations were moved to Cambridge and the Canary Islands. The telescope buildings were intact.

The castle added a new dimension to life at Queen's, providing studies in European politics, economics, law art as well as opportunities for astronomy and physics aided by the telescopes.

A standing ovation for German-born Delfs

[Delfs, from Page 1]

Maestro Delfs was born in Flensburg, Germany, a town not far from the border of Denmark. He was exposed to music from his very early years. Because his mother was an actress, he had the chance to be backstage and soak up the music all around him; he began taking piano lessons at the age of 5. But it was music of show tunes - not the classical masters - that he first heard at the theater.

"I grew up at the theater," he says, "I played piano for shows, coached the singers, played for the ballet training. Somebody gets sick, so you do your first operetta, then your first opera. I did everything."

Delfs first attended the symphony at the age of 12, and by age 17 he was conducting the Flensburg Stadt theater orchestra. As a young musician and a young man, he found guidance from his music teacher, Professor Stoterau, after his father died.

Teacher a father figure

"Without a father, it was very important for me to have an older man in my life who took my by the hand...He was a piano teacher and a journalist who wrote for the local newspaper, so he went to every concert. As soon as I was old enough, I toddled along with him."

His piano teacher also taught him a larger lesson: "Not only did he, from day one, teach me the scales and where to put my fingers, but he opened up the whole wonderful world of music for that little boy....He was a kind of Renaissance man who read everything, knew everything, and loved music his whole life. He shared that all with me."

Because of his diverse talents in both classical music and musical theater, Delfs viewed America as a land of opportunity. Even as a young child, he saw classic American TV shows as a little window into a new place:

America: open, big, flexible

"I loved the Brady Bunch, and Lassie, but especially I loved Flipper. I always had a certain idea of how America could be, and what I always loved about it was that it seemed open, big, and flexible."

And the rest, as they say, is history.

Today Andreas Delfs is one of the youngest conductors of a major American orchestra, but that suits him well. Early in his career he became the youngest music director of the Hamburg Symphony at the age of 20. He continued to gain experience, holding the post of guest conductor at the Bremen State Theatre in 1981. Later that year, he graduated from Hamburg Conservatory.

Andreas Delfs, MSO music director

He enrolled at The Juilliard School upon the recommendation of his teacher, Christoph von Dohnányi. During the program, he studied with Jorge Mester and Sixten Ehrling, and won the Bruno Walter Memorial Scholarship on the way to receiving his master's degree in 1984.

(Coincidentally, MSO Concertmaster Frank Almond was studying at Juilliard during that same time. "I always thought I'd run into him somewhere down the line," says Almond.)

Wife, Amy, an art historian

It was in Pittsburgh that Delfs met his wife, Amy, an art historian. He also worked as an assistant to Lorin Maazel, who gave him ample opportunity to prep world-class orchestras while also conducting pops and children`s concerts. His range of experiences as a guest conductor drew the attention of the Milwaukee Symphony Orchestra search committee. In 1999, SYMPHONY, the magazine of the American Symphony Orchestra League, ran a full feature on Maestro Delfs and his appointment to Milwaukee, written by Tom Strini.

His experiences in both Germany and America have highlighted different attitudes about funding the art form of classical music. In the U.S., orchestras are run more on a business model, rather than as a tax-funded service.

"I have also had the added classing of America and Juilliard," he noted, "where I got my first taste that there is something like an orchestra industry. If you spend your life in Germany, you have no idea."

His resume is full of prestigious posts in Europe and North America, growing before (and during) his

[Please turn to Delfs, Page 11]

A standing ovation for German-born Delfs

[Delfs, from Page 10]

tenure with the MSO: music director of the Saint Paul Chamber Orchestra (2001-2004), general music director of Hannover, Germany (1995-2000), music director of the Bern (Switzerland) Opera, resident conductor of the Pittsburgh Symphony (during the tenure of Lorin Maazel as music director), and music director, at an early age, of the celebrated Orchestre Suisse des Jeunes.

He has conducted other major orchestras and world premiered several pieces. In 1997, Delfs made his debut with the Sydney Symphony in Australia, and in November 2000 he debuted with the NHK Symphony in Japan. Among his most notable achievements in the world of opera is his highly-praised debut with the New York City Opera, conducting performances of "Carmen" during the 1995-1996 season and a production of the uncut version of Hans Werner Henze's monumental "Koenig Hirsch" for the Württemberg State Theatre in Stuttgart.

> **"I think it's not so terrible to sit down at the piano and play a Gershwin song. There is room for fun and enjoyment in music. In America it's never wrong to have fun."**
>
> **- Andreas Delfs**

Recently, he completed a collection of sacred songs for the Delta label with Renee Fleming and the Royal Philharmonic orchestra.

In Europe, Mr. Delfs has led distinguished ensembles from several countries, including: the Frankfurt Radio Symphony Orchestra, the Berlin Radio Symphony Orchestra, the Royal Philharmonic, the London Philharmonic, the Leipzig Gewandhaus Orchestra, the Dresden Philharmonic, the Tonhalle Orchestra of Zurich, the Danish National Symphony Orchestra, the Netherlands Philharmonic, the Leipzig Radio Orchestra and the Deutsche Kammerphilharmonie.

Additionally, he led a tour of Spain and France with the Schleswig-Holstein Festival Orchestra and soloist Mstislav Rostropovich, who immediately invited Delfs to conduct the Moscow Conservatory Orchestra at the inauguration of the new concert hall at the Evian Festival in France.

MSO
MILWAUKEE SYMPHONY
ORCHESTRA
ANDREAS DELFS MUSIC DIRECTOR

After a sabbatical during the 2004-2005 MSO season, the Delfs family has returned to Milwaukee. They had decided that a more extended amount of time in Germany would allow the children the chance to experience German culture and practice their language skills while attending German schools (he and his wife Amy have four children).

Although he wasn't in Milwaukee quite as often, that's not to say Maestro Delfs took a break from all conducting during his time away; he was in Milwaukee for six concert weekends and had guest conductor engagements at other orchestras.

He does note that his sabbatical has allowed him to come back to this season with a fresh perspective on some of the well-known pieces such as Beethoven's Symphony No. 9, coming up in May.

In his role as music director at the MSO, Delfs balances several considerations: public tastes, contemporary works, artistic vision, revenue goals, and talents and specialties of MSO musicians. As he noted in a recent article in the Milwaukee Journal Sentinel: "If I were the customer," he said, "the season would be different. But I'm not the customer. You have to stay flexible. You cannot have one formula and say 'This is what I do, and nothing else.' "

As a modern conductor who is fond of contemporary works, he balances his love of new music with favorite pieces that audiences enjoy hearing throughout the years. "I think it's not so terrible to sit down at the piano and play a Gershwin song. There is room for fun and enjoyment in music. In America, it's never wrong to have fun."

Welcome

Goethe House of Wisconsin is a non-profit German-American cultural institute serving Wisconsin since 1958. Our mission is to serve as a statewide resource for information about the past and present culture of all German-speaking people - especially those in the Federal Republic of Germany. Goethe House of Wisconsin invites the financial support of individuals, companies and organizations who share our mission and recognize the value of this important cultural exchange. Goethe House of Wisconsin is a not-for-profit (501) (c) (3) organization. Donations are tax deductible as the law allows.

Goethe House of Wisconsin is now online.
Visit us at and send your friends to:
www.goethehousewis.com
Information available on Goethe House events, membership and other resources.
Satisfy your need for German culture 24 hours a day.
Use our web site or e-mail address to send
Letters to the Editor:
Goethe@execpc.com

Germany excels in Olympics

Germany and the United States again won the most medals at the 2006 winter Olympics in Torino, Italy.

2006 WINTER GAMES: OLYMPIC MEDAL COUNT
Closing totals for 84 medal events:

COUNTRY	G	S	B	TOTAL	COUNTRY	G	S	B	TOTAL
Germany	11	12	6	29	Finland	0	6	3	9
United States	9	9	7	25	Czech Republic	1	2	1	4
Canada	7	10	7	24	Estonia	3	0	0	3
Austria	9	7	7	23	Croatia	1	2	0	3
Russia	8	6	8	22	Australia	1	0	1	2
Norway	2	6	9	19	Poland	0	1	1	2
Sweden	7	2	5	14	Ukraine	0	0	2	2
Switzerland	5	4	5	14	Japan	1	0	0	1
South Korea	6	3	2	11	Belarus	0	1	0	1
Italy	5	0	6	11	Britain	0	1	0	1
China	2	4	5	11	Bulgaria	0	1	0	1
France	3	1	4	9	Slovakia	0	1	0	1
Netherlands	3	2	4	9	Latvia	0	0	1	1

Associated Press

Biedermeier show set for Milwaukee Art Museum

Goethe House has a role in the exhibition of Central European art

Georg Friedrich Kersting, Germany
***A Maiden at an Open Window in Conversation with a Young Man,* 1817**
Museum Georg Schäfer Schweinfurt

Biedermeier refers to work in the fields of literature, music, the visual arts and interior design in the period between the years 1815 (Vienna Congress), the end of the Napoleonic Wars, and 1848, the year of the European revolutions and contrasts with the Romantic era which preceded it.

The term Biedermeier comes from the pseudonym Gottlieb Biedermaier, taken by Joseph Victor von Scheffel in 1848 from the poems Biedermanns Abendgemütlichkeit (Biedermann's Evening Cosiness) and Bummelmeiers Klage (Bummelmeier's Complaint). Later it was used by the country doctor Adolf Kussmaul and the jurist Ludwig Eichrodt in poems, printed in the Munich Fliegenden Blättern (Flying Leaves), parodying the poems of the Biedermeier era as depoliticized and petit-bourgeois.

- Wikipedia

Two members of the board of directors of Goethe House of Wisconsin will have roles in the exhibition *Biedermeier: The Invention of Simplicity* at the Milwaukee Art Museum from September 16 of this year to January 1, 2007.

They are Dr. Ronald J. Ross, professor emeritus of modern German history at the University of Wisconsin-Milwaukee, and Dr. Sylvester Kreilen, German teacher at Marquette University High School and past president of the Wisconsin Association of Teachers of German.

Additionally Goethe House of Wisconsin is a member of the Milwaukee Art Museum's Regional Advisory Committee formed to promote the exhibition and assist in the organization of related public events, entertainment, and education programs.

Ross and Kreilen will present a program on the historical background of Biedermeier, an umbrella term for the many styles and phases associated with Central European art in the first half of the 19th century. Their program will include the socio-political-economic aspects of the Biedermeier movement as well as literary, furniture and other areas. The date of their presentation is still to be determined.

Biedermeier: The Invention of Simplicity will focus on a core group of artworks from around 1820, when the elements of simplicity, natural beauty, and clarity of form predominated and gave shape to a new aesthetic vision in Central Europe. Up to 300 examples of German, Austrian, Czechoslovakian and Danish paintings, furniture, decorative arts and works on paper will demonstrate proto-abstract and proto-modern tendencies that inform art of this period.

The exhibition was organized by the Milwaukee Art Museum in partnership with the Albertina in Vienna and the Deutsches Historishes Museum in Berlin. The Milwaukee Art Museum is the only venue in the United States for this exhibition.

The exhibition will be displayed in the new exhibition buildings of the Milwaukee Art Museum (the Quadracci Pavilion designed by Santiago Calatrava).

Next year, the exhibition will travel to Vienna from January 25-April 29; Berlin from June 8-September 2; and the Louvre in Paris from October 1-January 7, 2008.

A new season, German rites of Spring

Mixing Christian influence, ancient pagan resilience

By Dr. Samuel Scheibler

Celebrations of Spring with the gradual awakening of nature and the preparations for the intense agricultural season ahead represent a colorful and interesting amalgam of Christian influence and ancient pagan resilience. As with most cultural phenomena, it is often difficult to discern where one tradition ends and another begins but together the colorful and unique vernal customs of Germany all speak of hope, growth and new life.

THE ANNUNCIATION/ MARIA VERKÜNDIGUNG

Exactly nine months before Christmas Day, Germans in Catholic regions of the country celebrate the Annunciation of the Blessed Virgin Mary (Maria Verkündigung). Logic dictates that if Jesus was born on 25 December then His miraculous conception must have taken place 270 days before (minus certain "black calendar days" such as All Souls' Day) or 25 March.

In some villages of Oberbayern and in Austria the Annunciation is known as "Feast of Swallows" since the swallows return on or around this day from their winter migration to North Africa. Swallows are known as "Mary's birds" in this region and are believed to have a special relationship to purity and peace. It is considered bad luck to remove swallows' nests or to disturb these small creatures in any way. Referencing the Archangel's announcement to Mary that she was going to have a child, a medieval Austrian rhyme still quoted on this day says:

When Gabriel does the message bring
Return the swallows, comes the spring.

As 25 March also falls close to the beginning of the planting season, German and Austrian Catholic farmers still paint pictures of the Annunciation on the barrels or crates that hold seed grain. They begin sowing their crops on 26 March having fulfilled their devotion and received assurance that their crops will prosper. The relationship of the conception of Christ to prayers for fertility is obvious. One example (from Oberbayern) of the prayer accompanying the dedication of the seed containers on the Feast Day is:

O Mary, Mother, we pray to you;
Your life today with fruit was blessed:
Give us the happy promise, too,
That our harvest will be the best.
If you protect and bless the field,
A hundredfold each grain must yield.

One further advantage of this Feast is the belief that the frost season will end if proper devotions are given. An ancient proverb from Austria relevant to the planting of crops on the morning following the Feast of the Annunciation promises:

Saint Gabriel to Mary flies:
This is the end of snow and ice.

EASTER EGGS

Under the strict form of Roman Catholicism practiced in Bavaria and Austria the consumption of eggs was forbidden during the 40 days of Lent. To mark this sacrifice, "Fastnachtshüner" (Shrove Tuesday Chickens) were butchered as a festive food on the night before Ash Wednesday. Some scholars believe that the Christian custom of killing and stewing a rooster on this night may have originated in an ancient Germanic sacrifice to the gods of winter to convince them to make a hasty departure. Regardless of the fate of roosters, however, hens were spared and the resulting glut of their labors

[Please turn to Spring, Page 15]

A new season, German rites of Spring

Mixing Christian influence, ancient pagan resilience

[Spring, from Page 14]

gave rise to the Easter Egg.

The custom and art of painting eggs was begun by the "Sorben," a Slavic minority of some 150,000 in Brandenburg and Saxony, and was perfected by the Hessians. The Hessians have become specialist in this tradition. Not only are Hessian eggs beautifully decorated, the Hessian Easter egg also boasts Bible verses and proverbs inscribed in beautiful script.

Numerous Easter games involve the egg: "Eiersuchen" (Easter egg hunt), "Eierwerfen" (throwing eggs), "Eierticken" (the egg that does not break, gets the broken one). "Eierlaufen" (egg running) are still part of the Easter tradition.

Osterhase (Easter bunny), introduced in 1682 by Georg Frank, professor of medicine in Heidelberg, still makes an appearance in most German towns.

Maifest/Walpurgis

Perhaps the least understood German holiday of the Spring (outside of Germany) is Maifest/Walpurgis. The day marks the final victory of Spring over Winter, but before departing, the witches and their cohorts have one last fling. The night from 30 April to 1 May is called "Walpurgisnacht", the night of Walpurgis or Walpurga. The festival is marked by numerous rituals to ward off evil. Legend has it that on Walpurgisnacht the witches would gather on the Brocken, the highest peak in the Harz Mountains. Because of the Walpurgisnacht scene in Goethe's Faust, in which Mephistopheles takes Faust to the Brocken and has him revel with the witches, the witches gathering became widely known.

Under Christian influence Walpurgisnacht became a fest to drive out evil spirits. Walpurgis derives its name from Walpurga or Walburga. Walburga, Abbess of Heidenheim near Eichstätt, a Catholic saint, was known as the protectoress against witchcraft and sorcery. On the eve of 1 May, bells may toll in some areas and prayers may be said; there may be blessings with holy water and blessed springs can be found in homes and barns. The most widespread remedy against evil spirits during Walpurgisnacht is noise. As soon as the sun sets, boys of all ages may make noise. Their equipment ranges from boards to beat onto the ground to pistols firing shots.

In Bavaria the night from 30 April to 1 May is called a Freinacht or Drudennacht. For youth it is an opportunity to play tricks. They may stroll in groups through the streets and wind toilet paper around cars, smear door handles with tooth paste, unhinge garden doors and carry them a few meters away, and they may displace shoe scrapers.

Excerpts from Goethe's *Faust* , "Walpurgis-Night"

The witches and their cohorts revel for one last fling before the final victory of Spring over Winter

Witches in chorus
The witches t'ward the Brocken strain
When the stubble yellow, green the grain.
The rabble rushes - as 'tis meet -
To Sir Urian's lordly seat.

O'er stick and stone we come, by jinks!
The witches f..., the he-goat s...

Voice
Old Baubo comes alone, I see;
Astride on farrow sow is she!

Chorus
So honor be where honor is due!
Dame Baubo first! To lead the crew,
A hag upon a sturdy sow!
All witches come and follow now!

Voice
Which way didst thou come here?

Voice
By Ilsenstein crest;
I peered into an owlet's nest.
Her wild eyes stared at me!

Voice
To hell, I say, with thee!
Why ride so furiously?

Voice
She almost flayed me!
See here, the wounds she made me!

Chorus of Witches
The road is wide, the way is long:
How madly swirls the raving throng
The pitchfork pricks, the broom us hurts;
the infant chokes, its mother bursts.

HEXEN (im Chor):
Die Hexen zu dem Brocken ziehn,
Die Stoppel ist gelb, die Saat ist grün.
Dort sammelt sich der groszeHauf,
Herr Urian sitzt oben auf.

So geht es über Stein and Stock,
Es farzt die Hexe, is stinkt der Bock.

STIMME:
Diealte Baubo kommt allein,
Sie reitet auf einem Mutterschwein.

CHOR:
So Ehre denn, wem Ehre gebührt!
Frau Baubo vor! Und angeführt!
Ein tüchtig Schwein und Mutter drauf,
Da folgt ganze Hexenhauf.

STIMME:
Welchen Weg kommst du her?

STIMME:
Übern Ilsenstein! Da guckt ich der Eule ins Nest hinein,
Die macht ein Paar Augen!

STIMME:
O fahre zur Hölle!
Was reitst du so schnelle!

STIMME:
Mich hat sie geschunden,
Da siehnur die Wunden!

HEXEN, CHOR:
Der Weg ist breit, der Weg ist lang,
Was ist das für ein toller Drang?
Die gabel sticht, der Besen kratzt,
Das kind erstickt, die Mutter platzt.

Excerpts from Goethe's *Faust* , "Walpurgis-Night"

The witches and their cohorts revel for one last fling before the final victory of Spring over Winter

Wizards, Semi-chorus
We creep as slowly as a snail;
Far, far ahead the witches sail.
When to the Devil's home they speed,
Women by a thousand paces lead.

The Other Half
Not so precise are we! Perhaps
A woman takes a thousand steps.
Although she hastes aas best she can,
One leap suffices for a man.

Voice (above)
Come with us from the rockbound lake!

Voices (below)
We fain would follow in your wake!
We've washed, are clean as clean can be;
Yet barren evermore are we.

Both Choruses
The wind is hushed, the starlight pales,
The dismal moon her features veils;
As magic-mad the hosts whiz by,
A myriad sparks spurt forth and fly.

Voice (from below)
Tarry! Tarry!

Voice (from above)
Who calls so loud from rocky quarry?

Voice (from below)
Take me too! Take me too!
Three hundred years I have been striving
To reach the peak - I'm not arriving;
I fain would join my equals too.

Both Choruses
The broomstick carries, so does the stock;
The pitchfork carries, so does the buck;
Who cannot rise on them tonight,
Remains for aye a luckless wight.

HEXENMEISTER, HALBER CHOR:
Wirschleichen wie die Schneck im Haus,
Die weiber alle sind voraus.
Denn, geht es zu des Bösen Haus,
Das Weib hat tausend Schritt voraus.

ANDERE HÄLFTE:
Wir nehmen das nicht so genau,
Mit tausend Schritten macht's die Frau;
Doch wie sie sich auch eilen kann,
Mit einem Sprunge macht's der Mann.

STIMME (oben):
Kommt mit, kommt mit, vom Felsensee!

STIMMEN (von unten):
Wir möchten gerne mit in die Höh.
Wir waschen, and blank sind wir ganz und gar;
Aber auch ewig unfruchtbar.

BEIDE CHÖRE:
Es schweigt der Wind, es flieht der Stern,
Der trübe Mond verbirgt sich gern.
Im Sausen sprüht das Zauberchor
Viel tausend Feuerfunken hervor.

STIMME (von unten)
Halte! Halte!

STIMME (oben)
Wer ruft da aus der Felsenspalte?

STIMME (von unten):
Nehmt mich mit! Nehmt mich mit!
Ich steige schon dreihundert Jahr,
Und kann den Gipfel nicht erreichen
Ich wäre gern bei meinesgleichen.

BEIDE CHÖRE:
Es trägt der Besen, trägt der Stock
Die Gabel trägt, es trägt der Bock
Wer heute sich nicht heben kann
Ist ewig ein verlorner Mann.

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Ted E. Wedemeyer Jr.

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Chemical Information

BULLETIN

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IN THIS ISSUE

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	William Town (2006-2008)

CINF Web Site: *www.acscinf.org*

MESSAGE FROM THE CHAIR

Dear Colleagues:

2006 was another successful year for CINF under Osman Guner's excellent leadership. Here are just a few highlights for 2006 to give you a flavor for the type of activities in which our members were involved last year:

- Our division won not one, but two, ACS Innovative Project Grants. The first one was given to the CINF-CIC (Chemie-Information-Computer division of the German Chemical Society) collaborative working group, for a pilot project to develop a depository of Chemical Information Educational Material. The second grant allows us to invest in equipment to podcast future CINF technical programming. Our very first podcasted session was held in Atlanta and hailed a great success in an ACS Chemical Biology article (*ACS Chem. Biol.* (2006) 1 (4), 195–197.
- Hugo Kubinyi received the 2006 Herman Skolnik Award at the San Francisco ACS Meeting, for his work on drug design and molecular modeling. The 2007 recipient will be Dr. Robert S. Pearlman, the Coulter R. Sublett Regents Chair in Pharmacy and Director of the Laboratory for the Development of Computer-Assisted Drug Discovery Software at the University of Texas at Austin. He is best known for developing CONCORD, a tool for conversion of 2D connection tables into 3D structures.
- A record number of papers (126) were presented at the San Francisco meeting. Some well-attended sessions were *Cyberinfrastructure in Chemistry, Information and Education: New Emerging Technologies* (organized by the CINF-CIC collaborative working group), *Library Watch: Hot New Areas in Chemistry, Chemical Information and Organic Chemistry: The Road Ahead* (sponsored by the Beilstein Institute), *Rediscovery of Older Information.*
- The division members organized a very successful program for the *Biennial Conference on Chemical Education* (BCCE) held at Purdue University. The CINF program featured two sessions: (1) *Information Obstacle Course: Successfully Incorporating Chemical Information Into Your Curriculum* and (2) *Teaching Students About Copyright and Plagiarism.*

2007 will be marked as the year of CINF strategic planning! One of the main goals in this process is to have as wide member input as possible. We will have a member survey, interview many of our active members, and 12-15 members will get together on the Friday before the Chicago ACS National Meeting to put it all together (with the help of an ACS facilitator). At the Boston ACS meeting, the strategic planning working group will present a final proposal on how our division should be moving forward in the next 2-3 years to the CINF Executive Committee.

At the Chicago meeting, as usual, Saturday is reserved for our committee meetings starting early in the morning, with breakfast and the long-range planning meeting. Most of our committee meetings are open to all. Welcome to our receptions on Sunday and Tuesday nights! Our ticketed Tuesday luncheon speaker will talk about the sustainability of the Great Lakes. I look forward to seeing you in Chicago!

Erja Kajosalo, M.S., MLIS
Chair, ACS Chemical Information Division

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LETTER FROM THE EDITOR

In the last issue (Fall 2006) we published a survey asking readers to give us their feedback about the *Chemical Information Bulletin* (*CIB*). We got only 16 responses, but there were some interesting suggestions about the format and content of the publication. All respondents said that they usually check the CINF Division Technical Program and the events calendar, as well as any other conference information related to ACS national meetings; they also read the news articles.

Almost all respondents would like to see both print and electronic versions of *CIB*; many supported the idea of having the issues loaded on a searchable database, and most of the people voted for a new design of the cover. Other things on the wish list were related to publishing more interviews (including such with CINF members), news about developments in the chemical information field, reviews of past conferences and information about upcoming ones; reviews of databases and other information resources (for example, "what five resources are a must-purchase for that particular year"), articles devoted to chemical information literacy programs, discussions of issues that chemistry librarians are facing at their particular institutions. One person suggested including a list of new CINF members, with short introductions about each one of them; another one asked for more information on how to contribute to the publication; and a third one suggested that the *Bulletin* could publish extended (or even full) versions of some of the presentations made at ACS national meetings.

This is what some of the respondents said:

- "I look for news about people that I know."
- "I would like to see information about advancing chemical information as a profession and assuring that it gets proper recognition."
- "On the whole, I think that the *Bulletin* is pretty good."
- "The *Bulletin* is really pretty good; keep up the good work."

As you could see, this issue of the *Chemical Information Bulletin* has a new cover. I hope that those who voted for it would be delighted. The design was done by Barb Swartz (Design One), who has been designing the employee newsletters of the ACS Headquarters and CAS for many years. The Chicago skyline on the cover of this issue is familiar even to people who have never visited this city. Many of you will be able to see it "*in vivo*" at the end of March, when the 233rd ACS National Meeting will be held there. In the future, we are planning to have a different picture on the cover of each new issue. This could be a picture of the city in which the imminent ACS national meeting will be held, or we could use other pictures relevant to the Division's activities.

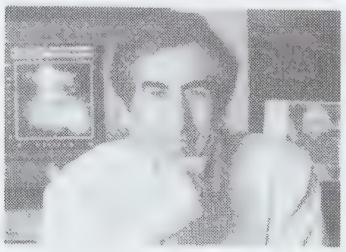
We would like to know what you think of the new cover and the content of the *Bulletin*. You can express your opinions and give us suggestions on how to improve the publication by going to the CINF Web page www.acscinf.org. You could also send me an email at the address shown below.

We look forward to hearing from you!

Svetla Baykoucheva, Editor
sbaykouc@umd.edu

AWARDS AND SCHOLARSHIPS

2007 Herman Skolnik Award Winner



Robert S. Pearlman, the Coulter R. Sublett Regents Chair in Pharmacy and Director of the Laboratory for the Development of Computer-Assisted Drug Discovery Software at the University of Texas at Austin, is the winner of the 2007 Herman Skolnik Award. This award is given by the Chemical Information Division of the American Chemical Society in recognition of outstanding contributions to and achievements in the theory and practice of chemical information science. The award ceremony will be held at the American Chemical Society National Meeting in Boston in September of 2007.

Dr. Pearlman is best known for developing CONCORD, a tool for conversion of 2D connection tables into 3D structures. Availability of CONCORD triggered the development of several 3D searching and pharmacophore perception technologies that revolutionized computer-aided molecular design capabilities in the pharmaceutical and agrochemical industries.

Dr. Pearlman was the 2006 recipient of the Society for Biomolecular Sciences Accomplishment Award for his work on the DiverseSolutions package which introduced novel concepts and descriptors related to clustering and diversity in chemistry-space. His BCUT-descriptors are widely used to help focus lead discovery efforts and guide the growth of corporate screening collections.

His more recent work includes innovative software for properly addressing both tautomerism and stereoisomerism in the contexts of cheminformatics and computer-assisted molecular discovery. Over the years, his Laboratory has developed and distributed a total of fifteen CAMD-related software packages.

When asked for comment regarding the Award, Dr. Pearlman said, "Obviously, I feel both honored and delighted to be recognized with such a prestigious Award. I am also very glad that our software has proven so useful to so many scientists around the world. However, I would be remiss if I, in turn, did not recognize at least a few of the many people who have worked with me over the years: Andrew Rusinko, Jeffrey Skell, and Renzo Balducci, for their work on Concord and Confort, our conformational analysis package; Karl Smith, for his work on both DiverseSolutions and EA-Inventor, our novel *de novo* design engine; Eugene Stewart and Hongyao Zhu, for their work on LibraryMaker, our 2D/3D library enumeration software; Felix Deanda, for his work on GSSI for modeling solution-phase properties; Yubin Wu and Brian Masek, for their work on our "Nature's Way" software for dealing with tautomerism and the resulting stereochemical consequences; and many others. This Award recognizes their efforts as well as my own."

Dr. Pearlman founded Optive Research, Inc. in July of 2003 to provide a more easily sustainable environment for CAMD software research and development. However, Optive Research was acquired by Tripos Inc. in January of 2005. Dr. Pearlman continues his research and teaching at the University of Texas at Austin. *Submitted by Guenter Grethe*

2008 Herman Skolnik Award—Call for Nominations

The ACS Division of Chemical Information established this Award to recognize outstanding contributions to and achievements in the theory and practice of chemical information science. The Award is named in honor of the first recipient, Herman Skolnik.

By this Award, the Division of Chemical Information is committed to encouraging the continuing preparation, dissemination and advancement of chemical information science and related disciplines through individual and team efforts. Examples of such advancement include, but are not limited to the following:

- Design of new and unique computerized information systems;
- Preparation and dissemination of chemical information;
- Editorial innovations;
- Design of new indexing, classification, and notation systems;
- Chemical nomenclature;
- Structure-activity relationships;
- Numerical data correlation and evaluation;
- Advancement of knowledge in the field.

The Award consists of a $3,000 honorarium and a plaque. The recipient is expected to give an address at the time of the Award presentation. In recent years, the Award Symposium has been organized by the recipient.

Nominations for the Herman Skolnik Award should describe the nominee's contributions to the field of chemical information and should include supportive materials such as a biographical sketch and a list of publications and presentations. Three seconding letters are also required. Nominations and supporting material should be sent by email to me (ggrethe@comcast.net). Paper submissions are no longer acceptable. The deadline for nominations for the 2008 Herman Skolnik Award is June 1, 2007.

Submitted by Guenter Grethe, CINF Awards Chair

2007 CINF Meritorious Award—Call for Nominations

Nominations are being sought for the 2007 CINF Meritorious Award. The award recognizes outstanding contributions to the Division and is open to CINF members who have performed activities benefiting the Division and deserve special recognition. Contributions to the Division might include, for example, the preparation of a major report, continuing leadership of the Division in a particular area, or sustained active contributions to a major task over many years. Chair, Chair-Elect, Treasurer and Secretary of 2007 are ineligible to receive the award.

Nominations should be sent by e-mail to Guenter Grethe, Chair of the CINF Award Committee, at ggrethe@comcast.net. The deadline for nominations is March 1, 2007. *Submitted by Guenter Grethe*

CINF- FIZ CHEMIE Berlin Scholarship for Scientific Excellence

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society (ACS) funded by FIZ CHEMIE Berlin is designed to reward graduate and post-graduate students in chemical information and related sciences, for scientific excellence and to foster their involvement in CINF.

Three scholarships valued at $1,000 were given out at the Fall ACS National Meeting in San Francisco. The winners showed their award-winning posters at the Sci-Mix session of the same meeting. They were presented with the cash awards by Dr. Jost Bohlen of FIZ CHEMIE Berlin at the divisional luncheon. The names of the recipients and the titles of their posters are:

Maciej Hanrańczyk, Department of Chemistry, University of Gdańsk, 80-952 Gdańsk, Poland, "*Quantum Mechanical Energy-Based Screening of Combinatorially Generated Library of Tautomers*"
Sally Mardikian, Department of Information Studies, University of Sheffield, Western Bank, Sheffield, S10 2TN, UK, "*Studying the Effects of Individual Interaction Energies in a Variety of Protein-Ligand Complexes*"
Robert S. Paton, Unilever Centre for Molecular Science Informatics, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW, UK, "*Understanding Stereochemistry: Molecular Modeling to Inform Organic Synthesis*"

FIZ Chemie Berlin will continue to support young scientists by again funding three scholarships valued at $1,000 each at the 234th ACS National Meeting in Boston, August 19 – 23, 2007. In order to apply for these scholarships please see the relevant announcement on the CINF website (http://www.acscinf.org) under "Recent Announcements". *Submitted by Guenter Grethe*

CINF Sponsors in 2007

January, 2007

The Division of Chemical Information was fortunate again to receive generous financial support from our sponsors to maintain the high quality of the Division's programming at the 2007 National ACS Meetings in Chicago and Boston, to promote communication between members at social functions, and to support other divisional activities during the year, including scholarships to graduate students in Chemical Information.

The Division gratefully acknowledges contribution from the following sponsors:

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Please feel free to contact me if you would like more information about supporting CINF.

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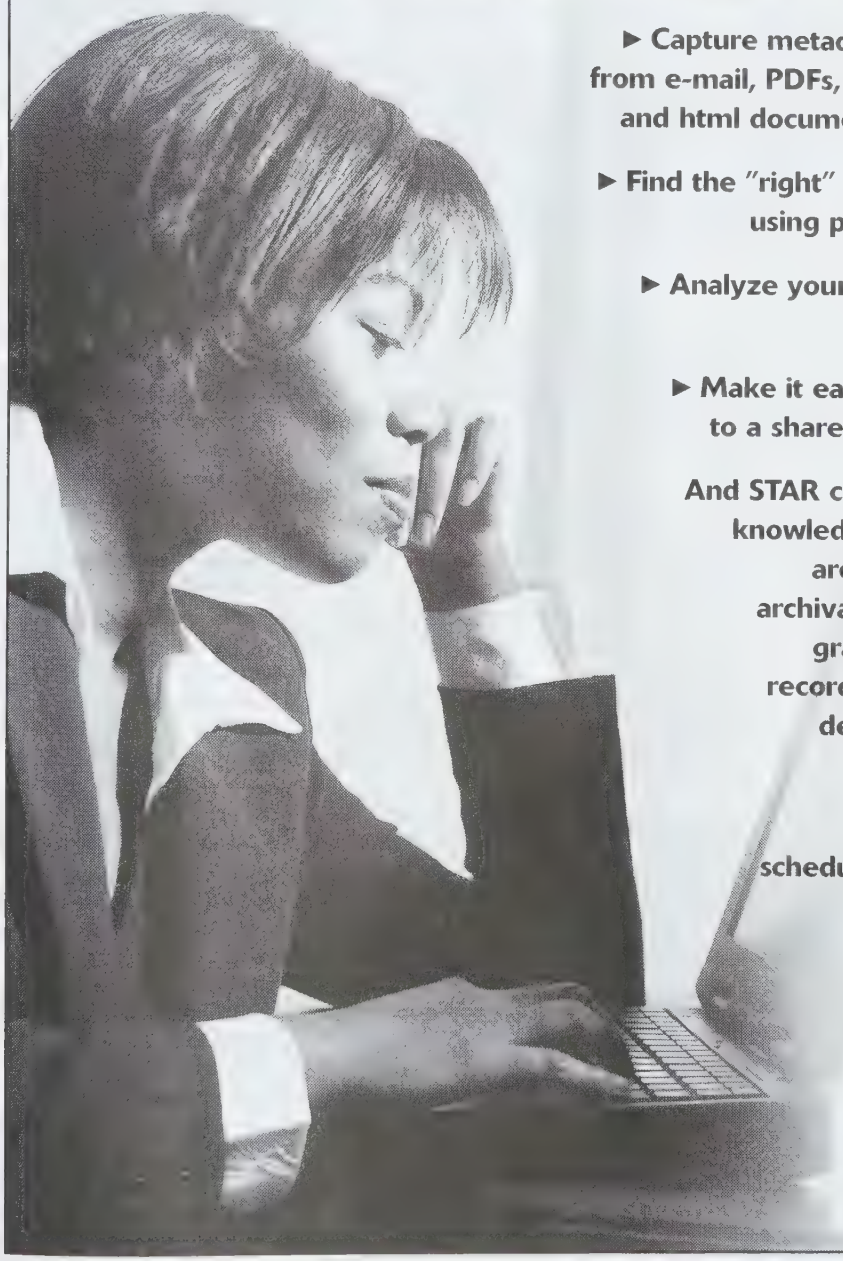

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CAS Observes its 100th Anniversary

By Eric Shively

Chemical Abstracts (*CA*) began publication on January 1, 1907, as the result of efforts of the American Chemical Society to bring more recognition to American chemists and chemical engineers, whose accomplishments seemed to be overshadowed by their European counterparts. The first issue contained just 502 abstracts, brief summaries of scientific papers and patents. By contrast, CAS added more than a million abstracts to its databases during 2006.

The Chemical Abstracts Service in Columbus, Ohio (*Photo courtesy of CAS*)

CA was first published at the National Bureau of Standards in Washington, D. C., where the Editor, William A. Noyes, Sr., was chief chemist. The *CA* editorial office moved to the campus of the Ohio State University (OSU) in Columbus in 1909, after a brief sojourn at the University of Illinois. Austin M. Patterson, the second *CA* Editor, had been invited to move to OSU by the chemistry department chairman, William McPherson. The *CA* office remained on the OSU campus for 56 years and today maintains close ties to the university.

In 1956 the organization became an operational division of the American Chemical Society and has been known ever since as Chemical Abstracts Service (CAS). By 1965 keeping up with the chemistry-related literature required a larger staff and facilities and CAS moved to a new building just north of the OSU campus. This site is still home to CAS and now comprises three buildings, including a data center constructed in 2001. E. J. Crane became the *CA* Editor in 1915 and the first CAS Director in 1956. Crane did much to establish the professionalism and commitment to excellence that made *CA* a model for secondary information services in the sciences.

Dale Baker succeeded in as CAS Director in 1958 and led the organization into the electronic age by encouraging the application of computers to the production of *CA*, database building, and the delivery of information services. A leading advocate of international cooperation in scientific information, Baker spearheaded the formation of the STN network in cooperation with Germany's FIZ Karlsruhe in 1983.

In 1995 at the dawn of the Internet era, CAS introduced SciFinder®, a revolutionary desktop research tool. SciFinder and CAS have been growing ever since. CAS' global revenues have grown steadily for more than a decade, even though price increases have been modest. Meanwhile, the scope and depth of CAS' indexed content has expanded rapidly, as CAS has added tens of millions of bibliographic and substance records, reactions, property data elements, citations, etc. In addition, analysis and visualization capabilities are now featured in STN AnaVist™, supporting the evolving role of information professionals, who have become management advisors, not simply corporate librarians.

Where will CAS go in its next 100 years? A series of forward-looking communications will appear on the CAS web site in 2007. With its unrivaled databases of literature, patents, and substance information and a team of skilled, analytical scientists, CAS looks ahead with confidence. More than ever, researchers must keep up with and build upon the work of fellow scientists worldwide, and CAS will continue serving that need.

CAS and CINF: A History of Cooperation

By W. Val Metanomski

CAS is celebrating its 100th anniversary in 2007. This article will highlight the very close cooperation, especially in the development of chemical information science, between CAS and CINF throughout the 58-year-old existence of CINF.

Both CAS and CINF are ACS Divisions, the former an operational division, the latter technical. CAS' vision is to be

"the world's best digital research environment to search, retrieve, analyze, and link chemical and related information,"

and the CINF mission is

"to provide leadership and an environment for the exchange of expertise among the producers and users of information in chemistry and related disciplines worldwide through high quality programs."

It is obvious that both complement each other admirably, and the history of the past 6 decades proves that this synergy worked very well for the chemical information profession and its practitioners.

At the very first symposium of the Chemical Literature Group (the predecessor of CINF within the ACS Division of Chemical Education) at the 106th ACS National Meeting in Pittsburgh in September 1943, E. J. Crane, the Editor of *CA*, presented a paper on "Abstracting and Indexing." Within the next 10-year period, there were a total of 14 papers presented by the *CA* staff on topics ranging from abstracting and indexing to chemical nomenclature to growth of chemical literature and distribution of scientific research activities to pitfalls of transliteration.

Thus, *Chemical Abstracts* (*CA*) and the Chemical Abstracts Service (CAS) as instituted in 1956, was in one form or another on the program of almost every CINF meeting. In the period 1949-1975, when the Division was still the Division of Chemical Literature, every aspect of CAS activities was reported at one time or another, including coverage of specific chemical fields, mechanization and computerization of CAS production operations, description of CAS publications and services, and planned expansions. The same continued for the next period starting in 1975, when the Division became the Division of Chemical Information. The CAS publications and services continued to be the subject of both formal and informal papers, and of occasionally heated discussions ranging in scope from technical content to online searching to pricing.

From the early 1960s to mid-1970s, CAS presented "Open Forums" at the ACS National Meetings. They were not officially part of the CINF activities, but their timing was carefully coordinated with Divisional activities. Many CINF members participated and did not shy away from expressing their opinion and concern. The early topics were CAS plans and progress, especially in the development of the CAS Chemical Registry and modernization of the CAS operations and services. The last such CAS Open Forum at the 169th ACS National Meeting in Philadelphia in April 1975 was devoted specifically to the first attempts at substructure searching of files derived from the CAS Chemical Registry.

The following symposia were selected to highlight close ties between CAS and CINF:

1. "*Chemical Abstracts*: Its Policies, Production, and Use," celebrating the CA 50th anniversary at the 130th ACS National Meeting, in Atlantic City in September 1956.

2. "*Chemical Abstracts* in Transition" at the 166th ACS National Meeting in Chicago in August 1973.

3. "User Reactions to CAS Data and Bibliographic Services" at the 169th ACS National Meeting in Philadelphia in April 1975.

4. "Communication and the Future of Science," celebrating the 75th anniversary of CAS, at the 184th ACS National Meeting in Kansas City in September 1982.

5. "Indexing Chemical Information," honoring Russell J. Rowlett, Jr., the Herman Skolnik Awardee, at the 186th ACS National Meeting in Washington, DC, in September 1983.

6. "Challenges in Moving Towards a New International Chemical Information Order," honoring Dale B. Baker, the Herman Skolnik Awardee, at the 191st ACS National Meeting in New York in April 1986.

7. Gerald G. Vander Stouw (1937-1995) Memorial Symposium at the 210th ACS National Meeting in Chicago in August 1995.

8. "Chemical Identifiers: Names and Structures," Kurt L. Loening (1924-2000) Memorial Symposium, at the 222nd ACS National Meeting in Chicago in August 2001.

For 10 years starting in 1976, CINF sponsored vendor workshops and/or seminars as part of their technical sessions. Unlike at the typical marketing presentations and demonstrations, the participants were asked to present technical-like papers prepared by their staff as well as by users. The first such two seminars were presented by CAS on "Using *CA* Volume Indexes" and "Using *CA* Condensates."

CINF recognized three CAS staff members for their contributions to the development of the theory and practice of chemical information science by giving the CINF Herman Skolnik Award to:

1978 - Fred A. Tate
1983 - Russell J. Rowlett, Jr.
1986 - Dale B. Baker

and others for their contributions to CINF:

1992 - Meritorious Service Award to W. Val Metanomski
1992 - Certificate of Appreciation to Gerard G. Vander Stouw
2006 - Lifetime Membership Award to W. Val Metanomski

CAS staff members who chaired CINF were:

1950 E. J. Crane. who received the highest ACS honor, the Priestley Medal in 1952.
1984 Ralph E. O'Dette
1987 W. Val Metanomski
1994 Gerald G. Vander Stouw
2005 Eileen M. Shanbrom

Other CAS staff members, Ralph E. O'Dette, John T. Dickman, Paul E. Swartzentruber, and Judith E. Watson, represented CINF on the Board of Directors of Documentation Abstracts, Inc.

CAS staff members have also participated in most, if not all, CINF Committees, and their number and different functions are too numerous to list.

Since 1994, CINF has had joint sessions with the ACS Society, later the Joint Board-Council, Committee on CAS, to improve communication between the ACS governance and the CINF members, and to provide a forum for exchanging views and comments on topics of mutual interest.

CAS sponsored many CINF receptions and social hours, among them celebrating the three Herman Skolnik Award receptions, the 75th CAS anniversary in 1982, the 25th CAS Registry anniversary in 1990, the Memorial Symposia receptions, and many others. Currently, CAS is listed on the CINF Web site as a past and current "Platinum Sponsor", which is the most generous category.

There is little doubt that the CAS-CINF cooperation will continue through 2007, the CAS 100th anniversary year, and for many years after that.

A division of the American Chemical Society

IN MEMORIAM

RUSSELL J. ROWLETT, Jr. (1920-2006)

Dr. Russell J. Rowlett, Jr., a former Editor of *Chemical Abstracts* (*CA*) and a pioneer in chemical information science, passed away on November 17, 2006, at the age of 86.

He graduated from the University of Virginia with three degrees, a B.S., a M.S., and Ph.D. in Chemistry. Dr. Rowlett first became associated with *CA* in 1946, when as an industrial research chemist he became a volunteer abstractor. It did not take long for the *CA* Editor E. J. Crane to invite him to join *CA* on a full-time basis. He worked there from 1947 to 1952 on indexing organic-chemistry abstracts. In 1952, he returned to his native Virginia and to industry as patent coordinator for Virginia-Carolina Chemical Corporation and rose to become its Director of Research and Development. In 1960, he became Assistant Director of the Virginia Institute of Scientific Research. He also resumed his association with CAS serving as a consultant to CAS on indexing. The subdivision of the large *CA* Index headings into "categories" and "qualifiers," as we know them today, was the result of his recommendations and experimentation. He presented the proposed improvements at the 5th CAS Open Forum at the 151st ACS National Meeting in Pittsburgh in March 1966.

When Dr. Rowlett returned to CAS in 1967, he became the CAS Editor, and in 1979 the Director of CAS Publications and Services, a position he held until his retirement in 1982. A farewell dinner was hosted by the ACS at the 184th ACS National Meeting in Kansas City in September 1982, where Jean G. Marcali, the 1982 CINF Chair, officially represented CINF and spoke about his achievements. He was an active member of the ACS Division of Chemical Information (CINF) and attended all the ACS and CINF meetings during that period. He participated in CINF symposia and presented papers, mostly related to the progress in modernizing the CAS operations, and on explaining and promoting CAS policies and practices. In 1983, Dr. Rowlett received the CINF Herman Skolnik Award, and the citation read: "For guiding Chemical Abstracts' transition from a manually produced abstracting and indexing publication to a computer-generated family of products and for his leadership in the improvement of patent coverage, the CAS Registry System, timeliness of *CA* Volume and Collective Indexes, and quality control through a shift from volunteer abstractors to full-time professional document analysts utilizing to the fullest extent man-machine interactions." Other honors included a Presidential Citation for research during World War II, the Distinguished Service Award of the Virginia Academy of Science, the Board of Visitors Research Award of the University of Virginia, and the Miles Conrad Lecture Award of the National Federation of Abstracting and Information Services (NFAIS). He was President of NFAIS in 1977-1978.

His earliest papers, published in the *Journal of the American Chemical Society* in 1946-1948 were on the synthesis of antimalarial drugs. His first paper related to chemical information science, published in 1968, on "Computer Pathways to Chemical Information" discussed at some length the path the CAS would take to make "chemical and chemical engineering information widely available to the scientific community in an economic, timely, and useable form." In the same year, he presented a paper on "Training Chemists in the Use of Chemical Abstracts' Services" at the CINF symposium at the 156th ACS National Meeting in Atlantic City in September 1968.

Dr. Rowlett was an outspoken promoter of CAS editorial practices and policies, especially in response to outside criticism of the revised *CA* Index names (more systematic) for the 9th Collective Period in 1972. At the CINF symposium on "User Reactions to CAS Data and Bibliographic Services", presented at the 169th ACS National Meeting in Philadelphia in April 1975, he said, among other things, that he regretted that he "just did not have the intestinal fortitude to go all the way" to eliminate all the trivial names such as formic acid, phenol, and hydrazine. It is not surprising that Dr. Rowlett was a strong advocate for creating and including abstracts in the chemical databases. His Miles Conrad Memorial Lecture, delivered at the NFAIS 23rd Annual Conference in Arlington, Virginia, in March 1981, was on the topic "Abstracts, Who Needs Them?", and his last published paper in the 25th anniversary issue of the *Journal of Chemical Information and Computer Sciences* in 1985, was on "Abstracts and Other Information Filters." After his retirement in 1982 to South Carolina, he enjoyed his hobby of color photography and the recipients of his Christmas cards can attest to his skills.

Those of us who knew him and worked with him will always remember his devotion to the profession and his ever present bow tie.

Submitted by W. Val Metanomski

Chemistry and Art: The Incredible Life Story of Dr. Alfred Bader

By Svetla Baykoucheva

It is not very often that you have a chance to interview someone who has become a famous chemist and businessman and who also happens to be an expert on Old Dutch Masters. In 1951 Dr. Alfred Bader founded the Aldrich Chemical Company. For decades, chemists around the world have been tearing off the covers of the Aldrich catalogs carrying reproductions of beautiful paintings (often from Dr. Bader's personal collection) to decorate the walls of their labs. Articles on art history and alchemical paintings have also appeared in the Aldrich catalog, written (anonymously) by Dr. Bader. Studying art and writing about it has become a passion for Dr. Bader, who is now considered by art historians and art dealers an expert in the field of the Old Dutch Masters. He was named a fellow of the Royal Society of Arts in London. During his life, Dr. Bader was able to combine his career of a distinguished chemist and businessman with his passion for the fine arts.

The extraordinary life story of Alfred Bader began in Vienna, where he was born in 1924. He made it to England in 1938, to avoid Nazi persecution, but in 1940 was suspected to be a Nazi sympathizer and sent to an internment camp in southern Quebec, Canada. Queen's University in Ontario was the only educational institution to accept him after he was released from the camp. After getting a Bachelor's degree in engineering chemistry there, he went to Harvard, where he earned an M.S. and a Ph.D. in chemistry.

Dr. Alfred Bader and his wife Isabel visited the Washington, DC, area in the Fall of 2006. The visit was sponsored by the Office of NIH History and the American Chemical Society. During this visit, Dr. Bader gave three lectures. The first one was held at the University of Maryland and what we heard from him took many of us by surprise. He challenged two major beliefs that chemists have lived with for so many years. Generations of students of chemistry have been taught that two great discoveries—the structure of the benzene ring and the theory according to which the element carbon has four valences—were made by the famous German chemist August Kekulé.

Dr. Bader presented evidence that when Kekulé published his paper on the benzene ring, he had already seen similar models proposed by an Austrian chemist, Josef Loschmidt [1]. According to the legend, Kekulé came to the idea of this particular (ring) structure of benzene after dreaming of a snake eating its own tail. His theory was published in 1865—four years after Loschmidt had already proposed a similar structure, which he published in a little-known book. Dr.Bader walked us through the investigative research that concluded that another chemist, Archibald Scott Couper was the first to propose the theory of the tetravalence of carbon, but it was Kekulé who published it just a month earlier (in May of 1858) than Couper[2].

In his lecture at NIH, "History of Aldrich and Sigma-Aldrich, with Advice to Young Scientists," Dr. Bader gave this advice: "Find a niche to explore in order to become successful entrepreneurs." Dr. Bader also gave a lecture at the Royal Netherlands Embassy, which was celebrating the 400th anniversary of Rembrandt's birth. The topic of the lecture was "The Rembrandt Research Project and the Collector." This project was started in 1968 by a group of experts on Rembrandt for the purpose of investigating whether paintings attributed to the artist were actually painted by him. Some paintings that had previously been considered painted by Rembrandt were re-classified by this group as ones painted by his students. Understandably, the conclusions made by these experts caused many problems for museums and private collectors.

Dr. Bader's collection of paintings currently consists of 130 paintings, including five Rembrandts. He and his wife have donated 150 paintings to Queen's University, which has received many other donations from them, including the 15th-century Herstmonceux Castle in Sussex, England. To pay tribute to his numerous contributions, Queen's named a campus road "Bader Lane," initiated a number of Alfred Bader fellowships, and created three Bader Chairs: the "Bader Chair in Southern Baroque Art," the "Bader Chair in Northern Baroque Art," and one in Organic Chemistry. The Queen of England has honored him with the title "Commander of the British Empire." Dr. Bader is a generous donor to other educational institutions, providing scholarships and awards to chemical students in the United States, Canada, England, the Czech Republic (he has Czech roots), and other countries. He and his wife support "Project Seed," an ACS program for underprivileged students.

Interviewing Dr. Bader for the *Chemical Information Bulletin* was a very unusual experience for me. Besides the fact that I was sitting next to someone who owns five Rembrandts, I was often frustrated with the answers I received to my questions. The most common answer from him was "You'll find the answer to this question in Chapter…of my book." The book he had in mind was his autobiography, "Adventures of a Chemist Collector" (London: Weidenfeld and Nicolson, 1995). I later sent him eight questions in writing that he was kind enough to answer. I am sure his reminiscences about chemistry, its future, and other topics will be of great interest to the readers of the *Bulletin*. In a tribute published in a recent Special Issue of the *Canadian Journal of Chemistry* (vol. 86, 2006) honoring Dr. Bader, Anne and Howard Alper wrote: "Alfred Bader, a true visionary, has had a profound effect on the way chemists do research."

References:

1. Wotiz, John H. (ed) (1993) The Kekulé Riddle: A Challenge for Chemists and Psychologists. Glenview Press, Vienna, IL.
2. Dobbin, Leonard (1934) The Couper Quest. *J. Chem. Educ.* **11**, 331

Interview with Dr. Alfred Bader

Svetla Baykoucheva, editor of the *Chemical Information Bulletin*, did this interview with Dr. Alfred Bader in the Fall of 2006.

SB: *Your life, achievements, and the recognition for these have been extraordinary. Of all the different things and passions that you have been through in your life, from lab research to becoming the founder of the largest and most profitable company for research chemicals in the world today, what have you found most rewarding and why?*

AB: I would like to answer this question on two levels. Professionally, it is the accomplishment of a dream. In September 1967 I wrote in an advertisement: "We can say with the prophet that we have dreamed a dream: to be the chemists' chemist, to save scientists throughout the world millions of man hours by having synthetic building blocks and reagents readily available; to become the world's most competent supplier of organic chemicals. We hope to accomplish this dream." We have accomplished that dream.

On a personal level, meeting Isabel and marrying her has been the most rewarding. She is a wonderful person, has improved me so very much, and together we have been able to help many people.

Alfred Bader with Madeleine Jacobs, Executive Director and Chief Executive Officer of the American Chemical Society.

(Photo by Rachel Petkiewich, adapted and reprinted with permission from *Chem. Eng. News*, October 23, 2006, 84(43), p 65. Copyright 2006 American Chemical Society.)

SB: *In your lecture at the NIH you advised young chemists to find a niche for entrepreneurship. With chemical and pharmaceutical companies merging and forming even bigger companies, isn't Sigma-Aldrich now similar to what Kodak used to be in the 50s for start-ups like Aldrich and how can start-ups compete and survive today, even if they find a niche?*

AB: I hope that Sigma-Aldrich now is totally different from what Kodak used to be in the 50s. Kodak focused on photography, and the fine chemicals business was almost incidental. Kodak left it altogether when real competition arose. To Sigma-Aldrich, supplying research tools of all kinds promptly and in high quality is all important. For a start-up to compete with Sigma-Aldrich, [it] would be very difficult, but I suggested that young entrepreneurs find a niche and that is certainly possible today. During the last years I have helped a number of these—for instance, JRD in England, supplying fluoroaromatics, and Fluorous Technologies in Pittsburgh. The early years are difficult but success is possible.

SB: *You have answered many questions during your presentations at the University of Maryland, NIH, and the Royal Netherlands Embassy in October, 2006. Are there questions that you would have liked people to ask you and that you have not discussed in your book?*

AB: A key question that should be asked by a young entrepreneur is "what are the essentials for success once you have found a niche." They are:

- Treat your customers well. Every question should be answered promptly.
- Try to find the ablest employees and treat them well. In that I often failed at Aldrich in its early days because we were short of cash.
- Try to keep venture capitalists away as long as you can, because most want to invest and control.

SB: *You have lived and traveled in many countries in Europe and North America; you had unique opportunities, through the positions you have had and your personal interests, to see many aspects of life in these countries. What was it like to be a scientist in the 50s and the 60s? Was there more idealism in doing science than it is now? Was there something more prestigious to be a scientist than it is now? And was it the competition between the two worlds that made science so important then? How has science endeavor changed since then and what motivated people then and what motivates them today to go into science and subject themselves to working in smelly labs and sweat over manuscripts?*

AB: I don't think that it was so very different to be a scientist fifty years ago than it is today. I still speak to many great chemists in North America and Britain and see real enthusiasm for research now as I saw it then. What has changed is the esteem in which chemistry is held. Ask the man on the street what first comes to mind when he heard the word chemistry. In 1950, it would have been penicillin and nylon, longer life through chemistry. Today it is pollution and global warming. Our chemical societies have not done as good a job as they could and should have. The situation is most serious in Britain where a number of universities have actually closed their chemistry departments—Kings College, Queen Mary College, and Exeter University. Recently, their five star chemistry department was almost closed down by the University of Sussex. Such adverse publicity has of course discouraged some able youngsters from studying chemistry.

SB: *For chemists who have always believed that Kekulé was the one who first recognized that carbon is tetravalent and also proposed a theory, according to which benzene forms a ring, it is quite shocking to learn from your presentations that, in fact, other people— Archibald Scott Couper and Johann Josef Loschmidt, respectively, were the first to have these ideas, but their contributions remained unknown. Why are you so passionate about this issue—are you on a mission to re-write the chemistry books?*

AB: I would simply like the truth to be known. There is almost certainty that Couper submitted his manuscript on the tetravalence of carbon before Kekulé did. And there is absolute certainty that Loschmidt illustrated over a hundred circular aromatic structures in his book of 1861, five years before Kekulé's paper. And Kekulé saw this book no later than January 1862 when he wrote about it to Erlenmeyer. Am I on a mission to re-write chemistry books? Well, if wanting the truth to be known is being on a mission, yes.

SB: *You are supporting many young scientists through your foundation. What do you see as the biggest challenges today in attracting young people to go into science?*

AB: Isabel and I are not supporting young scientists through our foundation, but through personal gifts. The biggest challenge in attracting young people into chemistry lies in convincing them that chemistry is essential to progress. Sadly, almost ridiculously, chemistry has become a dirty word, yet where would we be, whence could we progress without chemistry?

SB: *When you mention the Aldrich catalog to scientists, they remember the beautiful paintings by old masters on the covers of these catalogs that many of us used to tear off and put them on the walls in the labs. Could you tell us about your tastes in art and what you have in your collection?*

AB: My favorite paintings are Dutch 17th century, my favorite painter is Rembrandt, and my favorite subjects are Biblical. I was very happy when Dr. Jai Nagarkatti, the CEO of Sigma-Aldrich, asked me recently to suggest paintings from my collection for Aldrichimica Acta covers.

Isabel and I are leaving our collection to my alma mater, Queen's University in Kingston, Ontario. Later this year the University will publish a catalogue of that collection, part of which is already in Kingston.

SB: *The 2006 Nobel Prize for Chemistry was awarded to Roger D. Kornberg, a biochemist at Stanford University, for figuring out the way in which information in the DNA of a gene is copied to provide the instructions for building and running a living cell. Aren't they giving a second Nobel Prize for Biology and Medicine and not having one for Chemistry this year? Science is becoming more and more interdisciplinary, but isn't chemistry losing ground and becoming a sub-discipline of Molecular Biology and Biochemistry?*

AB: Chemistry, biochemistry and molecular biology are indeed closely interrelated. But you could not have biochemistry or molecular biology without chemistry, though you can of course have chemistry without biochemistry and without molecular biology. Chemistry is the backbone and I am not concerned when a great biochemist wins the Nobel Prize for Chemistry.

Paving the Road to More Open Access for Chemistry: Interview with Bryan Vickery, Editorial Director of Chemistry Central

Svetla Baykoucheva, editor of the *Chemical Information Bulletin*, talked with Bryan Vickery about Chemistry Central, a new service from BioMed Central publishing peer-reviewed open access research in chemistry.

SB: *Why was it necessary to create Chemistry Central from BioMed Central? What is the business model on which Chemistry Central is built and what are the potential challenges for such a model? How many people are currently employed by Chemistry Central (CC) and are there plans for hiring more people?*

BV: The open access movement has grown quickly over the past few years and took off first in the biomedical sciences. Here, open resources like PubMed and GenBank allowed biomedical researchers to understand the benefits of open access. Other fields have not had that advantage and most of the important resources for chemists are still locked behind subscription barriers. Chemists have traditionally been conservative (compared to biomedical researchers and physicists) in challenging the status quo, but with some areas of chemistry on the decline, and boundaries between disciplines blurring rapidly it is time to act. There has been increasing recognition that the benefits of open access for the publication of original research apply in all fields, and certainly foster collaborations in multidisciplinary areas.

BioMed Central was already publishing chemistry-related information through a variety of titles including *BMC Biochemistry*, *BMC Chemical Biology* and through partnerships such as *Geochemical Transactions* (ACS Division of Geochemistry) and *Beilstein Journal of Organic Chemistry* (published by the Beilstein Institut in cooperation with BioMed Central). We decided to launch Chemistry Central to support this activity, by promoting open access strongly within the chemistry community.

The business model is the same as that for BioMed Central—the *Chemistry Central Journal* that covers all areas of chemistry will levy an article processing charge for all manuscripts accepted for publication. The current major challenge is educating authors that the publication process is *not* free, and that someone, somewhere, needs to pay for it. As the rate of research increases, so does the number of articles being published – and yet many library budgets remain static or are being cut. Many are now acknowledging that publication is part of the research process, and should be supported through research funds.

Chemistry Central currently consists of me and an external Editorial Board of more than 120 highly regarded scientists including, at present, 30 Section Editors. We use the same systems as BioMed Central and share the expertise already built up in the other business units here including Editorial Production, Production, Marketing and Customer Service. As the volume of submissions grows, we will look to grow the chemistry knowledge within BioMed Central.

Bryan Vickery…likes challenges.

SB: *The field of chemical information is still dominated by commercial and societal publishers and open access publishing remains to prove itself as a business model. Is the author-pays model self-sustainable and what are its weaknesses? By the way, are there cases when authors pay from personal funds to publish in your journals?*

BV: The field is dominated by subscription products, be they from commercial or learned societies. These access barriers limit the usage of the information, stifle innovation, and lead to an ineffective marketplace. By introducing Article Processing Charges (the most well-known model for open access, often misleadingly referred to as "author-pays"), a true market is created whereby the author can see the price and judge the quality of service they will receive and compare this against other providers of the same service. Questioning the sustainability of open access seems bonkers to me. At most, this model has the same costs as the toll access model, and therefore they are equally sustainable. The traditional model of publishing is sustainable, by which I mean profitable, because the academic/research community still funnels vast amounts of money into it from library budgets – it is certainly not self-sustaining. The fact that libraries still pay excessive charges to access this literature shows that the market is broken, not that the toll access route is sustainable.

SB: *What will happen if it turns out to be unsustainable? Doesn't this make it possible for a significant part of the record of science to be lost?*

BV: BioMed Central takes archiving as seriously as all publishers do, and should. In fact, because of the open access business model that we operate it is possible for any individual or organization to make a copy of articles published in our journals. BioMed Central deposits the open access articles that it publishes in multiple digital archives around the world to guarantee long-term digital preservation. These archives include: INIST (France), Koninklijke Bibliotheek (The Netherlands), Potsdam University (Germany), PubMed Central. BioMed Central is also participating in the British Library's e-journals pilot project, and plans to deposit copies of all articles with the British Library.

BioMed Central makes article metadata available in compliance with Open Archives Initiative protocols, enabling automated "harvesting" of our research articles for inclusion in any other digital archives. We support non-exclusive digital archiving of research articles by as many international archives as possible, to ensure the security and permanent accessibility of that research. BioMed Central is a participant in the LOCKSS (Lots of Copies Keep Stuff Safe) initiative. LOCKSS will enable any library to maintain their own archive of content from BioMed Central and other publishers, with minimal technical effort and using cheaply available hardware. To facilitate data mining research, the full text XML of all BioMed Central open access research articles is available for ftp download as a ZIP archive.

SB: *Some people have expressed concerns that the open access author-pays model is "ethically flawed," because it raises the risk that bad science could be widely distributed without being subjected to more careful peer review.*

BV: That's an interesting question! All journals live and die by their reputation, and as such are motivated to weed out poor science through peer review. A journal will only attract submissions if it can convince authors that they will achieve credibility and kudos by publishing in it. In fact, many open access journals are demonstrating equally high standards as their toll counterparts (*BMC Bioinformatics*, *PLoS Biology* and *Nucleic Acids Research*). Many of those who have implied that open access journals are tempted to publish more because of the increased revenues work for traditional publishing houses, who at the same time justify increasing their prices by more than inflation because of the increasing number of pages they are publishing.

SB: *With more and more journals becoming freely available on the Internet, how is this going to affect the commercial publishers, as well as the secondary publishers and what could they do to survive?*

BV: All toll-access publishers are starting to feel the pressure from freely-available literature, not just commercial ones, but commercial publishers are likely to come under the greatest scrutiny because of the prices they charge. The transparency which open access brings to the costs of publishing will mean better competition and lower margins for publishers. Making a profit from offering publishing services is not the issue; it is the size of that profit that is in question. The Internet has significantly changed the way we find and access information. As more and more research articles and associated data become freely available, so free indexing services will spring up to support access to it – such as Google Scholar, PubChem. Many secondary publishers built significant revenues on the back of this need to access the primary literature. As technology advances, and communities of researchers build similar tools, on freely supplied data, secondary publishers need to cover more content, from more sources, in greater precision. At the same time, they must also offer broader and easier to use search interfaces.

SB: *How will the proliferation of freely accessible journals change the citation rates of authors and the impact factors of journals?*

BV: The way we measure the importance of an article is changing, but citation is still the major factor. Several studies have concluded that open access research articles have a citation advantage (they are cited earlier and more often) than toll access articles. Clearly, the number of citations will influence the impact factor of the journal.

SB: *How does the way chemists do their research, communicate with each other, and report their findings differ from the way researchers in other disciplines do it?*

BV: The role of chemistry is changing. Many of the areas we are currently most active in are multidisciplinary, and for this reason the way we communicate with other researchers (biologists, physicists, etc.) needs to change too. We do not have the same history of preprinting, for example, that the physics community has, though we did try this with some success at ChemWeb.com. As we continue to collaborate across subjects, we need to open up our information in the same ways. Open access publishing is just as relevant, therefore, to chemistry as it is to biology or medicine.

SB: *Are there any rules for refusing to publish an article in an open access journal just because the instrumentation used to obtain the results was expensive? I recently sent a pre-submission inquiry to an open-access peer-reviewed biomedical journal, to find out whether an article that I had been working on would be appropriate for publication in it. The purpose of the article is to educate biomedical researchers about the existence of some chemistry resources (PubChem, SciFinder Scholar, and DiscoveryGate) that could be very useful in their research. The response from the journal editors was that, as an open access journal, "it would be very unusual...to publish a*

paper that promotes expensive services such as DiscoveryGate, which are out of reach of most of our readers (especially in developing countries)." I don't see how discussing expensive information tools or resources in a paper would be different from discussing results obtained with a mass spectrometer or other expensive equipment. What is your opinion of the decision made by these editors?

BV: Educating a community of researchers about tools and services that could be of benefit to their research is useful, if the article tries to cover as many services as possible and the author has no competing interests. A discussion of what is currently available, both free to use and subscription based, is valuable if a detailed comparison of the services is given, e.g. breadth of coverage, number of compounds/reactions, frequency of updates, accuracy, indexing, use of thesauri and, just as importantly, cost. It is perfectly reasonable to conclude that a subscription service is the most beneficial, provided all alternatives have been assessed.

***SB:** On a personal note, could you tell us something about yourself—how have you come to be where you are now?*

BV: I am a chemist by training and joined ChemWeb.com at its inception in 1997. There I focused on community interaction, what we now call peer-to-peer. My drive was in using web technologies to improve the ways chemists create, access and share information. In many respects what we were doing was ahead of its time. Elsevier acquired ChemWeb.com in 1998, and I stayed with this team until 2002, learning about the migration from print to online publishing. As a marketing tool we offered "free access" to particular Elsevier journals at certain times. The traffic this generated demonstrated to me that a significant number of researchers simply had no access to the literature. I moved to Elsevier Engineering Information to broaden my understanding of secondary publishing, search and linking technologies, before taking charge of Elsevier Advanced Technology – a B2B unit with a portfolio of controlled circulation magazines, newsletters, handbooks and conferences.

My experience here taught me that researchers in commercial organizations, especially in SMEs, had limited access to the primary literature. I strongly believe that publishing is part of the research process, and that access to the primary literature should be free to those who wish to access it. It is this that led me to move to BioMed Central to lead the launch of Chemistry Central.

More information about Chemistry Central is available at *http://www.chemistrycentral.com*

Divisional Committee Meetings and Social Events
233rd ACS National Meeting
Chicago, IL
March 25-29, 2007

Committee Meetings

All meetings on Saturday, March 24 will be held in the McCormick Place (MCC). The CINF Executive meeting is a closed meeting but if you wish to attend, contact the division chair. CINF members are encouraged to attend any of the other committee meetings and all social functions. If you would like information on any CINF committees, contact the Committee chair or the CINF Chair.

CINF Program & Executive Committees (Room MCC E258)

7:30 am – 9 am	Breakfast & Long-Range Planning Meeting
9 am – 12 pm	Program Committee
12 pm – 1 pm	Functionaries Luncheon
1 pm – 5 pm	CINF Executive Committee

CINF Awards, Fund-raising, & Fundraising Committees (Room MCC E261)

9 am - 9:30 am	Awards Committee
9:30 am – 10:30 am	Fundraising Committee
10:30 am – 12 pm	Finance Committee

CINF Publications Committee (Room MCC E262)

9 am – 12 pm	Publications Committee

CINF Education Committee (Room MCC E263)

9 am – 12 pm	Education Committee

CINF Membership and Careers (Room MCC E259)

9 am – 10:30 am	Membership Committee
10:30 am – 12 pm	Careers Committee

Social Events

Sunday, March 25, 2007

6:30 pm – 8:30 pm	CINF Division Welcoming Reception InterContinental Hotel, King Arthur's Court

Tuesday, March 27, 2007

12 pm-1:30 pm	CINF Luncheon (Room MCC N136) (Tickets required)
6:30 pm - 8:30 pm	CINF Reception Hyatt Regency Chicago, Columbus AB

Please check the CINF web site at http://www.acscinf.org, *Chemical & Engineering News*, or the Meeting Program to verify times, locations, and room numbers.

DIVISION OF CHEMICAL INFORMATION (CINF)

Final Program

233rd ACS National Meeting
Chicago, IL, March 25-29, 2007
L. R. Solla, Program Chair

OTHER SYMPOSIA OF INTEREST

Educating for Sustainability (see SUST, Mon)

Sustainability: A World View (see SUST, Sun)

Pressing Challenges and Technical Opportunities for a Sustainable Future (see SUST, Mon)

BMGT Presents an Executive Overview of Energy Programming for the Chicago ACS Meeting (see BMGT, Sun)

SUNDAY MORNING

Section A

Symposium in Honor of Gary Wiggins
Hyatt Regency McCormick – 12 C/D
M. Trimarchi and A. Twiss-Brooks, Organizers

8:40— Introductory Remarks.
8:45—1. Fanfare for an uncommon man: A tribute to Gary Wiggins' contributions to the chemical information profession. F. B. Culp
9:30—2. Changing nature of academic librarianship: Implementing a distributed institutional repository. J. R. Garritano
10:00—3. Hands-on learning: Developing a creativity collection. T. Baldwin
10:30—4. Challenges in developing a global alerting system. L. Sandvoss
11:00—5. Corporate libraries: Evolving as the electronic resources evolve. M. J. Dunker

Computer Assisted Drug Design: Reminiscing about the Future, A Symposium Honoring Yvonne C. Martin
Hyatt Regency McCormick – 10 C/D
Sponsored by COMP, Cosponsored with CINF and WCC

Landmark Chemistry Books of the Twentieth Century: Authors from the University of Illinois
Hyatt Regency McCormick – 21 A
Sponsored by HIST, Cosponsored with Bolton Society, ACS East Central Illinois Section, CHED, and CINF

Using Social Networking Tools to Teach Chemistry
McCormick Place North, N230B, Level 2
Sponsored by CHED, Cosponsored with CINF

SUNDAY AFTERNOON

Section A

Symposium in Honor of Gary Wiggins
Hyatt Regency McCormick – 12 C/D
M. Trimarchi and A. Twiss-Brooks, Organizers

2:00—6. Toward a global chemical knowledgebase. P. Murray-Rust
2:30—7. Integrating text and literature sources with traditional chemoinformatics tools. D. J. Wild
3:00—8. When will the evolution of chemical information on the Internet turn into a revolution? S. R. Heller
3:30—9. The promise and reality of turning chemical literature into information. T. N. Doman
4:00—10. The present and future of informatics in chemistry. T. W. Heritage, P. McHale, T. Hoctor
4:30—Concluding Remarks.

Section B

Computer Assisted Drug Design: Reminiscing about the Future
A Symposium Honoring Yvonne C. Martin
Hyatt Regency McCormick – 12 B
Cosponsored with COMP, and WCC
A. Tropsha, Organizer; O. F. Güner, Organizer, Presiding

2:00—11. Bibliometric analysis of chemoinformatics. P. Willett
2:30—12. Still searching for the perfect fingerprint. R. D. Brown
3:00—13. Virtual screening for new chemotypes using compound similarity measures. I. A. Muegge
3:30—Intermission.
3:50—14. Lead-like, drug-like or "pub-like": How different are they? T. I. Oprea
4:20—15. Computer-aided drug design: The next twenty-five years. J. Van Drie
4:50—16. What I learned from a career in computer-assisted molecular design. Y. Martin

Landmark Chemistry Books of the Twentieth Century: Authors from the University of Illinois
Hyatt Regency McCormick – 21 A
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Using Social Networking Tools to Teach Chemistry
McCormick Place North, N230B, Level 2
Sponsored by CHED, Cosponsored with CINF

MONDAY MORNING

Section A

Chemistry Applications Involving Data Analysis and Visualization
Hyatt Regency McCormick – 12 C/D
Cosponsored with COMP
A. J. Trippe, Organizer

9:00—17. ChemDB: A public database of small molecules and related chemoinformatics resources. J. Chen, E. Linstead, S. J. Swamidass, D. Wang, Y. Dou, P. F. Baldi
9:30—18. Characterization of spectra and other analytical data via combination of two methods: Multivariate processing and overlap density heatmap visualization. G. M. Banik, M. D'Souza, M. Scandone
10:00—19. Novel visualization techniques for the analysis of molecular properties. J. Corkery, B. Kelley, K. Schmidt, M. McGann, R. Tolbert, A. Nicholls
10:30—20. Spectral clustering of chemical datasets. R. Guha, D. J. Wild
11:00—21. Data analysis and visualization: Some case studies. D. Walter

Section B

This One is Just Right! Information Resources for Small Colleges
Hyatt Regency McCormick – 12 B
Cosponsored with CHED
A. B. Twiss-Brooks, Organizer

8:25—Introductory Remarks.
8:30—22. Right now, approximating just right! Chemical information resources for small/all (Canadian) colleges and universities. L. I. Lancaster, B. M. Lynch
9:00—23. Information literacy in the chemistry major: Stretching our money at Augustana College. C. Ghinazzi, D. Jensen Jr., R. Narske
9:30—24. Delivering chemical information in the age of tight budgets: Faculty and librarian cooperation at Trinity University. S. M. Bachrach, B. MacAlpine
10:00—25. SciFinder Scholar, Chemical Abstracts Student Edition or General Science Abstracts: Which should you ask your library to purchase? P. Kirkwood
10:30—26. Make the most of what you have: Use Scifinder Scholar as a collection development tool. D. R. Resetar
11:00—27. Meeting the challenge of "The New Biology" for college libraries and librarians in the post-genomic era. F. Stoss

MONDAY AFTERNOON

Section A

Chemistry Applications Involving Data Analysis and Visualization
Hyatt Regency McCormick – 12 C/D
Cosponsored with COMP
A. J. Trippe, Organizer

1:30—28. Analysis of documents pertaining to the phenomena of RNA interference. B. Sweet
2:00 —29. Uncovering competitive technology intelligence from chemical information in patent databases. B. Stewart
2:30—30. Text visualization in chemistry: Roadblocks and rewards. J. D. Saffer
3:00—31. A new key-based molecular fingerprinter for visualization and data analysis in compound clustering, similarity searching, and substructure commonality analysis. N. E. MacCuish, J. D. MacCuish
3:30—32. Selection of commercially available lead discovery compounds potentially active against P. falciparum methionine aminopeptidase by substance analysis and clustering. A. J. Trippe
4:00—Intermission.
4:30—Open Meeting. CINF Division.
5:00—Open Meeting. Committees on Publications and Chemical Abstracts Service.

Section B

This One is Just Right! Information Resources for Small Colleges
Hyatt Regency McCormick – 12 B
Cosponsored with CHED
A. B. Twiss-Brooks, Organizer

1:55—Introductory Remarks.
2:00—33. Effective teaching requires comprehensive reaction databases. V. Eigner Pitto, J. Eiblmaier, H. Kraut, H. Saller, P. Loew
2:30—34. ChemgaPedia Enzyclopedia: A new electronic visualization program for teaching and learning organic chemistry. G. Grethe
3:00—35. Creation of an instructional module for small college science librarians highlighting free chemistry resources and their use in undergraduate instruction. S. K. Cardinal, C. L. Newsom
3:30—36. One answer: On-line access to chemical information at community colleges, but what are the questions? R. G. Landolt

Beyond the Bench: Non-Traditional Careers in Chemistry
McCormick Place South, S504A, Level 5
Sponsored by CHAL, Cosponsored with CHED, CINF, SCHB, WCC, and YCC

MONDAY EVENING

Section A

Sci-Mix
Hyatt Regency Chicago – Riverside Center
L. R. Solla, Organizer

8:00 PM–10:00 PM
37. A novel cheminformatics study of non-peptidic HIV protease inhibitors using machine learning and statistical tools. B. Bhhatarai, S. Alla, C. R. Bernier, R. Garg, S. Kumar
38. Pharmacokinetic modeling of anti-HIV protease ritonavir analogs. R. C. Kasara, B. Bhhatarai, R. Garg
39. Understanding the effect of benchmark dataset composition on the validation and optimization of ligand based virtual screening using self-organizing maps. S. G. Rohrer, K. Baumann
40. Data mining of NIH DTP human tumor cell line screen data for anticancer drug discovery. H. Wang, D. J. Wild
41. A method for calculating the pKa values of small and large molecules. J. Szegezdi, F. Csizmadia
42. NCL-3D: A 3-D natural compound library for computer-aided anticancer drug discovery. Z. Hu, W. M. Southerland
43. Classification of proteomics data by kernel methods. K. Tang, T. Li
44. Fabrication of chemical and engineering devices. K. Choi
45. Gas chromatography determining 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 in electrosynthesis reaction solution. S. Chengying, L. Zhisheng, W. Liucheng, Z. Jianhong, Z. Mingxing
46. Loop fitting with a combined force field and shape potential. B. P. Kelley, G. Skillman, M. Stahl, S. Wlodek, A. Nicholls
47. Optimization of LC/APCI-MS quinone isomer separation. A. Gonzalez, K. L. Foster, G. Hanrahan

17-18, 35,48, 68, 73, 79, 81. *See subsequent listings.*

TUESDAY MORNING

Section A

The Evolving Network of Scientific Communication
Hyatt Regency McCormick – 12 C/D
Cosponsored with COMSCI
D. P. Martinsen, Organizer

8:30—Introductory Remarks.
8:35—48. Implementation of scientific "blogging" into chemical laboratory research. A. C. Fahrenbach, A. H. Flood
9:00—49. Filling the void: Organizations and social networking. D. S. Loney
9:25—50. New global communication process in thermodynamics and its impact on quality of published experimental data. M. Frenkel, R. D. Chirico, V. V. Diky, C. D. Muzny, Q. Dong, K. N. Marsh, J. H. Dymond, W. A. Wakeham, S. E. Stein, E. Koenigsberger, A. R. H. Goodwin, J. W. Magee, M. S. Thijssen, W. M. Haynes, S. Watanasiri, M. Satyro, M. Schmidt, A. I. Johns, G. R. Hardin
9:50—51. Semantic chemical publishing. N. E. Day, P. T. Corbett, P. Murray-Rust
10:15—52. Data lifecycle and curation of laboratory experimental data. T. Hey
10:40—53. The semantic wiki as a model for an intelligent chemistry journal. H. S. Rzepa
11:05—54. Standard domain ontologies: The rate limiting step for the "Next Big Change" in scientific communication. A. Renear

Section B

Sustainable Resources: Science and Information Sources
Hyatt Regency McCormick – 12 B
Cosponsored with AGRO, FUEL, and SUST
B. Town, L. R. Solla, and S. Swann, Organizers

8:30—Introductory Remarks.
8:35—55. Designing a new industry for sustainability: Life cycle analysis for the emerging bioeconomy. B. E. Dale
9:15—56. Emerging technologies for renewable materials in the UK and EU. J. Tomkinson, A. Hamer
9:45—57. Biofuels: From an information perspective. K. Sands
10:15—58. Survey of information resources covering renewable fuels, chemicals and energy. S. Swann
10:45—Discussion.

Communicating Chemistry
McCormick Place North, N227B, Level 2
Sponsored by CHED, Cosponsored with CINF

TUESDAY AFTERNOON

Section A

The Evolving Network of Scientific Communication
Hyatt Regency McCormick – 12 C/D
Cosponsored with COMSCI
D. P. Martinsen, Organizer

2:00—59. Enhancing the web experience with ACS journals. E. Jabri, S. Tegen
2:25—60. Podcasting and social bookmarking at Nature. J. C. Scott, T. Hannay
2:50—61. Beyond searching: Adding increased value to today's scientific databases. M. Dennis
3:15—62. Google Scholar: The adventure continues. A. Acharya
3:40—63. Recommendation systems for research. M. F. Krellenstein
4:05—64. Collaborative filtering in a scholarly context. G. Papadopoulos
4:30—65. Modeling the scholarly community from usage data. J. Bollen

Section B

Advances in 3-D Pharmacaphores and 3-D Searching
Hyatt Regency McCormick – 12 B
O. F. Güner, Organizer

2:00—66. Ligand binding and circular permutation modify residue interaction network in DHFR. Z. Hu, D. Bowen, W. M. Southerland, Y. Pan, A. del Sol, R. Nussinov, B. Ma
2:30—67. Chemical superposition and pharmacophore elucidation by SCAPFOld: Self-consistent atomic property field optimization. M. Totrov
3:00—68. Surface interaction property based similarity searching with the eHiTS Filter. D. Reid, Z. Zsoldos, B. Sadjad, A. Simon
3:30—69. Effect of query structure on specificity for flexible 3-D searching. P. R. Wolohan, R. D. Clark
4:00—70. Adventures in shape space. P. Hawkins
4:30—71. New self-organizing algorithm for molecular alignment and pharmacophore development. D. Bandyopadhyay, D. K. Agrafiotis

5:00—72. Analyzing docking results by substructure search in Euclidean space. T. Zuhl, M. Gastreich, C. Lemmen, H. Claußen

Agricultural Biomass, Biobased Products, and Biofuels: Defining the Challenges
McCormick Place South – S103D, Level 1
Sponsored by AGRO, Cosponsored with FUEL, SUST, CELL, and CINF

Communicating Chemistry
McCormick Place North – N227B, Level 2
Sponsored by CHED, Cosponsored with CINF

WEDNESDAY MORNING

Section A

Advanced Mining and Use of Life Science Information
McCormick Place North – N134, Level 1
Cosponsored with CSA Trust, BIOT, BTEC, MEDI, and COMP; D. J. Wild, Organizer

8:25—Introductory Remarks.
8:30—73. Using text mining software to identify drug, compound, and disease relationships in the literature. D. A. León
8:55—74. Descriptive and predictive models for in-vitro human cancer cell growth screens. R. Kho, M. Correll, J. Ratcliffe
9:20—75. Toward linking small molecules to biological processes in RSC publications. C. R. Batchelor
9:45—76. Applying data mining approaches to further understanding chemical effects on biological systems. C. Yang, A. M. Richard
10:10—77. Pharmaceutically intuitive chemical space visualization: Enabling the discovery of structural relationships and associated biologically relevant properties between substances. A. J. Trippe
10:35—Intermission.
10:45—78. Mining and visualizing the chemical content of large databases. H. O. Villar, M. R. Hansen, J. Hodges
11:10—79. Developing semantic web service for chemical informatics. X. Dong, D. J. Wild
11:35—80. A tiered screening protocol for the discovery of structurally diverse HIV Integrase inhibitors. R. Guha, D. Dutta, D. J. Wild, T. Chen

Section B

On Beyond Keyword Searching: Advanced Instruction in Chemical Information
McCormick Place North – N135, Level 1
Cosponsored with CHED
F. B. Culp and L. R. Solla, Organizers

8:25—Introductory Remarks.
8:30—81. Something old, something new: Creating an undergraduate chemical information seminar. T. M. Vogel, B. A. Sawrey
9:00—82. Mmm...vanillin: Reaching graduate students through ice cream seminars. J. R. Garritano
9:30—83. Hands-on remote training in chemical information. P. Renery
10:00— Intermission.
10:10—84. Taking the graduate classroom teaching a step further. M. Shokeen, K. T. Powell, K. L. Wooley, C. J. Anderson
10:40—85. Educating graduate students in chemical information. E. Zass, M. P. Braendle
11:10—86. Librarian office hours: An old tool with a new use to improve graduate education. B. Wang
11:40—87. Deconstructing molecules in an organic information course. J. N. Currano

Agricultural Biomass, Biobased Products, and Biofuels: Process and Product Control
McCormick Place South – S103D, Level 1
Sponsored by AGRO, ed with FUEL, SUST, CELL, and CINF

Communicating Chemistry
McCormick Place North – N227B, Level 2
Sponsored by CHED, Cosponsored with CINF

High Throughput Screening and Drug Discovery
McCormick Place Lakeside – E353C, Level 3
Sponsored by MEDI, Cosponsored with CINF

WEDNESDAY AFTERNOON

Section A

Great Lakes Research: Environmental Issues for a Freshwater Ecosystem
McCormick Place North – N134, Level 1
Cosponsored with ENVR and SUST
A. B. Twiss-Brooks, Organizer

1:25—Introductory Remarks.
1:30—88. Fifty years of the International Association for Great Lakes Research. M. F. Simcik
2:00—89. Mass balance models for persistent, bioaccumulative, toxic chemicals (PBTs) in the Great Lakes: Application to Lake Ontario. J. V. DePinto, R. G. Kreis Jr.
2:30—90. Contaminant mass balance model applications in the Great Lakes: Lower Fox River/Green Bay and Lake Michigan. R. G. Kreis Jr., J. V. DePinto
3:00—Intermission.
3:10—91. PBDEs and PCBs in the sediments of the Great Lakes: Distributions, trends, influencing factors, and implications. A. Li, K. Rockne, N. C. Sturchio, W. Song, J. C. Ford, D. R. Buckley, W. J. Mills
3:40—92. The Great Lakes offshore biological dessert and the nearshore slime around the tub. D. C. Rockwell
4:10—93. Moving the region toward meaningful Great Lakes restoration. K. Meyer
Agricultural Biomass, Biobased Products, and Biofuels: Process Characterization
McCormick Place South – S103D, Level 1
Sponsored by AGRO, Cosponsored with FUEL, SUST, CELL, and CINF

THURSDAY MORNING

Section A

General Papers
Scientific Information Resources
McCormick Place North – N134, Level 1
L. R. Solla, Organizer

9:30—94. Index to physical, chemical and other property data: What's next? O. B. Sparks, L. Shackle
10:00—95. Open software and open standards may help cease the fire. T. Helmus, S. Kuhn, P. Murray-Rust, M. Rojas Cherto, H. S. Rzepa, O. Spjuth, C. Steinbeck, J. E. S. Wikberg, E. Willighagen
10:30—96. IUPAC name generation: Challenges and evaluation. D. Bonniot

Agricultural Biomass, Biobased Products, and Biofuels: Improving Bioproduct Design
McCormick Place South – S103D, Level 1
Sponsored by AGRO, Cosponsored with FUEL, SUST, CELL, and CINF

THURSDAY AFTERNOON

Section A

General Papers
New Developments in Chemical Information
McCormick Place North – N134, Level 1
L. R. Solla, Organizer

1:00—97. Information content in organic molecules: Brownian processing of ribonucleases. D. J. Graham, J. L. Greminger
1:30—98. Chemical Terms, a language for cheminformatics. G. Pirok, N. Máté, J. Szegezdi, Z. Mohacsi, S. Csepregi, I. Cseh, A. Szabo, M. Vargyas, F. Csizmadia
2:00—99. Accounting for 3-D descriptors of conformers in QSAR modeling. S. K. Dogra, A. Das, K. Subramanian

Agricultural Biomass, Biobased Products, and Biofuels; The Cellulosic Challenge
McCormick Place South – S103D, Level 1
Sponsored by AGRO, Cosponsored with FUEL, SUST, CELL, and CINF

ABSTRACTS

CINF 1 Fanfare for an uncommon man: A tribute to Gary Wiggins' contributions to the chemical information profession. F. Bartow Culp, Mellon Library of Chemistry, Purdue University, 504 West State Street, West Lafayette, IN 47907-2058, bculp@purdue.edu

For over 30 years, Gary Wiggins has ably served the information community as librarian, author, administrator, and mentor. He has been a trailblazer in many areas of our profession. Gary has been instrumental in the development of the Chemical Information specialty at the Indiana University School of Library and Information Science, authored a standard textbook on the subject of chemical information, and created the CHMINF listserv, among his many other accomplishments. In this symposium, we honor his contributions to our profession.

CINF 2 Changing nature of academic librarianship: Implementing a distributed institutional repository. Jeremy R Garritano, Mellon Library of Chemistry, Purdue University, 504 W. State St., West Lafayette, IN 47907, jgarrita@purdue.edu

Librarians at Purdue University are adapting to the implementation of a distributed institutional repository (DIR). Traditionally, a librarian's role in the cycle of scholarly communication has been focused on the products of research: books, articles, dissertations, etc. The DIR is pushing the librarian's role further back in the cycle by assisting and advising researchers on how their data can best be collected, tagged, and stored. In some cases, librarians are even becoming embedded within research groups. Once in the DIR, these data sets and other non-traditional types of information are just as accessible as books and journal articles. The DIR is opening up new avenues of research for librarians and allowing for renewed interactions with faculty across disciplines. This paper will look at how the role of an academic librarian is changing in regard to the implementation of a DIR on campus, including successes and pitfalls.

CINF 3 Hands-on learning: Developing a creativity collection. Ted Baldwin, College of Applied Science Library, University of Cincinnati, 2220 Victory Parkway, ML0103, Cincinnati, OH 45206-2839, Fax: 513-556-4217, Ted.Baldwin@uc.edu

Academic libraries are continuously expanding and redefining their roles, in order to retain their relevance and contribute to the learning objectives of their institutions. This presentation will describe how a library serving undergraduate students in the applied sciences has carved out a new role through the development of a creativity collection. The collection contains hands-on learning resources to spark learning and innovation, including chemical modeling kits, construction kits, scientific toys, and art supplies. These items feature prominently in the library, and have been utilized in both formal and informal learning settings. The speaker will detail sources of inspiration for the collection, the contents and collecting parameters, and the impact of the collection on undergraduate perceptions of libraries.

CINF 4 Challenges in developing a global alerting system. Leah Sandvoss, Research Informatics, Pfizer, 10677 Granby Way, San Diego, CA 92126

In the competitive environment of the pharmaceutical industry, keeping scientists, clinicians, and marketing professionals informed of the latest public information on competing products and companies is key to understanding the position of internal drug projects. In order to track this information, many companies have information specialists whose sole responsibility it is to deliver cutting edge information to end-users. The information in question can come from a variety of sources, and include content types such as news, literature, patents, and pipeline reports. The most up-to-date content is often called an "alert" and the delivery of such referred to as the "selective dissemination of information (SDI)". The alert sources combined often include overlapping references, and as such are delivered separately in a number of different formats. The differing formats can be somewhat overwhelming and confusing for the end-user. A plausible solution to this challenge is to create an overarching system to combine the delivery of the different information types from multiple sources. Ultimately, the results are presented in one unified interface, in a common format, with links to full-text articles where available. Although collating this information through such a system might seem a simple task, there are many challenges to overcome. This presentation will discuss some of the major issues which can arise in developing a global alerting system.

CINF 5 Corporate libraries: Evolving as the electronic resources evolve. Marilynn J Dunker, Intellectual Property & Business Information Services, The Procter & Gamble Company, 6280 Center Hill Ave, BB3N286, Cincinnati, OH 45231, Fax: 513-277-7219, dunker.mj@pg.com

Faced with serving a global community of researchers in a large consumer goods company, the libraries at Procter & Gamble have been evolving. What was once a series of local physical libraries with a few databases on a LAN has turned

in to a global information research organization providing a virtual library and service to researchers regardless of location. The development & evolution of electronic resources has been one of the driving forces.

CINF 6 Toward a global chemical knowledgebase. Peter Murray-Rust, Unilever Centre for Molecular Science Informatics, Department of Chemistry, University of Cambridge, Lensfield Road, CB2 1EW Cambridge, United Kingdom, pm286@cam.ac.uk

The world's approach to information is being transformed by pervasive resources such as Google, Flickr, YouTube, and many others. In our homes we presume instant access to knowledge - reference, news, services, etc. This is rapidly changing many aspects of scientific information, including semantic data, new methods or publication, automated and customised readers. The academic world is reacting patchily, with some exciting innovations in Open repositories and instant publication, but is also tied to conventional methods of scholarship and dissemination. This presentation will show live demos of what the future for chemistry might look like - a global knowledgebase without a fixed centre where machines remove the drudgery of search, calculation and analysis. The primary challenge is not technology but the social adoption of a radically new world.

CINF 7 Integrating text and literature sources with traditional chemoinformatics tools
David J Wild, School of Informatics, Indiana University, Bloomington, IN 47408, djwild@indiana.edu

This presentation will review developments in text searching, natural language processing and the semantic web that enable structures to be automatically extracted from documents and fed to chemoinformatics tools like docking, cluster analysis and similarity searching. Examples will be given of the use of web service workflows for performing scientifically interesting tasks on structures extracted from literature, and the potential future directions for the exploitation of text and literature information will be discussed.

CINF 8 When will the evolution of chemical information on the Internet turn into a revolution? Stephen R. Heller, Physical and Chemical Properties Division, NIST, Gaithersburg, MD 20899-8380, srheller@nist.gov

Decades ago computers were devices known and familiar to only a few people around the world. Today computers and the Internet are known and familiar to virtually everyone person on earth. In the area of chemistry, first computers and then the Internet have led to an evolution of information and data available to all. The Internet has also led to a revolution in the type and amount of information available. This presentation will describe where chemical information was just a few decades ago, where it is now, and when this slow, but mounting evolution of information and data are likely to become a revolution and change the world of information providers. Open Access journals (e.g., Beilstein Journal of Organic Chemistry and Chemistry-Central), Open Source standards (e.g., InChI), and Open Data (e.g., NCI and PubChem) will provide examples of this changing world.

CINF 9 The promise and reality of turning chemical literature into information. Thompson N. Doman, Eli Lilly and Company, Lilly Corporate Center, Indianapolis, IN 46285, DOMAN_THOMPSON_N@Lilly.com

The fields of computational chemistry and especially chemical informatics have advanced greatly in recent years, and vastly more sophisticated analyses of chemical results are possible these days. However, due to technical, business, and political realities, there are still significant barriers to conducting these analyses in a timely fashion. Using a recent case study, I will highlight the challenges in turning traditional 2D chemical graphs found in many chemistry-related publications into 3D molecular models.

CINF 10 The present and future of informatics in chemistry. Trevor W. Heritage, Chief Scientific Officer, Elsevier MDL, 2440 Camino Ramon, Suite 300, San Ramon, CA 94583, T.Heritage@mdl.com, Phil McHale, Solutions Product Management, Elsevier MDL, and Tim Hoctor, Academic, Government, & International Markets, Elsevier MDL

Chemistry has evolved from hardcopy textbooks and journals to online access and directly to actionable data. This program will outline how changing technology drives informatics systems. In particular we will examine the state of the art in terms of electronic access to chemistry data, including integrated content systems from commercial data providers, as well as a discussion of future trends such as Web services.

CINF 11 Bibliometric analysis of chemoinformatics. Peter Willett, Department of Information Studies, University of Sheffield, Western Bank, Sheffield S10 2TN, United Kingdom, p.willett@sheffield.ac.uk

Chemoinformatics has come to the fore as a specialist discipline quite recently. This presentation will review the place of chemoinformatics in the chemical literature, highlighting the core journals in which chemoinformatics articles appear and the current main areas of research, and conducting citation analyses of the principal research groups and research workers.

CINF 12 Still searching for the perfect fingerprint. Robert D Brown, SciTegic, Inc, 9665 Chesapeak Dr. #401, San Diego, CA 92123, Fax: 858 279 8804, rbrown@scitegic.com

In the mid 90s the author, together with Yvonne Martin, published research results that sought to identify the most appropriate structural descriptors and clustering methods for library design and lead optimization. The goal was to identify methods that were best able to group similarly active molecules together and separately from inactives. The results, which were somewhat surprising at the time, showed that fingerprints based on 2D structure outperformed those based on 3D, and that in particular a fingerprint from the MDL MACCS system was preferred. Brown and Martin then showed that the 2D descriptors better captured information relevant to ligand-receptor binding. The quest for better fingerprints has continued within many research groups since then and most recently circular substructure fingerprints have shown good utility in activity prediction. In this paper, we review the original fingerprint work, discuss some of the latest approaches to fingerprint descriptors, including the development of a tautomer-independent circular substructure fingerprint, and compare the original results to those from the latest descriptors.

CINF 13 Virtual screening for new chemotypes using compound similarity measures
Ingo A. Muegge, Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals Inc, 900 Ridgebury Road, Ridgefield, CT 06877, imugge@rdg.boehringer-ingelheim.com

Compound similarity-based virtual screening experiments have been conducted using a variety of different drug targets, 2D and 3D descriptors, and ranking approaches. Particular attention has been paid to assembling data sets such that each active compound represents its own unique chemotype. This condition guarantees that a similarity recognition event between active compounds constitutes a scaffold hopping event at the same time. In a series of virtual screening studies involving 7 drug targets with the number of actives varying between 4 and 13 and 9969 MDDR compounds as negative controls it has been found that atom pair descriptors, SciTegic fingerprints, and 3D pharmacophore fingerprints combined with ranking, voting, and consensus scoring strategies perform well in finding new bioactive scaffolds. The performance of descriptors largely depends on the structure of the database of compounds subjected to a virtual screen. If topological biases exist between actives, as is often the case when literature data sets are used in recall experiments, 2D topological fingerprints often perform best. However, if such biases do not exist as often the case when independent compound collections are screened, pharmacophore descriptors perform well. A comparison of virtual screening performances achieved with structure-based and compound-similarity based methods will be presented also.

CINF 14 Lead-like, drug-like or "pub-like": How different are they? Tudor I. Oprea, Division of Biocomputing, University of New Mexico School of Medicine, MSC 084560, 1 University of New Mexico, Albuquerque, NM 87131-0001, toprea@salud.unm.edu

Trends in probe, lead and drug discovery are evaluated using the following compound categories: 385 leads, and the 541 associated drugs; "active" (152) and "inactive" (1488) compounds from the Molecular Libraries Small Molecule Repository (MLSMR) tested by HTS; "active" (46) and "inactive" (72) compounds from Nature Chemical Biology (NCB) tested by HTS; MDDR drugs (phases I, II, III and launched); and medicinal chemistry compounds from WOMBAT, split into high-activity (5,787 compounds with nM activity) and low-activity (30,691 with ìM activity). Molecular weight (MW), complexity, flexibility, the number of hydrogen bond donors and acceptors, the octanol/water partition coefficient estimated by CLogP and ALOGPS, the intrinsic water solubility estimated by ALOGPS and Rule of five (Ro5) violations were considered. Using the 50% and 90% distribution moments, we noticed no difference between leads and MLSMR/NCB "actives". "Inactives" from NCB and MLSMR exhibit similar properties. These combined sets ("Actives", 569 compounds) are less complex, less flexible, and more soluble than drugs (1,688 drugs), and significantly smaller, less complex, less hydrophobic and more soluble than the 5,787 high-activity WOMBAT compounds. These trends indicate that chemical probes ("pub-like") are similar to leads with respect to complexity, solubility, and hydrophobicity

CINF 15 Computer-aided drug design: The next twenty-five years. John Van Drie, Novartis Institutes for Biomedical Research, 250 Mass Ave, Cambridge, MA 02139, johnvandrie@mindspring.com

In a somewhat-serious, somewhat-lighthearted way, prognostications will be made on what the future holds for our field. Drawing upon the past, and in particular on the many roles that Yvonne Martin has played in that past, some possible future evolutionary paths of this field will be sketched. The areas for greatest potential impact on drug discovery and design will be highlighted. Also, today's key outstanding issues will be framed, to draw attention to these issues for students and others new to this field, in the hope that they will be the biggest determinant of what the future holds for CADD.

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CINF 16 What I learned from a career in computer-assisted molecular design. Yvonne Martin, private consultant, 2230 Chestnut St., Waukegan, IL 60087, Fax: 847-937-2625, yvonnecmartin@comcast.net

A fads come and go in CAMD, certain truisms remain: 1.) It is better to use an old or inaccurate method to help solve the real problem of your experimental collaborators than to use a fancy method that solves a problem that they don't have. 2.) It is often more fruitful to use computational methods to help set priorities than to use them to suggest new, and potentially time-consuming, directions. 3.) Encourage your collaborators to come up with tests of your predictions. This way if the predictions are correct, everyone is happy and if they are incorrect, you have more work to do but have gained scientific respect. 4.) Pay attention to the needs of your collaborators. If you don't have a method to solve a particular problem, let it rest and someday someone, maybe you, will come up with a solution.

CINF 17 ChemDB: A public database of small molecules and related chemoinformatics resources. Jonathan Chen, Erik Linstead, S. Joshua Swamidass, Dennis Wang, Yimeng Dou, and Pierre F. Baldi, Institute for Genomics and Bioinformatics, School of Information and Computer Sciences, University of California, Irvine, Irvine, CA 92697, chenjh@uci.edu

ChemDB is a chemical database containing over 4M commercially available small molecules. The data is publicly available over the Web for download and for targeted search using a variety of powerful methods. The chemical data includes predicted 3D structure, ideal for docking and other studies, and physicochemical properties such as solubility. Recent developments include optimization of chemical structure (and substructure) similarity search algorithms enabling full database searches in less than a second. A text-based search engine allows efficient searching of compounds and over 65M vendor annotations, such as systematic and common names, and fuzzy text matching capabilities that yield productive results even when the correct spelling of a chemical name is unknown. Finally, built in reaction models enable searches through virtual chemical space, consisting of hypothetical products readily synthesizable from the building blocks in ChemDB. ChemDB is available at http://cdb.ics.uci.edu.

CINF 18 Characterization of spectra and other analytical data via combination of two methods: Multivariate processing and overlap density heatmap visualization. Gregory M. Banik1, Michelle D'Souza1, and Marie Scandone2. (1) Bio-Rad Laboratories, Informatics Division, 3316 Spring Garden Street, Philadelphia, PA 19104, gregory_banik@bio-rad.com, (2) Informatics Division, Bio-Rad Laboratories, Inc

The use of methods such as Principal Component Analysis (PCA) to perform multivariate analyses on spectral and chromatographic data has used for years in the field of analytical chemistry. In this study, we will introduce a new method that combines a second—patent pending—technology known as Overlap Density Heatmap (ODH). ODH allows the user to explore data similarities and dissimilarities in large databases by providing information about the most and/or least commonly occurring spectral or chromatographic features in a data set(s). In this session, the combination of these two approaches for spectroscopic analysis will be explored through a series of successful applications and case studies.

CINF 19 Novel visualization techniques for the analysis of molecular properties. Joseph Corkery, Brian Kelley, Kevin Schmidt, Mark McGann, Robert Tolbert, and Anthony Nicholls, OpenEye Scientific Software, American Twine Office Park, 222 Third Street, Suite 3211, Cambridge, MA 02142, Fax: 617-374-6575, jcorkery@eyesopen.com

Visualization remains an important tool in the analysis of molecular properties. We have developed new methods to aid in the small and large-scale analysis of molecular properties and the subsequent communication of information to others. For example, we now have a unique visual style of mapping specific atom, bond or molecule properties back onto the source atom or bond. Such mappings can be applied to properties from a variety of sources including pKa, solubility, strain energy, QSAR/reverse-QSAR, goodness-of-fit to electron density, docking scores, and many others. A potential-field style of visualization has also been developed for Cartesian-dependent properties such as ligand-protein interactions. These visual tools coupled to integrated data analysis can provide an excellent platform for elucidating specific areas for ligand optimization. Examples will be presented from docking, 3D shape comparisons, and crystallography.

CINF 20 Spectral clustering of chemical datasets. Rajarshi Guha and David J Wild, School of Informatics, Indiana University, 1130 Eigenmann Hall, 1900 E 10th Street, Bloomington, IN 47406, rguha@indiana.edu

Spectral clustering utilizes matrix decompositions to transform a dataset of n-dimensions to a lower dimensional subspace within which clustering can be performed. The

most common decomposition used is the SVD and it has been shown that the SVD of a data matrix represents a clustering. We investigate the use this approach in the clustering of an Ames mutagenecity dataset and an aqueous solubility dataset. We also investigate the use of the fast SVD algorithm which approximates the SVD of a matrix. Our results indicate that the approximation algorithm leads to an order of magnitude speedup. Furthermore the clustering results are similar to those obtained using traditional partitional clustering algorithms.

CINF 21 Data analysis and visualization: Some case studies. Donald Walter, Customer Training, Thomson Scientific, 1725 Duke Street Suite 250, Alexandria, VA 22314, Fax: 703 519 5838, Don.Walter@Thomson.com

Collecting, sorting and analyzing information from the technical and patent literatures to give an unbiased understanding of the scientific and competitive landscapes can be difficult. Each step involves choosing techniques which may skew the answers. Often one approach leads to hypotheses which must be tested with other approaches. In this presentation, we will compare and contrast different approaches to understanding the literature and competitive intelligence on a given question. For example, we will see whether, the patent and technical literatures lead to the same picture of the state of the art; illustrate the use of perhaps little known tools in common applications, as well as some specialized tools; and more.

CINF 22 Right now, approximating just right! Chemical information resources for small/all (Canadian) colleges and universities. Lai Im Lancaster and Brian Maurice Lynch, Department of Chemistry and Angus L. MacDonald Library, St. Francis Xavier University, 1 West Street, Antigonish, NS B2G 2W5, Canada, Fax: 902-867-2414, llancast@stfx.ca, blynch@stfx.ca

In earlier CINF presentations we illustrated low-cost recording/storage and possible integration of audio files with slide shows and movies. Now, we describe further applications providing background material relevant to our local chemical informatics resources ["cinf-R"] and to inter-university distribution of keynote research presentations at regional conferences. The cinf-R patterns differ in Canadian degree-granting institutions from most other countries; a national consortium [Canada Research Knowledge Network] provides free access for every college and university researcher. We will demonstrate local electronic access to the complete full text and abstracts sets of ACS and RSC journals, to the complete set of the Canadian Journal of Chemistry, and also to references accessed from the World of Science, Wiley InterScience, Elsevier, ProQuest Research Library et al., extrapolating to ACS conferences. Webcasting and podcasting of key files of our undergraduate senior research seminars for the 2005-2006 and 2006-2007 academic years will be illustrated, including videoconferencing aspects.

CINF 23 Information literacy in the chemistry major: Stretching our money at Augustana College. Connie Ghinazzi1, Dell Jensen Jr.2, and Richard Narske2. (1) Tredway Library, Augustana College, 639 38th Street, Rock Island, IL 61201, connieghinazzi@augustana.edu, (2) Department of Chemistry, Augustana College

Augustana College, a four year liberal arts institution with 2400 students, has an ACS accredited Chemistry department that routinely integrates literature research into their curriculum. In the past five years, Tredway Library at Augustana College has significantly changed its chemistry collection practices to meet the current and future researching needs of our students. This presentation provides a model for other small libraries to maximize their budgets by giving examples of effective faculty/librarian collaboration in assignment design, database selection, and reference collection purchases.

CINF 24 Delivering chemical information in the age of tight budgets: Faculty and librarian cooperation at Trinity University. Steven M. Bachrach, Department of Chemistry, Trinity University, 1 Trinity Place, San Antonio, TX 78212, Fax: 210-999-7569, sbachrach@trinity.edu, and Barbara MacAlpine, Coates Library, Trinity University

Trinity University chemistry faculty and librarians have followed a model of strong cooperation to beat the battle of the budget over information resources. Recognizing that shrinking financial resources requires creative solutions, we have explored new ways to insure that we deliver the appropriate combination of resources, principally databases and journals, to support information literacy for our undergraduate students and our active research program. The talk will discuss the difficult choices that were made and how the active participation of both faculty and library staff helped make implementation of these changes as seamless as possible.

CINF 25 SciFinder Scholar, Chemical Abstracts Student Edition or General Science Abstracts: Which should you ask your library to purchase? Patricia Kirkwood, University of Arkansas Libraries, University of Arkansas, 365 N. N. McIlroy Ave, Fayetteville, AR 72701-4002, Fax: 479-575-4592, pkirkwo@uark.edu

Small schools have limited subscription dollars and science databases are expensive. There are many possible options with newer plans for small institutions that share seats and pricing, SciFinder Scholar has become one possibility for undergraduate needs. It has the advantage of serving researcher needs as well as instruction for students. Is it the

better choice given the dollars and resources involved? Chemical Abstract Student Edition is available through OCLC FirstSearch with small college discounts as well. It has some advantages, like 24/7 availability and off campus access and it has two things non-science librarians understand -- the First Search interface and indexing for a selected number of journals that are more likely to be available to the student immediately. General Science Abstracts from H.W. Wilson, indexes all ACS journals including Journal of Chemical Education. It is an alternative that would allow the undergraduate chemistry student access to the most important literature of chemistry and be useful for other science students as well. Is it sufficient? This paper will discuss the advantages and disadvantages of these databases for lower division undergraduate course work. Committee on Professional Training guidelines will be addressed.

CINF 26 Make the most of what you have: Use Scifinder Scholar as a collection development tool. Donna R. Resetar, Christopher Center for Library and Information Resources, Valparaiso University, 1410 Chapel Drive, Valparaiso, IN 46383, Fax: 219-464-5204, Donna.Resetar@valpo.edu

Money and materials are not the only resources in short supply at the smaller academic institution. Staff are also limited and most librarians serve in multiple roles. Time for special projects is scarce. Under these circumstances, it is very difficult to do a citation analysis or journal use study as detailed as those published in the library literature. However, SciFinder Scholar can be used to learn where some science faculty and students publish and what journals they cite, and thus provide concrete data to help support or negate a subscription list. This presentation will describe how to use SciFinder Scholar to do an efficient journal-use/citation analysis for your institution.

CINF 27 Meeting the challenge of "The New Biology" for college libraries and librarians in the post-genomic era. Frederick Stoss, Science and Engineering Library, University at Buffalo - SUNY, Buffalo, NY 14260, fstoss@buffalo.edu

Sequencing the Human Genome was one of the greatest scientific achievements in history. The results unleashed a wave of research in molecular and structural biology giving rise to "The New Biology" of genomics, proteomics, bioinformatics, systems biology. Research universities have larger budgets than colleges to support libraries addressing these new endeavors. Four-year liberal arts colleges often serve as academic incubators for incoming cohorts of students into Masters and Doctoral programs at larger universities and must adequately prepare these undergraduates. This presentation provides insights for college librarians to access the new generation of genomic databases, describes development of essential monograph and journal collections, addresses reference services and librarian expertise in these subjects, and describes roles college librarians can play in innovative librarian-faculty collaborations. The later aspect of this presentation will outline various strategies for library and librarian outreach to college faculties and students, particularly among the life, physical, and computational sciences.

CINF 28 Analysis of documents pertaining to the phenomena of RNA interference. Brian Sweet, Product Marketing, CAS, Olentangy River Rd., Columbus, OH 43210, bsweet@cas.org

RNA interference (RNAi) prevents genes from being transcribed into proteins. The therapeutic potential of RNA interference for infectious diseases, cancer and a variety of illnesses is being actively explored by biotechnology and pharmaceutical companies throughout the world. The promise of this technology was recently recognized when the 2006 Nobel Prize in Physiology or Medicine was awarded to the discoverers of RNA interference, Andrew Fire and Craig Mello, only eight years after they made their discovery based on research involving the roundworm Caenorhabditis elegans. Based on the body of literature citing these authors' seminal paper on RNAi, and using analysis and visualization technology, we'll review the institutional leaders in exploiting their discovery, the leading researchers in this area, and show how this technology is being applied to pharmacology and medicine.

CINF 29 Uncovering competitive technology intelligence from chemical information in patent databases. Bob Stewart, Dialog, Thomson Scientific, 3501 Market Street, Philadelphia, PA 19104-3302, bob.stewart@thomson.com

There is a large amount of chemical information contained in commercially available patent databases. Uncovering that information is relatively straightforward, but converting it into intelligence is often more challenging. This presentation will examine several methods for turning chemical information from patents into actionable intelligence. At one end of the spectra are tools that are readily available to the majority of information professionals, such as Microsoft Excel and simple analysis tools that are built into commercial search engines. At the other end are sophisticated text and data mining tools that can uncover hidden intelligence from lists, matrices and relationship maps. The presentation will show that it is often possible to uncover intelligence with the simpler tools, while discussing situations where the more sophisticated tools add value.

CINF 30 Text visualization in chemistry: Roadblocks and rewards. Jeffrey D. Saffer, OmniViz, Inc, Two Clock Tower Place, Suite 600, Maynard, MD 01754, Fax: 978-461-1299, jsaffer@omniviz.com

Decision-making in chemistry can be effective only when done in context of all relevant information. With at least 75% of that information in the form of text documents - such as journal articles and patents, the volume of information that has to be assimilated is huge. Data visualization thus becomes a required step in making effective decisions. However, the ambiguities in language and the sheer volume of data are roadblocks to the process. I will discuss recent efforts to visualize extreme volumes of data and work to disambiguate chemical literature. These efforts lead to the reward of useful visualizations that support integrated analysis of text with experimental and clinical data.

CINF 31 A new key-based molecular fingerprinter for visualization and data analysis in compound clustering, similarity searching, and substructure commonality analysis. Norah E. MacCuish and John D. MacCuish, Mesa Analytics & Computing, LLC, 212 Corona St., Santa Fe, NM 87501, Fax: 509-472-8131, norah.maccuish@mesaac.com

We present a new, key-based fingerprinter designed specifically for the visualization and data analysis in clustering, similarity searching, and substructure commonality analysis. The use and efficacy of the fingerprinter in clustering and similarity searching is shown using an interactive hierarchical clustering tool and cost analysis ROC curves, respectively. Visualization and data analysis of substructure commonality analysis is explored with the interactive ChemTattoo program.

CINF 32 Selection of commercially available lead discovery compounds potentially active against P. falciparum methionine aminopeptidase by substance analysis and clustering. Anthony J. Trippe, New Product Development, Chemical Abstracts Service, 2540 Olentangy River Road, Columbus, OH 43202-1505, Fax: 614-447-5443, atrippe@cas.org

This presentation will demonstrate new developments in pharmaceutically intuitive methods for visualizing chemical space by organizing and clustering large numbers of chemical substances. A practical application of this technology will be provided in the form of a case study examining a recently identified methionine aminopeptidase enzyme. An inhibitor of this enzyme has been identified using high throughput screening. Additional, commercially available candidates will be identified using the substance clustering and visualization methods recently developed by CAS.

CINF 33 Effective teaching requires comprehensive reaction databases. Valentina Eigner Pitto, Josef Eiblmaier, Hans Kraut, Heinz Saller, and Peter Loew, InfoChem GmbH, Landsberger Straße 408, D-81241 München, Germany, Fax: +49 89 5803839, valentina.eigner-pitto@infochem.de

SPRESIweb is a Web application that enables access to the SPRESI data: a collection of 5 million molecules, 3.7 million reactions and 28 million factual data items abstracted from the most representative journals in the field of organic chemistry. In this lecture the experiences and opinions of teachers who are using SPRESIweb in undergraduate institutions in Europe and the US will be presented. Focusing on structure, reaction and reference searches in chemistry we will show the features of the Web application that are used most and, in particular, those aspects that help faculty in teaching students scientific information literacy skills. Examples given are the advanced options for defining specific query features (such as lists/not lists or R-groups) and the results of an optimized query submission on the hit list retrieved. Another significant feature is a new tool, Name Reactions that provides implicit definitions of complex reaction substructure queries, and assists teaching and retrieval of examples for reaction mechanisms.

CINF 34 ChemgaPedia Enzyclopedia: A new electronic visualization program for teaching and learning organic chemistry. Guenter Grethe, Consultant, 352 Channing Way, Alameda, CA 94502-7409, Fax: 510-865-5152, ggrethe@comcast.net

ChemgaPedia Enzyclopedia, a web-based program for e-learning and e-teaching, evolved from the German government sponsored project "Vernetztes Studium" to which 16 groups from European universities contributed their expertise and knowledge. The German version, covering all aspects of chemistry and related topics, features more than 15,000 pages with 25,000 media elements and 900 exercises as well as glossaries and biographical entries. Further development of this project is now in the hands of FIZ CHEMIE Berlin. Translation into English of the Organic Chemistry part is nearly completed. The informative text is illustrated with graphic representations and 3D models and supported by video clips, animations and exercises to enhance the learning process. The material is designed for self-studies on the undergraduate level as well as for instructors who can include their own material for a more personalized course. We will provide an overview of the system and discuss some examples.

CINF 35 Creation of an instructional module for small college science librarians highlighting free chemistry resources and their use in undergraduate instruction. Susan K. Cardinal, Carlson Science & Engineering Library, University of Rochester, Carlson Library, Rochester, NY 14627, scardinal@library.rochester.edu, and Carrie L. Newsom, Marston Science Library, University of Florida

The Chemical Education Committee of ACS CINF is creating modular instructional materials for the web. One module will teach science librarians of small colleges about free or nearly free resources and how the resources may used to teach chemistry undergraduates about chemical information. We will report on our progress and give a preview of the format and contents of the module.

CINF 36 One answer: On-line access to chemical information at community colleges, but what are the questions? R. G. Landolt, Department of Chemistry, Texas Wesleyan University, 1201 Wesleyan Street, Fort Worth, TX 76105, Fax: 817-531-4275, rlandolt@txwes.edu

From ACS Guidelines for Chemistry Programs in Two-Year Colleges: "Because of the increasing volume and complexity of chemical literature, students are no longer able to acquire skills in information retrieval without some formal instruction. ... This can be accomplished in many ways, such as cooperative library arrangements and electronic access. " Project UCAIR (Undergraduate Cooperative Access to Information Resources) has demonstrated how students may relate concepts learned in chemistry to published research, to attack "real-world" problems. A cost-effective Chemical Abstracts (CA) search process will be described in which Internet-based access has been used in undergraduate laboratories. Experience gained through UCAIR will be described, and feedback will be sought, to optimize benefits of using electronic journals as well as CA in the Community College environment.

CINF 37 A novel cheminformatics study of non-peptidic HIV protease inhibitors using machine learning and statistical tools. Barun Bhhatarai1, Srinivas Alla1, Chad R Bernier1, Rajni Garg1, and Sunil Kumar2. (1) Department of Chemistry, Clarkson University, 8 Clarkson Avenue, Potsdam, NY 13699-5810, bhhatarb@clarkson.edu, (2) Electrical and Computer Engineering department, SanDiego State University

A combinatorial approach (QSARomics) has been applied to study a large dataset of non-peptidic HIV protease inhibitors retrieved from literature. This fusion-based chem-informatic study integrates the results of models obtained using different statistical and machine-learning techniques. Descriptors were calculated (CODESSA, MOE) using SMILES input. Genetic Algorithm (GA) and Principal Component Analysis (PCA) were used for feature selection. Several linear and nonlinear QSAR models were developed using CODESSA, C-QSAR, WEKA, Matlab and others. The relationship between biological activity and the important descriptors/components obtained after feature selection was analyzed using Neural Network models. Comparative analysis of these results; with emphasis on similarities and differences, with Multiple Linear Regression (MLR) and Partial Least Square (PLS) results will be presented. We hope that the results of this research will be helpful in further optimizing the structure of non-peptidic HIV-PIs and provide lead for development of new drugs active against emerging mutant virus.

CINF 38 Pharmacokinetic modeling of anti-HIV protease ritonavir analogs. Raghava Chaitanya Kasara1, Barun Bhhatarai2, and Rajni Garg2. (1) Chemistry Department, Clarkson University, 8 Clarkson Avenue, Potsdam, NY 13676, Fax: 315-268-6610, kasarar@clarkson.edu, (2) Department of Chemistry, Clarkson University

Quantitative Structure-Activity Relationship (QSAR) study is being increasingly used to predict and rationalize pharmacokinetic and pharmacodynamic profile of drugs. The extension of QSAR technique to the pharmacokinetic data has led to emergence of new tool called QSPkR (quantitative structure pharmacokinetic relationship) studies, which can be employed at early stage of drug development to select potent molecule out of a series of biologically active molecules (congeners). QSAR and QSPkR models were developed using multiple linear regression (MLR) analysis method on antiviral and bioavailability data of HIV protease inhibitors (Ritonavir analogues). The biological data was taken from the literature. Our results show that the antiviral activity and bioavailability of these inhibitors is highly dependent on their hydrophobicity along with some other important parameters. Besides providing mechanistic insight, these models also have the potential to be used as in-silico virtual screening tool for predicting pharmacokinetic profile of HIV protease inhibitors.

CINF 39 Understanding the effect of benchmark dataset composition on the validation and optimization of ligand based virtual screening using self-organizing maps. Sebastian G. Rohrer and Knut Baumann, Institute of Pharmaceutical Chemistry, Technical University of Braunschweig, Beethovenstr. 55, 38106 Braunschweig, Germany, Fax: +49-531-3912799, s.rohrer@tu-bs.de

A common finding of many reports evaluating VS methods is that validation results vary considerably with changing datasets. It is assumed that these dataset specific effects are caused by the self-similarity and cluster structure inherent to those datasets. Self-Organizing-Maps (SOMs) were used to

analyze the structure of several published benchmark datasets. Utilizing the fact, that SOMs preserve dataset topology, a SOM-based quantitative measure for dataset diversity is introduced. It is shown, that the redundancy and inherent self-similarity of the datasets lead to general overestimation of all figures of merit. We demonstrate a linear relationship of the stability of VS validation results and dataset diversity, which can be used to quantify the robustness of a method. Furthermore, a quick and intuitive way to detect cases, when a method is not suited to model datasets with certain properties is provided. Our finding that a method's stability linearly decreases with dataset diversity has an important implication: when knowledge of active substances is sparse, which is usually the case at the beginning of real-life VS campaigns, the application of VS parameters optimized on self-similar datasets is misleading. We propose a procedure that finds a robust method for a given target by utilizing knowledge of a similar target protein with sufficient activity data. Target similarity is quantified by a spatial pharmacophore-hotspot guided alignment of binding pockets. Moreover, a methodology for conservative estimations of both expected hit rate and scaffold hopping potential is provided by statistical analysis of published case studies.

CINF 40 Data mining of NIH DTP human tumor cell line screen data for anticancer drug discovery. Huijun Wang and David J Wild, School of Informatics, Indiana University, 1200 S Rolling Ridge Way, #1001, Bloomington, IN 47403, huiwang@indiana.edu

The National Cancer Institute Discovery Therapeutics Program (DTP) maintains a database of compounds (currently over 40,000) which have been screened for activity as potential anticancer agents in 60 human tumor cell lines. Each of these cell lines has also been tested in a microarray assay to generate gene expression profiles. Those data are potentially useful in identifying lead compounds for a specific molecular target and studying the molecular mechanism action of a drug by appropriate data-mining methods. In our work, various statistical and artificial intelligence methods are used to analysis the screen data together with compounds fingerprint data and the microarray assay gene expression data. Mining those databases, which bridge chemical, biological and genomic information together, can provide useful information in finding the correlations between the chemical sub-structure and biology activity, selecting compounds most likely to interact with a specific molecular target and developing a genomic-based approach to the prediction of drug response.

CINF 41 A method for calculating the pKa values of small and large molecules. Jozsef Szegezdi and Ferenc Csizmadia, ChemAxon Ltd, Maramaros koz 3/a, 1037 Budapest, Hungary, Fax: +36-1-4532659, fcsiz@chemaxon.com

pKa is an essential factor of many drug disposal and lead development studies and considered to be as pivot parameter by synthetic and analytical chemists as well. Predicting the pKa of potential drug candidates in a huge data set or molecules with a large number of titratable groups requires a fast and an accurate method. There is significant interest in the development of an effective and accurate pKa prediction method. Some approaches apply the fragmentation of a molecule to predefined substituents, which is not unambiguous. This is why in our approach a molecule is not considered a finite set of fragments, but a set of partially charged atoms connected trough chemical bonds. Our purpose was to develop a new method for the calculation of macro ionization constants (pKa) of organic molecules in aqueous solution. This pKa calculation method pays special attention for molecules, which have a large number of ionizable groups. The ionization constants of the microspecies are estimated from empirically calculated partial charge distribution and the polarizabilities of atoms surrounding the ionizable centers (O, N, S, C). The number of microspecies is 2^N for molecules containing N ionizable atoms. Calculation is very time consuming for large N values, therefore, we have also developed an effective method for cases N>8. In these cases, instead of fixed microspecies, we defined a protocol for creating abstract groups of microspecies and pKa values calculated from this microspecies distribution at different pH values. Predicted and experimental values are in good correlation.

CINF 42 NCL-3D: A 3-D natural compound library for computer-aided anticancer drug discovery. Zengjian Hu and William M. Southerland, Department of Biochemistry and Molecular Biology, Howard University College of Medicine, 520 W Street, NW, Washington, DC 20059, zhu@howard.edu

Natural compounds and their derivatives have historically been invaluable as a source of therapeutic agents and have played a significant role in the anticancer drug discovery and development process. To facilitate the application of natural compounds in modern anticancer drug discovery process, we have developed NCL-3D, a searchable 3-dimensional (3D) structure library of natural compounds. NCL-3D will be useful for structure-based virtual screening to find lead compounds in anticancer drug discovery process. It can also be used in the ligand-based virtual screening method when the structure of the target protein is not available. The third application of NCL-3D is to perform ligand-protein inverse-docking for finding potential protein targets of a small molecule, which is applicable to the identification of multiple proteins to which a small

molecule can bind or weakly bind.). We anticipate the NCL-3D will be used as a powerful research tool for researchers to discover novel lead compounds for modern anticancer drug discovery projects and as a useful and inexpensive source of potentially therapeutic compounds. This work was supported by grant 2 G12 RR003048 from the RCMI Program, Division of Research Infrastructure, National Center for Research Resources, NIH

CINF 43 Classification of proteomics data by kernel methods. Kailin Tang and Tonghua Li, Department of Chemistry, Tongji University, Shanghai, China, tangkailin@hotmail.com

High-resolution mass spectrometry instruments are increasingly used for disease classification and therapeutic guidance. However, the analysis of immense amount of data poses considerable challenges. Here kernel PLS algorithm is presented and applied to the classification of the SELDI-TOF data of ovarian cancer and normal samples. This algorithm is a robust and nonlinear version of popular partial least square (PLS) method. In terms of process of SELDI-TOF data, the dimensionality reduction is critical stage before discrimination. We show that the Kernel-PLS method is capable of classifying SELDI-TOF proteomics data. Dimensionality reduction and classification can be carried out simultaneously. The method achieves an average sensitivity of 0.9833 and an average specificity of 1.0000 in leave-one-out cross-validations. This study demonstrates the potential applications of this algorithm for tumor diagnosis and the identification of candidate biomarkers.

CINF 44 Fabrication of chemical and engineering devices. KM. Choi, Lucent Technologies, Bell Laboratories, 600 Mountain Avenue, Room 1D-357, Murray Hill, NJ 07974

Since industry has been seeking for advanced nanotechnology, development of new nano-materials and nanofabrication techniques for information technology is a key contribute to this area. We present here a technological emergence of engineering and chemistry to explore new advances in nanotechnology by developing new materials. As an example, soft lithography has been widely used in the replication and fabrication of small features to fabricate engineering and chemical devices at the nano-scale with high performances. However, commercial stamp materials used in current soft lithography are limited in their capability on fabricating nano-scale devices due to their low moduli since conventional PDMS materials are initially produced for other purposes. We thus developed a new version of PDMS stamp materials to overcome the limitations and thus to extend this technology to the nano-scale regime. We also fabricate 'elastomeric photopatterns' at the micro-scale using the photocurable PDMS prepolymer for integrated circuits to fabricate devices with specific functions for information technology.

CINF 45 Gas chromatography determining 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 in electrosynthesis reaction solution. Song Chengying, Liu Zhisheng, Wang Liucheng, Zhao Jianhong, and Zhao Mingxing, Chemical engineering, Zhengzhou University, Wenhua 97th Road, Zhengzhou 450002, China, Fax: +86-371-63887327, liuzhisheng8106@sohu.com

The method for determination of 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 in electrosynthesis reaction solution by GC was studied, naphthalene was used as a internal standard. The chromatography conditions are as follows: column temperature 200°C, detecting instrument temperature 280°C, vapor temperature 280°C, amount of feed 0.5μl respectively. Contents of the title compound were determined adopting DB-1 capillary column, FID as detector. Under the conditions which have been optimized, each component can be well separated. The content of 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 in reaction solution were calculated by internal standard method, and the concentrations of 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 presented good linear relation with their areas of peak. The mean relative standard deviation of 2-methylnaphthalene and 2-methylnaphthoquinone-1,4 is 0.95% and 1.18%. The recovery of them is 98.65% and 101.58%, respectively.

CINF 46 Loop fitting with a combined force field and shape potential. Brian P. Kelley1, Geoffrey Skillman2, Matthew Stahl3, Stanislaw Wlodek4, and Anthony Nicholls4. (1) American Twine Building, 222 3rd St Suite 3211, OpenEye Scientific, 222 Thirs St, Suite 3211, Cambridge, MA 02142, kelley@eyesopen.com, (2) OpenEye Scientific Software Inc, (3) OpenEye Software, (4) OpenEye Scientific Software

Rapid solution of protein-ligand co-crystal structures is critical to successful structure-based drug design. Drug-like ligands often contain complex chemical motifs that are poorly handled by typical crystal refinement protocols, particularly those with force-fields designed toward protein refinement. Building high-quality, low-strain models from electron density can become a bottleneck in the process of garnering structural insights for ligand design. Thus reliable, automated methods for fitting ligands into electron density have long been sought. We have demonstrated that adiabatic mixing of a high-quality small molecule force field (MMFF) with a shape-based fit to electron density can reliably solve this problem*. Here we extend this method to fitting loop structures, as well as simultaneous fitting of ligands and nearby loops that have moved during ligand binding. *

"Automated Ligand Placement and Refinement with a Combined Force Field and Shape Potential", S. Wlodek, A.G. Skillman and A. Nicholls, Acta Crystallographica D, D62, pp. 741-749 (2006).

CINF 47 Optimization of LC/APCI-MS quinone isomer separation. Aidee Gonzalez, Krishna L. Foster, and Grady Hanrahan, Department of Chemistry and Biochemistry, California State University, Los Angeles, 5151 State University Drive, Los Angeles, CA 90032, agonza51@calstatela.edu

Polycyclic aromatic hydrocarbons (PAHs) are of health concern due to their mutagenic and carcinogenic properties. Incomplete organic combustion processes are the main source of this class of ubiquitous compounds. Oxidation of PAHs occurs in the natural environment and produces various products including isomers. A challenge faced while studying these compounds and their oxidized derivatives is their chromatographic separation. Isomers are the most difficult to separate because of their slight structural differences. High performance liquid chromatography separation of benzo[a]pyrene-1,6-, -3,6-quinones, oxidized products of the PAH model compound benzo[a]pyrene, have been optimized with a highly effective chemometric response surface designs. In particular, a Box-Behnken design was incorporated to study the effect of eluent composition, flow rate, and column temperature on experimental response. The response was measured as a combination of chromatographic resolution and retention time, and was interpreted with the aid of the Box-Behnken model results. The optimum predicted conditions were experimentally tested and offered resolved quinones giving the possibility for quantitative analysis by peak integration.

CINF 48 Implementation of scientific "blogging" into chemical laboratory research.
Albert C. Fahrenbach and Amar H Flood, Department of Chemistry, Indiana University, 800 East Kirkwood Avenue, Bloomington, IN 47405, fahrenbachus@yahoo.com

The advent of the computerized age in the latter half of the 20th century has revolutionized the way people communicate and how information is stored and presented, particularly in regards to science and engineering. The blogging of scientific research, such as experiment results and conclusions, as well as the incorporation of digitized laboratory notebooks and other high-tech devices into the research activity has been proposed by many as an expedient way to achieve greater productivity and cooperation among the scientific community. The implementation of these new technologies into the everyday lives of a research group would imply the use of digitized laboratory notebooks, RSS (Really Simple Syndicate) feeding of group progress into the scientific communal web, virtual meeting rooms, as well as computerized data storage and record keeping of experiments. We have shown that it is possible to create a platform to host several of these technologies while maintaining a high standard of professionalism and security at no extra costs to the research group.

CINF 49 Filling the void: Organizations and social networking. Dennis S. Loney, Department of Member Research and Technology, American Chemical Society, 1155 16th St., NW, Washington, DC 20036, d_loney@acs.org

Nonprofit organizations, specifically membership organizations, are actively seeking ways to engage and attract members via online community building and collaboration tools. In November 2006, the American Chemical Society launched BiotechExchange.org, a social networking site targeting the biotechnology community. This presentation will describe how the social networking community was established, how successful it was in attracting its target audience, how success is measured, lessons learned, and future versions and implementations.

CINF 50 New global communication process in thermodynamics and its impact on quality of published experimental data. Michael Frenkel1, Robert D. Chirico1, Vladimir V. Diky1, Chris D. Muzny1, Qian Dong1, Kenneth N. Marsh2, John H. Dymond3, William A. Wakeham4, Stephen E. Stein5, Erich Koenigsberger6, Anthony R. H. Goodwin7, Joseph W. Magee1, Michiel S. Thijssen8, William M. Haynes1, Suphat Watanasiri9, Marco Satyro10, Martin Schmidt11, Andrew I. Johns12, and Gary R. Hardin1. (1) Physical and Chemical Properties Division, National Institute of Standards and Technology, Boulder, CO 80305, frenkel@boulder.nist.gov, (2) Department of Chemical and Process Engineering, University of Canterbury, (3) Chemistry Department, University of Glasgow, (4) School of Engineering Sciences, University of Southampton, (5) Physical and Chemical Properties Division, NIST, (6) Division of Science and Engineering, School of Mathematical and Physical Sciences, Murdoch University, (7) Schlumberger Technology Corporation, (8) Acquisitions, STM, BRILL, (9) Aspen Technology Corporation, (10) Virtual Materials Group, Inc, (11) Software development, FIZ Chemie Berlin, (12) Oil, Gas & Chemicals Group, TUV NEL Ltd

Thermodynamic data are a key resource in the search for new relationships between properties of chemical systems that constitutes the basis of the scientific discovery process. In addition, thermodynamic information is critical for development and improvement of all chemical process technologies. Historically, peer-reviewed journals are the

major source of this information obtained by experimental measurement or prediction. Technological advances in measurement science have propelled enormous growth in the scale of published thermodynamic data (almost doubling every 10 years). This expansion has created new challenges in data validation at all stages of the data delivery process. Despite the peer-review process, problems in data validation have led, in many instances, to publication of data that are grossly erroneous and, at times, inconsistent with the fundamental laws of nature. A new global data communication process in thermodynamics and its impact in addressing these challenges, as well as in streamlining the delivery of the thermodynamic data from "data producers" to "data users" will be discussed.

CINF 51 Semantic chemical publishing Nick E Day, Department of Chemistry, Unilever Centre for Molecular Sciences Informatics, Lensfield Road, CB2 1EW Cambridge, United Kingdom, Fax: +44-1223-763076, ned24@cam.ac.uk, Peter T. Corbett, Unilever centre for Molecular Sciences Informatics, and Peter Murray-Rust, Unilever Centre for Molecular Science Informatics, Department of Chemistry, University of Cambridge

Modern informatics tools support, in principle, the complete publication of a chemical experiment: substances, procedures, timelines, observations and analysis. This is being rapidly enhanced by new social computing (blogs and wikis, Connotea, del.icio.us), feeds (RSS), reference works and collections(Wikipedia, Pubchem), ontologies (Goldbook-XML, GO, OBO, CheEBI, MeSH). These now support XML representations and we have enhanced all of them with chemistry though Chemical Markup Language. The challenge is populating them: through OSCAR3/OPSIN we use chemical linguistics to extract information from free-text. CIF2CML and CMLSpect support crystallography and analytical data. With Open publications machines can extract a large amount of semantic chemistry and we shall show live demos. This is merely an interim approach, however; the main requirement is for publishers to wake to the power of this and support the Open publishing of semantic chemistry.

CINF 52 Data lifecycle and curation of laboratory experimental data. Tony Hey, Microsoft Corporation, 1 Microsoft Way, Redmond, WA 98052-6399, Fax: 425-936-7329, Tony.Hey@Microsoft.com

There is an ongoing revolution in the collection of large volumes of experimental data in many fields of science, including chemistry. Early capture of digital data is vital for scientists to have the ability to integrate this data with other data and to search and analyze large amounts of such scientific data. This talk will use the UK e-Science 'CombeChem' project as an exemplar of a variety of technologies for dealing with the entire data lifecycle from acquisition, curation, publication and preservation.

CINF 53 The semantic wiki as a model for an intelligent chemistry journal. Henry S. Rzepa, Department of Chemistry, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom, rzepa@ic.ac.uk

Wikis are now recognized as excellent collaborative content authoring environments (provided the appropriate level of author-authentication is achieved). In chemistry however, one also needs to capture both data and metadata in a formal manner, with correct datatyping, and an associated ontology (machine processable vocabulary). Potentially at least, the so-called Semantic Wiki offers just such an environment in which to explore how an intelligent chemistry journal article might be authored, to achieve a so-called SPARQL endpoint for logical analysis. Initial experiences using the Semantic Mediawiki environment will be reported, as applied to capturing relationships and attributes in an article on mauveine. Careful logical analysis (by a human) of an article first published in 1879 by William Perkin reveals that the erroneous molecular structure of this species, as widely reported in the literature up to 1994, could have been inferred as wrong by making use of the facts reported in the original article, with the addition of only a minimum of modern knowledge. The analysis centres on what would be needed for an intelligent software agent, armed with a semantic expression of the original facts as reported by Perkin, to reach the same conclusion, and whether issues of scale, and communal agreement on the appropriate chemical ontologies to deploy for this purpose, are in fact a reasonable and achievable goal for the chemistry community over the next 24 years.

CINF 54 Standard domain ontologies: The rate limiting step for the "Next Big Change" in scientific communication. Allen Renear, Graduate School of Library and Information Science, University of Illinois at Urbana-Champaign, 501 E. Daniel St, Champaign, IL 61820, renear@uiuc.edu

The long awaited emergence of high-function scientific publishing may, finally, be near. There will soon be the tools, structured data, and communication infrastructure that will allow researchers to use new and innovative strategies for taking advantage of computationally available representations of scientific information. As this happens, the use of traditional publishing artifacts like journals, abstracts and articles will be increasingly away from simply finding and reading and towards more direct and efficient computer-supported exploitation. Several important social and technological trends are converging to make this possible. We focus here on the role of standard domain ontologies and their potential for interaction with changing user behavior in search environments.

CINF 55 Designing a new industry for sustainability: Life cycle analysis for the emerging bioeconomy. Bruce E. Dale, Dept of Chemical Engineering and Materials Science, Michigan State University, 2527 EB, East Lansing, MI 48824, Fax: 517-432-1105, bdale@egr.msu.edu

Strong evidence exists that we are in the early phases of a truly historic transition--from an economy based largely on petroleum to a more diversified economy in which renewable plant biomass will become a significant feedstock for both fuel and chemical production. The development of the petroleum refining industry over the past 150 years provides many instructive lessons for the future biobased economy...and also many reasons for supposing that the new biobased economy will be different from the hydrocarbon economy in many crucial ways. We assume a mature biobased economy--as the petroleum economy is mature today--and from that assumption we extrapolate likely features of the mature biobased economy. Among the technosocioeconomic forces that will drive the mature biobased economy we consider: 1) yield (using the whole "barrel of biomass"), 2) gradual diversification of biobased products, 3) the great diversity of biomass resources combined with their considerable compositional similarity, 4) possible/likely limits on agricultural productivity, 5) integration of biorefining and agricultural ecosystems in a local social and political context (the "all biomass is local" paradigm) and 6) the sustainability of the mature biobased economy and its most important underlying resource--productive soils.This presentation emphasizes the use of life cycle analysis to evaluate the sustainability of the emerging biobased economy. Life cycle analysis is a systems level tool to evaluate the environmental impacts of processes and products. For the first time in human history, by properly using life cycle analysis and related tools, we have the ability to analyze and design a major emerging industry so that it satisfies both environmental and economic criteria.

CINF 56 Emerging technologies for renewable materials in the UK and EU. Jeremy Tomkinson, Chief Executive Officer, National Non-Food Crops Centre (NNFCC), NNFCC Biocentre, York Science Park, Innovation Way, Heslington, York YO10 5DG, United Kingdom, Fax: +44 1904 435345, J.Tomkinson@nnfcc.co.uk, and Alison Hamer, Communications and Information Manager, National Non-Food Crops Centre (NNFCC)

The development of first- and second-generation fuels is driving a change to the wider use of renewable materials across a widening industry base. The pharmaceuticals, biopolymers and biofuels markets are all showing an increased market acceptance and uptake of renewable materials mainly through the enhancement of material property or through the provision of new functionality in traditional formulations. This presentation will introduce some of the emerging technologies in the UK and EU, indicating where real market uptake is occurring and also highlighting some of the future issues in respect to land availability and the management of new waste streams.

CINF 57 Biofuels: From an information perspective. Kathleen Sands, Information Centers, Agricultural Research Service, Room 108A, NAL BLDG, 10301 BALTIMORE BLVD, Beltsville, MD 20705-2351, kvazoulas@nal.usda.gov

Interest in biofuels is sweeping the nation due to a growing demand to relieve our nation's dependence on oil and to ease strains on the environment that are produced by using fossil fuels. In order for this industry to grow and become an integral part of our transportation and energy systems, people must be able to inform themselves of the issues, ideas and research activities associated with biofuels. Some of the leading public resources for obtaining the latest information on biofuels include the World Wide Web, libraries, online and in-print journals, and government and university research projects. The breadth of information found in these resources continues to expand because of the urgent need for research and development, advances in technology, and the push for additional public policy. These driving forces mandate the development of information coordination which, due to the subject's recent rapid growth, is not well established at the present time. This makes it difficult for researchers and the general public to navigate easily through the resources that are currently available. In addition, there are a broad group of stakeholders who have a wide range of information needs on biofuels. Chemists, biologists, scientists, farmers, private companies, engineers, environmentalists, economists, government officials and the general public all want information on the topic. To best serve all of these interested parties, a coordinated information system would create and provide central, organized, and easily accessible information resources. For many years, the National Agricultural Library (NAL) has served as a central hub of current agricultural information, providing for a diverse group of patrons. Some of our latest focuses have been on rural issues, alternative farming systems and technology transfer. This talk will present NAL's plans for improving the availability of information on biofuels as this important industry continues to grow.

CINF 58 Survey of information resources covering renewable fuels, chemicals and energy. Samantha Swann, Business Acquisition Editor, John Wiley & Sons, Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, United Kingdom, Fax: +44 1243 770432, SSwann@wiley.co.uk

The international Society of Chemical Industry (SCI) and John Wiley & Sons Ltd have undertaken a survey of information resources relating to renewable chemicals, fuels and energy. This paper describes the motivation for carrying out the survey, the methodology used, the results and the outcome of the study. The presentation will be illustrated with examples of print and online information resources relevant to this topic area. Statistics pertaining to the recent growth of literature on this subject will also be presented.

CINF 59 Enhancing the web experience with ACS journals. Evelyn Jabri and Sarah Tegen, ACS Chemical Biology, American Chemical Society, 1155 16th St NW, Washington, DC 20036, e_jabri@acs.org

Enhancing our understanding of scientific concepts will require creative and effective uses of web functionalities. At the journal level, we use the web to keep our readers up-to-date on cutting research. With the continued growth of new areas of science such as chemical biology, we must make our content accessible to a larger, more scientifically diverse set of readers. At ACS Chemical Biology we are using many web tools, such Podcasts, forums and Wikis to engage readers with our content. We have also improved our HTML pages with web enhanced objects such as interactive figures and 3D images of macromolecular structures. These enhancements and others coming soon improve our user experience and enhance their ability to understand the subject matter.

CINF 60 Podcasting and social bookmarking at Nature. Joanna C Scott and Timo Hannay, Web Publishing, Nature Publishing Group, 4 Crinan Street, N1 9XW, London, United Kingdom, Fax: 00442078433673, j.scott@nature.com

The Internet has created an array of options for publishers to support scientific communication. This talk will present two examples from Nature Publishing Group (NPG). Creating and distributing audio content is easier than ever before, allowing organisations that previously issued only written information to explore this new medium. The Nature Podcast was released in October 2005 and quickly gained tens of thousands of listeners. Since then the range and variety of NPG's audio output has increased greatly (e.g., the Chemistry Podcast), reflecting behind-the-scenes changes at NPG that have made audio a natural part of the editorial mix.The Internet also offers new opportunities for publishers to help scientists to collaborate with each other through participative websites. An example of this is NPG's own social bookmarking service, Connotea. This includes many features tailor-made for scientists, including automatic extraction of bibliographic details, support for DOIs and OpenURL, and privacy options.

CINF 61 Beyond searching: Adding increased value to today's scientific databases.
Michael Dennis, Planning & Development, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210, mdennis@cas.org

At the beginning of the twentieth century, secondary information sources such as Chemisches Zentralblatt and Chemical Abstracts helped scientists derive value from the published research of their colleagues. Even in the Internet era, search and retrieval of well indexed, timely comprehensive databases remains an important component of the research process. But information technology now affords new means of helping researchers and information professionals not only to identify relevant papers and patents and access the primary documents but also to recognize trends and patterns in the shifting infosphere that continues to grow in size and complexity. From the perspective of Chemical Abstracts Service's hundred years in the information industry, an overview of new directions in the visualization, analysis, and processing of data, text and substance information will be outlined. Technology has changed markedly, but the objective of helping scientists assimilate and apply the wealth of available information remains essential and can be achieved more effectively than ever before. Reliable, trusted, and well organized databases are an essential platform for further advances.

CINF 62 Google Scholar: The adventure continues. Anurag Acharya, Google, Inc, 1600 Amphitheatre Parkway, Mountain View, CA 94043, acha@google.com

Google Scholar is a fresh look at the traditional problems of discovering and accessing scholarly literature. It is currently being used by researchers all over the world. I will describe the general principles that underlie its design and will share some operational experiences. I will also present lessons learnt - both from building and running such a service and from seeing how people use it.

CINF 63 Recommendation systems for research. Marc F. Krellenstein, Elsevier, 30 Corporate Drive, Burlington, MA 01803, m.krellenstein@elsevier.com

As the relevant research literature expands at a rate beyond the ability of any one person to process, technology to recommend work related to your own interests is a valuable tool to help users discover possibly useful information. Collaborative recommendation systems leverage what

similar researchers have viewed or done and can provide excellent and reliable suggestions, though there are some obstacles to their use due to privacy considerations and the need for usage history. Content-driven recommendations, perhaps augmented with chemical structure or other similarity measures, do not leverage other (human) judgments but also don't share privacy and usage history limitations, relying only on the existence of available research content and appropriate statistical and natural language technology. These technologies have a good track record of success for similarity searching and are being enhanced to produce ever-better suggestions for related work of interest.

CINF 64 Collaborative filtering in a scholarly context. Georgios Papadopoulos, Atypon Systems, Inc, 5201 Great America Parkway, Suite 510, Santa Clara, CA 95054, Fax: 408-988-1070, georgios@atypon.com

Collaborative filtering is the technical term for the "other users who bought this book also bought these books" feature popularized by Amazon. Atypon has been tracking user behavior and experimenting with various algorithms since July 2005 and deployed the first implementation in July 2006 and a full implementation in late 2006. We have gathered ample data on the usefulness of such a feature specifically for scientific publications and how it can be best utilized in conjunction with other discovery mechanisms such as search.

CINF 65 Modeling the scholarly community from usage data. Johan Bollen, Research Library, Los Alamos National Laboratory, TA03 - P362 - STBPO-RL, Los Alamos, NM 87545, Fax: 505 665 6452, jbollen@lanl.gov

This presentation outlines efforts at Los Alamos National Laboratory to construct models of the scholarly community from usage data that has been recorded by online information services. I will discuss an architecture we developed to collect and aggregate usage data at a large scale. Associative networks of resource relationships are extracted from the resulting usage data. These networks then form the substrate for the definition of usage-based metrics of scholarly impact, the implementation of recommender systems, and mapping of the social network structure of the community for which usage was recorded. Results obtained from usage recorded at the California State University system will serve as a case-study. The presentation will conclude with a summary of the main issues in this emerging domain and an overview of the MESUR project, an Andrew W. Mellon Foundation funded project at Los Alamos National Laboratory to support the development of usage-based impact metrics.

CINF 66 Ligand binding and circular permutation modify residue interaction network in DHFR. Zengjian Hu1, Donnell Bowen1, William M. Southerland1, Yongping Pan2, Antonio del Sol3, Ruth Nussinov2, and Buyong Ma2. (1) Department of Biochemistry and Molecular Biology, Howard University College of Medicine, 520 W Street, NW, Washington, DC 20059, zhu@howard.edu, (2) Center for Cancer Research Nanobiology Program, Basic Research Program, SAIC, NCI-FCRDC, Frederick, MD 21702, Fax: 301-846-5598, mab@ncifcrf.gov, (3) Research & Development Division, Fujirebio Inc

Residue interaction networks and loop motions are important for catalysis in dihydrofolate reductase (DHFR). Here we investigate the effects of ligand binding and chain connectivity on network communication in DHFR. We carry out systematic network analysis and molecular dynamics simulations of the native DHFR and 19 of its circularly permuted variants by breaking the chain connections in 10 folding-element regions and in 9 non-folding element regions as observed by experiment. Our studies suggest that even though the cutting in the folding element area may not destroy the protein structure, chain cleavage in these regions may de-activate DHFR due to large perturbations in the network properties near the active site. Protected areas are often associated with protein folding; however, our study indicates that chain connection in protected areas may also be important for network interactions. Further, our network analysis reveals that ligand binding has "network bridging effects" on the DHFR structure. The protein active site is near or coincides with residues through which the shortest paths in residue interaction network tend to go. Our results suggest that ligand binding leads to a modification, with most of the interaction networks now passing through the cofactor shortening the average shortest path. Ligand binding at the active site has profound effects on the network centrality, especially the closeness. This work was supported by grant 2 G12 RR003048 from the RCMI Program, Division of Research Infrastructure, National Center for Research Resources, NIH

CINF 67 Chemical superposition and pharmacophore elucidation by SCAPFOld: Self-consistent atomic property field optimization. Maxim Totrov, Modeling and Drug Design, Molsoft, LLC, 3366 North Torrey Pines Court, S. 300, La Jolla, CA 92037

Accurate multiple ligand superposition and subsequent elucidation of the pharmacophoric features are the key steps in ligand-based drug design process. The proposed method is based on iterative optimization of a composite 7-component atomic property field. Ligand conformations and positions are optimized by montecartlo minimization procedure in internal coordinates in the property field potentials combined with the internal force field energy. Up

to several hundreds of ligands can be simultaneously flexibly superimposed. Rigid 'seed' structures can be included in the ligand set to drive the process towards preferred conformations deduced from experimental data such as X-ray structures. The resulting optimal self-consistent atomic property field can be used to elucidate a pharmacophoric model by locating the maxima of the field components corresponding to the classical pharmacophoric properties. The results are illustrated on Figure 1, depicting the conformations of 25 inhibitors of CDK2 flexibly superimposed by SCAPFOld procedure. Yellow, blue and red blobs are the isosurfaces contouring high potential value regions in space for, respectively, the hydrophobic, hydrogen bond donor and hydrogen bond acceptor components of the property field. Test results for several datasets will be presented and discussed.

CINF 68 Surface interaction property based similarity searching with the eHiTS Filter.
Darryl Reid, Zsolt Zsoldos, Bashir Sadjad, and Aniko Simon, SimBioSys Inc, 135 Queen's Plate Dr, Suite 520, Toronto, ON M9W 6V1, Canada

Ligand based similarity searching is a key process in many drug discovery pipelines. The goal is often to find structurally diverse ligands which have similar binding properties and thus find new lead scaffolds for further optimization. The eHiTS Filter tool uses different interaction surface point types to capture the chemical properties on the surface of ligands and thus describe the ligand. A neural network is then trained on known actives and used to search for similar ligands in a screening database. The training process will be described, along with results from several test sets. The measure of the "Goodness" of the hit lists obtained will be measured by the GH Score.

CINF 69 Effect of query structure on specificity for flexible 3-D searching. Philippa RN. Wolohan and Robert D. Clark, Informatics Research Center, Tripos, Inc, 1699 South Hanley Road, St. Louis, MO 63144, pwolohan@tripos.com

Pharmacophores were originally defined as distributions of generalized features in space that are required for activity against a particular biochemical target. Every active compound must exhibit every component feature in such an "essential" pharmacophore, which has the virtue of making clique detection and other deductive approaches to pharmacophore elucidation feasible. Unfortunately, the corresponding 3D search queries are often comprised of too few features too closely spaced to effectively discriminate between active and inactive ligands - i.e., queries that have a large false positive "hit" rate. But such queries can also be so complex that they are too specific. Searches based on them will only recover ligands very similar to those in the training set and will have a prohibitively high false negative hit rate. Including partial match constraints in a query makes it possible to strike a useful balance between these two extremes, especially when a mix of stringent and permissive constraints is used. In the former, most or all features are required to "hit", whereas in the latter only a few are required. This talk will describe a model for predicting the search specificity of a query from its geometry, feature composition and constituent partial match constraints.

CINF 70 Adventures in shape space. Paul Hawkins, OpenEye Scientific Software, 3600 Cerrillos Road, Suite 1107, Santa Fe, NM 87507, Fax: 505-473-0833, phawkins@eyesopen.com

A bedeviling problem in ligand-based design has been the nature of the conformation of the ligand(s) used to build a query and the conformations of the database compounds to be searched. Many assume the query should be the bioactive conformer or a similar low-energy conformer. We will present data to challenge this notion. Further, an approximation to an aqueous-phase ensemble is often used in multi-conformer databases, though evidence exists suggesting that ensembles of moderately unfolded conformers better reproduce crystal structures. In this paper the inter-relationship between conformer space and shape space of both queries and database compounds will be explored in the context of virtual screening with the shape-based similarity tool ROCS. The results will focus particularly on the impact of different conformer generation and sampling methods on success in shape-similarity virtual screening.

CINF 71 New self-organizing algorithm for molecular alignment and pharmacophore development. Deepak Bandyopadhyay and Dimitris K. Agrafiotis, Johnson & Johnson Pharmaceutical Research & Development, L.L.C, 665 Stockton Dr, Exton, PA 19341, Fax: 610-458-8249, dbandyop@prdus.jnj.com

We present a method for simultaneous conformational analysis and pharmacophore-based molecular alignment using a self-organizing algorithm called Stochastic Proximity Embedding(SPE). Earlier(2003) we used SPE to generate 3D structures by iterative rule-based adjustment of atom coordinates, achieving higher speed and conformational diversity than earlier programs. Here, we run SPE on an ensemble of 2D molecules to be aligned, with 1D correspondence between atoms/groups coming from automatically generated pharmacophore hypotheses or specified manually. We add distance terms to SPE to bring corresponding pharmacophore points and their associated direction vectors closer. Atoms/groups may also be constrained to lie near external coordinates from a binding site. The 3D structures of each molecule in the resulting

alignment are nearly correct if the pharmacophore hypothesis was chemically feasible; post-processing by distance and energy minimization further improves the structures and weeds out infeasible hypotheses. 3D pharmacophores extracted from a successful alignment can be used for database searching.

CINF 72 Analyzing docking results by substructure search in Euclidean space. Thomas Zuhl, Marcus Gastreich, Christian Lemmen, and Holger Claußen, BioSolveIT GmbH, An der Ziegelei 75, 53757 Sankt Augustin, Germany, Fax: +49 2241 25 25 525, Thomas.Zuhl@biosolveit.de, Holger.Claussen@biosolveit.de

The scoring problem remains unsolved for molecular docking. Target-specific scoring and other tweaks in the docking process are current work-arounds for this problem. Our Docking Database (DDB) provides a powerful analysis tool for this task. We have introduced a DDB substructure search in 3D that allows users to analyze spatial arrangements of substructures of docking poses. In addition to simple selection and filtering of particular substructures, the new mechanisms enable users to generate statistics of, for example, the distribution of functional groups within the active site and to test the effects of FlexX-Pharm constraints by eliminating unwanted results. In order to yield fast analyses, all 3D coordinates of both protein structure and all ligand poses are preprocessed and stored in an underlying ORACLE database. The substructures are specified as SMARTS expressions. We will present first test results and an outlook on further potential applications.

CINF 73 Using text mining software to identify drug, compound, and disease relationships in the literature. Darryl A. León, Active Motif, 1914 Palomar Oaks Way, Suite 150, Carlsbad, CA 92008, leon@activemotif.com

From national security agencies to drug discovery companies, these organizations find text mining an excellent approach for information retrieval and knowledge extraction. However, when analyzing life science abstracts, many text mining methods are challenged with such issues as multiple synonyms, inconsistent homonyms, and ambiguous acronyms. In the drug discovery arena, most scientists do not want to become experts in text mining techniques, but simply want to find key, published information and relationships about a drug, compound, or disease. This talk will introduce basic text mining approaches, describe how text mining software can help with extracting the relevant biochemical knowledge in life science publications, and give a short survey of select text mining tools for the life sciences. A few examples will be provided to show how text mining software is being used in research and discovery.

CINF 74 Descriptive and predictive models for in-vitro human cancer cell growth screens. Richard Kho, Mick Correll, and Jonathan Ratcliffe, InforSense, 25 Moulton St, Cambridge, MA 02138, rkho@inforsense.com

The recent explosion of data in the life sciences has served as an impetus for the application of classic data mining methods in analysis and prediction. Here, we compare and contrast various data mining techniques for analyzing and predicting the inhibition of cancer cell growth by small molecules. Data consisting of >40,000 screening results were obtained from the NCI's Human Tumor Cell Lines Screen of the Developmental Therapeutics Program. Cheminformatic methods were used to calculate descriptors for the screened compounds, and data pre-processing was performed to cull out redundant features. A suite of data mining techniques were applied to a random subset (the training set) and validated using leave-one-out or stratified three-fold cross-validation. The performance of these models in predicting cancer cell growth inhibition is described for potential use in early virtual screening of chemical libraries.

CINF 75 Toward linking small molecules to biological processes in RSC publications. Colin R Batchelor, Royal Society of Chemistry, Thomas Graham House, Milton Road, Cambridge CB4 0WF, United Kingdom, batchelorc@rsc.org

Chemical text mining is unlike biomedical text mining for all sorts of reasons. We contrast the main challenges and current techniques in both fields and evaluate their applicability to chemical publishing, as well as the impact of developments in chemoinformatics and large databases such as PubChem. We look at what will be needed to go beyond drug discovery into general chemistry and discuss the possibilities for deep parsing of chemical text from publishers' and end users' perspectives.

CINF 76 Applying data mining approaches to further understanding chemical effects on biological systems. Chihae Yang, Leadscope, Inc, 1393 Dublin Road, Columbus, OH 43215, cyang@leadscope.com, and Ann M. Richard, US EPA

Data mining methods require the technological framework of a relational database based on a rigorous data model, flexible searching and retrieval functions, and data analysis and visualization tools. A data model, consisting of a schema (hierarchy) and controlled vocabulary, provides the foundation for meaningful data mining, enabling mechanistic hypotheses to be generated and validated. Advances in the field of computational toxicology are being driven by expanding capabilities for mining the domains of biology and chemistry simultaneously. To break away from the current paradigm of analog searching solely based

chemical similarity, this paper presents informatics methods to finding chemical structures with biologically similar functions. A chemical stressor with particular biological attributes will seed the biology domain. The resulting biological profile will then be projected onto the chemical structure domain to broaden the concept of "analogs" and to assist in the understanding of hazard potential through iterative exploration of both chemical and biological analog space. The National Toxicology Program recently conducted high throughput screening of over 1400 chemicals in a series of cell-viability assays and made the data available through PubChem. This dataset will be used to illustrate various data mining techniques to biologically profile the chemical space. This abstract does not necessarily reflect EPA policy.

CINF 77 Pharmaceutically intuitive chemical space visualization: Enabling the discovery of structural relationships and associated biologically relevant properties between substances. Anthony J. Trippe, New Product Development, Chemical Abstracts Service, 2540 Olentangy River Road, Columbus, OH 43202-1505, Fax: 614-447-5443, atrippe@cas.org

This presentation will demonstrate new developments in pharmaceutically intuitive methods for visualizing chemical space by organizing and clustering large numbers of chemical substances. In addition, data mining experiments to provide individual bioactivity profiles to substances will also be discussed. These two activities will be brought together by way of a pharmaceutical industry case study to demonstrate how the combination can provide immediate and unique insight into a related substance collection.

CINF 78 Mining and visualizing the chemical content of large databases. Hugo O. Villar, Mark R. Hansen, and Jason Hodges, Altoris, Inc, 11575 Sorrento Valley Rd, Suite 214, San Diego, CA 92121, hugo@altoris.com

The dominant paradigm in drug discovery emphasizes techniques that generate large amounts of data. What was possible by simple inspection in the past cannot be effectively achieved nowadays without the aid of informatics techniques. The selection of compounds for synthesis in a medicinal chemistry program is founded on the identification of structural or physicochemical patterns that correlate with activity data, or negatively correlate with undesirable effects. The task is made extremely taxing when researchers are confronted with massive amounts of biological information, where instead of a few compounds, entire chemical classes may have to be assessed simultaneously. The assimilation of these data is a prerequisite for the identification of patterns and gathering of information. Therefore, there is a need in modern chemistry to organize data for the bench chemist in a manner that facilitates incorporation of all available information into their research in the simplest manner that retains accuracy. In this way, information from high throughput screening or other tests can be fully exploited to improve library design and lead optimization. Most tools for analysis currently in vogue are highly complex and limited to the hands of experts. We will discuss some methods and statistical approaches that can aid in the assimilation of the information by bench scientists.

CINF 79 Developing semantic web service for chemical informatics. Xiao Dong and David J Wild, School of Informatics, Indiana University, Bloomington, IN 47408, xdong@indiana.edu

As the use for web service technology has become more prevalent in chemical informatics, it also poses new challenges in the organization and discovery of available information and computation services. In the mean time, semantic web developments are aiming to make web content machine-processable, allowing semantic interoperability and meta-level exploitation of data and computation. Here we explain how to use semantic web service technology to support an existing chemical informatics cyberinfrastructure. More specifically we use OWL-S, the web ontology language for web service, to describe the generic properties for our chemical informatics web services, which we extend to develop domain-specific ontology for those services. In this presentation we will also discuss how to utilize autonomous agent technology within the semantic web service infrastructure to allow automatic discovery, composition, invocation and execution of workflows that are meaningful in early stage drug discovery.

CINF 80 Tiered screening protocol for the discovery of structurally diverse HIV Integrase inhibitors. Rajarshi Guha1, Debojyoti Dutta2, David J Wild1, and Ting Chen2. (1) School of Informatics, Indiana University, 1130 Eigenmann Hall, 1900 E 10th Street, Bloomington, IN 47406, rguha@indiana.edu, (2) Department of Computational Biology, University of Southern California

We report a virtual screening protocol for the identification of identifying diverse HIV inhibitors. We developed linear and non-linear classification models based on a 900 compound training set. The models were then used to predict the activity class of a large vendor library. The vendor compounds that were predicted active were then filtered based on similarity to the most active compound in the training set. The final hit list was prioritized according to similarity to the most outlying active compound in the training set. Our initial results did not lead to a significantly diverse set of hits. Furthermore, none of our hits were common to the set obtained previously using a pharmacophore model. However, relaxing the similarity

constraints identified four compounds which were very similar to a known inhibitor. We discuss possible reasons why this was the case and describe docking results for the hits obtained using our tiered screening protocol.

CINF 81 Something old, something new: Creating an undergraduate chemical information seminar. Teri M. Vogel, Science & Engineering Library, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0175E, Fax: 858-534-5583, tmvogel@ucsd.edu, and Barbara A. Sawrey, Department of Chemistry & Biochemistry, University of California, San Diego

For Spring quarter 2006, we taught the first undergraduate chemical information seminar at UC San Diego as a potential complement to efforts to increase course-integrated instruction. Twelve students, freshmen to seniors, took the six-session, one-credit course. We used ACS' undergraduate guidelines on chemical information retrieval as a guiding framework, while experimenting heavily with instructional technologies and teaching techniques to promote active learning. This presentation will summarize the challenges and opportunities we faced in designing and teaching the seminar; present a detailed breakdown of the learning objectives and chemical information resources covered during the seminar, including instructional technologies and in-class handouts; share the student evaluations; and describe the changes that will be incorporated into the Spring 2007 seminar.

CINF 82 Mmm...vanillin: Reaching graduate students through ice cream seminars.
Jeremy R Garritano, Mellon Library of Chemistry, Purdue University, 504 W. State St., West Lafayette, IN 47907, jgarrita@purdue.edu

While there is no required chemical literature course for graduate students at Purdue University, a series of library ice cream seminars is offered throughout the semester as an alternative. These seminars are targeted toward new graduate students to help them adjust to the wide variety of library resources now available to them. Each seminar is focused on either a particular resource (SciFinder Scholar, Beilstein, etc.) or a topical theme (patents, citation searching, spectral information, etc.). Implementation of the seminar series will be explained as well as content presented and effective marketing methods. Results of evaluations and future directions will also be discussed.

CINF 83 Hands-on remote training in chemical information. Peg Renery, Educational Services, Elsevier MDL, 2440 Camino Ramon, Suite 300, San Ramon, CA 94583, Fax: 925-543-7849, P.Pontier-Renery@mdl.com

The development and deployment of new training formats and delivery options can be challenging. At the same time, these initiatives offer significant organizational and productivity benefits. Over the last several years, Elsevier MDL Educational Services has expanded its training offerings and broadened its role to include: decision making in software/database acquisition; enabling others to support in-house training efforts; creating a self-service environment with multiple points of access; and delivering hands-on training using Web conferencing tools. In this presentation you will see demonstrations of our Learning Centers and Video Libraries showcasing interactive simulations. In addition, we will discuss our live, instructor-led training delivered via Webex and address the challenges of delivering successful hands-on training remotely. Our goal remains—to offer more scientists, librarians, faculty and students worldwide the benefits of our proven instructional methodology of "tell me, show me, let me do."

CINF 84 Taking the graduate classroom teaching a step further. Monica Shokeen1, Kenya T. Powell2, Karen L. Wooley2, and Carolyn J. Anderson1. (1) Division of Radiological Sciences, Washington University School of Medicine, 510 Kingshighway Blvd., Campus Box 8225, St. Louis, MO 63110, shokeenm@mir.wustl.edu, (2) Department of Chemistry, Washington University in Saint Louis

The scope of graduate classroom teaching can be significantly improved by increasing the interaction between different departments and schools. Present day science can metaphorically be referred to as a melting pot of different subject areas. At the college/graduate level, it seems highly appropriate to offer courses that have an overlap with various areas of science. The synergistic effect can be compounded by the extensive use of multimedia based communication tools. These novel principles were put into fruition by offering a course on the emerging field of nanomedicine that was available to students in different universities. The lectures were available live via teleconferencing and also videotaped. All the subject material including the videotaped lectures was made available to the students via internet based resources. The methodology, challenges, success, and lessons learned will be discussed.

CINF 85 Educating graduate students in chemical information. Engelbert Zass and Martin P. Braendle, Informationszentrum Chemie Biologie Pharmazie, ETH Zuerich, HCI J 57.5, CH-8093 Zuerich, Switzerland, zass@chem.ethz.ch

Formal chemical information instruction for Ph.D. and diploma (graduate) students started at ETH Zurich in 1984. Instruction at the undergraduate level began later in 2000, and was extended to a full series of courses integrated into appropriate lab sessions or lectures with the switch to the Bachelor/Master system 2004. As a consequence of these teaching activities, the original course at the master thesis/Ph.D. level (1 CP) underwent a major change in 2005 to advanced topics: from "Introduction to Chemical Information" to "Advanced Chemical Information". In between, at the master level, we are still experimenting with suitable courses and their integration in a similar fashion as in our bachelor program. We will discuss organizational and didactical aspects of such courses including the use of electronic tools, as well as their role in the mission of the Information Center.

CINF 86 Librarian office hours: An old tool with a new use to improve graduate education. Bing Wang, Library and Information Center, Georgia Institute of Technology, 704 Cherry Street NW, Atlanta, GA 30332, Fax: 404-894-3005, bing.wang@library.gatech.edu

With more and more digitalized information available on their desktops, graduate students tend to go to the library building less and less. Although phone, email, and other telecommunication tools can facilitate students asking questions, face-to-face reference interviews are still very helpful especially for those who have language challenges. Besides, students hesitate to attend library instructional classes due to the physical distance between their labs and the library. Here at Georgia Institute of Technology, the subject librarian for the School of Materials Science and Engineering (MSE) has been holding office hours weekly in the MSE building. Instead of waiting for questions during office hours, the librarian starts with short demonstrations on various databases and resources followed by question and answer sessions. Such an approach is not only pushing information out to more graduate students but is also attracting faculty and undergraduate students' interests as well.

CINF 87 Deconstructing molecules in an organic information course. Judith N. Currano, Chemistry Library, University of Pennsylvania, 3301 Spruce St. 5th Floor, Philadelphia, PA 19104, Fax: 215-898-0741, currano@pobox.upenn.edu

The Chemistry Department at the University of Pennsylvania requires all PhD students to complete a course in chemical information during the first year of study. The twelve-week course, taught by the Chemistry Librarian, has the students divided into sections based on their subject interest (organic, inorganic, biological, or physical). The organic section focuses on resources that support synthetic organic chemistry and techniques of locating substances and reactions in the literature. It relies heavily on substructure searching in many of the databases; and three to five lectures are devoted to this topic. The students are taught to analyze molecules, create generic substructures, adapt them to be more or less specific, and apply these theoretical skills to each resource studied. The duration of the course gives students time to learn advanced substructure skills, including the use of complex generic groups, repeating units, reaction mapping, and the combination of substructure search sets.

CINF 88 Fifty years of the International Association for Great Lakes Research. Matt F. Simcik, Division of Environmental Health Sciences, University of Minnesota, MMC 807, 420 Delaware Street SE, Minneapolis, MN 55455, Fax: 612-626-0650, msimcik@umn.edu

The International Association for Great Lakes Research is a scientific organization made up of researchers studying the Laurentian Great Lakes and other large lakes of the world, as well as those with an interest in such research. It was established in 1975 as a society of scientists interested in studying the Great Lakes. These scientists represent such diverse backgrounds as biologists, economists, physical oceanographers and chemists. Many of the early work on environmental chemistry was published in its journal and countless presentations on the chemistry of the Great Lakes ecosystem are presented every year at its annual meeting. The history, mission and seminal findings of research presented at its conference and within its journal will be presented.

CINF 89 Mass balance models for persistent, bioaccumulative, toxic chemicals (PBTs) in the Great Lakes: Application to Lake Ontario. Joseph V. DePinto, Limno-Tech, Inc, 501 Avis Drive, Ann Arbor, MI 48108, jdepinto@limno.com, and Russell G. Kreis Jr., National Health and Environmental Effects Research Laboratory, USEPA Office of Research and Development

Over the past 20 years, the Great Lakes research and modeling community has made great strides in the

development and application of process-oriented models to support the assessment and management of PBTs in large lakes. These models have been used to develop a quantitative relationship between the loads of chemicals such as PCBs from various sources and the concentrations of those chemicals in the water, sediments, and biota of the lake. Mass balance modeling for PCBs in Lake Ontario will be used to illustrate how mass balance models are developed by blending research, monitoring, and modeling. We will also present insights that have been gained by models. For example, current external sources of PCBs to Lake Ontario are mainly from atmospheric deposition and upstream loading through the Niagara River. But the response of fish PCB concentrations, while continuing to decline, is controlled by feedback from sediments that still have high levels from historical loads.

CINF 90 Contaminant mass balance model applications in the Great Lakes: Lower Fox River/Green Bay and Lake Michigan. Russell G. Kreis Jr., National Health and Environmental Effects Research Laboratory, USEPA Office of Research and Development, Mid-Continent Ecology Division, Large Lakes and Rivers Forecasting Research Branch, Grosse Ile, MI 48138, kreis.russell@epa.gov, and Joseph V. DePinto, Limno-Tech, Inc

Multimedia, mass balance forecast models have been applied to determine the sources, transport, fate, and effects of contaminants in the Great Lakes and to aid managers in the decision-making process. This presentation provides an overview of applications to the lower Fox River/Green Bay complex for PCBs, and to Lake Michigan, on a lake-wide basis, for PCBs and atrazine. The lower Fox River/Green Bay complex has a long history of PCB contamination. Modeling results indicated that sediments were the primary source of PCBs, and if remediated, fish consumption advisories could be relaxed after approximately 10-20 years. The Lake Michigan Mass Balance Study indicated that the primary source of PCBs to the system was through atmospheric routes; whereas, atrazine inputs were primarily from tributaries. Forecasts indicated that PCBs will continue to decline in lake trout and could be accelerated; however, forecasts for atrazine suggest continued increases at present usage and input rates.

CINF 91 PBDEs and PCBs in the sediments of the Great Lakes: Distributions, trends, influencing factors, and implications. An Li1, Karl Rockne2, Neil C. Sturchio3, Wenlu Song1, Justin C. Ford1, Dave R. Buckley4, and William J. Mills1. (1) School of Public Health, University of Illinois at Chicago, 2121 W Taylor St, MC 922, Chicago, IL 60612, Fax: 312-413-9898, anli@uic.edu, (2) Department of Civil and Materials Engineering, University of Illinois at Chicago, (3) Department of Earth and Environmental Sciences, University of Illinois at Chicago, (4) Department of Civil and Materials Engineering, University of Illinois at Chicago

The spatial distribution and temporal trends of PBDEs and PCBs in the sediments of the Great Lakes were investigated through retrieving sedimentary records. The accumulation of the 9 tri- through hepta-PBDEs (Σ9BDEs), BDE209, and the sum of 11 PCBs were 5.2±1.1, 92±13, and 69±10 tonnes, respectively, around year 2002. The inventories of both PBDEs and PCBs show strong dependence on the latitude, and to a lesser extent on the longitude, of the sampling sites. From the 1970s to 2002, the increases in PBDE input flux were exponential at all locations. In the same time period, PCB fluxes were dramatically decreased or leveled off depending on locations. The year of deposition, latitude, and organic matter content of the sediments account for about 70% of the variations in PBDEs. For PCBs, changes in congener patterns with sediment depth differ among lakes, and evidence of in situ dechlorination was observed in Lake Ontario.

CINF 92 The Great Lakes offshore biological dessert and the nearshore slime around the tub. David C. Rockwell, Great Lakes National Program Office, United States Environmental Protection Agency, 77 West Jackson Blvd, Chicago, IL 60604, Rockwell.David@epa.gov
Annex 3 of the Great Lakes Water Quality Agreement calls for the development and implementation of phosphorus control programs and measures to reduce algal biomass and to eliminate nuisance conditions, especially in Lakes Erie, Michigan and Ontario. The primary objective of reducing phosphorus loadings to the Great Lakes was to control algal abundance and species composition. Based on TP trends observed in the GLNPO long-term monitoring data and Environment Canada, for all five lakes, there has been a decline in spring total P over the last 3 to 4 decades. At the same time, green slime conditions have reemerged in the nearshore zones and are reported in various places in all Lakes except Lake Superior. This talk will discuss the chemical and biological conditions observed in the biological nutrient depleted offshore and nutrient enriched nearshore zone.

CINF 93 Moving the region toward meaningful Great Lakes restoration. Kristy Meyer, Lake Erie Program Director, Ohio Environmental Council, 1207 Grandview Ave., Ste. 201, Columbus, OH 43212, Fax: 614-487-7510, Kristy@TheOEC.org

In 2004, President Bush signed an Executive Order that established the Great Lakes Regional Collaboration (GLRC) to address nationally significant environmental and natural resource issues involving the Great Lakes. The GLRC is comprised of more than 1,500 people representing federal, state, local and Tribal governments, non-governmental entities and concerned citizens that worked together to develop strong recommendations tied to funding targets to restore the Great Lakes. On December 12, 2005 the GLRC Executive Committee released the GLRC Restoration Strategy. Since December of 2005 the Healing Our Waters® - Great Lakes Coalition, a coalition of 86 national, regional, state and local groups that was founded in 2004, has been working with Congress, state, local and Tribal governments, non-governmental entities and concerned citizens to push for funding for critical projects in the Great Lakes basin that helps the region meet the goals and objectives laid out in the GLRC Restoration Strategy.

CINF 94 Index to physical, chemical and other property data: What's next? Olivia Bautista Sparks and Linda Shackle, Noble Science and Engineering Library, Arizona State University, PO BOX 871006, Tempe, AZ 85287, Fax: 480-965-0883

The Index to Physical, Chemical and other Property Data webpage was created in 1998 to assist Arizona State University Libraries staff and students find property information. At ASU, the page is used in instruction sessions for chemistry courses such as organic and biophysical, and is highlighted in materials science and chemical engineering library orientations. Current work is focused on the expansion of definitions and symbols and the addition of a WorldCat link for resources listed. What is the future direction of this resource? Many libraries link to the website from their Chemistry Subject Guide or their own property page. Is there a way to combine our efforts into one global resource? Librarians unite! This presentation will highlight the history of the webpage and describe the evolution of a new concept in property indexing.

CINF 95 Open software and open standards may help cease the fire. Tobias Helmus1, Stefan Kuhn1, Peter Murray-Rust2, Miguel Rojas Cherto1, Henry S. Rzepa3, Ola Spjuth4, Christoph Steinbeck1, Jarl E. S. Wikberg4, and Egon Willighagen1. (1) Research Group for Molecular Informatics, Cologne University Bioinformatics Center (CUBIC), Zuelpicher Str. 47, D-50674 Cologne, Germany, c.steinbeck@uni-koeln.de, (2) Unilever Centre for Molecular Science Informatics, Department of Chemistry, University of Cambridge, (3) Department of Chemistry, Imperial College of Science, Technology and Medicine, (4) Department of Pharmaceutical Biosciences, Uppsala University

Recent open source developments in chemical informatics, together with open standards for coding analytical information, now allow for the easy creation of open source electronic lab notebook software. An ideal candidate for such an endeavor is our rich client workbench Bioclipse (http://www.bioclipse.net), an open workbench for I/O, display and processing of molecular, analytical and other types of data relevant for electronic lab notebooks [1]. As a second component we have developed the open standard CMLSpect, an extension of Chemical Markup Language (CML) towards representing spectral data [2]. In this presentation, we demonstrate Bioclipse for authoring of semantically rich XML documents, integrating textual, factual, molecular and analytical data into electronic laboratory notebook documents.
[1] Spjuth, O.; Helmus, T.; Willighagen, E. L.; Kuhn, S.; Eklund, M.; Steinbeck, C.; Wikberg, J. E., Bioclipse: An open rich client workbench for chemo- and bioinformatics. 2006, submitted. [2] Kuhn, S.; Murray-Rust, P.; Lancashire, R. J.; Rzepa, H.; Helmus, T.; Steinbeck, C., Chemical Markup, XML, and the World Wide Web: CMLSpect, an XML vocabulary for spectral data. 2006, submitted.

CINF 96 IUPAC name generation: Challenges and evaluation. Daniel Bonniot, ChemAxon, Budapest, Hungary, dbonniot@chemaxon.com

Names are widely used to describe molecules in a familiar and easily understandable way, and have been formalized by IUPAC. We introduce a new implementation of an automatic converter from molecular structures to IUPAC names that can generate the Preferred IUPAC Name in most cases. This generator is available as a module integrated in the chemical software tools provided by ChemAxon. We present challenging cases that needed to be addressed, in several areas including: parent selection, principal chain selection, optimal numbering computation. We also demonstrate the naming of large bridged ring systems with optimal locants. We consider the specific challenges in naming structures with aromatic rings, where dearomatization is required for naming and has to be performed in a controlled way to lead to minimal locants for

the double bonds. Finally, we evaluate the rate of correct names and performance for various publicly-available collections of structures.

CINF 97 Information content in organic molecules: Brownian processing of ribonucleases. Daniel J. Graham and Jessica L. Greminger, Department of Chemistry, Loyola University Chicago, 6525 North Sheridan Road, Chicago, IL 60626, Fax: 773-508-3086, dgraha1@luc.edu

The informatic properties of organic compounds have been the subject of research in this lab during the past several years. The present study focuses on an important class of globular proteins (RNases) whose information can be expressed and quantified using Brownian processing. Proteins are like other organic molecules in that their informatics hinge on the details of atom/covalent bond networks and possible collision sequences in disordered environments. The folding and chemical function of a given sample thus correlate with the message space articulated by the network, its size, structure, and subtleties. In Brownian processing, this space is charted via elementary random walks applied to the structure graphs which are representative of the protein. We present informatic data for several members of the RNase extended family. We examine the correlations between the catalytic specificity of the enzyme and its information distribution functions. Further, the informatic ramifications of select amino acid residue mutations are discussed. Overall, the research investigates protein structure/function relationships from a Brownian computational perspective. The results are significant as RNases control(in part)information transport in the organism.

CINF 98 Chemical Terms, a language for chemoinformatics. György Pirok, Nóra Máté, Jozsef Szegezdi, Zsolt Mohacsi, Szabolcs Csepregi, István Cseh, Attila Szabo, Miklos Vargyas, and Ferenc Csizmadia, ChemAxon Ltd, Maramaros koz 3/a, 1037 Budapest, Hungary

Flexibility and ease of use are important yet contradicting requirements in cheminformatics systems. Complex search criteria routinely used in database queries provide apparent examples. Beyond flexibility and ease of use efficient computability sets a third requirement. To meet all these demands we have designed and developed Chemical Terms, a chemical computation language constituted of hundreds of chemical functions (such as pKa, logP and many other chemical and structural calculations) and common mathematical and logical operators to combine these functions. The predefined set of functions can be extended using an open plug-in architecture. Successful applications of the language including advanced search filters in chemical databases, virtual reactions design and pharmacophore perception are demonstrated. The Visual Chemical Terms Editor that embeds the language in a user friendly graphical environment is also presented. The future development of the Chemical Terms language will introduce strong typing, functional abstraction and containers.

CINF 99 Accounting for 3-D descriptors of conformers in QSAR modeling. Shaillay K Dogra, Achintya Das, and Kalyanasundaram Subramanian, Cheminformatics, Strand Life Sciences Pvt. Ltd, 237, C. V. Raman Avenue, Raj Mahal Vilas, Bangalore, India, Fax: 918023618996, shaillay@strandls.com, kas@strandls.com

3D descriptors computed from a single conformer are used in QSAR modeling. However, the molecule may exist in various conformers. How do we incorporate this variation in 3D descriptors in the modeling process? Does this affect modeling significantly? Averaging of descriptors based on probability-weights derived from a Boltzmann-distribution has been used as a method to address this issue. In an extensive study on a Solubility dataset (1305 compounds, ~45k conformers, 634 3D descriptors), we found that this approach did not make a significant difference. Comparable models were obtained for the two sets – a Boltzmann-averaged descriptors set and a minimum-conformer descriptors set. Though the values for a given descriptor differed across the two sets, these changed in a strongly correlated manner eventually giving us similar statistical models. Is there a better measure to account for the differences in conformers? We investigate different means of sampling and averaging and check their performance.

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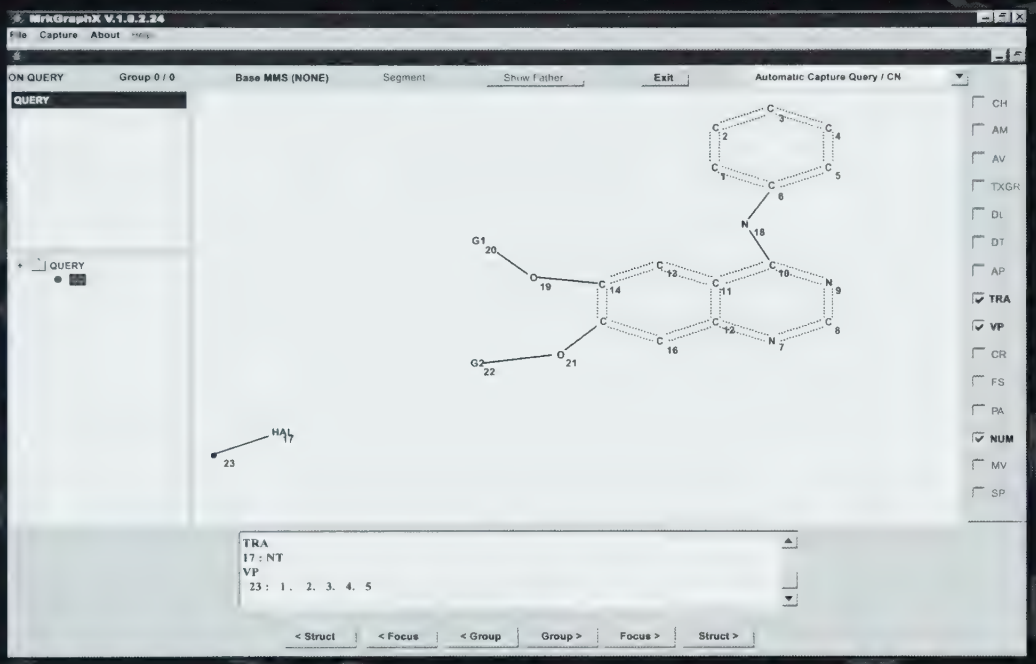

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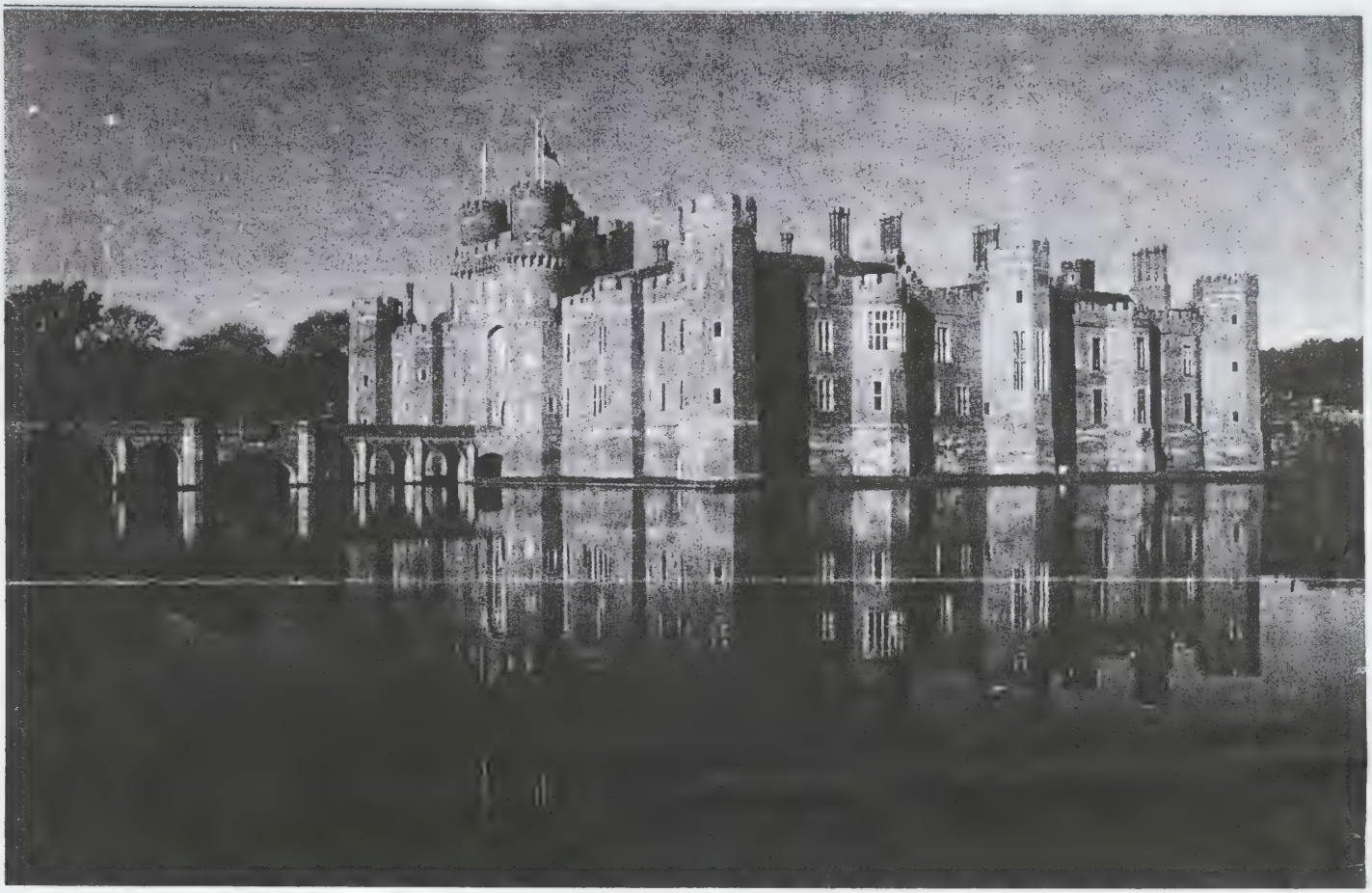

Julia Pearse Smith lived out a fairy tale of her own making while studying abroad at Herstmonceux Castle in southern England.

Moats, stars & ducks: My year in a castle

2008 Sylvia K. Burack Award winner

By Julia Pearse Smith

THE EXPERIENCE that has changed my life the most so far is not a particularly concise one. It wasn't an epic moment on a windy day on a mountain's peak in the Himalayas. Neither was it backed by orchestral accompaniment, swelling and fading with the emotions I experienced. It certainly didn't have a narrator, lending weight to the scene and making me into an epic heroine. At the time, however, it kind of felt like all of these things together couldn't compare to what I was actually living.

When I was 18, I was accepted to study at a place called Herstmonceux Castle in East Sussex, England. This international study center is run by Queen's University in Ontario and offered me the opportunity to study abroad —in my first year, no less—without having to worry about transferring credits. Truth be told, I couldn't have cared less about credits ... I was going to study in a castle. It had a moat. It had ducks, Canada geese, badgers, bunnies (by the thousands) and, delightfully, sheep. It had cantankerous English minibus drivers to bring us to Eastbourne and Brighton. It had official bus drivers to bring us to London and abroad. They wore suits but came home with

dozens of cases of beer from the ferry stowed away in the hold. In short, when I actually got there, it was more ridiculously amazing than I would ever have believed.

People at home said it sounded like Hogwarts—they asked me if I'd bought my wand and cape. When I got there, it actually felt like I might need both. The food turned out to live up to all the clichés about British cuisine, there were enormous "mansquitos" that swarmed our dormitory for a couple of months in the beginning, and the badgers turned out to be more terrifying than *Wind-in-the-Willows*-esque. But if I could give my own children one gift in life, I would send them to this place.

I had all the promised student experiences with my new best friends: the Roman Baths, Canterbury Cathedral and World War I trenches in Belgium, to name a few. What hadn't been in the brochure was the atmosphere in which I got to live for a year. When I looked out my window, I saw fields that would make Beatrix Potter yank out her pen and start writing. When I walked the castle grounds, there was a Shakespearian herb garden, a hidden Zen corner, a statue grove, and a grass bed with head and footboard. When I left the castle after dinner in the evening, the ducks that had come to know me well surrounded me by the dozen, vociferously demanding the bread they knew I had for them. They even sat on my knee sometimes, honking away, much to the amusement of the gardener.

At night, we lay out on the lawns and watched the stars. What made it particularly special was not only the vast unimpeded universe, only slightly polluted by the lights of London, but also the astronomical observatories sending up their green lasers into the night sky, making calculations as they came back through the atmosphere. The contrast of this mind-bending modern technology and the utterly beautiful night was both inspiring and humbling.

It would take me a whole book to explain everything with any accuracy of emotion. The most important part, I think, would be to try to explain the love I feel for that year. It was the happiest I've ever been, and the freest I have ever felt. What it gave me was not only a year's worth of experiences, however—it was the knowledge that my life could feel like that. I actually got to live and study in a castle on the most magnificent grounds I've ever seen, and feel like a character in a fantasy novel. I should have had a soundtrack and a narrator!

I didn't stand on a mountain top in the Himalayas with the wind howling, but I did stand on a rickety metal observation tower in the middle of nowhere with my best friend, 30 feet in the air, the wind so loud we couldn't hear each other even if we shouted. It was our last day in England before we came home for good. We stood next to each other, a little terrified and very cold, but needing to have one last epic moment together before we came home to Canada and had to go back to being regular people who didn't live in a castle. A few hours later, they'd finally gotten around to wrapping the death trap with barbed wire so that no one could kill themselves on it—but we'd already had our time in the wind.

Meet our award winner

JULIA PEARSE Smith is finishing up her degree in humanistic studies at McGill University in Montreal, her hometown. "After I graduate, I intend to open a destination hotel and vegetarian restaurant in Ireland, my mother's place of birth, where I've spent a lot of time living and working over several summers," she says. There she would like to offer cooking lessons and spa services. "I believe very firmly in the health benefits of relaxation and simple contentment," she says.

Her interest in writing developed in secondary school, when her short story was chosen for publication in *The WIER Tap*. "Whether it's fiction or creative nonfiction, writing is a record of what's banging around your mind, which can both surprise you later on, and remind you of parts of yourself that change and disappear with time," she says.

Julia Pearse Smith

She enjoys writing exercises because they "focus on the writing itself instead of the quest for originality." For the winning essay, she explains, "I chose to write about my year in the castle because it was a life-changing experience in so many ways—personally, academically and emotionally. [The experience was] irreplaceable to me."

Editor's note: *The Sylvia K. Burack Award is named for the former editor and publisher of* The Writer. *For 60 years she served the magazine and encouraged writers at all stages of their careers. We asked college students to write about the experience that most changed their lives, and Julia's essay was picked from more than 400 entries. She received $500 and a subscription to* The Writer.

www.WriterMag.com

Guidelines and entry information for the 2009 Sylvia K. Burack Award are available on *The Writer* Web site. This year we are asking college students to write a personal essay on a subject they feel passionate about.

Goodbye summer... hello school! Jacob Etches, a student in the graduate department of community health, standing outside University College, is one of thousands of new and returning students making their way back to U of T's three campuses this September. During orientation last week President Robert Prichard urged new students to take full advantage of "the great resources this university has to offer" — including everything from sporting facilities and events to theatres, libraries and campus clubs and activities — and to experience its immense diversity and excellent programs.

Inside

U of T Day is coming!

U OF T DAY IS HAPPENING ON Saturday, Oct. 3 at the St. George campus between 10 a.m. and 4 p.m. This year's attractions include a mock medical emergency, a petting zoo and a children's fair featuring an "outer space" adventure

Donors Give Victoria $6 Million

BY KATE ECCLES

VICTORIA UNIVERSITY HAS received the largest donation in its 162-year history — $6 million — from philanthropists Isabel and Alfred Bader.

The gift will enable the university to build a 500-seat theatre on Charles Street next to historic Burwash Hall. The Isabel Bader Theatre, tentatively slated for completion in the fall of 2000, will become home to The Bob Revue which began in 1874 and is Canada's longest-running annual theatre program. The facility will also double as a lecture hall for University of Toronto students from a wide variety of disciplines.

"Victoria University has a long tradition of amateur theatricals," said Victoria president Roseann Runte. "Norman Jewison, Donald Sutherland and Don Harron are examples of the many Vic grads whose show business careers began during their student days at Victoria."

The college's reputation in the humanities has also been forged by many Canadian academic and literary luminaries, Runte added, including literary critic Northrop Frye, poet E.J. Pratt and author Margaret Atwood.

"By making the theatre and lecture hall possible, Isabel Bader has brought her love of the humanities, theatre, education and people together on the Victoria campus," Runte said.

Isabel Bader, a 1949 graduate of Victoria College, spent 30 years in England as an English and history teacher and, while there, became an associate of the New Era Academy of Speech and Drama. A lover of the dramatic arts, she also co-founded a costume museum.

Alfred and Isabel Bader have helped reshape Victoria College's awards programs. In 1993 they established the Bader Scholarships to help talented students whose economic circumstances might deprive them of a university education. In addition the Baders have provided awards for students who wish to study abroad.

The Campaign for the University of Toronto, Canada's largest university fundraising effort, has set a goal to raise a minimum of $400 million in private support.

Profile

New Recruit

Florence Silver takes on challenge of attracting diverse student group

BY SUSAN BLOCH-NEVITTE

AFTER FIVE YEARS AS VICE PRESIDENT FOR exhibits and marketing at the Royal Ontario Museum, Florence Silver is no stranger to the art of selling. As a former superintendent of schools for the North York Board of Education who has spent most of her life somewhere near a classroom, U of T's first director of student recruitment looks like a pretty good fit for some pretty hefty university ambitions

Silver will develop and oversee a comprehensive recruitment strategy to continue attracting top students and to increase applications and enrolment of undergraduate and graduate students nationally and internationally. That's no small challenge for a campus that's stridently international in stature but decidedly regional in its student body.

Almost 79 per cent of first-year undergraduates at U of T come from the Greater Toronto Area, 16.1

~ *See NEW, Page 7* ~

May 8, 2007

Alfred and Isabel Bader asked me as a friend of theirs to attend this film performance to represent them. Allow me a few moments to explain our relationship and give you my personal comments on Alfred and Isabel's life.

Alfred and I have much in common and yet differ widely in many respects. I came to know Alfred in Internment camp and found him to be a charming, very bright young man who was curious about and interested in Judaism and our religion. We spent time in camp together discussing this and many other topics.

I come from an Orthodox, old established German Jewish background growing up in the midst of a large monolithic close family, attending Orthodox elementary and high school, until in my young age I left for England in 1937, ahead of my parents who followed penniless in late 1938 after Kristallnacht, robbed by the Nazis of everything they possessed, but lucky to escape alive with my sister before the war, thus escaping the Holocaust.

Fate brought Alfred and me together – first in internment and then four years at Queen's University in Kingston and we have remained friends ever since, though we traveled on different paths with very different personalities.

A "Canadian in Love" depicts Alfred as an incorrigible romantic soul which I never was. I got married some 57 years ago, meeting my wife by a fluke – she living in New York and I in Montreal. After a whirlwind courtship that brought us together a total of not more than 48 hours at several intervals we decided to get engaged and subsequently got married a few months later. By now we are blessed with three children in Toronto, New York and Jerusalem, twenty-one grandchildren and twenty-three great-grandchildren.

Alfred has two sons Daniel and David of whom he is justifiably proud and he has a number of grandchildren that give him much joy.

I always followed Alfred's spectacular business and art-collecting career with great fascination and from time to time we exchange thoughts and views on religion and on the social and political ills and woes of society.

What we have in common is our desire to help others and to try and make the world a better place by being charitable when and where it makes a difference, where our presence and our helping hand to society and individuals affects their life for the better.

Alfred is an impetuous and enormously innovative person, recognizing an opportunity and seizing it, be it a painting, a business opportunity, an old castle in Wales to buy and donate to his alma mater Queen's University to serve as a Centre of International Study, or helping victims of war and hunger, or endowing with extraordinary generosity Jewish education.

A quiet, reserved and personally very austere and almost stingy person, his great unselfish, selective personal philanthropy has been extraordinarily effective on the campus of Queen's University, in his city of residence Milwaukee, and assisting society in Israel, in the Middle East, in the Balkans and in the FSU, formerly Soviet Russia.

Isabel has had a very positive loving influence on Alfred and his life's activity. She is a true partner to him and a very exceptional person in her own right.

I wish them well and many more years of fruitful endeavour.

Kurt Rothschild

ILLUMINATION

Centuries of Knowledge at the University Libraries ~ University of Maryland

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UEEN ELIZABETH IS
INTRODUCED TO KING FOOTBALL"

"43,000 CHEER QUEEN, PRINCE
AND VICTORIOUS TERPS"

"MARYLAND PULLS UPSET
THAT'S FIT FOR A QUEEN"

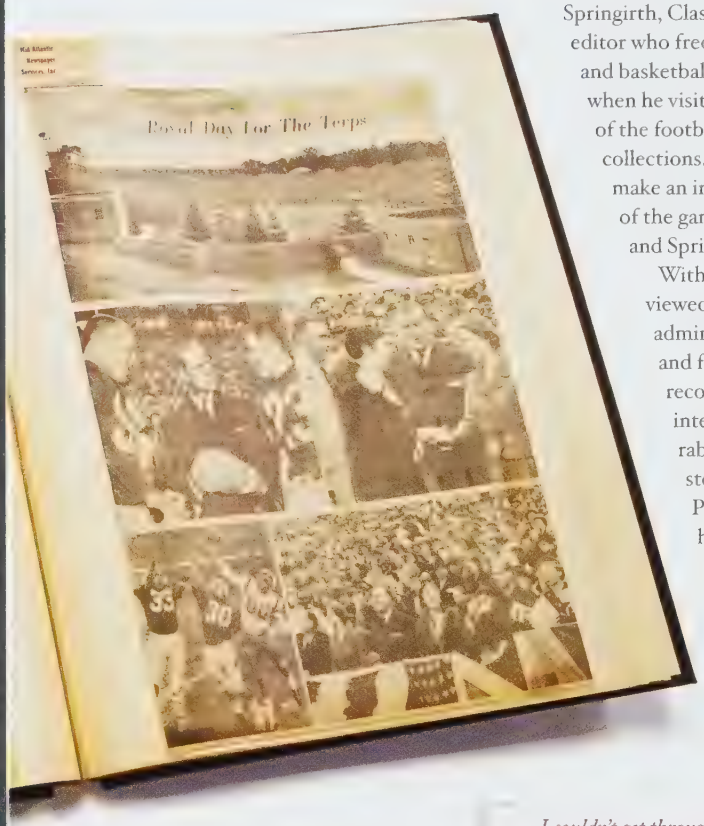
"QUEEN, PRINCE 'GO AMERICAN'" read the headlines in the Washington, D.C. area, across the nation, and around the world, marking a memorable event in University of Maryland history. On October 19, 1957, Her Majesty Queen Elizabeth II and her consort, Prince Philip, journeyed to Byrd Stadium on the University of Maryland campus to see "a typical American sport." As guests of University President Wilson H. Elkins and Maryland Governor Theodore R. McKeldin, they witnessed the Terrapins defeat the North Carolina Tar Heels 21 to 7 in a major upset touted by Maryland football coach Tommy Mont as "the most wonderful victory of my career."

Queen Elizabeth received many gifts at the game, including a huge bouquet of roses, a ceramic drummer horse, and two arrows signifying the colony of Maryland's annual debt to its sovereign

The Queen and Prince Philip followed the action closely throughout the hard-fought contest and enjoyed the halftime festivities, during which the Queen received many gifts from the university, including a diamond and ruby-studded terrapin-shaped brooch. After leaving the stadium, the Queen and Prince Philip visited the Giant Food store located on Queen's Chapel Road as they returned to the White House, an intriguing footnote to the day's events.

This fall the University Archives will celebrate the fiftieth anniversary of the "Queen's Game," as this special day has become known, by mounting an exhibit entitled "Royal Remembrances." The celebration will also feature a public reception on October 4th, 2007, honoring the 1957 Terrapin football team and the premier of a documentary chronicling many of the events of game day. This production is the brainchild of Maryland alumnus Mike Springirth, Class of 1978, a local freelance videographer, producer, and editor who frequently undertakes projects for the university's football and basketball teams. Springirth first learned of the "Queen's Game" when he visited the University Archives two years ago to film some of the football team memorabilia and photographs in the Archives' collections. University Archivist Anne Turkos felt this event would make an interesting project and regaled Springirth with the story of the game as well as her plans for celebrating the anniversary, and Springirth was hooked on the topic.

Page from a scrapbook of newspaper clippings about the game from around the world, compiled by the Office of University Relations.



With funding for the project from a close friend, he interviewed members of the 1957 team and the marching band, administrators involved in planning the Queen's visit, and fans in the crowd in Byrd Stadium, anyone who had recollections of or anecdotes about the day. Many of those interviewed described the day as one of the most memorable of their lives, and quite a number recounted amusing stories, among them Carole Elkins Neal, University President Wilson Elkins' older daughter. Neal recalled her displeasure at being forced to attend the game, much preferring to be on the sidelines of the football game at Northwestern High School, where she was a cheerleader. To add to her indignation, her mother insisted that she wear a hat to the game and promptly took her rebellious daughter to buy a new outfit, including a lovely white velvet beret. That beret never made it home to the President's House following the game, however. As Carole recounted,

> *I couldn't get through the day without one last rebellious action, so I rolled down the limo window and frizzbeed the white velvet beret out the window and onto the playing field. My parents ignored me and never said a word about it. Now I wish I still had that little white beret! Of course, I am very proud to have been a part of that historic day!*

Springirth, with assistance from Anne Turkos, was also successful in locating the manager of the Giant Food store, the policeman who suggested that the Queen visit the Giant, and one of the shoppers who spoke with the Queen that afternoon and was photographed with her. In addition, he incorporated moving and still images, publications, and objects from the Archives into his piece, for a comprehensive and engaging look at many aspects of this remarkable day.

MARYLAND • NORTH CAROLINA

HER MAJESTY QUEEN ELIZABETH II

Cover of the game day program

SATURDAY, OCTOBER 19, 1957 • BYRD STADIUM • COLLEGE PARK, MARYLAND

The exhibit, "Royal Remembrances," will encompass numerous images from the "Queen's Game" and the Queen's visit to the grocery store, as well as personal reminiscences from game day participants and memorabilia. Among the pieces on display will be the game day program; a Canadian flag, one of the many representing the British Empire that flew over the stadium; and a neckerchief worn by a member of a Boy Scout troop which served as ushers for the game. The installation will also feature the football helmet worn during the game by Terrapin Ron Shaffer, a sophomore end on the 1957 team, on loan from Shaffer for the exhibition.

Please join the University of Maryland Libraries and the Department of Intercollegiate Athletics on October 4, for the premiere of Springirth's documentary and a reception honoring "Queen's Game" participants.

ROYAL REMEMBRANCES EXHIBIT, open September 1 through December 21, 2007, will be mounted in the Audrey Armistead Ruckert Reception Foyer of Hornbake Library and the Maryland Room. See *www.lib.umd.edu/hbk/hornbake.html* and *www.lib.umd.edu/mdrm/mdhours.html* for the hours these facilities are open. Questions concerning "Royal Remembrances" and the October 4 event may be directed to University Archivist Anne Turkos (301.405.9060, aturkos@umd.edu).

The Elegance of language:

Poets Laureate & their Poetry

MORE THAN 100 family, friends, and guests attended an exhibition reception hosted by the University of Maryland Libraries on Thursday, April 26, to celebrate the Maryland Poets Laureate Roland Flint and Reed Whittemore, and their gifts of personal papers to the Special Collections' holdings of literary manuscripts. It was an unforgettable evening. Beautiful poetry, rich insights, and elegant language were brought to life by the gracious presence of Poets Laureate Lucille Clifton, Michael Collier, Michael Glaser, Linda Pastan, and Reed Whittemore.

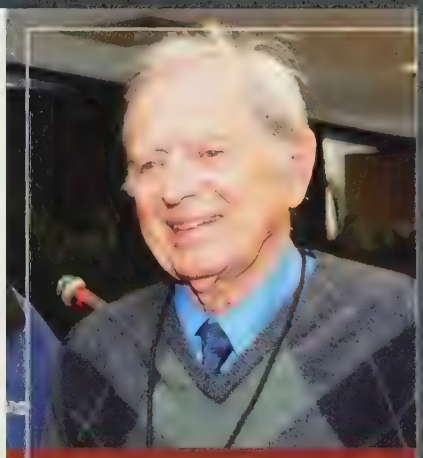
FROM LEFT TO RIGHT:
Mary Flint, Jim Hoyme, Roz Cowie, and Marjoie Hoyme; Michael Glazer, Lucille Clifton, Linda Pastan, Michael Collier, and Merrill Leffler.

PERHAPS THE MEMORIES that will live most vividly in the minds of the audience were the heart-warming stories and vignettes that gave a sense of the lives of Flint and Whittemore, and a feel for the experience of creating poetry. They were uplifting and fostered appreciation for the genius of those who create literature that refreshes thinking and broadens understanding.

It is vital that the records of such lives be kept, and the Libraries of the University of Maryland are deeply grateful for the gifts of papers of Roland Flint and Reed Whittemore to the literary manuscripts holdings of Special Collections. They join the records of other important literary lives such as Katherine Anne Porter, Djuna Barnes, Jesse Glass, Gianni-DeVincent Hayes, Roy Hoopes, Walter Howard Kerr, Mollee Kruger, John Pauker, Myra Sklarew as well as the Arthur J. Gutman Collection of Menckeniana. Literary Manuscripts also include materials documenting two small Maryland based presses—Dryad Press and SCOP Publications Inc.—and hold the Maryland Folklore Archives. In addition, significant small collections document American literary figures such as Laura Riding Jackson, Ferdinand Reyher, Karl Shapiro, and Gertrude Stein. These archives are organized for use through many, many hours of fine, detailed work, and are cared for so they will endure.

The collecting and processing of significant literary manuscripts is a quiet and steadfast commitment, but it is a challenge. The expertise required is costly and the support the University receives from the State of Maryland has shrunk. However, the Libraries are fortunate to have some special funding available to continue the care of the collection through individual gifts to The Kruger Fund. Established by alumna and donor Mollee Coppel Kruger and her husband Jerome, the Kruger Fund supports the building, maintenance and preservation of the literary manuscripts holdings of the University Libraries. Financial support from The Kruger Fund, augmented by support from the Friends of the Libraries Fund, made possible the April 26 event to honor the Maryland Poets Laureate.

It is a pleasure and an inspiration to glimpse the lives of those who create literature powerful enough to move the mind to nobler intent. To assure that future generations of thoughtful readers will also experience those lives, please consider a gift to the Kruger Fund. For more information contact the Office for External Relations at 301.314.5674 or libextrel@umd.edu

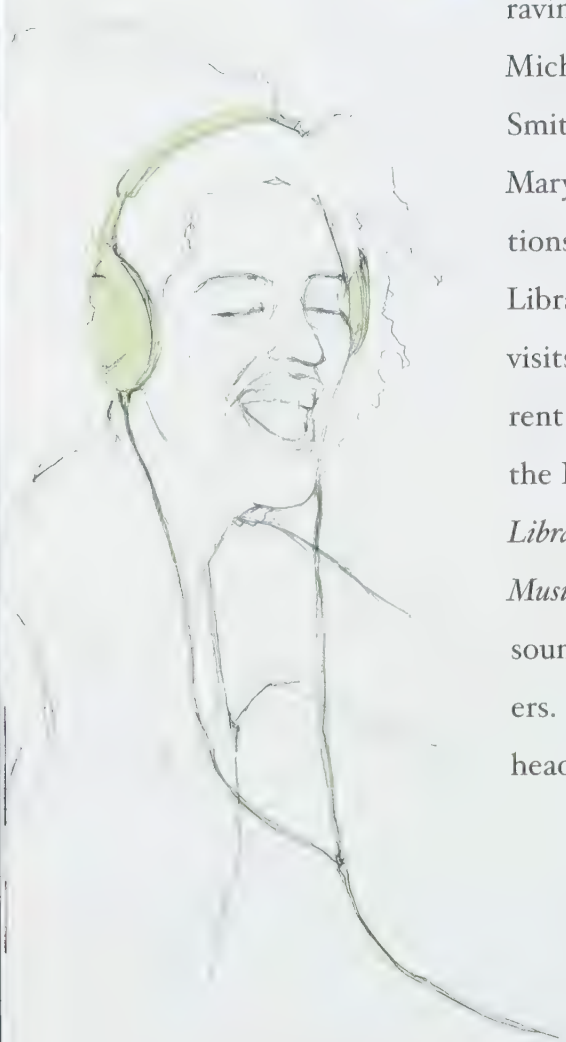


IT WAS A PLEASURE to have former Poet Laureate Reed Whittemore participate in the evening's activities. His memoir *Against the Grain: The Literary Life of a Poet*, is forthcoming.

They were uplifting and fostered appreciation for the genius of those who create literature that refreshes thinking and broadens understanding.

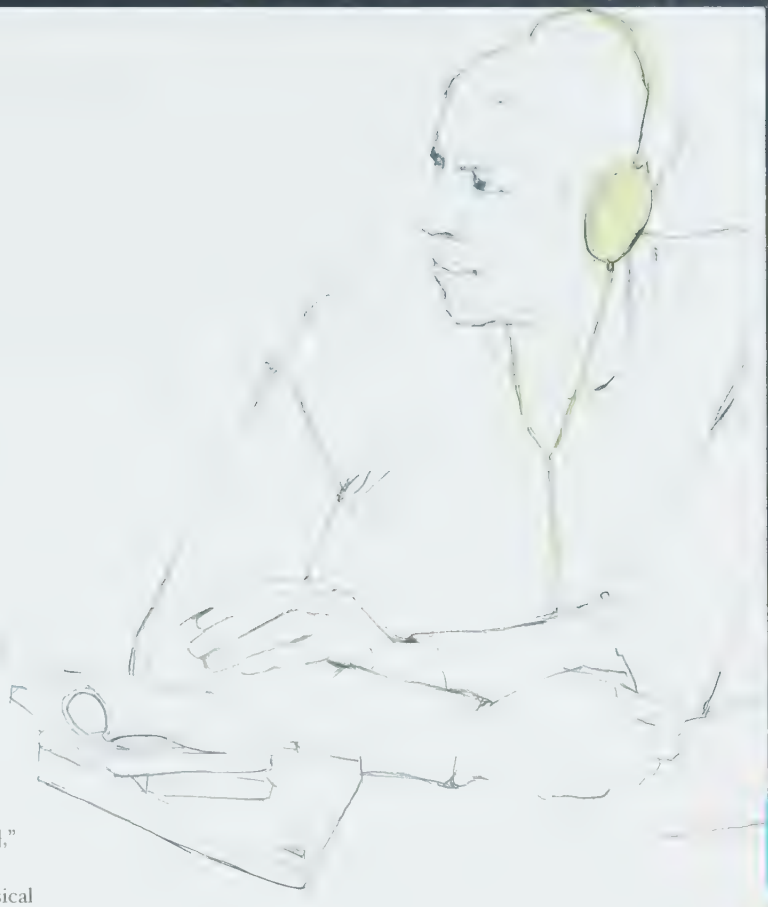
Listen

LIBRARIES ARE FAMOUSLY QUIET PLACES, but University of Maryland professors and students are raving about what they can hear in our Libraries. The Michelle Smith Endowment, created for the Michelle Smith Performing Arts Library at the University of Maryland, College Park, is being used for subscriptions to expensive music/audio databases which the Library could not otherwise afford. Anyone who visits the College Park campus Libraries or has a current student/faculty/staff UM ID card and accesses the Libraries remotely, may use them. *Classical Music Library*, *Digital Repository of American Music*, *Naxos Music Library*, and *Smithsonian Global Sound* deliver sound recordings on demand directly to computers. Users listen to them with desktop speakers or headphones.



illustrations by Brian Payne

in the LIBRARIES



"I USE THESE TO AUGMENT library recordings holdings, but also for convenience—rather than make a special trip to the library to check out CDs, it's nice to have them available via streaming [on personal computers]," says one music theory professor. "I find them very productive as a means to expand one's musical horizons—the easy access encourages acquaintance and familiarity with works and performances one either wouldn't otherwise be able to, or simply wouldn't, access. Having recordings online is, I understand, a BIG help for the students, allowing them to study from home and saving a lot of time instead of needing to physically be in the library to use the reserve desk." A musicologist said, "I've been using the Naxos Library regularly since it became available—it's saving my life and sanity!!! I mostly use it at home when I prepare lectures; ... the range of repertoire is superb. Really helpful, especially when I need access to a piece we only have one copy of in the library (probably the copy I've put on reserve for my students), or when I have a bright idea and need to hear something immediately—the flexibility is priceless. Thank you guys for making my job so much easier." Classrooms in the School of Music allow videos to run at the same time that music is playing on the computer, so during a recent class, the 1924 silent film *Entr'acte* was projected on the wall screen while a recording of music that Erik Satie composed for it was called up from one of the databases. Without the database subscription, the class could not have had such an experience, since the Libraries do not own a CD or LP of the orchestra version of this music and no one has produced a version of the film that puts Satie's music on the soundtrack.

Students find these databases "tremendously helpful." One voice major said he uses the classical music databases to listen to vocal works in preparation for lessons and another said, "I use them to listen either to pieces I'm thinking of learning (to see if the piece would fit into my voice well) or pieces that I am learning (to see how other artists performed them)." Others use them to study for listening exams when the library is not open, since they can access the music at all hours from their dorm or home. A graduate student said, "I love that we have these musical databases—I don't know what the University pays for us to have access, but what a great resource for students, and it is so much less time-consuming than having to look up/check out CDs from the library or purchase them from Amazon." A student who compared Mozart piano concertos using the databases testified, "For a paper I did last semester on 19 of Mozart's piano concertos, instead of getting each CD, I was able to listen using the database more quickly." A doctoral student said, "As I've searched for my dissertation theme, it's been particularly useful as I could listen

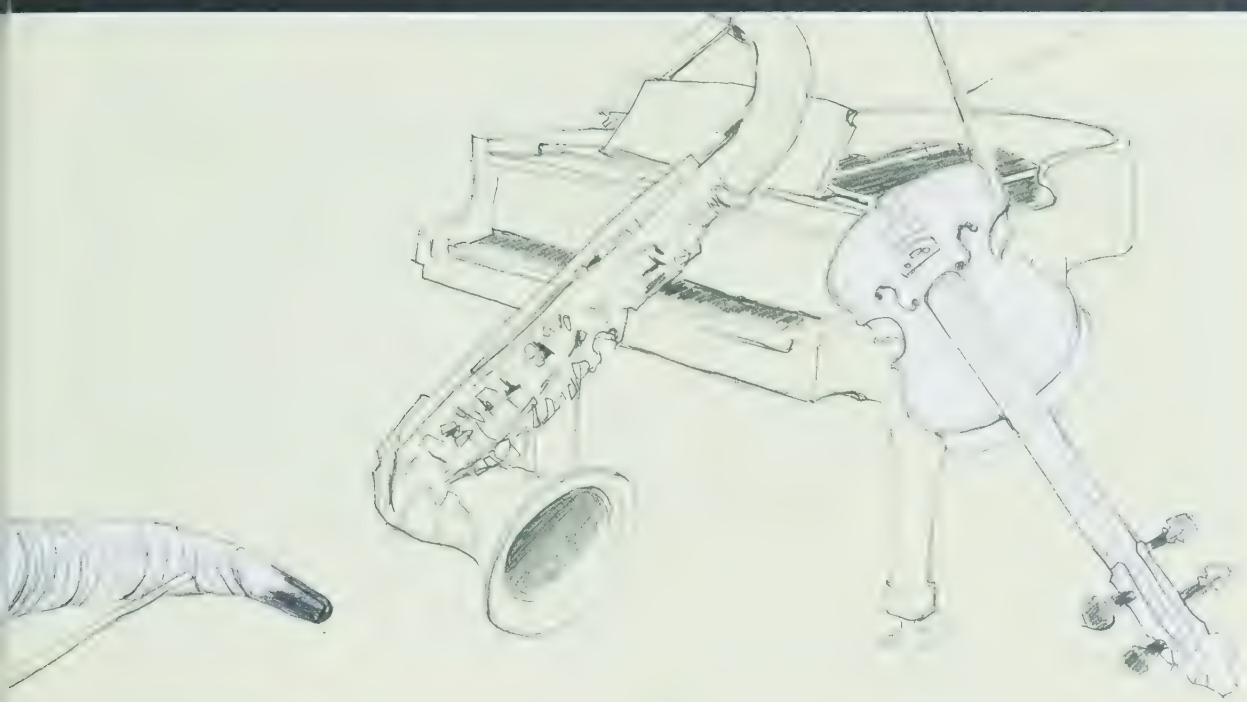
DRAM (*Database of Recorded American Music*) is a not-for-profit resource providing CD quality audio and complete original liner notes and essays from New World Records, Composers Recordings, Inc. (CRI) and other labels. This digital library of important American and international repertoire provides music and scholarly materials not otherwise accessible to students and researchers. Currently, more than 1,500 CDs (9,800 compositions) are in DRAM, the core of which is the diverse catalogue of American music recordings by New World Records. From folk to opera, Native American to jazz, 19th century classical to early rock, musical theater, contemporary, electronic and beyond, DRAM also includes music from other recording labels covering music of American composers. Music librarians consider this database essential for the study of American music.

to less studied music. In fact, this helped lead me to the topic I've decided to pursue: Ferdinand Ries's works for piano and orchestra." A master's student found his thesis topic by "using *Smithsonian Global Sound*—obsessively! It's the main topic of my research for my master's thesis, which developed out of my interest as a musician and customer. For the record, I emphatically support the idea of renewing the school's subscription." Another user of this database said, "Recently I had to provide a 'Jewish-sounding' tune for a theatre group and it was a great resource to immediately listen to authentic music from that genre."

Some faculty and staff use the databases to listen to music at their desks, while they work. Perhaps it makes them smarter!

Naxos Music Library has 87,000 tracks for online listening, including classical, jazz, world-music and historical releases. (Each movement of a multi-part work is on a separate digital track.) This database complements *Classical Music Library* and *Smithsonian Global Sound* and allows for more comparisons of performances of classical works. For example, one can compare performance of Handel's "Their Land Brought Forth Frogs" in *Classical Music Library* and *Naxos*. Both versions may seem far too polite to be believable, though—this music describes a frightening plague, after all—so LPs and CDs in the Michelle Smith Performing Arts Library remain important resources for all to explore.

Classical Music Library contains recordings of music written from the dawn of notated European music to the present. Repertoire ranges from vocal and choral music (including Gregorian chant), to chamber, orchestral, solo instrumental music, and opera. Works are continually added. CML wants to offer at least one recording of each work listed, though multiple recordings of most major works appear, enabling comparative listening. Coverage of repertoire is increasing as new labels are added. The collection for listening and searching is supplemented by reference texts (biographies, for example), but liner notes are not included.

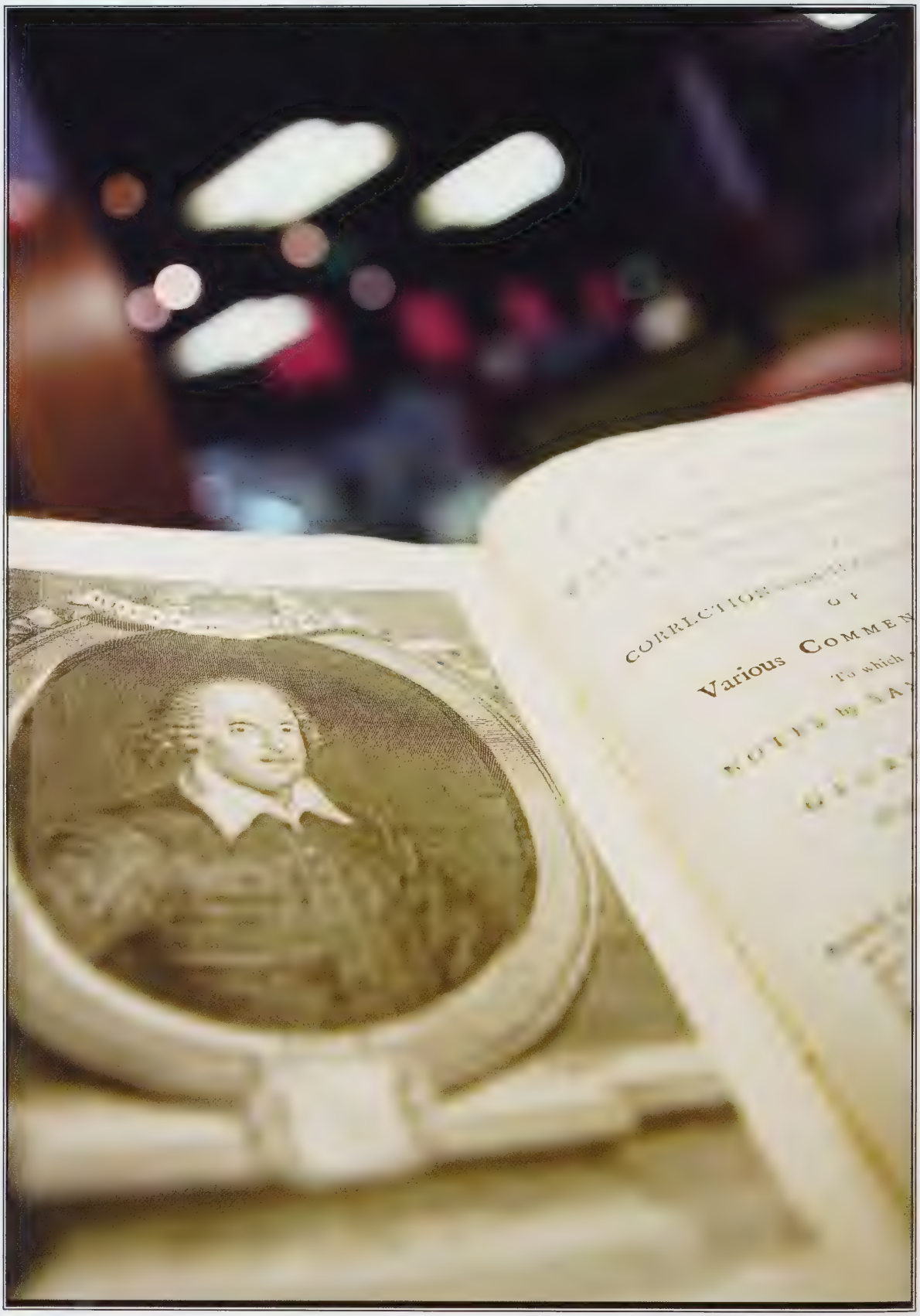


Smithsonian Global Sound for Libraries includes published recordings owned by the non-profit Smithsonian Folkways Recordings label and the archival audio collections of other folk music labels. It also includes music recorded around the African continent in the mid-20th century by Dr. Hugh Tracey for the International Library of African Music at Rhodes University. For each area of the world, but for Africa most meticulously, tracks are indexed and are searchable by type of instrument (percussion, vocal, wind, string), region of the continent, individual country, and specific cultural group, or tribe. Entire albums can be played through, album cover art is shown, and liner notes, many of which contain song lyrics, have also been scanned. Some experimental 20th-century composers (such as John Cage, Henry Cowell, and Charles Ives) could not land contracts with standard labels, but Folkways recorded them, so some of their music, not at all folkish, is in *Smithsonian Global Sound*. Besides music, spoken stories and memoirs such as Mahalia Jackson's nine-minute "Recollections of New Orleans music," are here, as are nature sounds. For example (speaking of frogs), one can listen to all tracks in succession of Folkways best-selling *Sounds of North American Frogs* and read the 22-page accompanying booklet online, too—it includes photographs of many of the singers on the album.

In some of the databases, users can create their own playlists or click on ready-made themed playlists that group tracks in various ways: in Classical Music Library some lists are by music textbook, some by composer, performer or style period, some by genre or pure whimsy: look for "Lover's Guide" or "Music for a Rainy Day." In *Smithsonian Global Sound*, the pre-set playlists may focus on a country, style, genre, or time period. The one titled "Mickey Hart's Musical Journey of Smithsonian Global Sound" offers percussion music from around the world. Faculty who have created playlists for specific courses can use tracks for listening tests by hiding track information. Students can also do this in their own playlist folders to test themselves.

Some music database tracks are available for sale, and people report having been able to buy recordings there that are not available elsewhere. These databases grow in popularity over time and will become even more important in future as they expand in size.

'Hear the Turtle' in the Libraries! *Smithsonian Global Sound* contains a Thai story-song that puts a non-competitive twist on Aesop's fable of the hare/tortoise race, a Venezuelan Yekuana Indian performer using a tortoise shell as a wind instrument, and a tortoise mating call (!) recorded in 1952 at the Brookfield Zoo near Chicago. On your next visit to our campus, have fun listening to frogs, turtles, or music by your favorite composer. The Michelle Smith Endowment is making it possible to subscribe to even more music and performing arts databases that are becoming available, so stay tuned to the Libraries. You never know what you might hear next.



PHOTOGRAPHS BY JOHN T. HOWELL

ALL
The Libraries Are a Stage!

WILLIAM SHAKESPEARE and the nation's capital have deep roots. The District is home to both the world's premier collection, in the Folger Shakespeare Library devoted to the Bard and his times, and the Shakespeare Theatre Company. It is not surprising to find the first half of 2007 devoted to a city-wide celebration of his work. The *Shakespeare in Washington* festival ran from January through June and featured hundreds of performances, exhibits, lectures, and other programs exploring the 400-year legacy of one of the greatest writers of all time.

INSPIRED BY WASHINGTON'S FESTIVAL, the University of Maryland Libraries organized their own *Shakespeare in the Libraries* exhibits and programs. Whether the topic was hard science, architecture, or more traditional historical and cultural subjects, all of the University Libraries "got into the act."

Shakespeare's words still inspire. As the Libraries discovered when exploring the topic, all academic disciplines can shed light on and deepen our appreciation for Shakespeare's genius. The University Libraries found that their diverse collections and areas of expertise could coalesce around the themes of William Shakespeare.

NONPRINT MEDIA SERVICES {HORNBAKE LIBRARY}

"SHAKESPEARE ON FILM," an exhibit presented by the Nonprint Media Services Library focused on the motion picture and television adaptations of Shakespeare's plays, along with documentaries and derivative works.

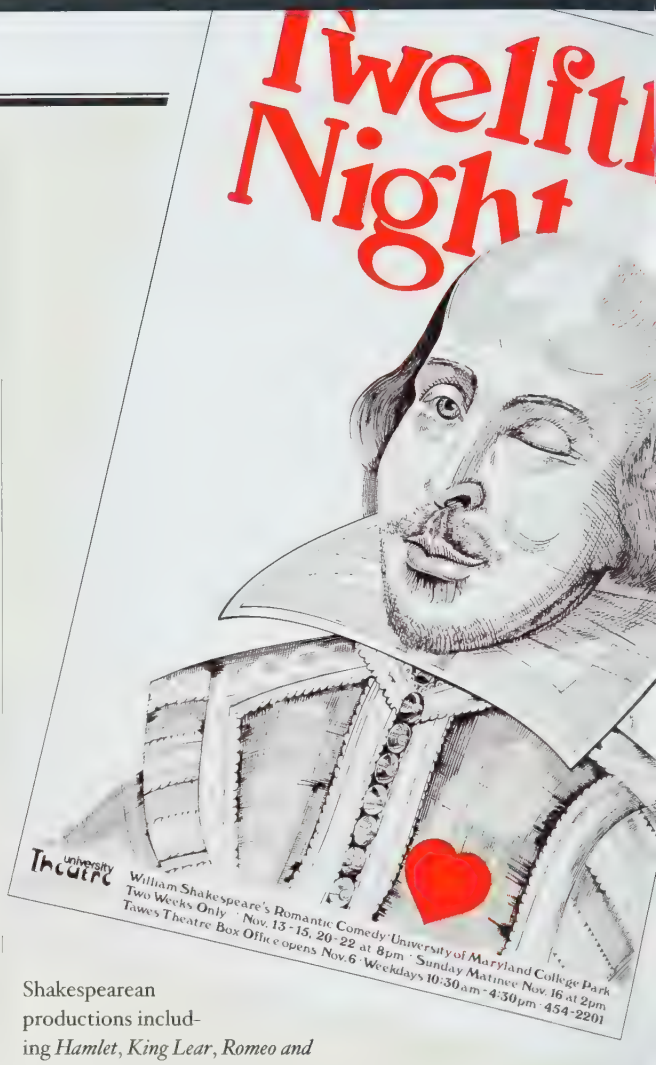
A featured collection was the BBC/Time-Life *Shakespeare Plays* series of all 37 official plays. This collection is amongst the earliest significant acquisitions of the Libraries. The series has come to be regarded as the canon against which other Shakespeare performances

on film are measured. Nearly 150 films in the collection are based on the plays, and include ballets, operas, science fiction, gangster movies, and animated films.

A highlight of "Shakespeare on Film" was the *Battle of the Shakespeare Superstars*. This showed, simultaneously in multiple theatres, different versions of the same play, giving the viewer the choice of either seeing a play in its entirety or sampling scenes across different versions. The *Battling Hamlets* was a great favorite; viewers compared the classic performances of Laurence Olivier, Richard Burton, Nicol Williamson and Richard Chamberlain with Kenneth Branagh, Mel Gibson and Ethan Hawke. Popular also were the comparative versions of *The Generations of Romeo & Juliet*, featuring a 1940s version with Laurence Harvey, the famous 1968 version directed by Franco Zeffirelli, and the wild 1997 version directed by Baz Luhrman starring Leonardo DiCaprio and Claire Danes.

ARCHIVES & MANUSCRIPTS
{HORNBAKE LIBRARY}

"Students do Shakespeare," an exhibit by the University Archives, revealed the role that Shakespeare has played in the lives of University of Maryland students throughout the university's 150-plus-year history. Shakespeare has been the focus of countless academic courses, and students have performed and attended his plays, reveled in his sonnets, and committed his poetry and prose to memory. Student groups fascinated by the famous bard's words, such as the University of Maryland Madrigal Singers and University Theatre, were a particular focus of the exhibit. The Madrigal Singers, founded in 1959, performed Renaissance-period music throughout the United States and abroad, including such venues as the Folger Shakespeare Library and the White House. University Theatre entertained the campus community with many



Shakespearean productions including *Hamlet*, *King Lear*, *Romeo and Juliet*, *Macbeth*, *A Midsummer Night's Dream*, *Othello*, *Julius Caesar*, and *Twelfth Night*, to name a very few. "Students Do Shakespeare" featured photographs, programs, flyers, a poster, and other materials from the University Archives, including a 1957 University Theatre program designed by Jim Henson, the renowned creator of the Muppets and University of Maryland alumnus.

MCKELDIN LIBRARY

"QUARTOS AND FOLIOS: The First Publications of Shakespeare's Plays" exhibited some of the Libraries' facsimiles of the earliest printed editions of Shakespeare's plays.

Shakespeare would not be famous today if his plays had not been printed during his lifetime, or soon after his death. No complete play in Shakespeare's actual handwriting has survived to the present. Fortunately, publishers in Shakespeare's time thought they could make a profit by making his plays available in print, thereby ensuring their survival.

During his lifetime, 18 (about half) of Shakespeare's plays were published not long after they were first performed, in editions known as quartos. (A quarto is a book formed of paper sheets that have been folded in half twice.) However, of Shakespeare's last fifteen plays, only two were published during his lifetime. The other thirteen almost surely would have been lost if his friends, John Heminge and Henry Condell, had not arranged to publish a collected edition of the plays in 1623. This edition is generally known as the First Folio (a folio is a book formed of paper sheets that have been folded in half just once and is therefore larger than a quarto). The First Folio has preserved for us some of Shakespeare's greatest plays, including *Macbeth* and *Julius Caesar*, *As You Like It* and *Twelfth Night*, *The Tempest* and *The Winter's Tale*.

MICHELLE SMITH PERFORMING ARTS LIBRARY

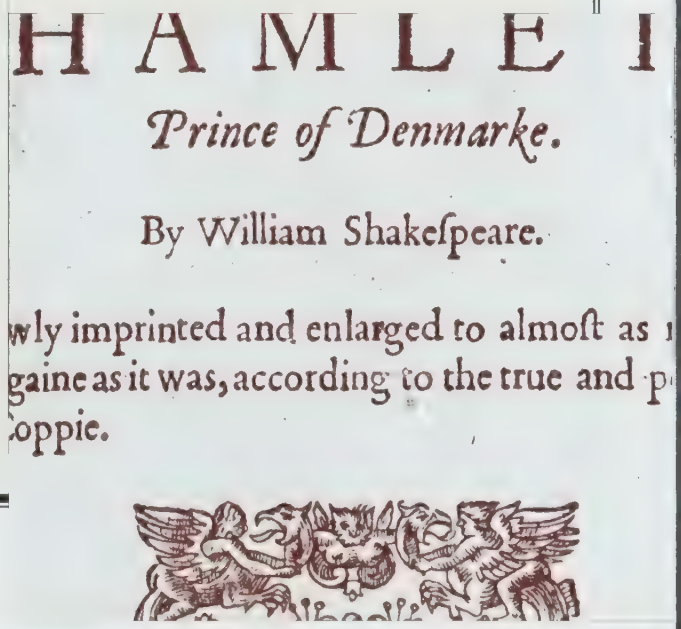
SHAKESPEARE has been a part of Washington's cultural life since the National Theatre opened in 1835. Today the Shakespeare theatre scene is alive and well with Shakespeare Theatre Company, The Folger Theater, and The Kennedy Center offering D.C. audiences world-class productions.

The University of Maryland has been a vibrant member of the larger D.C. Shakespeare scene for the past 35 years, and the theatre department faculty continues to have an active presence in the many regional theaters throughout the area. The exhibit in the Michelle Smith Performing Arts Library, "Shakespeare in the Washington Area," highlighted three faculty members' most recent contributions. Twelve screenshots of their creative work were taken from The James J. Taylor Collection of the Washington Area Performing Art Video Archives (WAPAVA), a collection held in the Michelle Smith Performing Arts Library. Included were department chair Daniel MacLean Wagner's lighting design for the Shakespeare Theatre Company's 1999 production of *A Midsummer Night's Dream*, which earned Mr. Wagner one of his twenty six Helen Hayes nominations for Outstanding Lighting Design; faculty member Daniel Conway's set for the Folger Theater's 2006 production of *Measure for Measure*, which earned him a sixth Helen Hayes award nomination for Outstanding Set Design; and adjunct instructor Elizabeth Forte's performances of Virgilia in the 2002 production of *Coriolanus*, and Lady Capulet in the 2000 production of *Romeo and Juliet*, a small sampling of her many appearances with the Shakespeare Theatre Company.

ENGINEERING AND PHYSICAL SCIENCES LIBRARY

THE "EARTHQUAKES, STORMS AND STARS: Shakespeare on Natural Phenomena" exhibit highlighted materials from the Engineering and Physical Sciences Library (EPSL) that demonstrate scientific understanding of phenomena expressed in Shakespeare works. For example, Shakespeare often used weather for dramatic effect and referred to celestial bodies and their movements. The five large, double-sided panels hanging from the Library's ceiling along the entry hallway displayed quotes from Shakespeare's plays. This inventive exhibit was seen by numerous library users who took a few moments to admire the beautiful, colorful images, to read the accompanying Shakespeare quotes, and to look at the book covers next to the panels. The topics ranged from earthquakes, hurricanes, and fires, to planets, and the moon. The exhibit was largely based on the book *Shakespeare and Science; A Study of Shakespeare's Interest in, and Literary and Dramatic Use of, Natural Phenomena*, Cumberland Clark, New York: Haskell House, 1970, held in the Engineering and Physical Sciences Library.

WHITE MEMORIAL



The Alchemist, by David Ryckaert (1612-1661). Courtesy of Dr. Alfred Bader.

CHEMISTRY LIBRARY

"Alchemy in Shakespeare's time" displayed literary works and reproductions of paintings depicting alchemists at work. It showed the connections between chemistry and art, serving as a vivid illustration of the roots of modern chemistry. The paintings from the 16th and 17th centuries, and the numerous literary works from that time, use concepts, allegories, and ideas related to alchemy revealing how modern chemical sciences were struggling to be born.

The initial goal of alchemists was to convert cheap metals to gold. The greatest aim of alchemy, though, was to discover the nature and composition of the so- called Philosopher's Stone - a medicine, a mixture, an element or a substance, which could cure the defects of any metal and produce the perfect one. In the 16th century, Paracelsus (a wandering scholar, physician and chemist born near Zurich) made the widely accepted claim that the real aim of alchemy should be to promote health by replacing certain elements in the human body rather than to convert base metals to gold. As extravagant as this idea might have sounded to his contemporaries, it is easy for us to see in it the roots of contemporary medicine and drug development.

The reproductions in the exhibit of the paintings related to alchemy were from the original paintings belonging to Dr. Alfred Bader, a chemist who founded the Aldrich Chemical Company (now Sigma-Aldrich), the largest supplier of reaction chemicals in the world.

Another event related to Shakespeare in the Libraries was a seminar presenting a variety of topics concerned with science in Shakespeare's time. *Leeches, Astrology, and Herbs: Medical Practices in the Time of Shakespeare* provided a snapshot of how physicians and other healers worked to restore health in the time of Shakespeare. *"Eye of newt and toe of frog": What Are Animals Doing in Shakespeare, and How?* explored the place of the natural world in Renaissance cosmology. *Alchemy and Drama in Shakespeare's Time* discussed why during Shakespeare's time there was so much interest in alchemy, why so many English authors used alchemical symbols in their works, and which alchemic themes transpired in dramas during that period of time. *"This Other Eden:" Shakespeare and Agriculture* presented Thomas Tusser's *Five Hundred Pointes of Good Husbandrie*, and other materials that provide useful descriptions of agricultural practices during Shakespeare's lifetime. *Development of the Compound Microscope* related the uncertain circumstances surrounding the development of the compound microscope during the late 16th and early 17th centuries.

RARE BOOKS {HORNBAKE LIBRARY}

"Shakespeare by the book", a selection of items on display in the Maryland Room from the Rare Books collection, featured the enduring popularity of the Bard over the centuries. Each generation has

reinterpreted Shakespeare's works, whether through romanticized Victorian-era portrayals of his heroines or by more recent fine press editions revealing Shakespeare in a fresh light. Among the most intriguing items in this exhibit was an 1803 printing of *King John* that commemorates a production by school boys of the Reading School in Britain, released during the patriotic fervor of the wars with Revolutionary and Napoleonic France.

ART LIBRARY

"Artists read Shakespeare" featured books from the Art Library's collections selected to showcase the Library's Shakespearean holdings and to illustrate the extent to which Shakespeare's literary themes have resonated in the visual arts through the centuries.

The books on view represented a variety of visual media—painting, drawing, illustration, engraving, lithography, glass—and included works from the seventeenth century to the twentieth century. Artists ranged from anonymous to illustrious—Eugene Delacroix, George Romney, Franz Marc, Benjamin West, John Singer Sargent, and even Louis Comfort Tiffany, represented by his 1915 *Shakespeare Window* installed at the Ladies Literary Club in Grand Rapids, Michigan.

A Catalogue of Paintings in the Folger Shakespeare Library: "As Imagination Bodies Forth," by William L. Pressly, Professor of Art in the Department of Art History and Archaeology, Yale University Press, 1993, was a spotlighted item and source of the many portrait images of William Shakespeare that appeared in the main display case.

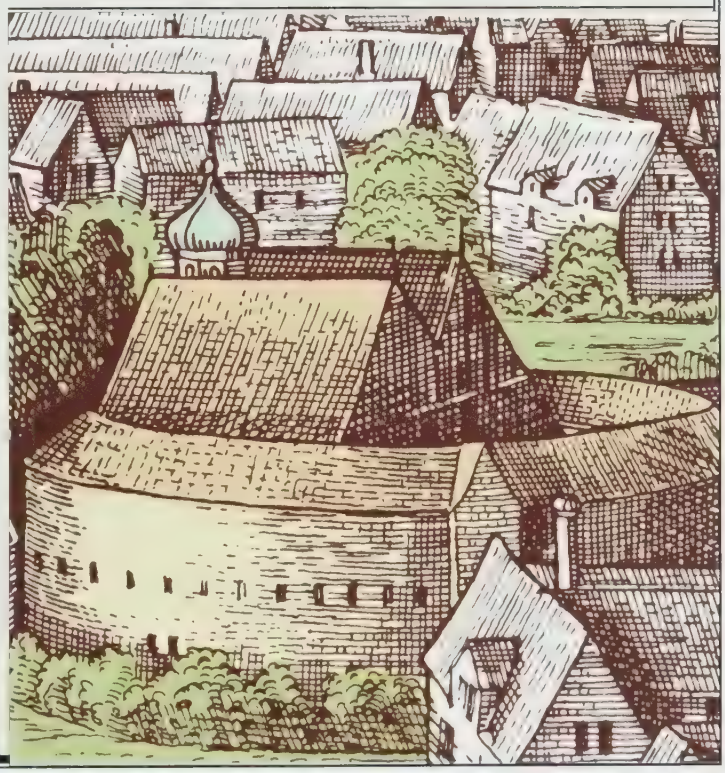
ARCHITECTURE LIBRARY

"Reconstructing Shakespeare's Globe Theatre", an exhibit in the Architecture Library underscored that the power of a dedicated donor to drive academic inquiry cannot be denied. The story of how Shakespeare's Globe Theatre in London came to be reconstructed in 1995 is the story of one such donor, Sam Wanamaker.

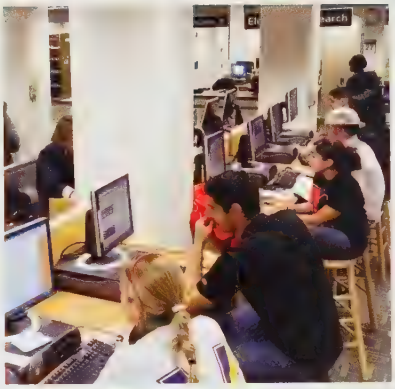
An American actor, Sam Wanamaker, found himself blacklisted by the House Un-American Activities Committee in 1952. He decided to make his home in Southwark, England, the neighborhood where Shakespeare's original playhouse had stood. Wanamaker's new life in England soon was entwined with Shakespearean theatre, as he became the director of the New Shakespeare Theatre and joined the Shakespeare Memorial Theatre company. In the 1960s and 1970s, he produced or directed several of Shakepeare's works. It is no wonder that he threw himself completely into manifesting a reconstruction of the Globe in London.

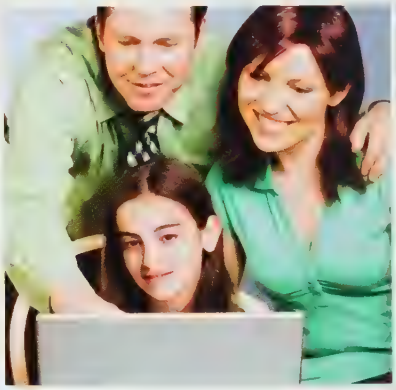
When he moved to Southwark, he set out to find the original site. Discovering only a battered plaque affixed to a brewery, he was disappointed. Two decades later, as an established passionate Shakespearean, Wanamaker founded the Shakespeare Globe Trust. Wanamaker met John Orrell, a Canadian scholar and theatre historian, who became the Globe project's chief academic supporter. At the request of Sam Wanamaker, Orrell began to assess the current state of scholarly knowledge about the original Globe. The results were of huge importance for the future of the project, and appeared as a book in 1983 entitled *The Quest for Shakespeare's Globe*. By this time Wanamaker had raised $36 million to fund the reconstruction of what has become London's most reliable tourist attraction.

The Architecture Library's exhibit, "The Globe Theater," pulled together from its own collections the historical maps and illustrations that informed Architect Theo Crosby's final designs and realized Sam Wanamaker's dream. ❧ *Finis.*



The University Libraries *What's in Them for You?*





The collections of the University of Maryland Libraries illuminate centuries of knowledge; they excite, provoke, inform, and ultimately inspire intellectual discovery. To explore the remarkable heritage of the recorded knowledge of man is a rich privilege and the wonders of the Libraries' collections are available to friends of the University of Maryland Libraries. Those who become friends of the University Libraries can read, use, and borrow from the collections, and even request that materials not found be obtained from libraries around the world. This privilege is available to friends who contribute $150 or more annually.

Friends can borrow materials from any of the University of Maryland College Park Libraries, and can request that materials already checked out to another borrower be recalled. The loan period is 56 days and can be extended through renewing.

If the University of Maryland College Park Libraries do not have the needed materials, they can be requested from libraries throughout the world using the Interlibrary Loan (ILL) service. Books, periodical articles, dissertations, microforms, government documents, and technical reports are just some of the materials ILL can obtain.

Increasingly, electronic databases are providing a wealth of information. The complete collection of the University Libraries' electronic resources is always available to the public on-site at any library on campus. However, friends can sign up for access from their home, office or other remote location to two electronic databases (see descriptions at right) made available by the University of Maryland Libraries, EBSCO Information Services, and the University of Maryland Alumni Association. This privilege is available to friends who contribute $200 or more annually to the University Libraries.

ACADEMIC SEARCH ALUMNI EDITION
This database provides the complete text for almost 1,500 publications, as well as indexing and abstracting for over 8,100 publications. There is information in nearly every area of academic study.

BUSINESS SOURCE ALUMNI EDITION
This database provides the complete text of almost 1,100 business magazines and journals.

Contact the Office for External Relations, McKeldin Library, Room 6131, 301.314.5674, libextrel@umd.edu or visit *www.lib.umd.edu/giving/borrowers.html*

a PICTURE is worth

THE UNIVERSITY OF MARYLAND Libraries are a wealth of books, journals, and databases. But, interestingly, they are far more than these traditional resources. Consider the case of Dr. Horng, pediatric dentist. Dr. Horng wanted to investigate whether there is sufficient access to dental services for children in Baltimore City through exploring the geographic distribution of dental providers relative to the location of public schools in Baltimore. So how did the UM Libraries help him get the answer? With GIS.

GIS stands for Geographic Information System. This is a combination of computer hardware, software, and geographic data that presents data visually—as a picture—rather than simply in textual form. A good example of GIS are the color maps used by news organizations to show up-to-the-minute Presidential voting; the map of 'red and blue states' is far more readily grasped than a list of state votes. Information presented visually is more powerful, more easily understood, than presenting the same information in text. Using GIS gives strong meaning to the phrase "a picture is worth a thousand words".

To help Dr. Horng, GIS was used to create a map showing the locations of dental practices and public schools (K–12) in Baltimore City. By representing schools and dental offices visually, Dr. Horng was able to look at the pattern of their relationship to each other. He then introduced data such as the name of each dental office, the phone number, whether the office accepted Medicaid, and the age range of its patients. For example, were pediatric dental offices that accept Medicaid clustered around schools, or around the geographic areas with children? He found that there is no correlation between the location of schools and dental practices. In some areas, there is a high concentration of schools, but no dental practices located in the same geographic areas and vice versa. Practices are concentrated in areas of the city which have heavier traffic, greater accessibility to transportation, or are located in areas with a greater retail presence, regardless of population density or school concentration. GIS is a great tool to identify these patterns by presenting the data visually.

Scott Turner, assistant professor in the Robert H. Smith School of Business, was interested in the kind of analysis that a GIS can provide. His project explored the effect of process consistency on customer satisfaction within the context of waste collection services. The work used data provided by the Environmental Services Department for the City of San Diego, including coordinates of waste retrieval locations using a global positioning system (GPS), the times at which the collections occurred, as well as customer satisfaction indicators. With GIS, Professor Turner was able to overlay the location of actual waste collections with the geographic boundaries for typical waste collection routes, so that within-route waste collections could immediately be distinguished from atypical ones. This process revealed several key employee workload variables which affected customer satisfaction. Working with tens of thousands of records, it was not realistic for Professor Turner to review the data for each address one at a time.

Information presented visually is more powerful, more easily understood, than presenting the same information in text.

Although GIS is becoming widely recognized as a powerful way to present and analyze data, many people have limited knowledge of the system and software, and can be overwhelmed. Dr. Horng agrees. "When I was initially approached about doing a project using GIS I was very excited, but once I had received the software I was overwhelmed with the daunting task of trying to implement it." The University of Maryland Libraries provided the needed help through the Government Documents and Maps Department. They not only provide data, and computers with GIS software, but very importantly offer services such as reference via phone, email, and one-on–one appointments to support a researcher. The services range from answering technical questions, to finding data, to software instruction.

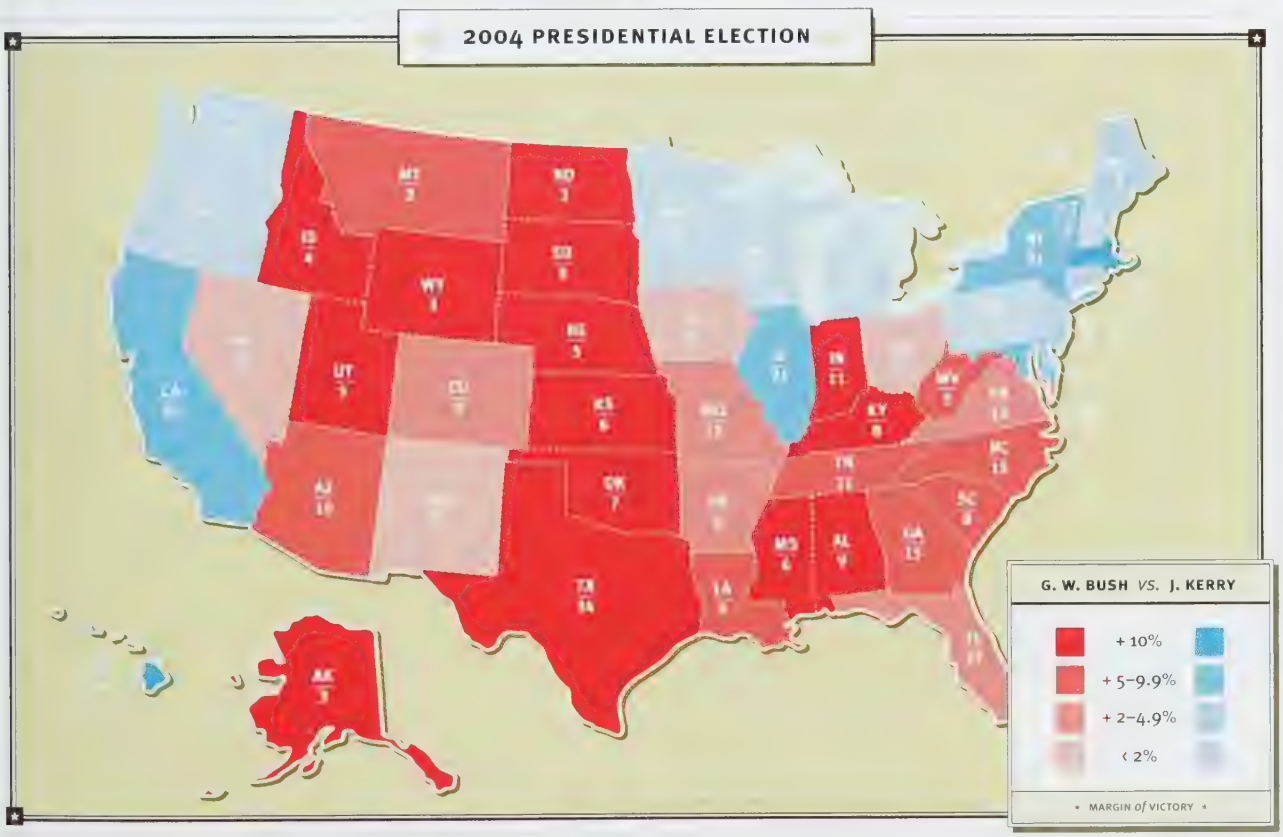
Dr. Horng stressed that "The guidance helped me complete my research project. The service was completely free and I was able to set up appointments that were flexible with my schedule."

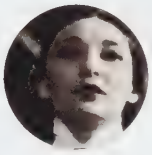
The University of Maryland Libraries' Government Documents and Maps Department is a Federal Depository. It receives publications and data produced by the federal government, the largest provider of data in a variety of areas, many of these being scientific. The Library's collection of over 2 million

a thousand WORDS

documents provides data in paper, micro fiche, microfilm, and electronic form. While the Government Documents and Maps Department has the responsibility to provide access to this extensive information, it also goes beyond access, and teaches users how to make use of the data through the power of GIS. This service is extended to the University of Maryland community and to the general public, and as Dr. Horng discovered, is free. "Even though I was no longer affiliated with the University of Maryland at College Park, they were still willing to help me," says Dr. Horng. "I thought perhaps some training in GIS would help so I tried to attend courses that were offered in the area but they were either too expensive or just didn't fit my work schedule." The Government Documents and Maps Department of the University of Maryland Libraries offers two free GIS workshops: Introduction to ArcGIS Desktop 9.2 and Introduction II to ArcGIS Desktop 9.2: Adding Data. These 2 ½ hour workshops are hands-on, and teach the fundamentals of GIS and how to get started using ArcGIS Desktop—a popular GIS software. At each class participants receive color instructional workbooks they can take with them for reference. These classes are extremely popular. Interested in strengthening his dissertation, Economics graduate student Lixing Li reflects on the GIS instruction offered, "This course, while it takes only 5 hours in total, teaches me some basic, yet very useful skills. It increases my confidence in learning other advanced GIS skills in the future."

GIS services are a groundbreaking way to help both students and experts in their fields use a very effective tool for data presentation and analysis. As Professor Turner says, "The University of Maryland Libraries have been a wonderful resource.... I have benefited in multiple ways, from taking an instructional course on the GIS software to utilizing reference materials from the lab. But I have most appreciated the key insights and one-on-one support. I have and will wholeheartedly point colleagues seeking GIS assistance to their door."





AN **EXTRAORDINARY FAMILY** IN MUSIC

are many important parts. To know the man Bob Sherman, you know his devotion to his family—promoting the legacy of those who came before, while closely bound to those who are following. To know the professional Bob Sherman, you know his work as a broadcaster, moderator, author, television personality, narrator, host and educator—embracing a wide spectrum in the world of music. Sherman is the son of pianist Nadia Reisenberg and Isaac J. (Sasha) Sherman, a successful international banker, and the nephew of renowned thereminist Clara Rockmore.

Sherman began his career in broadcasting as the Music Director and Program Manager for WQXR in New York. A regular columnist for *The New York Times* starting in 1964, he went on to publish several books on music. Sherman began lecturing at New York University by 1969, initiating an active career as an educator that involved him with institutions such as Yale University, The Juilliard School, Oberlin Conservatory of Music, The Manhattan School of Music and the Aspen Music School.

In 1970, Sherman began hosting the nationally-broadcast program "Listening Room", devoted to classical music and artisits, on WQXR. Following the addition of other programs, including the popular "Woody's Children", a folk music program, he expanded to television hosting "Vibrations" on PBS and appearing as a commentator for CBS "Camera Three". Sherman continues to broadcast today on Sirius XM Radio.

In recent years, Sherman has devoted much of his energy to preserving the legacy of his mother and aunt through memorial events, overseeing the production of biographical works, and writing program notes for their recordings. With his brother Alex, they compiled the materials for *Nadia Reisenberg: A Musician's Scrapbook*, published by the International Piano Archives at Maryland. Most recently, Sherman participated in the release of *Clara Rockmore's Lost Theremin Album* on Bridge Records in 2006.

The preservation of Bob Sherman's own legacy is now underway at the University of Maryland's Michelle Smith Performing Arts Library. Beginning in August 2005, recordings from his collection began to arrive at Special Collections in Performing Arts (SCPA) with nearly 500 CDs from his "Young Artist Series" programs. In August 2006, almost 1,500 open reel tapes from "Listening Room" and "Woody's Children" arrived. Both shows, like much of his programming, feature live interviews combined with performance and the playing of representative recordings. To have these unique instances of oral history and performance documentation is a great privilege for the Performing Arts Library, and make the Sherman Collection one of the Library's gems for students of musicology and performance.

To celebrate this new collection, the Library opened a gallery exhibition on July 1, 2007, *Reisenberg, Rockmore, Sherman: An Extrordinary Family in Music*. This exhibition focuses on the lives and careers of this family as depicted through photographs and objects from their respective collections. Later in July, Bob Sherman moderated three live artist conversations during the Clarice Smith Perform-ing Arts Center's William Kapell International Competition & Festival.

The exhibit can be seen in the gallery at the Michelle Smith Performing Arts Library. For information call Vin Novara at 301.405.9220 or email vnovara@umd.edu

Sherman interviewing acclaimed folk musician Burl Ives for "Woody's Children" at WQXR in New York, ca. 1984; Reisenberg, late 1930s; Rockmore playing theremin, ca. 1945

To know the man Bob Sherman, you know his devotion to his family. To know the professional Bob Sherman, you know his work embracing a wide spectrum in the world of music.

Our Heritage so Rich

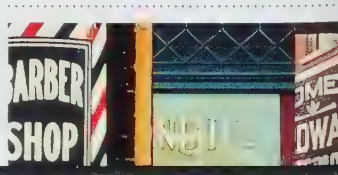
"If the preservation movement is to be successful it must go beyond saving bricks and mortar. It must go beyond saving occasional historic houses and opening museums ... It must attempt to give a sense of orientation to our society, using structures and objects of the past to establish values of time and place."

—From *With Heritage so Rich*

This call to action from 1966 came at a critical time for America. Small towns were losing population due to economic changes while urban renewal programs, meant to alleviate blight, were destroying the historic core of many cities. At the same time sprawling suburban growth created a physical and psychological barrier as Americans lost their connection to a sense of the past. In response to this crisis, landmark federal legislation in the 1960s set a new direction for historic preservation in the United States. With a broad mandate to preserve not only historic buildings and places but also communities and environments that enrich the lives of all Americans, the American preservation movement and its leading preservation organization, the National Trust for Historic Preservation, witnessed a dramatic rebirth. Forty years later, the historic preservation movement is firmly rooted in the mainstream of American life.

From rustic barns on the verge of collapse to buildings that have outlived their usefulness, preservationists are concerned with saving places that provide a sense of identity and heritage for communities across the country. To achieve effective results, historic preservationists rely on the lessons of past experiences that are preserved in the many reports, studies, and other materials created during projects. A key mission of the National Trust for Historic Preservation Library Collection (NTL) is to identify and make available the publications and documents important to the field. The collection, which began as the in-house library of the National Trust for Historic Preservation, was donated to the University in 1986. Today, the National Trust Library is the premier collection of preservation materials in the United States, collecting books, periodicals, films, videos, images, and archival materials that document the theory and practice of historic preservation. Using these materials researchers can help tell the stories of communities and places across the country.

One such place whose history is told in the reports and photographs of the NTL is the Queen City Hotel in Cumberland, Maryland. This hotel was a magnificent relic of the golden era of railroad travel. With its large, high-ceilinged rooms, long covered porches and superb decorative ironwork, it was a fine example of the American railroad station hotel. However, by the 1960s the hotel was abandoned and in poor shape. Local preservation groups in Cumberland rallied to prevent its demolition but the size of the building, the difficulty of finding an alternative use for it, the enormous cost of restoring the deteriorated structure, and the inexperience of the local and national preservation community led to the failure of the rescue attempt. In 1972, this grand old hotel was destroyed, leaving only photographs behind. Today, historic preservationists consider the fight to save the Queen City Hotel a galvanizing



Examples from the Historic Postcard Collection in the National Trust Library

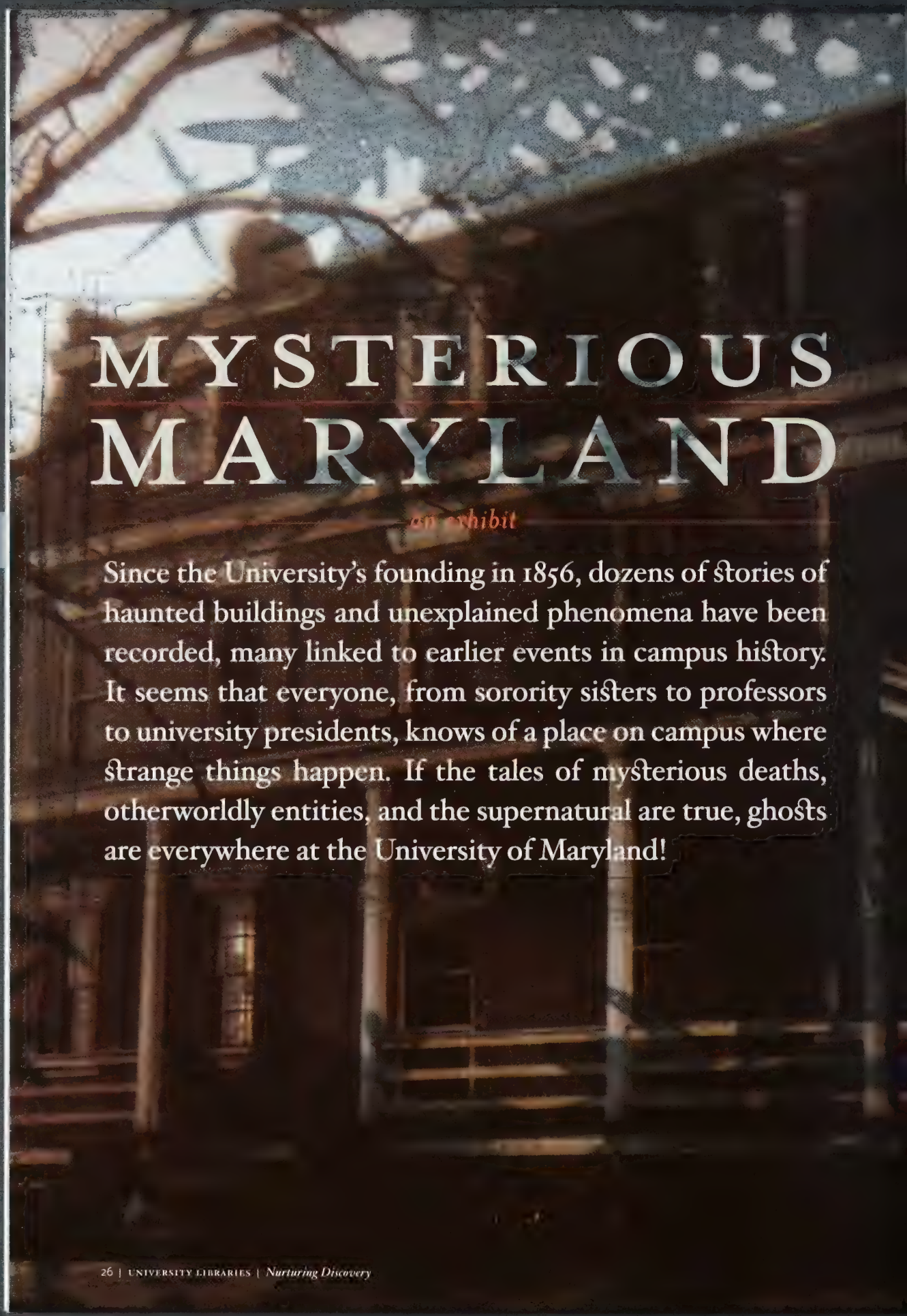
turning point in the preservation movement. So important was this battle that it was featured as a preservation case study published by the National Trust. The photographs held by the Library not only show the destruction of this architectural gem but coupled with the case study shed light on a pivotal time in the preservation movement.

Unfortunately, as the story of the Queen City shows, many wonderful and important historic sites have vanished over the years, victims of progress and the wrecker's ball. Photographs and the fading memories of people who enjoyed these historic buildings are all that survive. Images and postcards in the NTL collection offer researchers visual documentation of how a structure or place looked at a certain point in time and provide information about architectural features and alterations to sites over time. The postcard collection held by the library is one of the highlights of NTL's holdings, showing not only visual information about places across the country but also providing an authentic view of the society in which they were produced.

The messages on the cards can reveal important attitudes and ideas of the time period as well as providing additional information about the image on the card. The postcard quoted above informs the viewer that the house is not depicted accurately on the card and offers the reader the correct color and material for the building. One interesting use of postcards is the examination of the images for examples of landscaping used in earlier periods. This year a student researching the U.S. Treasury Building in Washington D.C. found clues about plants, trees, and open space around the building by examining postcards dating from the turn of the century.

"I wonder if you have a Sears kit house?" This is one of the most frequent questions received by the Library from the general public. Kit homes were sold in the early part of the twentieth century through mail order catalogs as ready to assemble homes. The most well-known manufacturer was the Sears, Roebuck Company although Aladdin Homes, Wardway Homes (Montgomery Ward), Harris Homes, the Ready Built House Company, and Robinson's also produced kit homes. Thousands of kit homes are still in existence across the country and in the last decade there has been an increased interest in studying, saving, and restoring kit homes. Homeowners and architects contact the National Trust Library to learn how to identify a kit home and the best way to preserve and restore their homes. Drawing on a collection of kit home catalogs and the papers of Katherine Stevenson and H. Ward Jandl, the authors of *Houses By Mail a Guide to Houses from Sears, Roebuck and Company*, researchers can identify their homes, obtain copies of floor plans, and see original architectural features. Many researchers even order photographic images of their homes from the catalogs to hang on their walls!

The National Trust Library, part of the University Libraries' Special Collections is located in Hornbake Library. For more information about the collection visit the website at: *www.lib.umd.edu/ntl/* or call 301.405.6320



MYSTERIOUS MARYLAND

an exhibit

Since the University's founding in 1856, dozens of stories of haunted buildings and unexplained phenomena have been recorded, many linked to earlier events in campus history. It seems that everyone, from sorority sisters to professors to university presidents, knows of a place on campus where strange things happen. If the tales of mysterious deaths, otherworldly entities, and the supernatural are true, ghosts are everywhere at the University of Maryland!

FACING PAGE:
The Rossborough Inn is haunted by a female apparition in a yellow dress.

LEFT:
Morrill Hall, home to ghostly sights, sounds, and smells.

BELOW:
The 1912 fire consumed the Barracks and old Administration building.

Prince George's County also has its share of weird tales. In 1685, a jury convicted Prince George's County resident Rebecca Fowler of witchcraft, and sentenced her to hanging. Historical sites such as the Surratt House, home to an alleged conspirator in the Lincoln assassination, are rife with supernatural activity. Abandoned buildings like the Glenn Dale hospital provide an ideal location for satanic rituals and mysterious religious cults. Fearsome creatures, such as the Goatman, are sighted throughout Prince George's County.

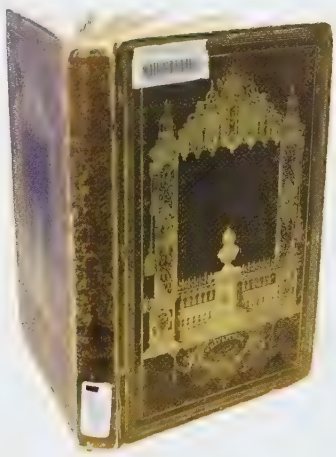
The exhibit, which will be featured in the Maryland Room Gallery of Hornbake Library in Fall 2007, brings together the most mysterious, haunting, and macabre legends in the history of the University of Maryland and surrounding areas. Illustrated with items from the University of Maryland Libraries Special Collections, these tales document centuries of local life—and death. Visit the gallery to learn more about College Park's most compelling unsolved mysteries and haunted places, and to see fascinating Special Collections items including cryptic turn-of-the-century yearbook illustrations, eerie theater ephemera, and even a coffin owned by a renowned author! Which of these tales of monsters, murders, and mystery are factual, and which are simply urban legends?

SHARE YOUR STORIES!

The curators of Mysterious Maryland are eager to hear your stories of hauntings and mysterious sightings on the College Park campus or surrounding neighborhoods. To share your personal scary stories, visit the exhibit blog at *www.lib.umd.edu/blogs/mystery/*, or contact Jennie Levine, Curator for Historical Manuscripts, at levjen@umd.edu or 301.314.2712.

SAVE THIS RARE BOOK

The Female Characters of Shakespeare
Engraved under the direction of Charles Heath (1785–1848)
New York: Wiley and Putnam, 1848



Recently on display as part of the *Shakespeare in the Libraries* series of exhibits, the University's copy of the *Female Characters of Shakespeare* from 1848 needs help. Bound in a classic example of a publisher's decorated cloth binding, this title was a keepsake or gift book for the Shakespeare enthusiast. Its high Victorian sensibilities—engraved portraits that idealized Shakespeare's female heroines, and an elaborately decorated binding that "enshrines" the Bard of Avon—speak to the aesthetic tastes of the mid-nineteenth century. Unfortunately, this book's popularity may have contributed to its present condition. Reversing the wear and tear evident in the frayed edges, partly detached spine, loose binding, and disfiguring library labels is possible in the hands of an expert book conservator. Our preservation staff estimates the cost for this treatment to be $750.00.

To sponsor the preservation of this exceptional rare book, please call Diana Grose in the Office for External Relations at 301.314.5674 or email libextrel@umd.edu

CONNECTIONS *Calendar of University Libraries Exhibitions and Events*

EXHIBITIONS

Through July 31, 2007
"THE CATBIRD SEAT: POETS LAUREATE IN MARYLAND"

This exhibition highlights the work of Poets Laureate in Maryland and the lives of two especially accomplished among them, Reed Whittemore and Roland Flint, whose papers are held by the University Libraries.

FREE | R. Lee Hornbake Library, Maryland Room Gallery

Beginning July 1, 2007
"REISENBERG, ROCKMORE, SHERMAN: AN EXTRORDINARY FAMILY IN MUSIC"

This exhibition focuses on the lives and careers of a musical family, including pianist Nadia Reisenberg, thereminist Clara Rockmore and broadcaster, moderator, author, television personality, narrator, host and educator Robert Sherman.

FREE | Michelle Smith Performing Arts Library Gallery

September—December, 2007
"MYSTERIOUS MARYLAND"

The exhibit brings together the most mysterious, haunting, and macabre legends in the history of the University of Maryland and surrounding areas. Special Collections items on display will include cryptic turn-of-the-century yearbook illustrations, eerie theater ephemera, and even a coffin owned by a renowned author!

FREE | R. Lee Hornbake Library, Maryland Room Gallery

September 1, 2007—December 21, 2007
"ROYAL REMEMBRANCES"

This exhibition commemorates the 50th anniversary of the Queen of England's legendary visit to the University of Maryland to attend a Terrapin football game in Byrd Stadium. The exhibit also honors all members of that 1957 team. Memorabilia on display include the game day program, a neckerchief worn by a Boy Scout ushering the game, a Canadian flag that flew over the stadium to represent the British Empire, and the football helmet worn during the game by Terrapin Ron Shaffer, a sophomore end on the 1957 team.

FREE | R. Lee Hornbake Library, Audrey Armistead Ruckert Reception Foyer

January—June 2008
"THE WELL-DRESSED BOOK: CLOTH BOOK BINDING IN THE UNITED STATES 1830-1920"

This exhibit will focus on publishers' cloth book bindings from 1830 to 1920 and explore the themes of stylistic and design development, the people and equipment that produced the bindings, marketing strategies, issues in preserving fragile bindings, and an examination of bindings produced in Maryland.

http://www.lib.umd.edu/mdrm/gallery bindings/clothbinding.html

FREE | R. Lee Hornbake Library, Maryland Room Gallery

EVENTS

Thursday, October 4, 2007
"QUEEN'S GAME 50TH ANNIVERSARY CELEBRATION"
5:30 p.m.–8:30pm

A special program and reception will commemorate the 50th anniversary of the Queen of England's legendary visit to the University of Maryland to attend a Terrapin football game in Byrd Stadium. This event will feature the public premiere of a documentary film chronicling the memorable event, and an exhibit from the University Archives will be on display

FREE | R. Lee Hornbake Library

Spring 2008
"THE WELL-DRESSED BOOK CLOTH BOOK BINDING IN THE UNITED STATES 1830-1920"

This symposium, and accompanying exhibit, will focus on publishers' cloth book bindings from 1830 to 1920 and explore the themes of stylistic and design development, the people and equipment that produced the bindings, marketing strategies, issues in preserving fragile bindings, and an examination of bindings produced in Maryland.

http://www.lib.umd.edu/mdrm/gallery bindings/clothbinding.html

FREE | R. Lee Hornbake Library, Maryland Room Gallery

FOR MORE INFORMATION
Please email libextrel@umd.edu or call 301.314.5674

The Maryland Room and Gallery is open Monday through Friday 10:00 a.m.– 5:00 p.m.; hours are extended during the academic year.

Michelle Smith Performing Arts Library Gallery is open Monday through Thursday 8:30 a.m.–10:00 p.m., Friday 8:30 a.m.– 6:00 p.m., Saturday 12:00 p.m.– 5:00 p.m., and Sunday 1:00 p.m.–10:00 p.m.

Between 1908 and 1940 over 100,000 kit homes were sold by Sears Roebuck and other companies. Prospective home buyers could select their model from a catalog and have the components delivered for assembly. Kit home catalogs, such as those featured on the front and back cover from the National Trust for Historic Preservation Library Collection, are valuable sources for residents of historic communities wishing to discover if they own a "Sears house."

ILLUMINATION — [illegible] — University of Maryland

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WEDNESDAY

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Inside TODAY

Pittcon Bureau Helps Job Seekers Despite Recession

Pittcon's free on-site employment bureau has been active this week with employers matching their job criteria to qualified candidates seeking jobs throughout the industry.

Dr. Dean Tzeng, the bureau's chairman, said his team of 30 Pittcon volunteers juggle the network of 128 participating employers and more than 500 job seekers.

Tang emphasized that the bureau's mission is unique in that it does not have follow-up services after Pittcon closes. Additionally, the confidential inter-action takes place at the conference and no records are archived or electronically stored.

Pittcon's 60-year reputation makes the employment bureau a place where fledgling job seekers and others from the ranks of the recently laid-off can congregate at a low-key pace and a reliable place to pursue positions.

The mixed demographic also allows the experienced attendees to make good suggestions for improvements to the bureau's future operations.

Biotechnology and nanotechnology are among the most active fields where jobs seem most available, Tang said, adding that a recent recruiting trend in the pharmaceutical industry shows an uptick in analytical positions available for job candidates.

Dr. Dean Tzeng

Students have fun participating in at Pittcon's science activity at Science Week, see story on page four.

Industry Leaders Predict Challenges of Today Create Opportunities for Tomorrow

The challenges in store for the chemical industry will also create opportunity for major growth, according to executives of Agilent Technologies's Life Sciences and Eli Lilly & Co. speaking at *C&EN*'s annual Pittcon Breakfast Tuesday.

Consolidation within the industry will continue to force equipment manufacturers to be resilient and flexible, said Agilent's Nick Roelofs, vice president and general manager. Along with consolidation will come re-deployment of equipment and geographic displacement—both of which companies like Agilent will have to respond with assistance, Roelofs said.

"Relocating R&D means relocating infrastructure. When a pharmaceutical company moves to India, for example, you have support and you will feel pressure to embed in those countries, too," he said.

Once there, the challenges do not stop, he warned. "In emerging countries, the challenge is also the local infrastructure. In remote sites, the reliability of instrumentation becomes even more critically important.

Equally important is the training of employees in the emerging countries, he said. While the

Continued on page 4 ►

Bader Continues To Make Headline News

From the perspective of a venerable and celebrated career, Alfred Bader, who has been a Pittcon 2009 centerpiece as the recipient of the Pittcon Heritage Award, made a cameo appearance at the *C&EN News* annual Pittcon Breakfast—and shared a few of his hard-won "rules of the road" to success.

His advice has come at the price of making a few

Continued on page 4 ►

Kids Tackle Science with Gusto, Enthusiasm

A back-to-back schedule of science workshops is leaving little time for young minds to wander this week. More often than not, those inquiring minds—of middle and high school students from around the Chicago metropolitan area—are brimming with wonder as they negotiate Science Week's series of half-hour workshops.

The program appears to be invigorating and challenging for students and workshop leaders, alike.

William Weller, a fourth year student at the University of Pittsburgh Greensburg, said the experience of teaching kids at Science Week's workshops has inspired him to rethink his original career plan of becoming a doctor. Instead, he said, he is redirecting his focus toward chemistry research. "I have always wanted to help cure disease—and with chemistry, I think I can do that on a bigger scale," he said.

Celebrating a third year as a volunteer at Pittcon's Science Week, the biology and chemistry major is spending mornings this week wrangling a roomful of middle-school and high school students, many impressed with his hands-on instruction about electrochemistry. Sessions in adjoining workshops cover such topics as astronomy, acids, bases and indicators, as well as chromatography, spectroscopy, and the behavior of gases.

Most students were delighted with the field trip and intrigued by the opportunity to unwind the mysteries of chemistry. Some are still not convinced that chemistry holds much promise as a major role for them. At least one admitted his dream is to be a pro basketball player, but conceded that chemistry is "cool."

For others, like seventh grader Lucy Aguirre, chemistry is the centerpiece of her career goal to be a chemistry teacher, she said.

"Chemistry is exciting because you get to figure out everyday things that you didn't know how they worked," she said. "Some things can be so simple and yet have a complex explanation, while other things—like electricity—seem complicated, but are actually easy to make happen."

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News Bites from Press Conferences

Grace Launches Flash Chromatography System

W.R. Grace & Co., a manufacturer of specialty chemicals, materials, and formulation technologies, has launched its Reveleris flash chromatography system. A technique used to separate mixtures of molecules into individual constituents, flash chromatography is frequently used in the drug recovery process. Grace's system was created to help synthetic and medicinal chemists streamline purifications of mixtures during the design and synthesis of promising new chemical entities. **Booth 1413.**

The Latest LIMS Upgrade from Accelerated Technology Labs

Accelerated Technology Laboratories release of the Sample Master LIMS 8.5 upgrade adds new functionality to its existing management system. Many of the new enhancements in the 8.5 version are a result of positive customer feedback and ATL's efforts to keep current with the regulatory compliance requirements associated with the fields the program services which include, environmental, food and beverage, agriculture, public health and biotechnology. ATL expects to rollout the software next month. **Booth 1054.**

JEOL Celebrates Their 60th Anniversary Along with Pittcon

This year marks JEOL's 60th year in the field of electron microscopy as they introduce the JEM-ARM200F atomic resolution analytical microscope.

With advanced analytical capabilities, the JEM-ARM200F enables both atom-by-atom imaging resolution and spatial resolution for atom-to-atom chemical mapping of materials, including EDS and EELS. The new electron column design integrates S/TEM with Cs correction for atomic spatial energy resolution combined with high probe currents for microanalysis. **Booth 3948, 4048.**

Tempshield Cryo-Protection Partners with the Susan G. Komen Foundation

Tempshield is offering their Cryo-Gloves, Cryo-Apron and waterproof Cryo-Gloves in a pink color in support of Susan G. Komen for the Cure and the fight against breast cancer. The Pink Cryo-Poducts are available for a limited time and can be ordered online at www.cryopink.comm or call 1-888-910-PINK. **Booth 1854.**

FaceBook for Scientists

LabRoots, a free online network composed of scientists and engineers, is angling to raise the bar on communications within the scientific community. After creating a profile that summarizes their research, experience, and accomplishments, participants are able to connect, collaborate with, and learn from each other—across geographic boundaries and fields of expertise. **Booth 3734.**

Picarro Launches Integrated Isotope Analyzer for Total Organic Carbon

Picarro Inc. has partnered with O.I. Corp. to introduce a turnkey analyzer to measure total organic carbon, as well as the carbon stable isotope ratio. The *i*TOC-CRDS is an integrated system that can either perform wet oxidation on the carbon content of aqueous solutions or combustion of solid/semi-solid organic materials to generate CO_2. **Booth 2606.**

ChemImage Seeks 'First-to-File' Status with FDA

ChemImage, a chemical and biological imaging technology solutions company, is set to help generic drug makers become the first to achieve bioequivalence for nasal spray suspensions and inhalation products by providing a way to determine drug particle size distribution in a drug product. The strategy—utilizing ChemImage's Falcon II Wide-Field Raman Chemical Imaging System—would help generic companies improve their time-to-market and perform chemical imaging of particles in droplets to distinguish the chemical identity, particle size distribution of drug and other substances. **Booth 2810.**

Kenneth Carroll, Director of Sales, ACS Publications, Publisher Pittcon Today, Nick Roelofs, Vice President and General Manager of Agilent's Life Sciences Solutions Unit, Horst Hemmerle, Director, DCRT, Eli Lilly and Company, Dean Baldwin, Regional Sales Manager, ACS Publications, Associate Publisher Pittcon Today.

← ***Industry Leaders*** *from page 1*

prospective employees have a certain level of education, they may not have had direct access to analytical equipment. "It's so important to bring those people up to speed as quickly as possible," he added.

Among future projects, multi-omics data analysis on single platform is becoming increasingly important—a strategy to assure that the workflow and data migration will become an easier proposition, he said.

At Eli Lilly and Co., DCRT director Horst Hemmerle said his company—founded in 1876 and posting $20 billion sales in 2008—is not a candidate for consolidation as it moves to develop partnerships with numerous entities.

"Partnering supports our growth with a host of new products expected in the next decade," he said. "We are a fully integrated network distributing across the globe to key markets."

← ***Bader*** *from page 1*

mistakes along the way, said the founder of the Aldrich Chemical Co.

Among his caveats is to keep control of the company as much as possible. He remembered how relieved he was when he refunded an early investor's $15,000 stake—and was able to regain control of one-third of his company.

When it comes to employees, he urged, "Get the best people to work for you. Have the best profit sharing and health care you can offer." He still recalls the angst he suffered in 1968 when a prized chemist left his employ for another job paying twice the salary. Bader was delighted to welcome the prodigal employee back to the fold 10 years later when the employee returned acknowledging that the salary may have been higher but the politics were brutal.

To ensure he kept the best employees through decades of up-and-down markets, Bader kept a promise to never lay off employees no matter the extent of a recession. "Instead, we would cut work week hours or trim executives salaries," he said.

Another mistake he has learned from is the tendency to check up on everything. "It isn't necessary when you have really good people," he said.

Treat customers fairly is another Baderism. "Answer promptly every query—even if you have to say 'no,'" he said. He recalled an experience as a Harvard University graduate student requesting a crucial compound he needed to complete his thesis. Kodak Chemical responded to his desperate query with a dismissive postcard notifying him "Don't write us again. If we have that material, we will send it."

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PLENUM: Dienstag, 17. Februar • ~~Donnerstag, 12. März~~ *Wegen der Teilnahme des Präsidenten an der Generalversammlung der* US Friends of the IKG in New York, *verschiebt sich die Sitzung auf* Dienstag, 26. März

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Dr. Alfred Bader: Vom Briefmarkenverkäufer zum Chemiker, Millionär und Kunstförderer

Von Ida Labudovic
Übersetzung: Karin Fasching-Kuales

Am Tag, als Alfred Baders Mutter, eine katholische Aristokratin, ihre Liebe zu seinem Vater, einem Juden aus der Mittelschicht, offenbarte, wollten sie ihre Eltern ins Asyl schicken. Doch trotz aller Widerstände heirateten die Liebenden wenig später in London, ließen sich in Wien nieder und bekamen zwei Kinder. Zwei Wochen nach Alfreds Geburt 1924 starb sein Vater und hinterließ Frau und Kinder ohne jegliches Einkommen. Alfreds jüdische Tante kümmerte sich daraufhin um den Jungen, bis er nach der „Kristallnacht" 1938 als einer von 10.000 jüdischen Kindern und Jugendlichen mit einem „Kindertransport" nach Großbritannien flüchten musste. Doch auch dort durfte er nicht lange bleiben – im Jahr 1940 kam er als einer der „enemy aliens" zwischen 16 und 65 in ein Internierungslager nach Kanada.

Der gerade erst 16 gewordene Alfred Bader wurde in Fort Lennox, Quebec, festgehalten. Erst im Herbst 1941 entließ man ihn in die Obhut eines religiösen sephardischen Juden in Montreal, der ihn zur Wiederaufnahme seiner Ausbildung ermunterte. Nachdem die Universitäten von Toronto und McGill ihn aufgrund ausgeschöpfter Quoten für jüdische Studenten abgelehnt hatten, begann Bader sein Studium als Chemie-Ingenieur an der Queen´s University in Kingston, Ontario. *„Ich war entschlossen, mein Bestes zu geben."*, erinnert er sich. Er erwarb mehrere wissenschaftliche Diplome an der Queen´s University, bevor er 1950 sein Doktorat in Organischer Chemie in Harvard abschließen konnte. Noch im selben Jahr ging Bader nach Milwaukee, um dort Forschungsarbeit für die Pittsburgh Plate Glass Company zu leisten und im Jahr 1951 gemeinsam mit seinem Freund Jack N. Eisendrath seine eigene Firma, die Aldrich Chemical Company, zu gründen, die Forschungschemikalien in kleinen Mengen produzierte und verkaufte. Das Unternehmen wuchs rasch zu einem für die Qualität und Vielfalt seiner Chemikalien weltbekannten Unternehmen an und schloss sich 1975 mit der Biochemikalienfirma Sigma aus St. Louis zusammen, mit Alfred Bader als Präsident der Sigma-Aldrich. Ein Konflikt im Jahr 1991, bei dem man ihm vorwarf, durch den Verkauf von Sigma-Aldrich-Aktien *„gegen das Unternehmen zu wetten"*, zwang ihn zum Firmen-Ausstieg. Bader wies diese Vorwürfe allerdings zurück.

Alfred Baders Geschichte ist eine Erfolgsgeschichte mit positiver Einstellung zum Leben. In diesem Sommer war er mit seiner großen Liebe, Isabel, in Wien:

Herr Bader, wie war das Leben in der Wiener Praterstraße vor dem Krieg, als Sie mit Ihrer Adoptivmutter dort gelebt haben? Was war für Sie entscheidend, als Sie zum überzeugten Juden wurden?

Meine Adoptivmutter und die Familie Mayer. In der Wohnung über uns lebten orthodoxe ungarische Juden, die Mayers, die starken Einfluss auf mein religiöses Leben hatten. Die Mayers waren wunderbare Nachbarn und luden mich an vielen Freitagabenden zum Essen ein, auch an den beiden Pessachabenden. Meine biologische Mutter war katholisch und hat mir oft gesagt, dass ich in die Hölle kommen würde, wenn ich nicht Katholik werde, aber sie hatte Unrecht, da bin ich sicher. Meine erste Frau war auch keine Jüdin, sie kam aus einen protestantischen Familie, doch sie konvertierte, bevor ich sie gebeten habe, mich zu heiraten. Meine Schwester wurde allerdings katholisch erzogen, sie verliebte sich in einen Engländer, kam nach England und heiratete anglikanisch.

Sie wurden am 10. Dezember 1938 mit dem ersten Kindertransport nach England geschickt. Welche Erinnerungen haben Sie an diesen Abend?

Ich hatte keine Ahnung, was mich erwartet. Um neun Uhr abends kamen wir zum Bahnhof Hütteldorf, meine Mutter, Mama, Hilda (die Gouvernante) und ich. Ich stieg schnell ein, fand einen Sitzplatz am Fenster und lehnte mich hinaus, um zum Abschied zu winken, als der Zug den Bahnhof verließ. Hilda starb während des Krieges an Krebs. Mutter wurde gezwungen, ihre Wohnung zu verlassen und in ein jüdisches Altersheim zu ziehen, bevor man sie im Juni 1941 nach Theresienstadt deportierte, wo sie fünf Monate später starb. Mama schied nach einem Schlaganfall 1948 aus dem Leben. An jenem Abend im Jahr 1938 umarmten wir uns zum letzten Mal. Ich sah keine von ihnen jemals wieder.

England war für Sie ein Ort des Exils. Welche Erfahrungen haben sie von dort mitgenommen, besonders was die Menschen betrifft?

Wir hatten in England eine entfernte Verwandte, durch meine jüdische Großmutter aus Prag. Frau Emanuel und ihr Ehemann fanden für mich eine Unterkunft bei einer jüdischen Familie. Ich ging dort ein Jahr lang in die Schule und fühlte mich sehr wohl. Dann ermöglichte Frau Emanuel mir den Besuch des Technik-Colleges, von Januar bis Mai 1940, als man mich schließlich internierte. Am 2. November 1941 wurde ich aus dem Internierungslager frei gelassen und zwei Wochen später wurde ich an der kanadischen Queen´s University aufgenommen, das hat mir sehr gut getan.
(Daraufhin wirft Isabel ein: „Sie fragten Alfred nach seinen Eindrücken von den Menschen in England. In der Familie, in der er lebte, gab es zwei Töchter und zwei Buben, jüdische Flüchtlinge aus Deutschland, die von einem Onkel Taschengeld erhielten, während Alfred sich sein Geld selbst verdienen musste. Die eine Tochter hat ihn nicht immer nett behandelt, obwohl das nicht ganz ernst gemeint

Isabel und Alfred Bader

war – für einen Jungen, der seine Heimat verlassen musste, ist das sehr unangenehm. Er begann, sich für Briefmarken zu interessieren, als er 8 Jahre alt war, denn er wusste: Je mehr er über die Briefmarken lernte, umso mehr würde er damit verdienen können. Er war ein Junge, der nicht gerne spielte, er arbeitete lieber, verkaufte seine Briefmarken, was er als Herausforderung sah. So beschaffte er sich sein Taschengeld. Ebenso war es, als er nach Kanada kam. Er arbeitete gern, deshalb lief das Geschäft auch so gut. Auch seine erste Frau, Danny, half mit, indem sie sich allein um das Haus und die Söhne kümmerte und ihn nicht mit Alltagsproblemen behelligte.)

Wie schafften Sie es, der Beste zu werden?

Durch schwere Arbeit und zwei gute Frauen, die mir viel geholfen haben. Jetzt habe ich Söhne, die mir enorm viel helfen und drei Leute, die mich in finanziellen Dingen beraten: Yechiel Bar-Chaim des American Jewish Joint Distribution Committee in Paris, Adina Shapiro in Jerusalem und einen Chabad-Rabbiner in Milwaukee. Meine Firma ist enorm gewachsen, dennoch hat man mich 1992 (aus der Sigma-Aldrich, Anm.) hinausgeworfen. Das war eigentlich mein großes Glück, denn jetzt arbeite ich mit Leuten, die ich gerne habe und es geht mir finanziell viel besser.

(Was das Geld betrifft, fügte Isabel hinzu: Alfred gehört nicht gern einer Gruppe von Menschen an, die ihm Geld geben, es ist ihm lieber, selbst etwas auf die Beine zu stellen, etwas Individuelles. Er mag es auch nicht, wenn jemand ihn um Geld bittet, denn das passiert ständig und man wird dessen irgendwann müde.)

Sie haben eine sehr erfolgreiche Firma gegründet. Was würden Sie Menschen raten, die ebenso erfolgreich sein möchten?

Wir hatten viel Glück. Mein Freund Jack Eisendrath, ein Anwalt aus Milwaukee, und ich gründeten ein Unternehmen, das Forschungschemikalien herstellte. Das war 1951, mit einem minimalen Kapital von US$ 250,- pro Person. Wir losten, wer über den Namen der Firma bestimmen darf – und ich verlor. Jack war damals mit einem charmanten Mädchen verlobt, Betty Aldrich, und so benannten wir unsere Firma in Aldrich Chemical Company. (Alfred liebte seine Arbeit, sagt Isabel. Er reiste zu Chemiefirmen in Europa, um ihnen seine Produkte zu verkaufen. Das machte ihm große Freude. Auch die Kodak-Leute machten ihre Arbeit, doch sie verstanden sich nicht darauf, die Bedürfnisse ihrer Kunden zu erfüllen – und genau das war Alfreds Spezialität: Die besten Chemikalien zu verkaufen und die Kunden zufrieden zu stellen. Außerdem war die Nachkriegszeit für dieses Geschäft wirklich gut. Die Nachfrage war sehr groß!)

Isabel, auf einer Reise von Quebec ins englische Liverpool 1949 trafen Sie sich zum ersten Mal, neun Tage später machte Alfred Ihnen einen Heiratsantrag, doch Sie lehnten ab, weil Sie dachten, dass Ihre religiösen Unterschiede zu groß sein könnten. Ihr Buch „A Canadian in Love" enthält die 80 Briefe, die Sie Ihrem späteren Mann zwischen Ihrem ersten Treffen im Juli 1949 und Ihrer Trennung ein Jahr darauf geschrieben haben. 1952 heiratete Alfred Helen Daniels (Danny), die ihm seine zwei Söhne Daniel und David gebar. Erst 1981 ließen sich die beiden wieder scheiden und Alfred war frei für die Ehe mit Ihnen. Wie sind Ihre Erinnerungen und Gefühle über diese Zeit?

Als wir uns im Juli 1949 zum ersten Mal begegneten hatten wir nur sehr wenig Zeit zusammen. Alfred musste zurück in die USA, während ich in England blieb, ich hatte keine Ahnung, wie es weiter gehen würde. Ab dem Jahr 1949 unterrichtete ich in Bexhill in Sussex, wo ich eine Schauspielschule und später ein Kostümmuseum mitbegründete. Die Stücke faszinierten mich, weil ich durch sie mehrere Leben leben konnte.

Wir haben uns am Mittwoch, dem 14. Juli, kennen gelernt und einen Tag später geküsst. Neun Tage später bat er mich ihn zu heiraten, aber ich habe nicht geantwortet. Erst 32 Jahre später sagte ich „Ja".

Wollen Sie weiter erzählen, Herr Bader?

Über ihren Bruder konnte ich dann erneut Kontakt aufnehmen. Als wir uns nach all den Jahren wieder trafen, war Isabel ganz erschüttert. Ich schrieb ihr daraufhin einen langen Brief, auf den sie nur antwortete: „Schreib mir nicht wieder, besuch mich nicht. Du bist glücklich verheiratet und hast Kinder." Sie wollte nichts mit mir zu tun haben und meine Ehe brechen. Aber ich bin ein sehr sturer Mann und habe nicht aufgegeben.

Isabel, haben Sie in dieser Zeit intensiv an Alfred gedacht?

In den Jahren, in denen wir getrennt waren, habe ich sehr oft an Alfred gedacht, doch ich wusste auch, dass er Jude war und eine Familie wollte, weil er ja nie wirklich eine ei-

gene Familie gehabt hätte. Ich war nicht bereit, über eine Konversion zum Judentum nachzudenken, um ihn heiraten zu können. Ich war nicht strikt dagegen, aber ich konnte auch nicht von einem Tag auf den anderen einfach die Seiten wechseln. Über so etwas muss man nachdenken können. Ich hatte auch erwartet, dass Alfred heiraten wollen würde. Er war ja auch älter als ich. Seine große Lebenserfahrung überstieg mich bei weitem. Ich bin eine ganz gewöhnliche Frau, doch Alfred war verrückt nach mir. Eines Tages traf ich einen seiner besten Freunde in England und er überzeugte mich, Alfred wieder zu sehen, mit den Worten: „Sein Leben liegt in deinen Händen". Was für eine Aussage! Ich verbrachte daraufhin einige Stunden mit Alfred, doch das genügte ihm nicht. Er rief mich an, schrieb mir. Danny wusste das es muss sehr schwer für sie gewesen sein. Doch er konnte nicht damit aufhören, obwohl ich ihm begreiflich zu machen versuchte, dass er aufhören musste. Auch für mich war es sehr schwierig, ich war innerlich zerrissen. Als Danny irgendwann nach England kam, sprachen wir miteinander und ich sagte ihr, dass ich mich am liebsten irgendwo verstecken würde. Sie antwortete: „Es würde nichts nützen, Isabel, er würde versuchen, dich zu finden."

Wie wirkte sich die spätere Scheidung auf Ihre Familie aus?

Materiell war die Scheidung sehr einfach, denn ich teilte immer alles, was ich hatte, 50:50 mit meiner ersten Frau. Emotional war es für Danny sehr schwer.

Um Alfred heiraten zu können, sind Sie dann doch konvertiert, Isabel. Wie war das für Sie?

Bis zur tatsächlichen Konversion hat es eine Weile gedauert. Und es machte eigentlich keinen Unterschied für mich, da Kinder ja kein Thema waren. Wir haben 1982 standesamtlich in Milwaukee und zehn Jahre später, nach meiner formellen Konversion, orthodox geheiratet.

Wie verbringen Sie nun Ihre Zeit?

Wir leben sehr einfach und spenden jedes Jahr mehrere Millionen, das macht uns große Freude. Wenn wir einmal sterben, wird es eine Isabel und Alfred Bader Foundation geben. Als wir im Juli 1992 mit dem Zug von London nach Bexhill fuhren, entdeckte ich eine Anzeige in der London 'Times' über den Verkauf eines Schlosses für fünf Millionen englische Pfund und ich fragte Isabel, ob sie es haben wolle. Ihre Augen strahlten, als sie sah, dass es Herstmonceux war, nur wenige Kilometer von Bexhill entfernt, doch sie war nicht interessiert – zu viele Räume, die geputzt werden mussten. Trotzdem wollten wir es uns anschauen und hatten dabei denselben Gedanken: Was für ein wundervoller Besitz es für die Queen´s University wäre. Also kauften wir es für sie.

Wir haben kein besonders umfangreiches Gesellschaftsleben. Wir sind gerne zu Hause. Seit ich 1982 nach Milwaukee gezogen bin, treffen wir hauptsächlich Menschen, die zur Synagoge gehören. Die meisten wissen, wie wir leben und erwarten nicht von uns, anders zu sein, als wir tatsächlich sind. Die Dinge, die wohlhabende Menschen üblicherweise tun, interessieren uns nicht. Unser Lebensmotto lautet: „Wir brauchen so wenig, und wir besitzen so viel."

Und was interessiert Sie, Isabel?

Musik und Theater. Als ich nach Milwaukee kam, habe ich Theaterkostüme gemacht. Jetzt helfe ich Alfred bei seiner Arbeit. Wir reisen viel, Alfred gibt Vorlesungen, wir diskutieren über Veranstaltungen, er schickt mir Briefe und Artikel, die ich durchlese. Es gibt genug zu tun.

Was waren Ihre Intentionen, den Ignaz Lieben Preis wieder zum Leben zu erwecken?

Ignaz Lieben, der den Preis in den 1860er-Jahren gestiftet hat, war ein jüdischer Bankier, dessen Nachkomme von den Nazis in Buchenwald ermordet wurde. Viele jüdische Geschenke basieren auf der Zahl 18, im Hebräischen „Chaj" (das Leben). So war der Liebenpreis ursprünglich mit US$ 18.000 dotiert. Aufgrund des fallenden Dollarkurses haben wir diesen verdoppelt und er beträgt nun US$ 36.000.
Außerdem haben wir der Österreichischen Akademie der Wissenschaften noch zwei andere Preise in der Höhe von US$ 18.000 gestiftet.

Sie sind auch ein leidenschaftlicher Sammler von holländischen Malern aus dem 17. Jahrhundert. Warum gerade aus dieser Zeit?

Einfach weil es mir am besten gefällt. Ich bin kein Kunsthistoriker, ich schaue mir die Bilder an, besonders Rembrandt und seine Schüler. Sie gefallen mir am besten. Wir haben unserer Universität zwei sehr schöne Rembrandts geschenkt. In der Einleitung für einen Katalog von Gemälden, die wir der Queen´s University überlassen haben, schrieben Isabel und ich: „Man hofft, dass die Signatur die Authentizität garantiert und das mag für ein Erwerbskomitee und manche Sammler wichtiger sein, als Schönheit, die doch so schwierig zu bewerten ist. Und hier liegen die Chancen von Sammlern, wie wir es sind."

Sie sagten: „Das Leben hat mir viel Freude bereitet." Wie sieht nun ihr Fazit über das Leben und die Liebe aus?

Das Wichtigste im Leben ist, den richtigen Partner zu finden und das habe ich. Wenn der Herr uns noch genügend Zeit gibt, können wir mit Isabels Weitsicht noch weitere großartige Projekte finden, die es zu finanzieren lohnt. Denn wir wollen unser Geld nicht für uns selbst ausgeben – und mitnehmen können wir es auch nicht.

Literaturhinweis:
„Alfred Bader: Chemie, Glaube und Kunst. Fundamente meines Lebens"
Böhlau Verlag 2008,
Herausgegeben von Gerhard Botz

buch-tipp

Panorama

Direktflüge Israel-Brasilien

Ab April 2009 wird die El Al Direktflüge zwischen Israel und Brasilien anbieten. Drei wöchentliche Flüge werden Tel Aviv und Sao Paulo verbinden, außerdem wird es Anschlussflüge zu verschiedenen südamerikanischen Destinationen geben, darunter Argentinien, Chile, Uruguay, Bolivien und Ecuador sowie andere große Städte innerhalb Brasiliens.
Etwa 30.000 brasilianische Touristen haben Israel im Jahr 2007 besucht. Diese Zahl soll sich mit dem neuen Flugangebot nun noch erhöhen.

Kiev begeht 150. Geburtstag von Sholem Aleichem

Das Museum der Bücher in Kiev begeht 2009 den 150. Geburtstag des jiddischen Schriftstellers *Sholem Aleichem*, der in der Ukraine geboren worden war und den Großteil seines Lebens dort verbracht hatte. Bekannt wurde Aleichem für Bücher wie „Tevje der Milchmann", das die Vorlage für das Musical „Anatevka" lieferte, oder „Menachem-Mendl". Er starb 1916 in New York.
Gleichzeitig wird in dem Museum eine Ausstellung über Leben und Werk des Künstlers zu sehen sein, darunter verschiedene Übersetzungen seiner Arbeiten, Manuskripte, Fotos, Portraits und Dokumente. Im März wird außerdem das Kiewer Sholem Aleichem Museum eröffnet.

EJC bekommt israelisches Büro

Der Europäische Jüdische Rat (EJC), Dachorganisation von 40 jüdischen Gemeinden Europas, bekommt nun auch ein israelisches Büro und wird damit seine Aktivitäten in Israel ausweiten können.

Gilad Shalit wird Ehrenbürger von Paris

Der israelisch-französische Soldat Gilad Shalit, der seit 2006 von der Hamas als Geisel gehalten wird, wurde von der Pariser Stadtregierung mit dem Tiltel des Ehrenbürgers ausgezeichnet. Die Nachricht wurde bei den für die Freiheit Shalits kämpfenden Aktivisten mit großer Freude aufgenommen.
Bereits im November hatte die französische Stadt Raincy Gilad Shalit zum Ehrenbürger erklärt, während sein Konterfei wiederum die Fassade der Stadthalle von Grenoble zierte.
Auch die italienische Hauptstadt Rom will Shalit zum Ehrenbürger machen, als „Zeichen der Solidarität mit der jüdischen Gemeinde", so Roms Bürgermeister Gianni Alemanno.

Juden begehen Todestag von tunesischer Rabbiner-Legende

So viele Menschen wie nie zuvor – zwischen 500 und 700 - versammelten sich am Friedhof von Tunis, um des Todes von *Rabbi Hai Taieb* zu gedenken, der sich der Legende nach zu Tode getrunken haben soll, nachdem seine Frau sämtliche seiner Arbeiten verbrannt hatte.
Der Rabbiner soll von der Mitte des 18. bis zur Mitte des 19. Jahrhunderts ein g'ttesfürchtiges Leben geführt und den Großteil seiner Zeit mit dem Studium der Torah, dem Verfassen von Kommentaren und Wundertätigkeit verbracht haben. Dies alles in einem Raum, den seine Frau niemals betreten durfte. Eines Tages jedoch soll sie heimlich in diesen Raum geschlüpft sein, als Taieb nicht zu Hause war. Sie war so geschockt von den Unmengen an Papieren und all dem Chaos dort, dass sie alles in Flammen aufgehen ließ. Daraufhin verfiel der Rabbiner dem Alkohol und starb. Doch seine Lehren und Weisheiten blieben unvergessen, weshalb auch auf seinem Grabstein „Lo Mait" geschrieben steht – „Niemals gestorben".
Tunesiens jüdische Gemeinde zählt heute etwa 1.500 Mitglieder.

Digitaler Siddur am iPhone

iPhone Besitzer können nun auf einen besonderen Service zurückgreifen: einen digitalen Siddur, der Gebetstexte in verschiedenen Versionen sowie Erinnerungen an Gebetszeiten je nach Standort aufs Handy liefert. Mittels eingebauter Datenbank kann auch der nächstgelegene Minjan ermittelt werden. Kostenfaktor: US$ 9,99.

Umfrage: Holocaust gehört nicht zur jüdischen Diasporaidentität

Die meisten jüdischen Jugendlichen, die in der Diaspora leben, geben an, dass der Holocaust zwar ihre Weltsicht verändert hätte, aber keine Rolle in ihrer jüdischen Identität spiele, ergab eine Umfrage. 60.000 jüdische Teenager zwischen 15 und 17 Jahren aus mehr als 20 Staaten wurden dazu über einen Zeitraum von 12 Jahren befragt. Die Ergebnisse wurden an der israelischen Bar-Ilan Universität im Zuge der Konferenz *„Representing the Holocaust: New Perspectives"* vorgestellt.
Mehr als 90% der befragten Jugendlichen meinten, der Holocaust hätte Einfluss auf ihre Sicht der Welt – über ein Drittel von ihnen bezeichnete diesen Einfluss sogar als „sehr wichtig".

Quaker News

A quarterly update on Quaker work in the care of Britain Yearly Meeting

Committed to caring for peace and planet

No 80 Autumn 2011

Contents

Cover photo: One small step for peace – children at Yearly Meeting Gathering make peace banners using prints of their hands and feet (story: page 8). © Mike Pinches

Editorial

"Peace is about everyday life," says Leicester Quaker Annette Wallis. "How you deal with controversy and conflict." She is among Quakers featuring on posters marking Quaker Week (1–9 October). Read on the back cover how her family makes peace a way of life.

Quakers in Burundi might agree with her. Clean water is essential for everyday life: indeed water is life. Clean water is scarce in central Burundi. So is trust and co-operation in communities where neighbours have witnessed horrific acts of violence. Now a pioneering project (page 6) – backed by Quakers – to build simple water filters is powerfully transforming lives. Along with clean water, a new sense of trust is flowing. "I am glad of my water filter," says one villager. "As we say that water is life, we are offering life to people from all groups of the community. My neighbours come to ask for filtered water."

The project shows that peace, security and sustainability are inextricably linked. Quakers at Yearly Meeting Gathering in Canterbury understood that message when we made a commitment to Quakers in Britain becoming a low-carbon sustainable community. We didn't just talk about sustainability: some of us made a small but tangible contribution to sustainability on the University of Kent campus by digging trenches and laying a new water pipe for the kitchen garden (page 4). The minute recording our commitment urged us to keep in our hearts that "this action must flow from nowhere but love". We agreed that it is not fear for the future that motivates us but love for all life on our planet.

Three hundred and fifty years ago such love for all life prompted Quakers to declare to the King that "We are a people that follow after those things that make for peace, love and unity". The Peace 350 project (page 8) suggests what a new text for today's Quakers might say: "We know a life and power which enables us to be both peaceable and powerful."

Like the children carefully painting each other's feet to create the peace banner on page 8, to reduce our carbon footprints and to become a low-carbon community we will need to be gentle and encourage one another to take bold steps. Peaceable and powerful.

Paul Parker
Recording Clerk

Quaker News

A quarterly magazine about work supported by Britain Yearly Meeting.

Britain Yearly Meeting works on behalf of Quakers in Britain, supporting the Quaker faith and putting Quaker values to work in the world. It is a registered charity, number 1127633.

Quakers try to live simply and sustainably, promoting peace, equality and truth. Putting faith into action is central to our way of life and we meet weekly for quiet worship, usually on Sunday, in more than 475 locations across Britain.

You are welcome to any Quaker meeting for worship. Find your local meeting, and more information about us, at www.quaker.org.uk.

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Quakers contribute to historic ruling on conscientious objection

Photo: Council of Europe Credits

In a landmark case, the European Court of Human Rights has ruled that conscientious objection to military service is protected under the European Human Rights Convention. Rachel Brett reports on the culmination of 50 years' Quaker work on conscientious objection at the United Nations.

A recent ruling by the European Court of Human Rights means that conscientious objection is protected under the European Human Rights Convention for the first time in the convention's 60-year history.

In its judgment, the court specifically cited the "third party intervention" from Quaker United Nations Office (QUNO) Geneva, together with Amnesty International, Conscience & Peace Tax International, the International Commission of Jurists, and War Resisters' International.

The intervention supported the UN Human Rights Committee's argument that conscientious objection to military service is protected under the right to freedom of thought, conscience and religion (Article 18 of the International Covenant on Civil and Political Rights). QUNO Geneva, largely funded by Britain Yearly Meeting, has been instrumental in persuading the committee to recognise this protection, paving the way for the European Court's ruling.

The ruling is significant for all 47 members of the Council of Europe, who can no longer argue that they are not required to provide for conscientious objectors.

The binding legal judgment was made in the case of *Bayatyan v. Armenia*. Vahan Bayatyan, a Jehovah's Witness, was imprisoned for refusing to serve in the Armenian army on conscientious grounds. The ruling is significant not only for Vahan Bayatyan but for all 47 members of the Council of Europe, who can no longer argue that they are not required to provide for conscientious objectors.

Within the Council of Europe, Turkey and Azerbaijan will be directly affected by the European Court's judgment since they do not provide for conscientious objectors. The Constitutional Court of the Republic of Korea may take note of it when considering the latest legal challenge to the lack of recognition of conscientious objection in South Korea. It is also likely to influence the consideration of asylum claims from conscientious objectors fleeing persecution, and to be followed by the Inter-American Human Rights System when considering conscientious objection cases in the Americas.

www.quaker.org.uk/quaker-united nations-office-geneva

About QUNO

The Quaker United Nations Office works to address Quaker concerns at an international level, and has a presence at the UN in Geneva and New York.

QUNO has 'general consultative status' with the UN, which means it can make formal representations to UN institutions on a wide range of issues.

Flowing from nowhere but love: Making a commitment to sustainability

Friends at Yearly Meeting Gathering work to improve the water supply at University of Kent's kitchen garden, leaving a lasting contribution to sustainability on the campus. Photos: © Mike Pinches

Quakers in Britain have made a commitment to becoming a low-carbon sustainable community. Alison Prout considers what this might mean for Friends, what has changed, and how we can support each other on our journey.

For a week in August, Canterbury was home to a community of over 1,600 Quakers. We came together for Yearly Meeting Gathering to grow in the spirit and to consider changing the way we live to sustain the world we live in. At the end of the week Quakers in Britain made a corporate commitment to become a low-carbon sustainable community.

Most Friends already try hard to live sustainably, avoiding over-consumption and waste. Our founding predecessors were committed to living simply as a symbol of their belief in religious integrity and equality. So what's changed?

This commitment takes us beyond that. It embeds care for our environment as a key part of being a Quaker. It reminds us that reducing our carbon impact links directly to our work for peace and equality – because environmental damage most hurts the poor and vulnerable and often contributes to violent conflict.

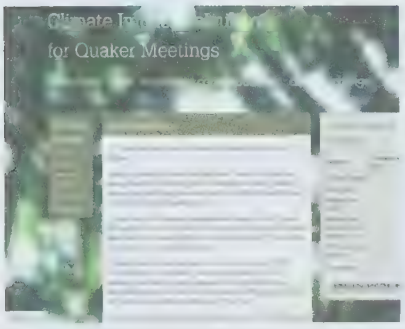
The minute recording our commitment urged us to keep in our hearts that "this action must flow from nowhere but love". We agreed that it is not fear for the future that motivates us but love for all life on our planet.

The commitment goes wider and deeper than a reduction in carbon emissions. Peace, justice and equality both lead to and result from a sustainable community. Our consumer-focused culture and the wider injustices within the economic system worsen environmental damage and contribute to alienation. Promoting equality and speaking out against injustice and violence are important parts of the process we have embarked upon. As we learn as a community how to live differently we will be able to speak from our experience and encourage others.

To ensure our progress is measurable, baselines must be recorded and a reporting structure put in place. Meeting for Sufferings, the national representative body for Quakers in Britain, will be looking at how these structures can be established and asking questions such as "how low is low?" and "what do we mean by sustainable?". They will report back at our Yearly Meeting in May 2012.

Transforming ourselves and our Quaker community will take time. Some changes will come easily, others will not. Mutual accountability and love will have to go hand in hand. Over the next few months a framework for corporate action will begin to emerge; in the meantime there are many different things that individual Friends, meetings and Britain Yearly Meeting can do to help build our low-carbon sustainable community, and to help discern what this community might look like.

Measure and reduce: Climate impact calculators



Working with Quaker sustainability organisation Living Witness, we have produced two easy-to-use climate impact calculators to help us understand and reduce our effect on the climate.

The calculators – one for individuals and one especially designed for Quaker meetings – will be available at www.quaker.org.uk/climate-impact-calculators from the end of October, and are included in the sustainability toolkit.

Sustainability toolkit: becoming a low-carbon sustainable community

The new sustainability toolkit aims to support Quaker meetings on their journeys to become low-carbon sustainable communities.

Developed in partnership with Living Witness and produced by Britain Yearly Meeting, the toolkit is packed with ideas to help meetings take their next step, including group activities, reflection pieces, learning resources and Friends' stories.

The toolkit will be launched at the end of October and a copy offered to each meeting. If you'd like a personal copy, contact Sunniva Taylor on 020 7663 1047 or at sunnivat@quaker.org.uk.

Sustainability stories

Many Quakers and Quaker meetings are already taking positive action on sustainability. You can read about the inspiring work that has been happening at www.quaker.org.uk/sustainability-stories.

We'd love to hear your sustainability stories too:

[illegible]

Exploring sustainability and spirituality

This year's Swarthmore Lecture, *Costing not less than everything: Sustainability and spirituality in challenging times* by Pam Lunn, made a big impact at Yearly Meeting Gathering.

Pam explored the role of theology, religion and spirituality in our human response to the current environmental situation, stressing "the absolute need for serious and sustained spiritual discipline if we're to develop the inner resilience to meet the challenges and demands that face us."

The book of the lecture features a study/reflection guide and is available from the Quaker Centre Bookshop, costing £8.

[illegible]

Creating a just and sustainable world: ideas for action

A new page on the Britain Yearly Meeting website pools resources for learning and opportunities for action.

At www.quaker.org.uk/creating-just-and-sustainable-world you'll find suggestions for actions you can take as an individual – even if you only have two minutes to spare – as well as things you can do together with your meeting.

Great journeys start with small steps – start your sustainability journey today.

Greening Friends House

Friends House, the London offices of Quakers in Britain, has taken a big step towards reducing its carbon footprint by 45% before 2015. The refurbishment of its upper floors is now complete, providing a better working environment for staff and creating new commercial conference space that will generate income for Quaker work. Some of the green elements are:

- solar panels fitted to the roof provide hot water
- walls that have 15cm of insulation and windows with full secondary glazing
- lighting that is more efficient, with light-level and motion sensors and greater user control
- blinds that allow sunlight through but prevent screen glare
- natural ventilation systems that improve the working environment and consume less energy
- fixtures and fittings that have been chosen for their green credentials
- refurbished desks, storage units and under-desk pedestals that have been sourced using old furniture in part-exchange
- existing chairs reused and re-covered using fabrics that are almost entirely made from recycled materials
- the use of renewable hardwood and sustainably grown eco-ply in all construction, and of Ecosure paint for decorating
- the introduction of energy-use monitoring systems.

Surplus furniture has been donated to partner organisations, and all waste either recycled or sent to waste-to-power schemes. The next step is to introduce more efficient heating and ventilation services and extend the use of renewable energy sources to further reduce our carbon footprint.

Healing water in Mutaho

Mutaho, like many villages in Burundi, is still struggling in the aftermath of a civil war that left the community divided. John Fitzgerald reports on a pioneering project that aims to replace hatred and suspicion with love and trust.

Suppose the only source of water for your village was a single and unreliable tap, or an unclean river a long walk away. That is the situation faced by Hutu villagers and Tutsi refugees in Mutaho, central Burundi. Scarce water puts a strain on the community as people struggle to share what little clean water is available.

Earlier this year Britain Yearly Meeting provided funding and support to a pioneering water filter project that has helped build peace and reconciliation between the two communities. Run by local partner organisation Healing and Rebuilding Our Communities (HROC), the project encouraged Tutsi and Hutu residents to work together, promoting harmony in the community at the same time as improving access to clean water.

"This kind of co-operation is vital in Burundi because it helps to bring about reconciliation between different sections of the community."
—Gerald Conyngham

We became involved with the project through Elin Henrysson, a peaceworker funded by Britain Yearly Meeting and placed with HROC in Burundi. Elin supports HROC by securing funding for, monitoring and evaluating projects, and by raising awareness about their work.

The project began with installing a few filters in people's homes. The filters are a simple design involving low-tech materials. The main structure is built of concrete and the water is filtered through locally available sand and pebbles that only need to be replaced every five years. Those who have filters in their homes are encouraged to share them with their neighbours, whichever community they are from.

Gerald Conyngham of Devon Area Meeting visited the project on behalf of Quaker Peace & Social Witness in February: "I saw two filters in different houses, both a source of great pride to the people involved. In the second house belonging to a local pastor, neighbours were coming in to make use of the filter." Gerald was impressed at the way the new water sources were already promoting sharing and neighbourliness.

Later in the spring, HROC ran a workshop on how to build the water filters. Elin Henrysson observed the training: "It was clear that trust and healthy relationships were encouraged by doing something practical together. One man told me that another participant had at one point wanted to kill him but that they had been reconciled during the HROC trauma-healing workshop. The water filter project is allowing them to build on this relationship."

HROC made sure that Hutus and Tutsis were represented equally in the workshops, helping to build the trust that is vital for a sustainable peace. Around half the participants were former combatants from the 12-year civil war that divided so many communities in Burundi. By learning how to build and install the water filters, the ex-combatants are picking up valuable skills, and an opportunity to earn money by developing filter construction into a business. The hope is that this will help them reintegrate successfully into society.

The workshop participants have so far built 41 of 50 filters planned for donation to local institutions and households, including three hospitals, 11 schools and a university. The next step for HROC will be to support the participants as

Learning how to build water filters.
Photo: AfID (Accounting for International Development)

Quaker peaceworker Elin Henrysson (second left) watches children from Mutaho use a water filter in the home of local pastor Sebastien (right). Photo: Gerald Conyngham

they form their own co-operative to build a further 100 filters for sale.

At a community celebration day in the summer, people who had used the water filters spoke about their impact on the community. "There was much suspicion between my neighbours and me," said Kanuma, an ex-combatant. "But now people come to filter their water in my house. I feel I am well integrated into the community through this project."

"... I am glad of my filter and I am confident that I drink clean water. As we say that water is life, we are offering life to people from all groups of the community. My neighbours come to ask for filtered water."
– Celine Mbonihankuye

Ernest, a Tutsi refugee living in Mutaho's camp for internally displaced persons, said: "It is amazing to see Hutus living nearby the camp coming to filter water in my house. This is what the crisis stopped in our country: sharing food and drink, which was the essence of our culture in Burundi."

Following the success of the pilot, the water filter project is now expanding to other locations in Burundi. Gerald summed up the importance of the work: "This project is clearly meeting an important need for water, as well as bringing people from different parts of the community together, as they build the filters and then share the clean water. This kind of co-operation is vital in Burundi because it helps to bring about reconciliation between different sections of the community."

"One man told me that another participant had at one point wanted to kill him but that they had been reconciled during the workshop."
– Elin Henrysson

What is HROC?

Healing and Rebuilding Our Communities (HROC) was founded in 2002 to respond to the tremendous need for post-conflict reconciliation in Burundi. Its trauma-healing workshops bring people together across ethnic divisions to learn about the effects of trauma, talk about the inner wounds that are left behind, and reconcile with one another. HROC also runs practical resource-sharing projects such as the goat-sharing programme reported in Quaker News 78.

HROC is connected to the Quaker church in Burundi and one of the core principles behind the work is the belief that there is something good in everyone – this can seem a radical notion in communities where many people have witnessed neighbours and even family members committing horrific acts of violence.

War or ice cream? Celebrating our peace testimony

Children making a peace banner at Yearly Meeting Gathering. Photos: © Mike Pinches

"War or ice cream?" asked a small group of five- to eleven-year-old Quakers in a session about peace at Yearly Meeting Gathering this August. "ICE CREAM!" shouted the rest of the children at the top of their voices, with a couple opting for war in jest.

Their session was part of a year-long celebration of the Quaker peace testimony that was launched at Yearly Meeting 2010 and ended at Yearly Meeting Gathering. The celebration was timed to mark the 350th anniversary of the first written declaration of the Quaker peace testimony – a commitment to peace that was addressed to Charles II and printed as a pamphlet.

The children were treated to a lively presentation from Chris Nickolay, Children's Officer for Britain Yearly Meeting. He explained how the declaration to Charles II came about, beating a drum to show the turmoil in Britain, waving a sword as the soldiers arrested the Quakers, and ripping paper as the first edition of the declaration was destroyed straight from the printing presses. He explained why twelve Quakers felt they had to "utterly deny… all outward wars" and why this matters to Quakers still. Afterwards, the children expressed what peace means to them by painting, sewing, sticking, drawing or hand- and foot-printing peace banners.

We ran sessions on the peace testimony for all ages at Yearly Meeting Gathering, based on our workshop *Peace 350 years on: What does the peace testimony mean today?*. More than 50 Quaker meetings ran one of these workshops during the course of the year. The workshop challenges Friends to work in groups to produce a 21st-century version of the peace declaration. Responses were sent to the Peace, Campaigning & Networking Group of Quaker Peace & Social Witness, who drew the threads together into a new text. This was read out in the concluding session of Yearly Meeting Gathering, bringing the Peace 350 project to a close:

The full text of the statement is available www.quaker.org.uk/350, as is the Peace 350 workshop pack, which remains an excellent opportunity for meetings to reflect on the peace testimony.

Flying the flag for peace at Yearly Meeting Gathering. Photo: © Mike Pinches

A 21st-century peace declaration: ideas from meetings

- We declare, guided by the light, to conduct our lives peacefully in truth and harmony with every living thing in the world. We are led by the spirit to reject war and arms.
- We declare that the spirit is crucial to the achievement of peace. That spirit is rooted in the solidarity of all people which we believe exists. That inter-relatedness is itself based on love, a universal love, which has the power to provide the wisdom which can change individuals and nations.
- To the government and the United Nations: Selling arms and weapons to other countries stirs up conflict. It is not done for our protection, but to make profits and jobs. There is alternative work to be created in new green industries. Sourcing raw materials and environmental damage are global issues causing more conflict. There are bans on land mines and cluster bombs. Extend this to all weapons, including nuclear ones.

What is the peace testimony's challenge to me? – responses from Friends

- To actively wage peace.
- To hold compassion for those whose eyes are closed, whose backs are turned, or whose behaviours I reject.
- To be still, be calm, listen, try to find the truth. Be an example.
- To put aside hypothetical situations. I want to be a pacifist, so I will act as one until I can do so no longer.

Creating peace in a violent world

Peace is not just the absence of violence. To truly commit to peace, we must make it central to the way we live our lives. In *Holding faith*, a new title from Britain Yearly Meeting's Quaker Books, David Gee explores how peace can come naturally from feeling and respecting the dignity of our common being; from living together more authentically as human beings.

"I hope the book might invite people into a fuller commitment to peace," says David. "I hope it might also help lay to rest a common misconception that the Quaker peace testimony is a sort of party-line ideology about the moral error of violence – it's what we do, not just what we think, that makes its mark in the world as a 'testimony' of faith."

Holding faith: creating peace in a violent world is available to buy from the Quaker Centre Bookshop now, priced at £8. David will give a talk about the book at the Quaker Centre in London on Wednesday 5 October at 6pm.

Contact:
Quaker Centre Bookshop
quakercentre@quaker.org.uk
020 7663 1030
www.quaker.org.uk/holdingfaith

Quakers support ecumenical submission on UK nuclear weapons policy

Quakers in Britain have worked with Baptists, The Methodist Church, The Church of Scotland and the United Reformed Church to produce a paper expressing the churches' united belief that the UK should relinquish its nuclear weapons.

Britain's Vanguard-class submarines can each carry up to 192 Trident nuclear warheads. Photo: Julian Merrill; © UK MoD Crown Copyright 2007

The paper has been submitted to the British American Security Information Council (BASIC), who set up an independent commission earlier this year to examine the UK's nuclear weapons policy and the proposed renewal of the Trident nuclear defence system.

Trident comprises four submarines armed with nuclear warheads. The submarines are due to be decommissioned in the 2020s. Although the government is committed in principle to the renewal of Trident, the construction

"This is a golden opportunity to demonstrate an ecumenical momentum for nuclear disarmament."
- Michael Bartlet

of replacement submarines has been postponed until after the 2015 general election, creating a window for further debate.

The ecumenical submission considers the renewal of Trident in the context of Christian ethics, international humanitarian law, the Nuclear Non-Proliferation Treaty and the UK's relationships with the US and NATO. By working together with other non-conformist churches we have been able to deliver our message with greater impact.

"This is a golden opportunity to demonstrate an ecumenical momentum for nuclear disarmament," says Michael Bartlet, Parliamentary Liaison Secretary for Quakers in Britain. "We encourage all local meetings to raise the issue with their constituency MPs."

Visit www.quaker.org.uk/dont-replace-trident to read the submission and to find out more about Quaker work on Trident.

Contact:
Sam Walton
samw@quaker.org.uk
020 7663 1067
www.quaker.org.uk/disarm

Quaker opposition to nuclear weapons

Quakers in Britain have been campaigning against the renewal of Trident since it was proposed in 2005. Quaker opposition to nuclear weapons dates back almost as far as the technology itself. In May 1955, less than a year after the British government announced its intention to build nuclear weapons, Quaker representative body Meeting for Sufferings issued a public statement arguing that "To rely on the possession of nuclear weapons as a deterrent is faithless; to use them is a sin."

Boycotting illegal settlement goods

In April this year Meeting for Sufferings, the representative body for Quakers in Britain, took the decision to boycott products from illegal Israeli settlements in the occupied West Bank. The decision was seen as a nonviolent move for peace for Israelis and Palestinians.

Since then we have been contacting major supermarket chains on behalf of Quakers in Britain to raise the issue, asking them how they are labelling settlement products and to what extent they trace the exact origins of imports from the area. Many of them now seem to be reducing the number of lines they stock from the illegal settlements.

We have also produced a guide to taking action on the issue, which you can download at www.quaker.org.uk/settlement-produce. It includes advice on identifying settlement goods and speaking out about the boycott. You can keep up to date on this issue by signing up via settlementproduce@quaker.org.uk.

Contact:
Suzanne Ismail
settlementproduce@quaker.org.uk
020 7663 1055
www.quaker.org.uk/economic-justice

Helping our children to grow in the spirit

"Close your eyes and think carefully... Be still and be calm... Imagine your favourite living being." Thoughtful silence. "What might that being say to us about caring for the earth?" Long pause. "Now, come back to the circle so we can listen..." And that's how some of the youngest children at Yearly Meeting Gathering convened a 'Council of all beings'. And we listened, as whales, tiger cubs, a gorilla, a rabbit, an elephant, a spider, and more told us, please, to stop [illegible] the planet.

Children's activities at Yearly Meeting Gathering. Photos: © Mike Pinches

The council was part of a carefully planned programme that enabled more than 260 children to think about caring for each other and for the world, to have fun and to be serious, and to grow in the spirit. The programme was planned and run by Britain Yearly Meeting staff, with plenty of help from volunteers.

Participants in Junior Yearly Meeting, the programme for 15- to 18-year olds, met with the adults in 'chat rooms', exploring the relationship between faith and action. "One of the highlights of the event was interacting with other Quakers and getting their opinions and thoughts," said one participant. "It helped me, a confused teenager, to know what I believe in."

The 11- to 15-year-olds in the Young People's Programme explored the Quaker way through music and dance. They also learned about economic justice and joined in with some of the main Yearly Meeting sessions.

"One of the highlights of the event was interacting with other Quakers and getting their opinions and thoughts," said one participant. "It helped me, a confused teenager, to know what I believe in."

Children under 11 spent their time in five age groups. The Spiritual Warriors (9–11 years) learned about Quaker history and staged a mini Olympics. The Light Explorers (7–9) talked about sustaining the earth and tried Godly Play. Crafts and fair-trade activities were organised for the Penn Friends (5–7), while the Fox Cubs (3–4) had music and stories. The New Shoots (0–2) enjoyed walks and messy play.

Comments from participants show just how valuable dedicated programmes for children and young people can be, helping them to feel supported and to explore their beliefs:

"Being at YMG gave me the chance to understand Quakerism more and develop my understanding of what I really believe."
– a Junior Yearly Meeting participant

"It helped me feel more like a Quaker."
– a Light Explorer

"Gathering has moved me so much – global warming, sustainable living, things like that."
– a Spiritual Warrior

"I feel completely included and supported, it really has made me feel like I belong as a Quaker."
– Young People's Programme participant

"I'd like to keep my sense of energy and belonging. I want to give my spirit and Quakerism more time."
– Junior Yearly Meeting participant

[illegible]

A promising partnership: Working with the National Trust at Peckover House

Peckover House. Photo: National Trust

Britain Yearly Meeting staff are working with the National Trust on a new project at the historic Peckover House. Alistair Fuller reports on this fantastic opportunity for outreach and the exciting possibilities the partnership brings.

On a handsome Georgian street in Wisbech, Cambridgeshire, stands Peckover House, an elegant property overlooking the river at the front and with generous, richly planted gardens at the rear.

Since 1943 the house has been the property of the National Trust. Before then, it belonged to the Peckovers, a family of Quaker bankers, who had owned it since the 1790s. The house was the centre of the Peckovers' banking business and the base from which generations of the family campaigned for causes that included peace, the abolition of slavery and improvements in education.

Having maintained the site as a popular attraction for decades, the National Trust is now beginning a major project to restore and open-up the old banking hall at Peckover House. They approached us earlier this year about working with them on the development of this project.

The Trust is interested in the domestic detail of Quaker families such as the Peckovers. How would their Quaker principles have influenced the decoration and appearance of their house and the shape of their daily lives? How might we understand the prevailing social attitudes that once barred them from areas of public life and yet also allowed them to thrive as business people with a reputation for integrity and trustworthiness? The Library at Friends House is looking forward to being involved in this venture, informing and giving detail to the historical aspects of the project.

The Trust are keen to show the way in which those things that are distinctive about Quaker living – simplicity, integrity, peace, equality – were lived out by the Peckovers and are central to the lives of Quakers today.

The Trust is also interested in the connections between the work of earlier generations of Quakers and our work and witness today. As well as being great campaigners and activists, the Peckovers were prolific readers and prodigious travellers; energetic philanthropists who were deeply engaged in the life of their community. How can we illustrate Quakers' ongoing commitment not only to causes around peace, social and economic justice and equality, but also to intellectual endeavour, investigation and discovery? The Trust are keen to show the way in which those things that are distinctive about Quaker living – simplicity, integrity, peace, equality – were lived out by the Peckovers and are central to the lives of Quakers today.

The National Trust has a commitment to community engagement and social involvement, especially in the areas of equality, education and access. For example, they work with schools, prisons and those living with substance abuse. It is hoped that our new relationship will offer wider opportunities to work together in some of these areas, to share some of our experience and to demonstrate the connections between the historic and contemporary expressions of Quaker witness.

We are excited by the possibilities of working with the Trust, not just on the Peckover House project, but also on the potential links between the Trust's community work and our own projects and programme areas. We look forward to what this new relationship might bring and hope that Friends will visit Peckover House to see the Quaker banking hall.

Contact:

Alistair Fuller
alistairf@quaker.org.uk
020 7663 1016
www.quaker.org.uk/outreach

to promote our work today

A new chapter for Swarthmoor Hall

Jane Pearson, who took over as manager of Swarthmoor Hall in June following the retirement of Bill Shaw, writes about new developments at the powerhouse of the early Quaker movement.

Swarthmoor History Group conducting its first onsite archaeological dig. Photo: Des Brady

It's a joy to welcome visitors to Swarthmoor Hall and share with them our Quaker history. Although the hall is a place of peace, beauty and stillness, there is plenty going on and developments are in the pipeline.

We are working with Woodbrooke Quaker Study Centre to produce a series of events in 2012 – 'Woodbrooke @ Swarthmoor Hall' – to help nurture the spiritual life of Quaker meetings. We are also talking with the National Trust about a potential partnership, though it is too soon to say exactly what this might involve.

The gardens and grounds are evolving. A new contemplative garden has been planted with species that may have been grown here in the 17th century, and we are planning a similar scheme for the recently cleared courtyard garden.

Our group projects are flourishing. The History Group recently conducted its first on-site archaeological dig, which was well attended by local people. The Patchwork Group have completed a new covering for George Fox's travelling bed and the work of the 17th Century Clothes-Making Group continues. A new conservation report will produce a plan of action for our Furniture Group.

Our ability to do all this depends on people. Swarthmoor Hall has an extraordinary group of talented and committed volunteers and staff. We are always looking for house guides and other volunteers and are happy to reimburse travel from a reasonable distance.

Contact

Jane Pearson
info@swarthmoorhall.co.uk
01229 583 204
www.swarthmoorhall.co.uk

Swarthmoor Hall

Swarthmoor Hall is a 16th-century house in Cumbria that was the home of Margaret Fell and George Fox, early leaders of the Religious Society of Friends. In the 1650s it was the powerhouse of the burgeoning Quaker movement.

Now owned by Britain Yearly Meeting, Swarthmoor Hall hosts a busy calendar of events and courses as well as offering holiday accommodation and conference facilities.

Opening up our history

The Library at Friends House holds a large collection of museum objects, pictures and photographs which reflect the activities of Quakers over the years, including prison reform, wartime relief work and the campaign to abolish the slave trade.

We know that there are similar materials in many meeting houses and some in private hands. We are interested in building up a detailed picture of Quaker artefacts held around the country. This would help us to encourage greater lending between parts of the Society and to plan exhibitions to communicate our values and history to the wider world. It would also pave the way for working collaboratively with other organisations, as we are currently with the National Trust at Peckover House.

This work would be taken forward by our new Visual Resources Development Officer, Melissa Atkinson, who started in the Library in August. She will also be curating, expanding and raising the profile of the Library's collections.

Contact

Melissa Atkinson
[illegible]@quaker.org.uk
020 7663 1129
www.quaker.org.uk/library

News in brief

New resources for Quaker employers

How can we be effective and supportive employers? What are our obligations to employees? How do we deal with difficult employment situations?

In response to the many questions we receive from meetings who employ staff, we have put together an online resource that covers all the issues Quaker employers need to know about.

At www.quaker.org.uk/employers, you'll find a wealth of information set out in an accessible question-and-answer format. This resource will be updated regularly, and is equally useful for Quaker employees.

Contact:
Richard Summers
richards@quaker.org.uk
020 7663 1096
www.quaker.org.uk/employers

Ways to connect with young people in your meeting

Ways to connect is a new resource to help Friends engage with young people in their meeting. Available as a booklet or a series of leaflets, it contains advice on communicating with young Friends, engaging them in the life of the meeting, keeping in touch when they move away, and running all-age events.

'Connecting as a community' is a special edition of our popular youth-work resource *Journeys in the Spirit*, featuring group activities that the whole meeting can share.

Both resources are on our website, and paper copies are available free of charge.

Contact:
Bevelie Shember
bevelies@quaker.org.uk
020 7663 1013
www.quaker.org.uk/cyp

Support Quaker work when you subscribe to Ethical Consumer

Ethical Consumer magazine is offering a £10 donation to Britain Yearly Meeting's Economic Issues Programme for every Quaker who subscribes before the end of October. Mention 'Quaker' on the phone or enter it into the online subscription form.

Contact:
Ethical Consumer
www.ethicalconsumer.org
0161 226 2929

Get involved

Celebrating our work in the world

Together we have something to celebrate. Quaker Peace & Social Witness (QPSW), funded by your contributions to Britain Yearly Meeting, is working today to put our faith into action in the world. But how much do you know about this inspiring work? If the answer for you and your meeting is "not much", then help is at hand.

We have 10 QPSW committee members who are keen to share the latest news about our work on sustainability and peace and crime, community and justice; about our presence at the United Nations and our witness in Israel–Palestine, and about our peaceworker placements in the UK and Burundi. They are ready to come to your meeting and talk about the areas that interest you most. Let's celebrate that we are making a difference in the world. And let's find out how our money is being spent. Book your speaker now.

Contact:
Helen Bradford
helenb@quaker.org.uk
020 7663 1071

Volunteer at the Quaker Centre

The Quaker Centre at Friends House, London incorporates a bookshop, café, resources area and worship space. An active group of volunteers helps to run the centre and meet people who drop in to learn about Quakers.

New volunteers are always welcome, so please get in touch if you'd be interested in this rewarding service.

You can see a video of one of our volunteers talking about his role at www.quaker.org.uk/quaker-centre.

Contact:
Amanda Woolley
amandaw@quaker.org.uk
020 7663 1041

Help shape the future of outreach gatherings

Have you attended one of our gatherings for enquirers or for attenders considering membership? If so, we'd love to hear from you. We are reviewing the way we run these gatherings and your feedback could help shape future events. All comments will be gratefully received and treated in confidence.

Contact:
Alistair Fuller
alistairf@quaker.org.uk
020 7663 1016

Find out more about the Quaker way

Enquirers' gatherings offer an opportunity to find out more about Quakers within a supportive and spiritually enriching environment:

- Charney Manor, Oxford: 28–30 October 2011
- Swarthmoor Hall, Cumbria: 11–13 November 2011

You can approach your meeting about bursary help.

Contact:
outreach@quaker.org.uk
020 7663 1017

Supporting the work

Alfred Bader is an extraordinary man with a rags-to-riches story who has given generously to Britain Yearly Meeting for the last decade. Kate Cargin visited Alfred and his adored wife Isabel at their British home to find out why someone of a different faith gives so much support to Quakers.

Alfred and Isabel Bader. Photo: Kate Cargin

"You want to know why I give money to the Quakers?" asks Alfred Bader, one of almost 10,000 Jewish children evacuated to Britain from Nazi Europe at the dawn of World War II. "In 1938 when we arrived on the Kindertransport there were 18,000 Quakers in Britain and 300,000 Jews. The Quakers took care of about half of us; the Jews didn't do very much."

Born in Austria in 1924, Alfred came to England at the age of 14 on the first Kindertransport leaving Vienna. His life story is a fascinating one of rising by his own efforts and considerable talents to head his own company in the United States.

I first encountered him after he met Brenda Bailey during the filming of *The children who cheated the Nazis*. Through Brenda he learned the story of her parents Leonhard and Mary Friedrich, who were wardens at Bad Pyrmont Quaker Meeting in Germany. Their efforts to rescue Jewish families from the Nazis culminated in Leonhard's imprisonment at Buchenwald concentration camp. This story reawakened Alfred's interest in Quakers and the huge part Quakers played in the Kindertransport.

He called into Friends House asking to make a donation. "I never thanked the Quakers," he announced as he took out his cheque book. Since that day, he has faithfully supported several parts of our work. First our peace work in Uganda, because he felt such empathy with children suffering from the effects of war. Later, he supported our work with children and young people and outreach because he wants Quakerism to continue into the next century.

So why does a man of another religion care so much for the Quaker faith? "Because they are good people," he says. Isabel expands on this: He feels that many Christian groups were compromised and had supported Nazism. He is happy to support Quakers because those particular people helped Jews.

The Baders live simply and frugally. They make their money count: the list of beneficiaries is long and various, and we are very grateful to be on it.

Contact

[redacted]

The Kindertransport

The Kindertransport was a remarkable operation to evacuate Jewish children and young adults from Nazi Europe just before the outbreak of World War II. Quakers were involved at all stages of the rescue, and many British Quakers provided homes, education and employment for the young refugees who made it to the UK.

Giving *chai*

The Hebrew word *chai* means 'life'. Each Hebrew letter has a numerical value, and the letters that make up *chai* have a combined value of 18. For this reason, many Jewish people give gifts of money in multiples of 18: this is called 'giving *chai*'. Alfred Bader feels he owes Quakers his life for rescuing him from Nazi Europe. He explains why he gives $72,000 [about £45,000] each year to Quakers: "The number 18 is *chai*, and *chai* means life. There are four in my family: my wife, my two sons and me. Four 18s are 72. Everything has a meaning."

Quakers make peace a way of life

Quakers share a way of life, not a creed or beliefs. Our unity is based on shared understanding and a shared practice of silent worship, where we seek a communal stillness. We seek to experience God directly within ourselves and in our relationships with others and the world around us. We seek expression for worship in local meetings which are inclusive and open to all.

We try to live according to the deepest truth we know. This means speaking the truth to all, including people in positions of power.

Our commitment to peace arises from our conviction that love is at the heart of existence and that all human beings are unique and equal. This leads Quakers to put their faith into action by working locally and globally to change the systems that cause injustice and violent conflict.

We try to live simply. We are concerned about the excesses and unfairness of our consumer society, and the unsustainable use of natural resources.

To find out more about the Quaker way visit www.quaker.org.uk or request a free information pack using the form below.

Request a free information pack

Your name

Your address

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Please send completed form to:

Quaker Life Outreach Team (QN)
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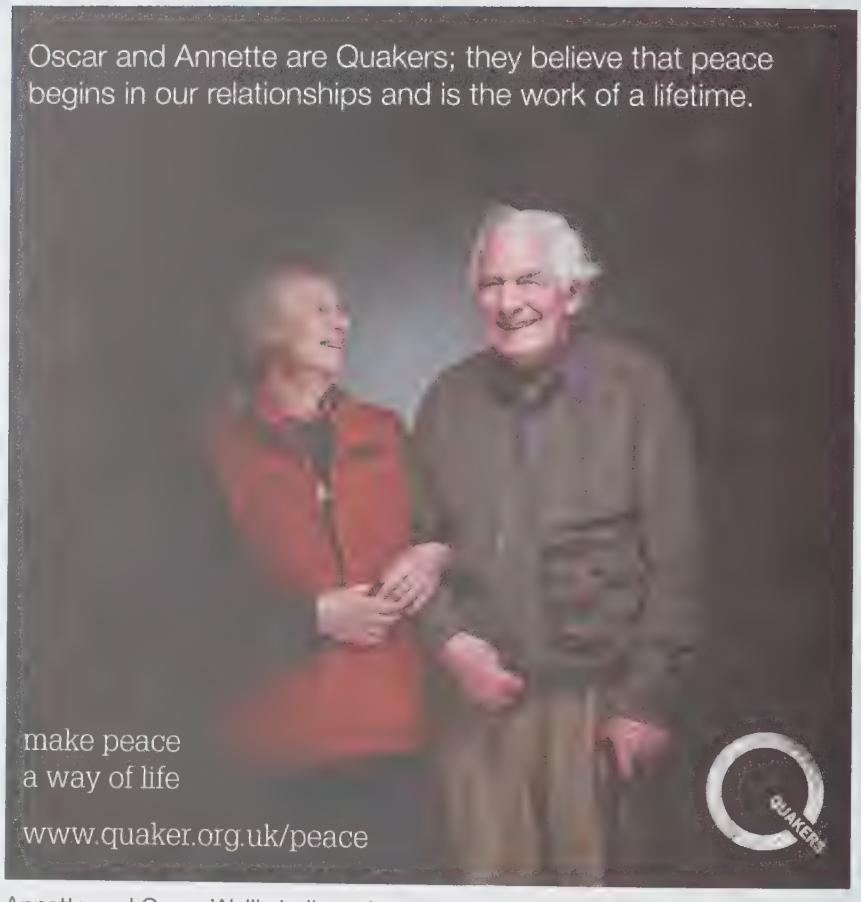
Friends House
173 Euston Road
London NW1 2YS
FREEPHONE: 0808 109 1651
Email: outreach@quaker.org.uk

Meet Annette and Oscar



Annette and Oscar Wallis believe that peace is the work of a lifetime. They are Quakers and for more than 60 years they have been campaigning for peace.

They grew up in families whose Quaker beliefs led them to stand up for treating people equally and finding alternatives to violence. Oscar says war is wrong. In World War II he refused to take up arms and instead served on a hospital ship. Like many Quakers, he and Annette's father were both conscientious objectors.

They married in the 1950s when a very real fear of nuclear conflict gripped Europe. That fear gave rise to the birth of the Campaign for Nuclear Disarmament in 1958. One of CND's first actions was to organise the first Aldermaston march. Oscar was among the 4,000 who walked fifty miles from London to Aldermaston Atomic Weapons Research Establishment.

Since then the Wallis family has campaigned together against nuclear weapons at Aldermaston, Greenham, Molesworth, Upper Heyford and Faslane.

They believe peace begins in our relationships. "Peace is about how you deal with everyday life," says Annette. "How you deal with controversy and conflict." She says we need to acknowledge differences and live with them and accept flaws in ourselves as well as others.

Oscar and Annette follow in the footsteps of centuries of Quakers who declared to the King in 1660: "We are a people that follow after those things that make for peace, love and unity." Commitment to peace and equality meant Quakers were a driving force in abolishing the slave trade and they helped set up modern charities like Amnesty International, Greenpeace, Oxfam and Campaign Against Arms Trade.

Read more and find your local meeting at www.quaker.org.uk/peace

APRIL 28, 2014

C&EN

CHEMICAL & ENGINEERING NEWS

CAPTURING CO_2
Enhanced oil recovery may be coal's unlikely savior **P.23**

NEW HUES
Exploiting nanostructure to create novel pigments **P.28**

TOP INSTRUMENT COMPANIES

Acquisitions alter size, not ranking **P.10**

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C&EN

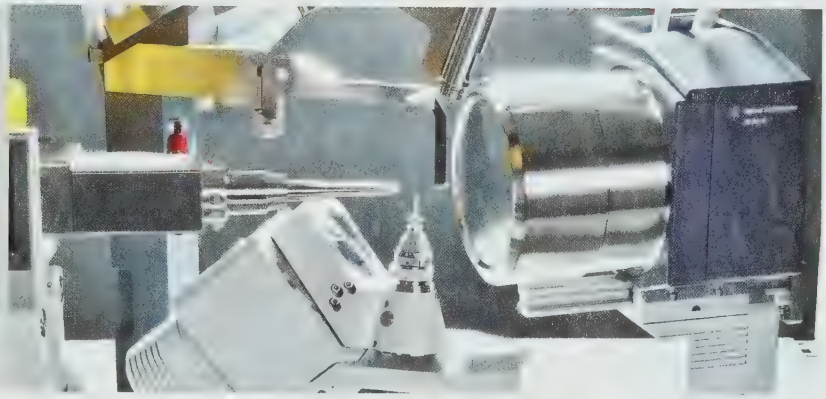
CHEMICAL & ENGINEERING NEWS

Serving the chemical, life sciences, and laboratory worlds

COVER STORY

TOP INSTRUMENT COMPANIES

The biggest firms in C&EN's annual ranking held on to top spots and grew organically and through acquisitions. PAGE 10



QUOTE OF THE WEEK

"It would seem unlikely that any person could be a renowned authority on paintings and fine artworks, synthetic chemistry, science history, and running a major science-based corporation. But I can say, 'Yes, it's possible,' and that person is Alfred Bader."

ELIAS J. COREY, EMERITUS PROFESSOR OF CHEMISTRY, HARVARD UNIVERSITY PAGE 34

NEWS OF THE WEEK

BUSINESS

GOVERNMENT & POLICY

SCIENCE & TECHNOLOGY

ACS NEWS

PEOPLE

THE DEPARTMENTS

COVER: *Close-up view of Agilent Technologies' GV1000 X-ray Diffractometer with the Atlas S2 CCD detector. Agilent*

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LETTER

WHAT'S IN A NAME?

"OBSCURE CHEMICAL Taints Water Supply" features a timeline about MCHM (C&EN, Feb. 17, page 10). I remain mystified by the naming of the compound. The names of two separate compounds (4-methylcyclohexane and methanol) are simply joined together. Why isn't the name 4-methylcyclohexylmethanol a methanol derivative?

Charles Feldmann
Cincinnati

BREAKING GOOD, NOT BAD

ALTHOUGH the final episode of the Emmy Award-winning AMC television series "Breaking Bad" has aired, discussion of its influence on society continues. Questions range from "Will it increase interest in science generally among both U.S. students and the general public?" to "Will it encourage our younger generation to synthesize meth?"

Students sometimes can't distinguish between fact and fiction. Students see negative characteristics in Walter White, the fictional high school chemistry teacher portrayed on "Breaking Bad." Then they wonder if their own real-life high school teachers have similar characteristics. Students have reportedly asked high school teachers, "Do you make meth?"

Being confronted with such a negative parallel can be disappointing. But such a teachable moment can be transformed into an opportunity to demonstrate the good that chemists do.

One can point to personal experiences and those of other chemists in sometimes heroic efforts to improve human lives. The visibility and high-quality narrative of "Breaking Bad" could greatly impact the image of chemistry teachers.

Without commentary and interpretation, young people might infer that chemistry teachers spend their evenings cooking methamphetamine. What will be the perception of our students?

We can confront the issue head-on and inspire rather than apologize. We can point out the ways in which chemists and chemistry teachers have shaped our world, making our contemporary society possible. When students ask this type of question, we should be ready. We want to inspire them to reach positive goals by offering positive role models.

chemistry teachers questions with, ... and we teach." ... to be chemistry teac...

Donna ...
Norman ...
Sally Mitchell
East Syracuse

Note: Donna Ne..., a professor of chemistry at the Univ...ity of Oklahoma, Norman, served as a sc...ence adviser to the producers of "Breaking Bad." Sally Mitchell is a teacher at East ...yracuse Minoa High Scho...

TRANSPARENCY IS A GOOD THING

REGARDING ... "Transparency's Sake," ... a good thing overall (C&EN ... page 28). Given events over the ... several years, it has become increasingly clear that there are multiple standards ... transparency." The environment is an important yet fragile force that can affect ... everyone around the world. As such, we should not put our trust in black-box scientific results.

The article speaks of "patient privacy rules," but I fully understand that, in order to have ... detailed disclosure is required ... anyone can verify its claims. Software patents protect the methodology that the code uses to attain a result, and a copyright can protect the duplication of the code itself. With these protections in place, I see no problem with full disclosure.

It is surprising that Rep. Suzanne Bonamici (D-Ore.) proclaims that secret data or secret software is "valuable" and the "best available science to inform regulatory actions" when she and the rest of us do not and cannot know how the results are attained. I am equally surprised that the Environmental Protection Agency had been making policy since 1990 based on two key studies that weren't available for scrutiny. So on what basis do we make policy decisions? On the words of a few researchers?

How about we just accept the words of researchers from pharmaceutical companies instead of requiring proof of drug safety and efficacy before approval? The Food & Drug Administration requires complete information disclosure of all clinical subjects for drug approvals. EPA can require the same for the studies on which its policies are based. EPA can easily code subject

identity of any study for the purposes of public disclosure.

Whoever owns the modeling software leased (no doubt at a high price) to EPA should get a patent and a copyright and release the information required for public transparency. I want to know why I should trust their model, especially if it affects the environment. Frankly, I don't trust politicians or agencies that do not care to know the workings behind the science from which they make policy.

Pete Nirchio
Lebanon, N.J.

RECONSIDERING ETHANOL

THE PATENT PICKS item "From Cellulosic Ethanol to Butanol" begins with the statement, "Blending ethanol into gasoline oxygenates the fuel, reduces pollution, and stretches petroleum supplies" (C&EN, Feb. 24, page 39). This statement is wrong on two counts.

First, ethanol-containing fuel may create less pollution per gallon of fuel burned, but because it requires more fuel to drive 1 mile, it actually calculates to create more pollution per mile driven.

Second, numerous studies show the total energy required to grow the corn, convert it to ethanol, transport it to the refiners, and blend it into the fuel is greater than the energy generated. So we actually end up having to import more petroleum when using ethanol in gasoline than when using straight gasoline.

Your statements are commonly made by the businesses that benefit from the ethanol and corn business, but I would hope a science magazine would get the science right.

David Berkebile
Landenberg, Pa.

A 'KNEADED' CONSIDERATION

AS INSIGHT into the desirability of using azodicarbonamide in bread making, consider how many of C&EN's readers would use this ingredient when making bread for themselves (C&EN, Feb. 17, page 9). Few would, I daresay. There are two reasons: First, it is unnecessary. Although it functions as a dough conditioner, azodicarbonamide's purpose is to decrease the cost of making large amounts of bread quickly. Second, with the notable exceptions of salt, water, and a few necessary minerals, many people, if not most, find the use of ingredients in their food that are not derived by simple processes from living things to be offensive.

The focus solely on the safety of ingredients is often used to frame the discussion of an issue so as to preclude consideration of this second point as a valid reason for opposition to their use. This is usually followed up by claims that the public is uneducated in such matters, implying that they are not fit to make decisions about what they eat.

David Lane
Davis, Calif.

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- Our fax number is (202) 872-8727.
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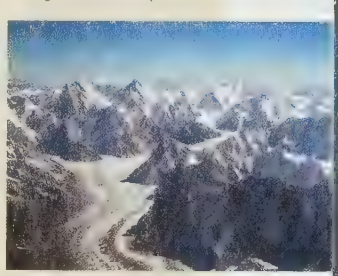
& THIS WEEK ONLINE

Speaking Of Chemistry

To showcase its most intriguing stories in minutes, C&EN has launched a Web-based program, Speaking of Chemistry. In the most recent podcast episode, C&EN Associate Editor Lauren Wolf and Senior Editor Carmen Drahl present highlights from stories on ways to make spider silk without spiders, the health risks of e-cigarettes, and milk proteins used as flame retardants.
http://cenm.ag/two43

Tracing The Loss Of Himalayan Glaciers

Scientists want to estimate how fast glaciers in the Himalayas are disappearing. But the task is difficult because of the region's treacherous terrain and high altitudes. Now, oceanographers report a new strategy that involves monitoring changes in the salinity and oxygen isotope composition of the Bay of Bengal, which receives most of the region's glacial meltwater.
http://cenm.ag/two44



GUILHEM VELLUT/WIKIMEDIA COMMONS

Stories Of The Aldrich Handbook

When it's time to buy research chemicals, chemists usually reach for the Aldrich Handbook. But the catalog also has sentimental value for many chemists. This March, at the ACS national meeting in Dallas, C&EN Senior Editor Linda Wang asked chemists to share their favorite memories of using the ubiquitous catalog. Check out a video of their responses.
http://cenm.ag/bader

Antifungal Coating For Medical Devices

Fungal films coat surfaces around us, and a fog of microscopic spores permeates the air. For people with compromised immune systems, some opportunistic fungi species can start dangerous infections. To combat one hot spot for invading fungi, a team of researchers has developed a coating for the rubber surfaces of medical devices that releases antifungal drugs when fungi are present.
http://cenm.ag/two45

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OVERVIEW

Monitoring and maintaining water purity are important to the power and electronics industries. In the both of these industries, impurities must be minimized and monitored to prevent corrosion or scaling, and degradation in demineralization processes Corrosion on a power plant scale can be catastrophic: broken pipes leaks, contamination, costly unplanned maintenance, and power interruptions. In the electronics industries, the impurities can be just as catastrophic, causing contamination, production problems, and product failures.

Here we demonstrate analysis of ppb concentrations of ionic contaminants using two easy methods: a direct large volume injection and concentration of a large volume injection, using electrolytically generated hydroxide eluents on a Reagent-Free™ Ion Chromatography system (RFIC™).

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KEY LEA… …OBJECTIVES

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Demo… …Scientific IC innovations around… … methods

APRIL 28, 2014 EDITED BY WILLIAM G. SCHULZ & SOPHIA L. CAI

PHARMA FIRMS SWAP ASSETS

PHARMACEUTICALS: Novartis, GSK, and Lilly trade businesses to create more focused companies

NOVARTIS IS EXITING vaccines, GlaxoSmithKline is shedding oncology drugs, and Eli Lilly & Co. is boosting its animal health business through a suite of multi-billion-dollar transactions with each other. All told, the big pharma companies expect the swaps to strengthen their market positions at a time when all three are struggling to grow.

In the biggest transaction, Novartis will pay up to $16 billion to acquire GSK's oncology products business. The deal includes R&D related to GSK's approved cancer drugs and rights to its AKT protein kinase inhibitor, currently in Phase II clinical trials. Novartis will also get commercialization opt-in rights to GSK's oncology R&D pipeline for 12.5 years.

The addition will make Novartis the second-largest company in the oncology drug field, according to Frank Orthbandt, corporates director at credit-rating firm Fitch Ratings. Roche is number one.

Meanwhile, GSK will buy Novartis's vaccines business excluding flu vaccines, where Novartis is looking for a separate buyer. The acquisition will give GSK a vaccines business with more than $7 billion in annual sales and more than 20 candidates in development.

In a third transaction, Novartis and GSK will combine their consumer health businesses into a joint venture. It will have about $11 billion in annual sales of mostly over-the-counter drugs.

"Opportunities to build greater scale and combine high-quality assets in vaccines and consumer health care are scarce," GSK CEO Andrew Witty said when announcing the deals. With the transactions, "we will substantially strengthen two of our core businesses," he said.

Novartis had one more move up its sleeve after its deals with GSK. The Swiss firm agreed to sell its animal health division to Lilly, which will combine the business with its Elanco unit to create a $3.3 billion animal health company. It will be the world's second-largest such business after Zoetis, the company spun off by Pfizer last year.

This acquisition will be Lilly's eighth since 2007, when it decided to invest in its then-number-eight-ranked animal health business.

"Elanco has been a key growth engine during the time when we suffered the ill effects of patent expirations on several of our major human pharmaceutical products," Lilly CEO John C. Lechleiter told analysts last week.

For its part, Novartis was looking for ways to turn good businesses that lacked scale into ones that could compete, CEO Joseph Jimenez told stock analysts. When it completes the transactions in 2015, Novartis will be about 7% smaller in sales, but it will be focused on what he calls the "growth engines" of pharmaceuticals, eye care, and generic drugs.

The asset trades "highlight the industry's growing emphasis on efficiency through more focused R&D and the pursuit of scale in consumer healthcare," Fitch's Orthbandt wrote in a review of the deals.

While Novartis, GSK, and Lilly were preparing to announce their deals, an article in the U.K.'s *Sunday Times* stated that Pfizer had made a $100 billion bid to acquire AstraZeneca, which reportedly rejected it.

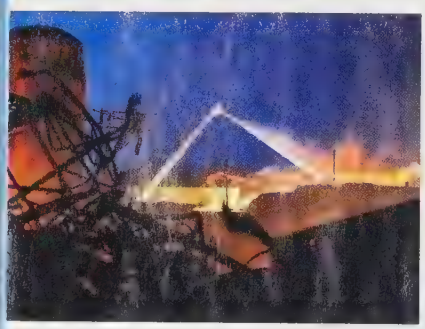
Such a deal, if it came to pass, would make sense for three reasons: taxes, cost-cutting, and an improved R&D pipeline, Leerink Swann stock analyst Seamus Fernandez told clients in a report.

AstraZeneca CEO Pascal Soriot declined to comment directly on a proposed deal when reporting first-quarter 2014 earnings last week. Instead, he emphasized that AstraZeneca is "very committed to creating value on an independent basis." But, he added, the company will look for partners for roughly $4 billion worth of noncore businesses in the areas of neuroscience and infectious disease.—ANN THAYER

EXCHANGE RATE Big pharma companies shuffle divisions to create more profitable combinations.

RULES LACKING FOR REACTIVE CHEMICALS

CHEMICAL SAFETY: Inquiry faults company, regulators for deadly Texas explosion



The aftermath of the April 17, 2013, fertilizer facility explosion in West, Texas.

ON THE ONE-YEAR anniversary of the West Fertilizer Co. explosion, the Chemical Safety & Hazard Investigation Board (CSB) returned to the West, Texas, community where the retail fertilizer warehouse had been located. There, at a public meeting on April 22, CSB released its preliminary accident report that proposes changes to federal laws overseeing reactive chemicals.

CSB's investigation found severe shortcomings in existing regulations and standards for ammonium nitrate at the federal, state, and county levels as well as a "failure by the company to take necessary steps to avoid a preventable accident," CSB Chairman Rafael Moure-Eraso said.

The West accident occurred when some 40 to 60 tons of ammonium nitrate fertilizer held in a wooden building caught fire and exploded, killing 14 people—12 volunteer firefighters and other emergency responders and two residents. Another 226 citizens of West were injured. Some 150 homes were destroyed by the blast, and twice that many were damaged. An apartment complex, three schools, a nursing home, and a hospital were also damaged.

Moure-Eraso noted that Texas lacks a statewide fire code, which could have encouraged county fire departments to closely monitor safe storage and handling of chemicals. Such codes, CSB said, could have also kept populations away from hazardous facilities, such as the warehouse.

The CSB investigation found that the community was largely unaware of the threat posed by the supply of ammonium nitrate in the warehouse, as well as another 100 tons that was held in a railcar adjacent to the facility. When built in 1961, the warehouse was surrounded by open fields, but CSB said that, over the years, homes, schools, and other buildings had been located nearby.

In its investigation, CSB found that throughout the nation some 1,351 facilities, similar to the one in West, held ammonium nitrate fertilizer. Most are in 10 southern agricultural states.

CSB proposed changes to federal laws, including adding reactive chemicals, such as ammonium nitrate, to substances regulated by the Environmental Protection Agency and Occupational Safety & Health Administration. It also recommended inherently safer design principles be required for these facilities.—JEFF JOHNSON

BUILDING RINGS WITH LIGHT

PHOTOCHEMISTRY: Catalyst pair forges cyclobutanes enantioselectively

BY COMBINING TWO CATALYSTS, researchers have used photochemistry to build enantiomerically enriched rings in high yields. The advance could add to the tool kit for building motifs present in agrochemicals and pharmaceuticals.

For more than a century, chemists have talked about generating chirality with photochemistry because it can access products not available by other routes. But photochemistry's march toward enantioselectivity has lagged behind those for transition-metal catalysis or organocatalysis. The reason is that once a molecule absorbs a photon of light, it reacts before it can be reined in by a stereochemistry-controlling catalyst, explains Tehshik P. Yoon, who led the new work. The few existing enantioselective options require specialized light sources or carefully designed catalysts.

Because it uses visible light, the new method works even with substrates with weak C–Br bonds.

Yoon and his coworkers at the University of Wisconsin, Madison, reported in *Science* a different approach. Their method makes chiral cyclobutanes from the visible-light-promoted [2 + 2] photocycloaddition of α,β-unsaturated ketones (2014, DOI: 10.1126/science.1251511). It requires two catalysts: $Ru(bpy)_3$, a transition-metal complex that absorbs visible light, and a chiral Lewis acid made from the lanthanide element europium.

"We're using wavelengths of light that pass through organic molecules," so they don't enter the excited state that leads to willy-nilly reactivity, Yoon says. It's $Ru(bpy)_3$ that absorbs this light, which comes from a compact fluorescent bulb, and then "spits out an electron" to trigger cyclobutane ring formation, Yoon explains. The reaction occurs under chiral control because the chiral Lewis acid coordinates to the ketone substrate.

The work cleverly mimics photosynthesis in that it decouples the harvesting of light energy from bond-breaking and bond-forming steps, explains University of Neuchâtel, Switzerland, chemist Reinhard Neier in an accompanying commentary (DOI: 10.1126/science.1252965).

"I think the concepts are general" and will yield more than just cyclobutanes, Yoon says.—CARMEN DRAHL

EARNINGS WEATHER LATE-WINTER CHILL

FIRST QUARTER: Shrugging off weather impact, chemical executives see a strong 2014

THE POLAR VORTEX may be America's most hated phrase so far this year, but the U.S. chemical industry overcame the extreme winter weather with first-quarter earnings that met or beat analyst expectations. Celanese, Cytec Industries, Dow Chemical, DuPont, and Praxair all boosted earnings compared with last year's first quarter, thanks to diversity of both product line and geographic footprint.

Dow's earnings shot up 17.7% to $964 million on almost flat sales but significant cost controls. The results, the sixth consecutive quarter of earnings growth for the company, were achieved despite the weather, CEO Andrew N. Liveris said. In a conference call with analysts, he reported higher sales of packaging plastics, improved fundamentals in the construction sector, and increased interest in new crop protection chemicals.

Bad weather in North America caused $100 million in higher feedstock and energy costs for Dow, but unseasonably warm weather in Europe boosted sales of agriculture products, Liveris pointed out.

A rebound in overseas construction markets contributed to an unusually strong quarter at Celanese, which raised earnings 39.0% to $196 million compared with first-quarter 2013. The firm said strong demand in Europe and Asia for emulsion polymers, used in paints and coatings, resulted in that business's best performance in years. Celanese's earnings per share of $1.33 beat expectations, according to Charles Neivert, a stock analyst at investment bank Cowen & Co.

Meanwhile, DuPont's earnings per share of $1.58 missed earnings expectations by a penny, as the firm fended off high feedstock costs and a slow planting season, both weather related. Still, DuPont raised earnings for the quarter by 6.6% to almost $1.5 billion. The company reported higher earnings for electronic chemicals, enzymes, and safety products.

DuPont CEO Ellen J. Kullman said her firm is well positioned for future growth—and that growth may be on its way. The Chemical Activity Barometer, a leading economic indicator maintained by the American Chemistry Council, a trade group, reached 95.2 in April, its highest level since March 2008. "This suggests further growth momentum in the broader economy in the months ahead," said T. Kevin Swift, ACC's chief economist.

In Europe, however, growth is recovering slowly, according to the European Chemical Industry Council. Although chemical output was up 3% in January compared with the previous January, prices shrank 2.8%. Trends in capacity utilization and chemical employment were negative at the end of 2013, and confidence levels remained unchanged in March, the trade group reported.—MELODY BOMGARDNER

FIRST-QUARTER CHEMICAL RESULTS

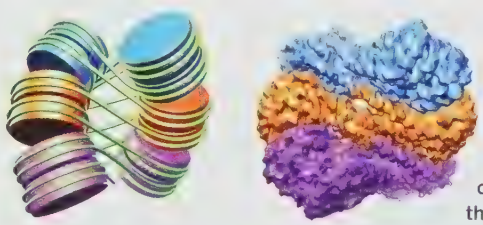
Most chemical firms boosted sales despite impact from lousy weather

	SALES	EARNINGS[a]	CHANGE FROM 2013		PROFIT MARGIN[b]	
	($ MILLIONS)		SALES	EARNINGS	2014	2013
Air Products	$2,582	$284	3.9%	-2.4%	11.0%	11.7%
Albemarle	657	77	2.3	-7.2	11.7	12.9
Celanese	1,705	196	6.2	39.0	11.5	8.8
Dow Chemical	14,461	964	0.5	17.7	6.7	5.7
DuPont	10,128	1,457	-2.7	6.6	14.4	13.1
W.R. Grace	745	50	4.9	-15.3	6.7	8.3
Praxair	3,026	448	4.8	8.2	14.8	14.3

a After-tax earnings from continuing operations, excluding significant extraordinary and nonrecurring items. **b** After-tax earnings as a percentage of sales.

STRUCTURAL BIOLOGY Researchers get first glimpse of how an animal genome is packaged

The human cell nucleus is home to a phenomenal feat of packaging: Two meters of genomic DNA are wound neatly around protein spools called nucleosomes and packed into an overall parcel called chromatin.



SCIENCE

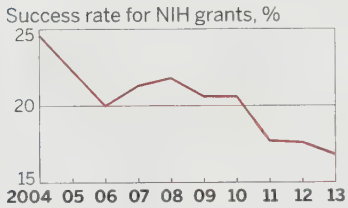
The first peek at the 11-Å structure of a well-studied chromatin fiber comes courtesy of cryoelectron microscopy (cryoEM) and a research team led by Ping Zhu and Guohong Li at the Chinese Academy of Sciences in Beijing (*Science* 2014, DOI: 10.1126/science.1251413). Scientists have long argued about how DNA is packed into chromatin. This is in part because so many forms of chromatin exist, from DNA packed for long-term storage to gene sequences that must be regularly accessed by cellular transcription machinery, comments Andrew Travers at the MRC Laboratory of Molecular Biology in Cambridge, England.

The Chinese team solved the structure of a chromatin form found in certain chicken and mammalian cells that no longer divide or differentiate. They found that DNA (green in schematic at left) winds around each nucleosome (colored cylinders) twice and that three sets of four nucleosomes (blue, orange, purple) stack tightly together in the cryoEM structure (right). The structure could better explain how epigenetic marks such as methylation and acetylation modify chromatin structure and thus gene expression, Travers adds.—SARAH EVERTS

NIH ADAPTS GRANT RESUBMISSION RULE

RESEARCH FUNDING: Community concern that too much good science was being rejected fuels change

SEEKING SUCCESS
Falling grant success rates have in part prompted NIH to allow applicants to submit rejected grants a second time.



NOTE: Success rates are for grant applications NIH wide. **SOURCE:** NIH

THE NATIONAL INSTITUTES of Health will allow scientists whose research grants have been rejected to resubmit funding requests a second time, the agency announced earlier this month.

Applicants who have rewritten their research grants once (stage A1) and had them rejected will be able to submit essentially the same application a second time. But they will have to submit the application as though it is a new grant (A0), with no reference to suggestions from previous peer reviewers.

The move comes in response to an outpouring of concern from the scientific community that limiting grant submissions forces scientists—especially vulnerable early-career researchers—to abandon successful research pathways. The issue has become even more pronounced in recent years, as NIH grant success rates have dropped to record lows because of federal budget cuts.

"We wanted to be supportive of your concerns," NIH Deputy Director Sally Rockey explained in announcing the policy change. "We believe this is a very positive move for our applicants."

Until five years ago, grantees were allowed to submit essentially the same grant application multiple times. NIH changed that policy in 2009 in an attempt to lessen the burden on peer reviewers and to encourage reviewers to fund good grants the first time around.

"The policy that allowed only two strikes was very harmful to early-career investigators who were just learning their craft, and it was unfair to people who barely missed the payline," says Howard Garrison, public affairs director for the Federation of American Societies for Experimental Biology.

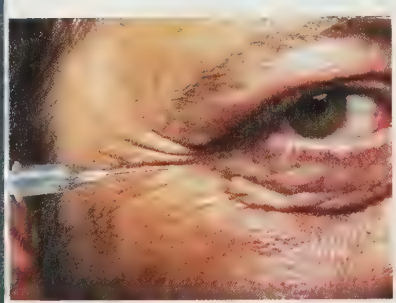
The result was that scientists were often rewriting grants to make work they thought was important look new, even if it wasn't. Now, "you don't need to artificially reinvent the science," says Seth M. Cohen, chair of the department of chemistry and biochemistry at the University of California, San Diego.

As a member of an NIH study section, which will likely receive an increase in applications, Cohen says, "It is probably a good policy change and a good compromise." But it could force NIH funding rates even lower because of an increased number of grants. "It could make what is a difficult situation even worse."—ANDREA WIDENER

HOSTILE BID FOR ALLERGAN

BUSINESS: Activist investor joins Valeant in seeking maker of Botox for $47 billion

Allergan expects sales of more than $2 billion in 2014 for Botox botulinum toxin.



SHUTTERSTOCK

VALEANT PHARMACEUTICALS has made a $47 billion cash-and-stock offer to buy specialty pharmaceuticals maker Allergan in a deal backed by activist investor William A. Ackman.

Adding Allergan's $6.3 billion in 2013 sales to Valeant would create a firm with revenues of $11.7 billion. Valeant would save some $2.7 billion by combining headquarters, eliminating duplicative operations, and cutting research spending.

Allergan, the maker of Botox wrinkle reducer, says it is examining Valeant's proposal. However, on April 22, the same day that Valeant made its hostile bid, Allergan also adopted a shareholder rights plan intended to make a deal more costly for a hostile acquirer and to provide Allergan's board more time to assess the Valeant offer.

The combined firms would be a leader in ophthalmology, dermatology, aesthetics, and dental markets, according to Valeant CEO J. Michael Pearson. Together, the two companies can achieve "significant synergies by applying Valeant's unique operating model to a combined set of assets," he says.

That model, applied in previous acquisitions, involves radical cost cutting and a sharp reduction in R&D. In Allergan's case, Valeant would eliminate early-stage research programs. On its own, Allergan plans to increase R&D spending from about $1 billion in 2013 to $1.5 billion by 2018. Valeant, in contrast, anticipates a $300 million R&D budget for the combined firm.

Ackman, who heads private equity firm Pershing Square Capital Management and has amassed just under 10% of Allergan's shares, says the proposed deal is "the most strategic and value-creating transaction I have ever analyzed." He has committed his shares to the takeover.

The activist investor has influenced others firms including Air Products & Chemicals, which in September decided to replace its CEO, John E. McGlade. But the Allergan bid marks the first time that Ackman has formed an alliance with an acquirer to target another firm.

In a note to clients, Marc Goodman, an analyst with investment banking firm UBS, says he doesn't believe Allergan's management has any interest in selling. But if Valeant succeeds in its bid, "it should be a wake-up call to the investment community that no company is untouchable."—MARC REISCH

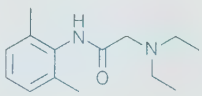
METHOD TRACKS CHEMICALS ON SKIN

DRUG DELIVERY: Mass spectrometry technique could help studies of transdermal compounds

A **MASS SPECTROMETRY** technique gaining popularity for medical applications such as imaging tumor surfaces can also be used to study the migration of small-molecule compounds applied to the skin (*J. Am. Chem. Soc.* 2014, DOI: 10.1021/ja5016351u).

Because skin is such a complex organ, the method could be a boon for researchers developing transdermal drugs.

Stanford University chemistry professors Richard N. Zare and Justin Du Bois, postdoc Livia S. Eberlin, graduate student John V. Mulcahy, and colleagues show that desorption electrospray ionization-mass spectrometry (DESI-MS) imaging has numerous advantages over other methods that require complicated preparation of skin samples.



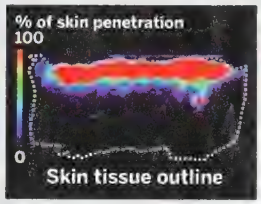
Lidocaine

What's more, DESI-MS imaging can be performed under ambient conditions, instead of in a vacuum environment, as other MS methods require. In addition, test compounds don't have to be radioactively labeled or tagged with cumbersome dye molecules that could affect the compounds' normal migration through skin.

"That's why this method is very appealing," says Mark R. Prausnitz, a chemical and biomolecular engineering professor who heads the Laboratory for Drug Delivery at Georgia Tech.

DESI-MS was developed a decade ago and involves spraying charged solvent droplets at a surface. Backsplash droplets containing dissolved molecules are then captured and analyzed using a mass spectrometer. The method has been used for medical applications such as imaging drugs in tissue samples.

The Stanford group selected a number of small molecules that alter sodium channels in skin cells, including lidocaine and a shellfish toxin. They applied them to the surface of skin samples and were able to track the compounds' migration to a depth of 1.2 mm.



J. AM. CHEM. SOC.

This DESI-MS image shows the percentage of penetration of lidocaine on a skin sample (red = 100%).

Such investigations of drug migration are needed to expand the limited repertoire of transdermal drugs, Prausnitz says. Only about 30 drugs, such as nicotine, have transdermal versions. The drugs must be small, lipophilic, and effective at a low dose.

With this newly adapted tool, however, scientists could more readily study methods to enhance skin permeation, Prausnitz says. "We're very interested in the pathway—which part of the skin did the drug go through?"—ELIZABETH WILSON

LEARNING NEXT DOOR TO INDUSTRY

SITE MAP: Thousands of schools are located within a mile of chemical plants

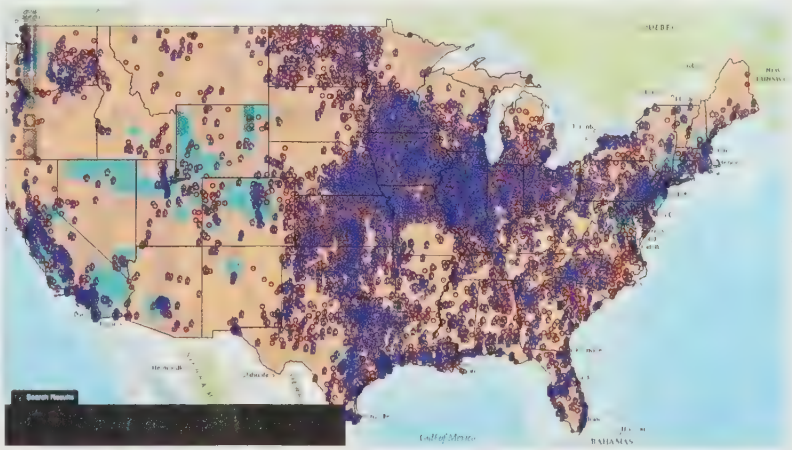
ONE IN 10 U.S. CHILDREN attends school in the shadow of a potentially dangerous chemical facility, according to a report issued by the advocacy group Center for Effective Government.

The analysis, displayed through an interactive map on the group's website, shows that 4.6 million children at nearly 10,000 schools across the U.S. attend class within a mile of a facility that produces, uses, or stores chemicals that can pose a risk to human health if they are spilled, released into the air, or involved in an explosion.

"The number of children who are potentially in harm's way is deeply troubling," says Katherine McFate, president of the center.

The center and other activist groups have called for stronger chemical information disclosure standards, more oversight by federal and state agencies, and better emergency response planning.

The chemical industry, however, says more regulation is not the answer. "We need better coordination at the state and local level, including access to key health and safety data by first responders," says Lawrence D. Sloan, CEO of the Society of Chemical Manufacturers & Affiliates, an industry trade association.—GLENN HESS


CENTER FOR EFFECTIVE GOVERNMENT

This map shows schools (blue markers) that are located within 1 mile of a high-risk chemical facility (red markers).

THERMO FISHER

TECH SAVVY A scientist at Thermo Fisher's Biomarkers Research Initiatives in Mass Spectrometry Center adjusts a Nanospray Flex ion source on the Orbitrap Fusion Tribrid MS.

TOP INSTRUMENT FIRMS

The big companies in **C&EN'S RANKING** continued to get bigger in 2013 as they sought dominant positions in the analytical and lab instruments market

ANN M. THAYER, C&EN HOUSTON

LEADING INSTRUMENTATION companies believe bigger is better. Through a mix of acquisitions and internal growth, the top analytical and laboratory instrument makers have been growing into billion-dollar behemoths. Industry consolidation is creating a top-heavy lineup of companies.

Size can present challenges to speed and agility. Major instrument suppliers are bullish, however, about their ability to perform, especially as the instrumentation market seems to be improving. Smaller companies, meanwhile, are trying to grow in the shadow of the heavyweights, maybe only to become acquisition targets.

Companies in C&EN's annual ranking of the top 25 instrumentation firms had 2013 instrument sales ranging between $162 million and $6.3 billion. For 2013, Danaher solidly held on to the top position it gained when it acquired Beckman Coulter in 2011 for $6.8 billion. Danaher's sales figure does include the Radiometer acute care business, which falls outside the traditional lab instrumentation arena.

The most notable change between this year's top 10 list and last year's, which was based on 2012 sales, is the absence of Life Technologies, previously number four. Thermo Fisher Scientific acquired the company in early 2014.

Although Life Technologies' sales were not included in Thermo Fisher's reported 2013 results, the company kept the number-two slot. And new to the top 10 this year is Roche Diagnostics, which moved up to sixth place after a corporate reorganization altered how it reports sales.

Even looking back five years, not much has changed in the composition of the top 10 firms, except their sizes. In that time, Danaher has grown through acquisitions, such as that of AB Sciex in 2010, and moved

Even looking back five years, not much has changed in the composition of the top 10 firms, except their sizes.

from ninth to first place. Although Thermo Fisher has stayed in second place, it has nearly doubled in size, with major purchases including Dionex and Phadia in 2011. Buying Varian in 2010 and Dako in 2012, Agilent Technologies has grown by 75% and remains third.

Combined sales of the top 10 firms grew 65% between 2008 and 2013, while sales of the top 25 grew about 40%. As a result, the top 10 accounted for 78% of the group's sales in 2013, compared with 66% in 2008. In 2013, the top four firms—Danaher, Thermo Fisher, Agilent, and Waters—together accounted for more than half of the market held by the top 25. In 2008, the top four had a 37% share.

Despite the growing concentration, the life sciences and diagnostic tools sector remains fragmented, especially compared with industries such as wireless and airlines, and could benefit from further consolidation, according to Isaac Ro, a Goldman Sachs stock analyst who covers the instrumentation industry. But acquisitions aren't the only path to growth.

"Unlike mature industries where consolidation was a vehicle used to restore pricing power and margins, tools offers ample innovation and an expanding addressable market to support continued pricing power," Ro told clients in a recent report.

For example, he calls Thermo Fisher "an underappreciated innovator." Although the company's R&D spending as a percentage of sales is toward the low end among its peers, Thermo Fisher has an R&D budget that is significantly larger than most. "Given the company's now-increased scale, we see continued opportunity for Thermo Fisher to out-invest competition on a dollar basis and drive organic growth via innovation in select markets," he said.

With a postmerger R&D budget exceeding $700 million per year, "clearly innovation will be important for us," says Dan Shine, president of chromatography and mass spectrometry at Thermo Fisher. The Life Technologies merger "really does align perfectly with our growth strategy," he argues. "It adds capabilities we didn't have before, especially in the genomics and next-generation sequencing areas."

Life Technologies is the bulk of Thermo Fisher's new Life Sciences Solutions unit, which today accounts for about 26% of the firm's sales. Its other segments are analytical instruments, 18% of sales; specialty diagnostics, 19%; and lab products and services, 37%. Notably, the acquisition expanded Thermo Fisher's consumables and services side to the point that today nearly 75% of its revenues are derived from these recurring revenue streams, Shine adds.

THE RIGHT BALANCE between equipment and consumables sales can help a company weather slow periods such as the one the industry endured in 2013. The market grew just 2.0%, lower than the 3.6% initially forecast, according to the Los Angeles-based market research firm Strategic Directions International (SDI). Overall, the market was worth about $46 billion.

"Widespread economic malaise and disruptive budgeting" contributed to uncertainty around equipment purchases, SDI notes.

The pharmaceutical and biotech sector is the largest end market. Worth about $11 billion, it has been growing 4–6% per year, according to Agilent's annual assessment of the instrumentation market. Big pharma R&D budgets have been constrained in recent years, suppliers say, but smaller biotech and contract research firms have picked up some of the slack.

Academic and government research is the second-largest market, at about $10 billion, and is growing 3–5% annually, Agilent reports. In recent years, purchases by academic researchers in the U.S. and Europe have been crimped by government funding caps. But signs of improvement began appearing in late 2013 with the end of sequestration in the U.S., a rising National Institutes of Health budget, and greater government-funded R&D in Europe.

More challenging are the industrial and applied markets, which include chemicals and energy. Even so, a few positive areas stand out. Instruments for assessing food safety make up a $4 billion market that is growing 5–7% annually. And environmental testing, at about $5 billion, is growing up to 4% per year. Food safety, environmental testing, and health care are particularly strong outlets in developing countries.

The Japanese economy also slowly recovered in 2013, driven by government stimulus programs. Not only were sales stronger within the country, but depreciation of the yen helped Japanese firms sell overseas. Japanese companies such as Shimadzu, Nikon, Olympus, and

TOP 25 INSTRUMENTATION FIRMS

Industry leaders largely kept their relative places in C&EN's ranking

RANK 2013	RANK 2012	COMPANY	INSTRUMENT SALES 2013 ($ MILLIONS)	% CHANGE FROM 2012	INSTRUMENT SALES AS % OF TOTAL SALES	HEADQUARTERS COUNTRY
1	1	Danaher	$6,279	4.6%	32.8%	U.S.
2	2	Thermo Fisher Scientific	4,125	2.7	31.5	U.S.
3	3	Agilent Technologies[a]	3,894	9.9	57.4	U.S.
4	5	Waters	1,904	3.3	100.0	U.S.
5	6	Shimadzu	1,754	10.0	58.7	Japan
6	11	Roche Diagnostics[b]	1,733	-0.9	15.4	Switzerland
7	7	Bruker	1,710	2.6	93.0	U.S.
8	8	PerkinElmer	1,625	13.0	75.0	U.S.
9	9	Mettler-Toledo	1,094	1.6	46.0	Switzerland
10	10	Carl Zeiss[c]	835	-3.2	15.0	Germany
11	13	Bio-Rad Laboratories	725	3.0	34.0	U.S.
12	12	Hitachi High Technologies[d]	680	4.6	11.4	Japan
13	15	Eppendorf	668	-3.3	100.0	Germany
14	17	Nikon[d]	635	14.8	6.1	Japan
15	16	JEOL[e]	578	4.8	70.9	Japan
16	18	Merck Millipore[b]	576	-4.6	16.4	Germany
17	19	Spectris	570	4.0	30.2	England
18	14	FEI	500	9.2	53.9	U.S.
19	20	Olympus[d]	449	10.9	6.1	Japan
20	21	Illumina	372	20.0	26.2	U.S.
21	22	Xylem Analytics[b]	295	1.4	100.0	U.S.
22	23	Tecan	275	-5.2	66.0	Switzerland
23	—	Sartorius	238	-0.6	20.2	Germany
24	24	Horiba	235	12.3	16.6	Japan
25	25	Qiagen	162	-4.1	12.4	Netherlands

NOTE: Results are for the calendar year unless otherwise stated. Some figures were converted at relevant average exchange rates for 2013. **a** Fiscal year ended on Oct. 31, 2013. **b** Results for instrumentation sales in this division alone. **c** Fiscal year ended on Sept. 30, 2013. **d** Company estimates for fiscal year that ended on March 31, 2014. **e** Fiscal year ended on March 31, 2013.

Horiba posted healthy sales gains in 2013.

Overall, Goldman's Ro pointed out, "the global macroeconomic outlook supports positive end-market trends." Goldman's economists expect the world's economy to improve in 2014 versus 2013, led by the U.S. and Europe.

Although 2013 didn't live up to expectations, Mike McMullen, president of Agilent's chemical analysis group, remains bullish on the long-term outlook for the major instrumentation segments. "All these markets are being driven by key global macroeconomic trends," he explains, including human health, quality of life, resource scarcity, and emerging-market growth.

"You will see some level of ups and downs, quarter to quarter," McMullen says. "But I think it would be hard to argue against these macro trends as drivers for what will continue to be very attractive markets to be in."

R&D SPENDING Instrument makers reinvested in 2013 to grow their businesses.

Company	R&D spending: As % of sales	R&D spending: $ Millions
Thermo Fisher Scientific[a]	5.6	736
Danaher[b]	7.6	476
Agilent Technologies[c]	8.0	310
Illumina	19.5	277
Bruker	10.4	191
Spectris	7.4	147
PerkinElmer	5.5	133
Mettler-Toledo	4.2	113
FEI	11.0	102
Waters	5.3	101
Tecan	11.7	51
Eppendorf	5.6	38
JEOL[d]	5.7	34

a Includes Life Technologies. **b** For life sciences and diagnostics business. **c** Excludes electronic measurement business. **d** For scientific and measurement instruments business. **SOURCE:** Company data

TO SHARPEN ITS FOCUS, Agilent decided last fall to split into two companies by November 2014. Its life sciences, diagnostics, and applied markets (LDA) businesses will keep the Agilent name, while its electronic measurement group (EMG) will become Keysight Technologies. The split makes sense, McMullen explains, because EMG is a highly cyclical, equipment-related business, whereas LDA, which also includes consumables, software, and services, is less cyclical and more growth-oriented.

"Over the last several years, capitalizing on the strength of our EMG business as a funding source, we have been able to grow a very sizable and credible LDA business," McMullen says. In 2006, LDA had sales of $1.4 billion. Through a combination of acquisitions and organic growth, sales are almost $4 billion today. LDA "has the scale and scope to compete with anybody in a consolidating marketplace," he adds.

The top four companies now account for half of the sales of the top 25.

When it comes to growth, Agilent is banking on its diagnostics business, which accounts for less than 20% of its total sales today. Agilent predicts the $7 billion clinical and diagnostics market to grow 8–10% per year. "Fully integrating the Dako diagnostic business into Agilent was a key milestone for us in 2013," McMullen says. "Not only does it open up very attractive end markets, but our genomics technology could be applied directly in diagnostics."

Indeed, Goldman's Ro believes that a lucrative opportunity in the clinical market is unfolding. Diagnostics, particularly those targeting oncology and neonatal screening, will be a significant driver for the adoption of next-generation gene sequencing beyond academic and government research markets. Longer term, consumer genomics could be an even larger market.

Sales of the top 10 companies expanded from **66%** of the market in 2008 to **78%** in 2013.

Ro considers Illumina, number 20 in C&EN's ranking, to be "uniquely suited to benefit from and drive the uptake of next-generation sequencing in the clinical and diagnostic fields." As a result, he believes Illumina will likely remain the "unchallenged leader in the next-generation sequencing market for the next few years."

Illumina has a long-standing strategy of focusing on technology development, explains Kirk Malloy, general manager of the company's life sciences business. At nearly 20%, Illumina's R&D spending as a percentage of company sales outranked all major instrument suppliers.

The firm's instrument development programs can take up to two years. "We're constantly planning out several years into the future and trying to anticipate what the

THEN AND NOW

Sales ballooned for several of the top instrument firms over the past five years

	2008		2013	
RANK	COMPANY	INSTRUMENT SALES ($ MILLIONS)	COMPANY	INSTRUMENT SALES ($ MILLIONS)
1	Life Technologies	$2,317	Danaher	$6,279
2	Thermo Fisher Scientific	2,200	Thermo Fisher Scientific	4,125
3	Agilent Technologies	2,195	Agilent Technologies	3,894
4	Shimadzu	1,667	Waters	1,904
5	Waters	1,575	Shimadzu	1,754
6	Roche Diagnostics	1,206	Roche Diagnostics	1,733
7	PerkinElmer	1,185	Bruker	1,710
8	Bruker	1,074	PerkinElmer	1,625
9	Danaher	875	Mettler-Toledo	1,094
10	Mettler-Toledo	868	Carl Zeiss	835

SOURCE: Company data

market is going to need," Malloy says.

At the same time, Illumina has been making an effort to branch out beyond its core customer base of the life sciences community, including academia and government labs. Revenues had been coming primarily from government-supported research, and "that's not the diversified mix of customers we want," Malloy says. Today, about half of the company's instrument sales, which grew 20% in 2013, come from consumer, agriculture, applied, and clinical customers.

To help it access these markets, Illumina made a few recent acquisitions. In late 2012, it bought sequencing technology firm Moleculo. In early 2013, the company purchased clinical diagnostics provider Verinata Health. Midyear, Illumina purchased Advanced Liquid Logic, and this year it anticipates launching a sample preparation instrument based on the digital microfluidics technology it gained. Late in 2013, Illumnia also acquired clinical and genomic informatics firm NextBio.

From 2008 to 2013, sales of the top five companies grew **80%,** while sales of the top 25 grew **40%.**

ILLUMINA GENERALLY acquires new technologies and extends them into markets it knows, Malloy explains. But some customers, such as the cancer genomics company Foundation Medicine, are creating completely new businesses around its technology.

"One of the bigger drivers of our business is the creation of small start-ups that are using the technology in a variety of ways that on our own we probably wouldn't be able to address," he says. This year, Illumina created a business accelerator program to help early-stage companies rapidly bring gene-sequencing applications to market.

In January, Illumina launched two instruments that are selling faster than expected. Its HiSeq X Ten, a $10 million system composed of 10 ultra-high-throughput sequencers, can sequence a human genome for about $1,000. The new NextSeq 500, meanwhile, addresses users wanting a less powerful system but more capability than Illumina's workhorse desktop instruments. The company expects about 16% growth for its entire instrument and consumables business in 2014.

Illumina's growth hasn't gone unnoticed. Roche launched a hostile takeover attempt in 2012. It pursued Illumina for months, eventually raising its bid to $6.8 billion, but gave up when Illumina rejected that offer. The following year, Roche dissolved its applied science unit, cut about 170 jobs, and canceled two sequencing technology development programs.

Along with Illumina, other small players participated in industry consolidation in 2013. Malvern Instruments bought NanoSight, an England-based maker of nanoparticle characterization instruments, for $24 million. The Dutch firm Qiagen acquired Ingenuity Systems, a genomics data analysis software firm, for $105 million and the bioinformatics company CLC Bio for

an undisclosed amount. Just recently, FEI acquired Lithicon, based in Norway and Australia, for $68 million.

Although 2013 didn't bring any acquisitions for Xylem Analytics, the business is the product of more than a dozen of them over the past decade. As part of the water technology company Xylem, the analytics business, which is number 21 in C&EN's ranking, sells field, lab, portable, and online instruments for water, environmental, food, and life sciences applications.

"OUR STRATEGY is to continue to grow organically as well as through acquisition," says Ron Geis, vice president of Xylem Analytics Americas. Although the market environment was challenging in 2013, the group did launch several new products and is anticipating growth in 2014. "We are seeing a definite uptick," Geis says about customer interest.

Small instrumentation businesses such as Xylem Analytics try to compete with large suppliers through tried-and-true strategies for technology development, customer service, and niche applications (see page 20).

"It would be hard to argue against these macro trends as drivers for what will continue to be very attractive markets."

The industry giant Thermo Fisher, in contrast, may still need to persuade the marketplace that its acquisition of Life Technologies makes sense, according to Goldman's Ro. "Some competitors are not convinced the 'supermarket' approach of Thermo Fisher's combined offerings will have a material impact on high-end equipment sales," he wrote.

Other companies, Ro said, are focusing on strengthening leadership positions where Thermo Fisher still has less dominant franchises, such as high-performance liquid chromatography and applied markets.

Executives at small firms also believe they can compete because instrumentation users tend to show strong brand loyalty. "When we acquire companies, we want to maintain the customer relationships and provide the same level of technical support," Xylem's Geis says, suggesting that these aspects may get lost when a large company absorbs a smaller one.

At the same time, an acquired business can benefit from access to greater resources within Xylem. "We not only maintain the legacy brand, but can actually grow it through our internal capabilities and know-how," he adds.

For their part, large companies maintain that their mergers benefit the customer as well. Agilent's McMullen, for example, points to ease of service and better software connectivity across various instruments.

"There are multiple technologies used in laboratories," he says, "and consolidation allows the customers to work with fewer vendors who are in much stronger positions to provide a broader suite of technologies to meet their application needs." ■

FYI

materials SCENE

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ETHANE EXPORT CENTER SET FOR GULF COAST

Gas processing firm Enterprise Products is planning what it claims will be the world's largest ethane export facility. When it opens in 2016 on the Texas Gulf Coast, the plant will have the capacity to export 240,000 barrels per day of ethane, enough to support nearly 4 million metric tons of annual ethylene production. A world-scale ethylene cracker has about 1.5 million metric tons of capacity. European companies including Ineos and Versalis want to import cheap ethane from the U.S. to feed their crackers. Enterprise says U.S. ethane capacity exceeds demand by 300,000 bbl per day. And even though chemical firms plan to build 11 new U.S. ethylene crackers, the glut will expand, Enterprise projects, to 700,000 bbl per day by 2020.—AHT

START-UP FIRM CLAIMS CATALYST BREAKTHROUGH

Catalytic Technologies Ltd. says its titanium-based catalysts are being tested commercially in Asia as a replacement for antimony oxide catalysts now used to make polyethylene terephthalate (PET). In addition to eliminating a heavy metal, the catalyst can yield high-quality PET for bottles with less plastic, high thermal stability, and improved clarity, the British firm says. Its target is to capture 50% of the PET catalyst market within five years.—MM

CATALYTIC TECHNOLOGIES

PET bottles made using Catalytic Technologies' new catalyst.

PLASTICS RECYCLING FOR THE DUTCH

The new company Quality Circular Polymers plans to build a $100 million plant for recycling postconsumer waste plastic at the Chemelot industrial park in Sittard-Geleen, the Netherlands. The plant is set to be built in three phases with a total capacity for 100,000 metric tons per year of recycled polyethylene and polypropylene. The first phase is scheduled to be commissioned by the end of 2015. The firm's founders are former executives of the chemical makers DSM and SABIC Europe.—AS

CELLULOSIC ETHANOL SLAMMED

After accounting for the reduction of organic carbon in the soil due to the removal of corn residues normally left in the field, cellulosic ethanol fuels can emit 7% more carbon dioxide into the atmosphere than can gasoline, according to a study published in *Nature Climate Change* (2014, DOI: 10.1038/nclimate2187). A team of University of Nebraska researchers led by assistant professor Adam Liska simulated the effects of making the fuels from residues on 128 million acres. The researchers found that removing the residues would release 50 to 70 g of CO_2 per megajoule of energy contained in the biofuels produced. Total emissions generated from producing biofuels, the report says, amounts to 100 g of CO_2 per MJ, which is higher than federal emissions reduction requirements for biofuels and even tops the levels from gasoline. The Renewable Fuels Association, a trade group, attacked the study's methodology. The assumption that farmers would remove 60–75% of residues is out of line with the 40–50% generally regarded as the sustainable limit, RFA says. "At a fundamental level, the farmer's livelihood depends on sustaining or improving soil health," RFA says. "Growers strive to ensure their most valuable asset (soil) is properly protected and managed."—AHT

CHEMICAL MAKER CABB CHANGES HANDS AGAIN

European private equity firm Permira has agreed to buy CABB International, a German maker of specialty and custom-synthesized chemicals. The company is a leading supplier of monochloroacetic acid, which it produces in Germany, India, and, soon, China. Spun off from Clariant in 2005, CABB has for the past three years been owned by Bridgepoint Capital, another private equity firm. From 2007 to 2011, it was owned by AXA Private Equity, now known as Ardian.—JFT

SHIN-ETSU TO MAKE MAGNETS IN VIETNAM

Shin-Etsu Chemical will spend $117 million to build a rare-earth magnet plant in Hai Phong province in northern Vietnam, where it opened a rare-earth refining facility last year. With annual capacity of 2,000 metric tons, the magnet plant will be built in two phases, opening in 2016 and 2017. Shin-Etsu says the new Vietnamese facilities will help it meet market growth while improving its customers' security of supply. The firm currently produces the magnets only in Japan. Rare-earth magnets are used in applications including hybrid cars, energy-saving air conditioners, and hard-disc drives.—JFT

ASHLAND'S O'BRIEN TO RETIRE THIS YEAR

ASHLAND

O'Brien

James J. O'Brien, who has led Ashland since 2002, plans to retire at the end of the year. The company has launched a search for his replacement. O'Brien, 59, transformed Ashland from a small conglomerate of oil refining, chemical distribution, water treatment, and construction materials businesses into a sizable specialty chemical company.—AHT

NOVOZYMES SLATES MICROBE R&D CENTER

Novozymes will build a $36 million research center in Cary, N.C., to study microorganisms that improve crop yield, soil fertility, and pest control. About 100 researchers will work at the new facility when it is completed in three years. Some of the research conducted at the site will advance an alliance Novozymes announced in December with

Monsanto. That deal calls for the two firms to join forces in developing microbial technology to increase crop productivity.—MSR

SEC CHARGES THREE WITH INSIDER TRADING

The Securities & Exchange Commission has charged a former executive of biotech firm Genta and two Genta stock owners with insider trading. According to a complaint filed in U.S. District Court for the District of New Jersey, Genta President Loretta M. Itri tipped off a friend about poor Phase III clinical trial results for Genasense, a melanoma treatment, a day before publicly releasing the results in 2009. The friend and an acquaintance sold their Genta shares for a gain of $139,000. Itri agreed to pay a $64,000 fine and will be barred from serving as an officer of a public firm for five years. The two others agreed to pay fines and return gains totaling $262,000. Genta filed for bankruptcy in 2012.—MSR

CELGENE PAYS BIG FOR ANTISENSE DRUG

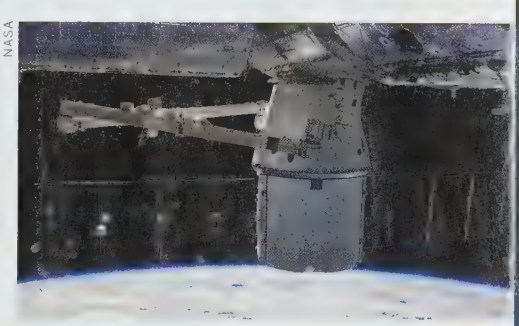
Celgene has agreed to pay $710 million to Ireland's Nogra Pharma to license GED-0301, an oral antisense DNA oligonucleotide being developed for the treatment of Crohn's disease. The drug works by shutting down messenger RNA that encodes for a protein, Smad7, involved in inflammation. On the basis of the results of a Phase II clinical trial, Celgene plans to initiate a Phase III program by the end of the year. If the drug is approved and successful, milestone payments to Nogra could reach $1.8 billion.—MM

AMRI WILL CLOSE SYRACUSE FACILITY

In an effort to consolidate resources and reduce costs, Albany Molecular Research Inc. plans to close its Syracuse, N.Y., drug discovery and development services facility by the end of June. Services in Syracuse include chemical process R&D, custom synthesis, and scale-up of pharmaceutical intermediates and final drug products. Activities will be transferred to company facilities in Albany, N.Y.; Grafton, Wis.; Holywell, Wales; and Hyderabad, India. The site currently employs about 45 people, some of whom will relocate.—RM

MERCK EXPERIMENT REACHES SPACE STATION

The SpaceX-3 Dragon space capsule reached the International Space Station last week carrying an experiment for Merck Research Laboratories. Merck is seeking to crystallize a human monoclonal antibody to help determine its physical structure.



NASA

The SpaceX-3 Dragon shown docked last week to the International Space Station.

Protein crystals grown in zero gravity can achieve larger sizes and more nearly perfect structures than those grown under the influence of Earth's gravity, NASA says.—MM

ABBVIE DRUG FILING IS ENANTA WINDFALL

Enanta Pharmaceuticals received a $20 million payment from AbbVie after AbbVie filed for FDA approval for an all-oral regimen that treats the hepatitis C virus. The drug includes the NS5A inhibitor ABT-267, the nonnucleoside polymerase inhibitor ABT-333, and the boosted protease inhibitor ABT-450/ritonavir, which was developed in collaboration with Enanta. The Watertown, Mass.-based biotech firm stands to receive another $20 million in May, when AbbVie expects to file for approval in Europe.—LJ

BUSINESS ROUNDUP

BASF will invest up to $8 million this year to enhance its facilities in Mortara, Italy, for making photoinitiators, materials used to speed up the drying of coatings and inks in the presence of ultraviolet light. The photoinitiator plant in Mortara is one of the largest in the world, BASF says.

FONTAROME Chemical has been acquired in a bankruptcy-court sale by the investment group SFM Investments. Milwaukee-based Fontarome, a maker of active ingredients for pharmaceuticals, flavors, and fragrances, entered receivership in January.

MEREDIAN, a privately held biopolymer maker, says it has successfully piloted production of polyhydroxyalkanoate in collaboration with the fermentation specialist Tate & Lyle. The firm says the pilot campaign "opens the door for mass production of completely biodegradable plastics on a commercial scale."

PETER GREVEN, an oleochemical producer based in Germany, is expanding its metallic stearates and oleates capacity with a new plant in Venlo, the Netherlands. The new facility will meet growing demand for the products across the drug, food, feed, and cosmetics industries, the firm says.

VERSALIS, the chemicals arm of Italian energy firm Eni, plans to increase capacity for ethylene-propylene rubber at its site in Ferrara, Italy. The expansion, which will raise capacity to 130,000 metric tons per year, is set to be completed in the second half of 2016.

CEM, a microwave laboratory instrument maker, has licensed a line of resins that can be used to synthesize high-purity peptides from Cheshire, England-based SpheriTech. CEM plans to manufacture the SpheriTide resins at its Matthews, N.C., headquarters.

AASTROM Biosciences, an Ann Arbor, Mich.-based specialist in multicellular therapies for cardiovascular disease, has agreed to acquire Sanofi's cell therapy and regenerative medicine business for $6.5 million. Aastrom will get rights to three products as well as production centers in the U.S. and Denmark.

EPIZYME has gained a $4 million milestone payment from GlaxoSmithKline, which has chosen a lead candidate against a histone methyltransferase (HMT) target. In 2011, GSK paid $20 million up front to work with Epizyme on small molecules that block HMT, a class of epigenetic enzymes implicated in cancer. The candidate is the third to emerge from the collaboration.

SAMSUNG BIOLOGICS will manufacture several biologic drugs for Bristol-Myers Squibb under an expanded agreement between the two firms. They joined in July 2013 to manufacture a single antibody in development to treat cancer.

SYNTHESIS ENERGY SYSTEMS

OPPORTUNITIES Foreign firms are offering clean technologies to China's coal-to-chemicals sector. Shown here is a gasification unit in Yima, China, part-owned by U.S.-based Synthesis Energy Systems.

CHINA'S FEEDSTOCK REVOLUTION

Dependent on imports for oil and gas, China is developing **COAL AS A RAW MATERIAL** for a range of chemicals

JEAN-FRANÇOIS TREMBLAY, C&EN HONG KONG

SINOPEC ENGINEERING, a subsidiary of China's state-owned oil conglomerate Sinopec, signed a $3 billion contract last December to build what it bills as the world's largest complex using coal to produce chemicals and plastics. Scheduled to open in late 2015 in Inner Mongolia, China, the project will implement several unique technologies developed in the country.

China has become the world leader in the use of coal to produce chemicals and liquid fuels. While the U.S. chemical industry experiences a rebirth with the help of natural gas extracted from shale, China is building large-scale facilities based on coal, which it has in abundance.

Although unconventional, the coal-based technologies appear to be competitive with traditional routes to petrochemicals. And the Chinese government supports them as a means of reducing the country's dependence on imported oil and gas. But coal is an environmentally challenging raw material for chemicals, just as it is for electric power, and China faces calls to dial back its use.

China already uses coal on a large scale to produce several important industrial chemicals, but it is now expanding into materials that aren't traditionally made from coal. The country is heavily investing in projects that gasify coal into methanol and then on to ethylene and propylene, two olefins that are usually made from oil or gas. China is also commercially implementing an indigenous process to produce ethylene glycol from coal.

According to the consulting firm IHS Chemical, more than 50 coal-based chemical projects are being considered across China. The company forecasts that the share of olefins produced from coal or methanol in the country will rise from essentially zero in 2009 to 30% by 2017. Coal-based ethylene glycol will capture close to 40% of the Chinese ethylene glycol market, IHS expects.

At least 10 coal-to-olefin complexes are now under construction in China, according to Yansheng Li, a senior engineer who is assistant to the president of Wison Engineering, a Shanghai-based engineering firm.

Wison has tied its fate to China's coal conversion industry. One of the largest oil and chemical engineering contractors in China, the company has in recent years derived most of its sales from the coal chemicals sector, Li says. So far, Wison has built five methanol-to-olefins facilities in China.

Working on its own or in collaboration with others, Wison has developed several processes related to coal chemicals, including some for reducing water and energy consumption during the production of methanol, Li claims. Last November, it opened a demonstration coal gasification plant in Nanjing that implements a pilot Shell technology.

Shell is one of several foreign firms seeking to sell coal conversion technology in China. General Electric is another. Last November, Jiutai Group selected GE's gasification technology to expand its output of methanol as a raw material for dimethyl ether, a cooking and heating fuel. Using GE's technology will reduce operational costs while producing methanol in a more environmentally friendly manner, Jiutai said.

COAL HAS BEEN PART of the global chemical industry since its earliest days. Calcium carbide, for instance, is made by reacting lime with coke, a coal derivative. Acetylene derived from calcium carbide yields a range of materials including vinyl chloride and butanediol. Although the rest of the world has largely switched to petrochemical-based vinyls, to this day a major portion of China's polyvinyl chloride is made from acetylene, particularly in the Chinese hinterland where coal mines are located.

Food supply security has been a historic driver of the use of coal by China's chemical industry, says David S. Jiang, president of Sinodata Consulting, a Beijing-based chemical market research firm that is an alliance partner of IHS Chemical. Coal can be gasified into synthesis gas, a mixture of carbon monoxide and hydrogen that is the starting material for producing ammonia. Ammonia, in turn, is converted into urea, the main source of nitrogen fertilizer for China's agricultural sector.

"When you're talking about urea use in China, you're talking about 70 million tons per year," Jiang says. "The government supports coal-based production of urea because it doesn't want to have the country depending on imports in a large proportion."

Synthesis gas is also the key starting material for methanol. Methanol has long been used to produce single-carbon chemicals such as formaldehyde and acetic acid, but Chinese firms have started using it to make two- and three-carbon chemicals via methanol-to-olefins technology. Sinopec, for example, says its Inner Mongolia project will use an in-house-developed silicoaluminophosphate catalyst that con-

verts methanol into ethylene and propylene with improved carbon selectivity.

MANY OF CHINA'S current methanol facilities are economically uncompetitive. Average operating rate of the industry is below 50%, according to Sinodata, because first-generation fixed-bed coal gasification plants are small and work only with lump anthracite, a premium grade of coal. The newest coal gasification technologies have much more flexibility in the type of coal they use, he notes. "If your plant is based on these gasifiers, you are more competitive," Jiang says.

Synthesis Energy Systems (SES) wants to help China make its coal-based methanol production both economically competitive and environmentally friendly. The U.S. firm is offering a coal gasification process licensed from the Gas Technology Institute, based in Des Plaines, Ill. The process can use any grade of coal as feedstock. It consumes little water and has low emissions, the firm says.

"China has huge reserves of low-quality coal," says Robert W. Rigdon, chief executive officer of SES. "We allow coal converters to operate in a cleaner manner."

Rigdon, a former GE executive who spends about half of his time in China, says the country offers vast opportunities for SES. The company already operates two methanol plants in the country through joint ventures, and earlier this month it formed a venture with Zhangjiagang Chemical Machinery, a Chinese manufacturer of pressure vessels for the coal and chemical sectors. The partnership is intended to help SES reach potential customers throughout the country.

Foreign companies active in China's coal conversion sector all stress the environmental attributes of their technologies, no doubt aware that China's increasing use of coal to make fuels and chemicals is controversial.

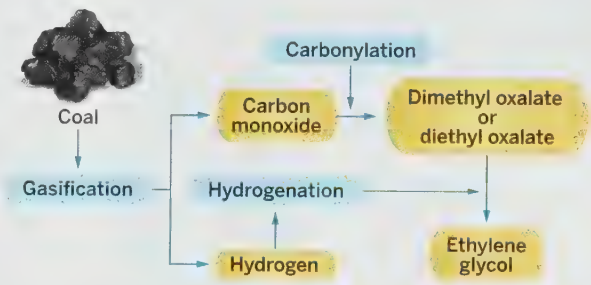
Last July, the environmental group Greenpeace issued a field report showing how a coal-to-liquid fuels project implemented by Shenhua Group in Ordos, Inner Mongolia, was creating pollution and contributing to desertification by consuming large quantities of water. State-owned Shenhua is China's largest coal producer. In an update last month, Greenpeace reported that Shenhua had pledged to process its wastewater and reduce its water usage.

Carbon dioxide emissions are another issue that could threaten the growth of the coal conversion sector, according to Sinodata's Jiang. Producing energy from coal generates twice as much carbon dioxide as producing it from natural gas, according to the U.S. Environmental Protection Agency, and a similar problem clouds coal-based chemical production.

"Some investors are so concerned about carbon emissions that they don't want to put money in that sector," Jiang says. It's even possible that, in response to international pressure, the Chinese government would impose a tax on carbon dioxide generation, although Jiang considers the risk small. "I don't think they can suddenly charge a high tax, because it could force some very capital-intensive plants to shut down," he says.

Ultimately, China's desire to reduce its reliance on imported oil and gas means coal-based chemicals will endure, provided that the environmental impact can be mitigated. In fact, China is implementing new regulations mandating that coal-to-chemicals plants be both larger in scale and environmentally less harmful, SES's Rigdon reports. "Demand for these chemicals will grow," he says. "We don't see China backing off." ■

ALTERNATIVE APPROACH China is pioneering the use of coal to produce ethylene glycol, a polyester raw material.



ADAPTED FROM SINODATA

AN INSTRUMENTALLY BETTER MARKET

Positive expectations outweighed competition concerns at **ANALYTICA,** Europe's largest lab instrumentation expo

ALEX SCOTT, C&EN LONDON

LAB INSTRUMENTATION executives exhibiting at Analytica, a huge trade show held earlier this month in Munich, had a spring in their steps. The exhibition halls were busy and the technical sessions well attended, despite the sunshine outside. Most said demand for their products is on the rise. Even with a strike at the German airline Lufthansa, 34,400 visitors made it to the show, a 13% rise over the last Analytica, held in 2012.

The largest instrument makers in attendance exhibited an avalanche of new products for analyzing faster and better everything from foods to polymers. Notably present were new instruments for studying nanomaterials and "omics" fields such as proteomics and genomics. But not everyone at Analytica was smiling: A couple of small firms voiced concerns that, after a spate of acquisitions, the biggest players are now so large that independent companies could be squeezed out of the market (see page 10).

The 2014 forecast for the European lab instrumentation market as a whole is "very good," said Mathis Kuchejda, chairman of Germany's Technical Society for Analysis, Biotechnology & Laboratory Technology. It's a stark contrast to the conditions of two years ago, when European sales for many instrument companies were flat. "We expect the market to pick up because of pent-up demand," Kuchejda told journalists at Analytica.

The improved forecast was reflected in the number of firms exhibiting at the event: 1,142, up 11.3% compared with the 2012 show. The big instrument makers Agilent Technologies and PerkinElmer—which have chosen not to exhibit in recent years at the Pittsburgh Conference on Analytical Chemistry & Applied Spectroscopy, or Pittcon, in the U.S.—made sure they were high-profile exhibitors at Analytica.

"For the past six months, the European Union market has been quite good," said Bruker's chief executive officer, Frank H. Laukien. "It's not boom time, but it is getting better." After a flat period, sales have been particularly strong in the U.K. Still, although major economies in Europe, such as France, continue to be steady spenders on instruments, "demand is rather better in the U.S. and Asia," Laukien said.

Bruker unveiled six new machines at the show. They included a compact spectrometer for atmospheric measurements and a unique large-format micro-X-ray fluorescence spectrometer that could be used for applications such as art conservation.

FLOORED Some small instrumentation firms are concerned that they are being outmuscled by a few dominant players in the sector.

Laukien's comments about the European market were echoed by a string of lab instrument makers at Analytica. Danilo Cazzola, vice president and general manager for Europe and parts of Asia at Agilent, also said Europe's demand for lab instrumentation is picking up. He speculated that it's partly a result of pent-up demand after constrained spending in recent years.

Jon DiVincenzo, president of PerkinElmer's environmental health business, said he is "looking forward to strong EU and global demand." At Analytica, PerkinElmer rolled out several novel products, including the NexION 350 ICP-MS, its newest atomic spectroscopy product. The machine accurately characterizes nanoparticles with a data acquisition rate 10 times that of any other inductively coupled plasma mass spectrometer on the market, according to DiVincenzo. "Nanotechnology analysis is a very large opportunity for us," he said.

Thermo Fisher Scientific executives at Analytica were bullish about the firm's ability to develop the lab technology that scientists really need. The firm spends $700 million annually on R&D. "That's 40% more than any of our competition," said Kornelia Weidemann, head of the firm's operations in Germany.

A GOOD SLICE of the spending is being funneled into the development of machines for proteomics and other "omics" activities. "There are probably hundreds of Thermo Fisher employees involved in developing instruments for this kind of chemistry," said Dan Shine, president of chromatography and mass spectrometry.

The firm is keen to provide scientists with bespoke solutions from its raft of products. "We can put it together like a Lego kit," said Klaus Lindpaintner, Thermo Fisher's chief scientific officer. Another key area for the firm "is the whole 'big data' challenge," Lindpaintner said. "Informatics will become an increasing thrust for the company."

Thermo Fisher released new software for liquid and ion chromatography control as well as for gas chromatography coupled to mass spectrometry. Specialist instrumentation software developers, including U.S.-based ACD/Labs, also were present at Analytica, offering products designed

"It's not boom time, but it is getting better."

to store and manage the increasingly large data sets that scientists generate.

Waters Corp. likewise is responding to the explosion of data coming out of modern research labs. The big U.S. firm brought new machines and software to Analytica including instruments for "omics" research such as its Acquity UPLC M-Class System, which it introduced commercially in January.

Waters' flagship application in this field is in association with the U.K.'s National Phenome Centre (NPC) at Imperial College London, where it provides a series of ultraperformance liquid chromatography-MS instruments. Ballooning data generation is an issue for NPC. The center handles 365,000 MS assays per year as well as 100,000 NMR samples and may generate about 1.6 quadrillion bytes of data over five years, equivalent to the memory held in about 256,000 Apple iPads.

Less happy about the advances trumpeted by major lab instrument makers was Jaroslav Klima, CEO of Tescan Orsay, a Czech instrument company with annual sales of about $55 million, mostly in the area of charged-particle optics. In a briefing to journalists at Analytica, Klima berated regulatory agencies, including the European Commission, for allowing the biggest instrument makers to keep merging, outmuscling smaller competitors in the process.

"We expect the lab instrumentation market to be controlled by several multinational groups," he warned, claiming that the "most aggressive" are U.S. companies such as Thermo Fisher and Agilent. If smaller firms are to survive, they need to partner up, Klima said.

AS IF TO PROVE Klima's point, at Analytica, Tescan Orsay and Germany-based WITec unveiled a jointly developed Raman imaging and scanning electron microscope. The firms say it is the first microscope to provide both ultrastructural and chemical images of nanostructures.

To compete against the major firms, Spain's Polymer Char, which has fewer than 30 employees, has chosen to specialize in the narrow field of instruments for analyzing polypropylene. The firm's latest product is Crystex QC, a machine that can measure the soluble fraction in polypropylene in just two hours, compared with the six hours it takes using standard methods, according to Aleyda G. Monzón, the company's marketing and communications manager.

Polymer Char's response to the rise of the mega instrumentation firms is to be innovative and provide high-quality service, Monzón said. "In many cases it is also true that being bigger takes away flexibility when needing to make decisions, slowing down the response rate to changes in customers' needs," she added.

For now, smaller instrument makers such as Polymer Char and Tescan Orsay are anticipating sales growth. The real test for them—as well as for the major companies they compete against—will come when the market slows once again. ■

FORENSIC SCIENTISTS TO CREATE STANDARDS

NIST is calling for scientists to join a new organization to unify and standardize the scientific basis for forensic science. The Organization of Scientific Area Committees (OSAC) will include 23 committees aimed at creating scientific standards for specific forensic disciplines, including a half-dozen chemistry-related fields. OSAC was created earlier this year through an agreement between NIST and the Department of Justice in an attempt to address concerns raised in a 2009 National Academy of Sciences report that many forensic disciplines have little or no scientific underpinning. OSAC is taking over the duties of many ad hoc scientific working groups that studied specific areas of forensic science and made recommendations on best practices. The NAS report said these groups were uneven in their quality.—AW

MERCURY FOUND IN FISH LIVING IN PRISTINE LAKES

Federal researchers have found mercury in all fish tested from remote lakes and streams in 21 national parks in 10 western states, but the mercury levels in most of the fish were below the threshold for potential health effects in fish, birds, and humans. The study was conducted by the National Park Service and the U.S. Geological Survey from 2008 to 2012. More than 1,400 fish, including brook, rainbow, and lake trout, from 86 lakes and rivers were tested. Smaller fish consumed by wildlife were also sampled. Mercury levels varied greatly from park to park and within each park. Grand Teton and Great Basin National Parks had the lowest percentage of fish exceeding the threshold for unlimited human consumption, and Glacier National Park had the highest, with 100% of its fish exceeding that threshold.—BEE

SHUTTERSTOCK

Mercury was found in fish living in the lakes surrounding Mount Rainier, in Washington.

ARCTIC OIL SPILL PREPARATION INADEQUATE, REPORT FINDS

"Current personnel, equipment, transportation, communication, navigation, and safety resources for overseeing a spill response in the Arctic are not adequate," according to a report released last week by the National Research Council. The report notes that the warming climate will increase pressure by oil companies to commercially develop drilling sites in Arctic waters. But a difficult challenge lies ahead for such projects because of extreme weather and environmental settings, limited available operational support, and the vast Arctic geographic area, which contains vulnerable species, ecosystems, and culture, the report says. It recommends development of a "full suite of proven oil response tools" as well as an additional spill response infrastructure. New testing protocols should also be developed, the report says, which may include "carefully controlled" field experiments that release oil into Arctic waters.—JJ

DOCTORAL SCIENTIST UNEMPLOYMENT RISES

The percentage of doctoral-level scientists and engineers who were unemployed in 2010 hit a 10-year high of 2.4%, according to a recent NSF report. Physical scientists had the highest unemployment rate of any field at 3.5%, up from 2.4% in 2008, the last time NSF's Survey of Doctorate Recipients was conducted. The unemployment rate for doctoral degree holders was still far below that of the general population, which saw unemployment in 2010 of 8.2% for those over age 25. The report also shows that the overall number of doctoral scientists in the labor force continues to rise, going from 582,500 in 2001 to 709,700 in 2010. Nearly 18% of this 2010 labor force were physical scientists.—AW

GOVERNMENT ROUNDUP

E-CIGARETTES would be subject to FDA regulation under a proposed rule announced last week. FDA currently regulates cigarettes, cigarette tobacco, and smokeless tobacco, but the agency wants to extend its authority to cover additional products, including electronic or e-cigarettes, cigars, pipe tobacco, waterpipe or hookah tobacco, and nicotine gels.

ATTORNEYS GENERAL from 13 states are against draft legislation recently released by Republicans in the House of Representatives to reform the 1976 Toxic Substances Control Act. They oppose the draft's provisions that would preempt state chemical laws.

THE U.S. SUPREME Court has declined to review a ruling against ExxonMobil that ordered the company to pay $105 million in damages for polluting New York City's groundwater with the gasoline additive methyl *tert*-butyl ether. The decision leaves intact a 2013 appellate court ruling that upheld the judgment.

CHINESE OFFICIALS say they will appeal a World Trade Organization ruling that the country illegally restricted trade in rare-earth minerals. China claims that the rules protect the environment, but its competitors say the restrictions help Chinese companies.

FDA'S DRUG REVIEW divisions vary widely in the time they take to approve new drugs, concludes a report from Manhattan Institute, a policy think tank. From 2004 to 2012, the time for approval of cancer and antiviral drugs was roughly twice as fast as average and three times as fast as drugs for neurological disorders.

EPA last week agreed with two oil industry petitioners and significantly lowered the amount of cellulosic ethanol required to be blended with gasoline in 2013 from 6 million gal to 810,185 gal. The change matches the level actually produced in the U.S.

NEW OIL At a Core Energy/DOE enhanced oil recovery facility in Michigan, compressed CO_2 is used to increase oil well production and store CO_2 underground.

A CARBON COMMODITY

Advocates say **ENHANCED OIL RECOVERY** using CO_2 can drive carbon capture and sequestration technologies

JEFF JOHNSON, C&EN WASHINGTON

AT FIRST GLANCE, using a greenhouse gas to produce more fossil fuel appears to offer a futile and counterproductive solution to today's climate-change crisis. But that is exactly what the Department of Energy, the oil industry, and some environmental groups are advocating.

They are touting enhanced oil recovery (EOR) as a pathway to reduce atmospheric CO_2 emissions. EOR is a method used by the oil industry to produce more oil by injecting highly pressurized supercritical CO_2 into partially depleted oil fields to recover oil left behind from previous drilling operations.

Oil companies have found that about half of the CO_2 used in the EOR process stays underground, geologically entombed in pores that originally held oil. Consequently, EOR is being considered as a sequestration technology for CO_2, the most common and pervasive anthropogenic greenhouse gas.

But EOR is not a magic bullet. Even if as much as half of the CO_2 used in EOR stays underground, the gas can leak back to the surface when pockets are disturbed. Also, and perhaps most important, EOR yields more oil, the combustion of which generates more CO_2.

Because EOR increases oil production, the oil industry's use of the method is expected to grow, according to industry and DOE analysts. That growth should fuel demand for CO_2, potentially creating a lucrative market for the gas, which could help kick-start stalled commercial development of technologies needed to capture CO_2 from large industrial sources, particularly coal- and natural-gas-fired power plants.

EOR could become the "technology bridge" to deployment of cost-effective plant-scale carbon capture, said Julio Friedmann, DOE deputy assistant secretary for clean coal, earlier this year when testifying at a House of Representatives Energy & Commerce Committee hearing. Many House members listened closely, particularly those from coal states who are trying to block a new Environmental Protection Agency proposal to cap CO_2 emissions from new power plants. For coal-fired plants, those CO_2 emissions levels could be achieved only with carbon capture and sequestration (CCS) technologies.

EPA says in its proposal that its carbon emissions limit was based on projections for three U.S. and one Canadian coal-fired power plant that are now under development. Critics in Congress and industry have complained that the agency should not base limits on unproven technologies.

These four power plants would all use carbon capture technologies that would be set up to feed CO_2 to EOR operations, Friedmann noted, saying that approach is the "most near-term and most commercially attractive utilization option for captured CO_2."

Friedmann acknowledged that electricity generated by power plants using CCS technologies would be 80% more expensive than the electricity from the current fleet of coal-fired power plants as well as from natural-gas-fired plants. For him, revenue from selling the captured CO_2 for oil recovery could offset the high cost for early adopters of expensive CCS technologies.

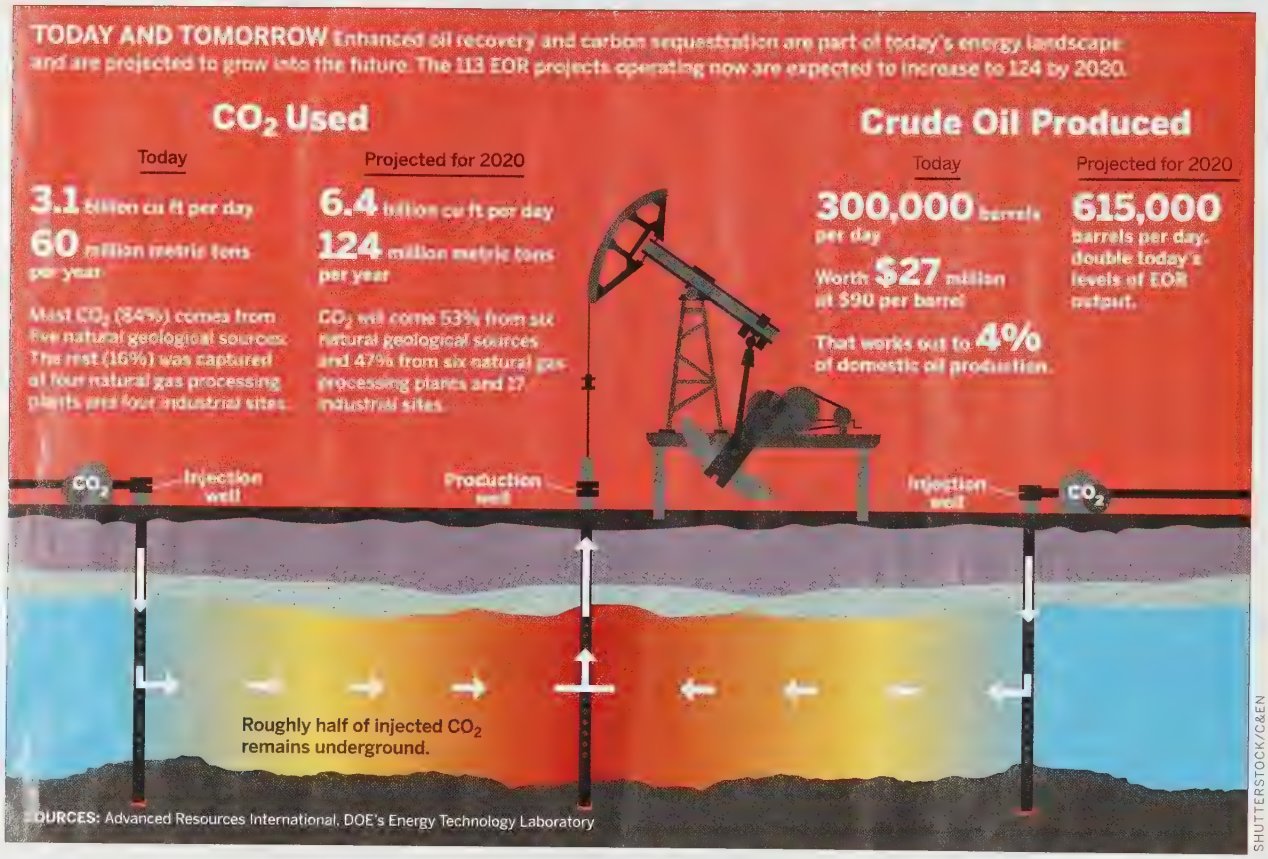
His views are echoed by Bruce Hill, chief geoscientist with Clean Air Task Force, an environmental nonprofit group working to reduce greenhouse gas emissions. "Today, we have no carbon cap-and-trade program, no price on carbon, and no driver that might lead to commercial CO_2 capture development," he tells C&EN. "That is why I am bullish on EOR."

The oil produced through EOR applications, he says, "is going to be produced anyway. We want to see capture and sequestration grow. We can start with EOR."

OVER THE PAST half-dozen years, DOE has poured more than $6 billion into CCS projects, according to the Congressional Research Service. Small demonstration projects and a few small-scale industrial applications are just getting under way; none of the larger coal-based power plants are in commercial operation.

The furthest-along DOE-supported project is Southern Co.'s Kemper gasification facility in Mississippi, which may fire up later this year. Kemper will generate

"It is like opening a can of Coke. The CO_2 just bubbles out of the oil."



SHUTTERSTOCK/C&EN

582 MW of electricity and produce 3 million metric tons of CO_2 annually for EOR applications. However, the $5 billion facility has been delayed and is over budget, and Southern has expressed doubts that it could serve as a model for CCS application.

CURRENTLY, 113 EOR projects are operating in the U.S. Some 3.1 billion cu ft of CO_2 is used daily in the process, which works out to 60 million metric tons per year. About 84% of this CO_2 comes from natural underground sources, according to a report by industry analysts with Advanced Resources International and DOE's National Energy Technology Laboratory (NETL). The rest was captured at some eight U.S. industrial plants and natural gas treatment and processing facilities, which remove CO_2 from the natural gas stream.

The Advanced Resources International/NETL study says the 16% share from gas processing plants and industrial sources is expected to grow to 47% by 2020. Much of the new CO_2 is likely to come from industrial sites along the Gulf of Mexico coast, where it will also be injected underground, likely in depleted oil fields.

"The potential for CO_2 use in EOR is huge," says Joseph P. (Phil) DiPietro, an NETL engineer. "The 60 million metric tons used today produces about 300,000 barrels of crude oil daily. That works out to 4% of total U.S. oil production," he explains. "We predict it could double to 600,000 bbl per day and more than 120 million tons of CO_2 by 2020. About half that CO_2 would come from industrial processes."

DiPietro says oil production from EOR has the potential to grow further. "I can say with a straight face that we could get to 2 million to 3 million bbl a day of oil production using EOR, and that would draw 500 million metric tons a year in CO_2 demand."

The use of EOR began in the 1970s as an oil industry niche technology using naturally occurring CO_2 to recover more oil. Most of the action has been in the Permian Basin formation of Texas and Oklahoma. Applications now run down the center of North America with an infrastructure that includes some 350 miles of CO_2 pipelines.

DiPietro sees CO_2 from industrial sources doubling over the next 10 years, while oil industry demand for CO_2 increases and natural sources tap out. "That is where DOE's technology development work with the coal-fired power plants comes in," he says. "It may take 10 to 20 years to develop these coal CCS technologies, but it will also take the oil industry 10 or 20 years to run out of inexpensive CO_2." When that happens, he says, CO_2 capture technologies for coal-fired power plants will be ready to compete.

To sustain this CO_2 demand for EOR, oil prices have to remain high, making CCS

"I can say with a straight face that we could get to 2 million to 3 million bbl a day of oil production using EOR."

advocates really just hopeful interlopers on an oil industry cash cow, explains former oilman Jeffrey N. Phillips. Phillips is now a senior program manager in the advanced coal group for the Electric Power Research Institute, a utility-funded research organization.

"You may get 25–30% of potentially available oil in a first drilling," Phillips explains. "In the past, the next step was to use a 'waterflood,' pumping water down one hole and trying to force oil and water out another one."

Because water and oil don't mix, he notes, water tends to slide by without collecting too much oil. Instead, the oil industry began exploring the possibility of shifting from water to CO_2.

WHEN CO_2 IS USED, it mixes and dissolves into oil and, at 2,000 psi, the gas expands into oil making it less viscous, Phillips says.

"With pressurized CO_2, drillers are getting 50% of the reserve," he says. When the high-pressure CO_2-oil mixture comes to the surface, it depressurizes and the oil and CO_2 separate. "It is like opening a can of Coke," Phillips explains. "The CO_2 just bubbles out of the oil."

Oil producers using CO_2 then try to recapture the gas and repressurize it for use in other holes, Phillips says. They found that roughly half the CO_2 stayed underground, trapped in geologic pores. So EOR began to be examined as a storage mechanism.

But sometimes CO_2 doesn't remain contained underground.

In August 2011, a CO_2 release occurred in an EOR operation run by Denbury Resources, an oil producer, in Yazoo County, Miss. The release lasted 27 days and suffocated wildlife. It was caused by an inadequately capped old well bore, according to a report from the Mississippi Commission on Environmental Quality. As Denbury cleaned up CO_2, water, and oil at the leak site, it also plugged 30 other old wells in the oil field, according to the state report. The state fined Denbury $662,500. Denbury did not return C&EN's calls and e-mail seeking comment. Other leaks have been reported in Louisiana and Wyoming.

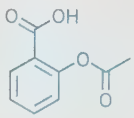
Because of leaks, the Sierra Club is challenging a DOE-supported proposed project in Kern County, Calif.—the Hydrogen Energy California gasification facility. It would use coal and petroleum coke to generate hydrogen, fertilizer, and 300 MW of electricity while capturing and selling 3 million metric tons of CO_2 per year for EOR.

In a letter to the California Energy Commission, Sierra Club attorney Andrea Issod cited the Mississippi and Louisiana leaks, pointing to documents showing that more than 1,000 old wells penetrate the oil and gas reservoir where EOR is being proposed in California. Issod wants a thorough examination of all abandoned and capped wells at the proposed injection site, looking at age, well integrity, and accuracy of well records before EOR begins.

What this examination reveals, as well as what occurs when the Kemper facility begins operating later this year, may determine whether EOR will become part of a climate-change solution or be part of the fossil-fuel problem. ■

HOW ASPIRIN REDUCES COLON CANCER RISK

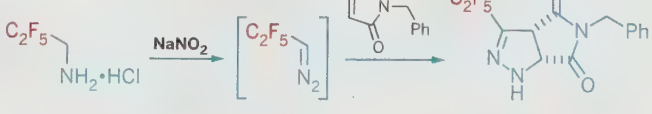
A variety of studies have suggested that taking aspirin can decrease the risk of colon cancer. But the mechanism by which the common painkiller exerts its protective effect has eluded researchers. A team led by Andrew T. Chan of Massachusetts General Hospital and Sanford D. Markowitz of Case Western Reserve University now reports that aspirin's colon cancer protection is linked to levels of an enzyme called 15-PGDH (*Sci. Transl. Med.* 2014, DOI: 10.1126/scitranslmed.3008481). The researchers note that the enzyme plays a role in the degradation of prostaglandins, which are important lipid messenger molecules that can also be involved in certain colon cancers. Aspirin appears to reduce prostaglandin levels by inhibiting the activity of another enzyme involved in prostaglandin synthesis. The researchers examined tissue samples from 270 cases of colon cancer stemming from two studies that tracked aspirin use of 128,000 people for three decades. They found that people who consumed at least two 325-mg aspirin tablets per week lowered their risk of colon cancer by 50%—but only if their 15-PGDH levels were higher than average. The finding could help identify people who can reduce their colon cancer risk with aspirin. Likewise, identifying individuals who won't benefit from aspirin's protection could help them avoid the drug's side effects, which include gastrointestinal bleeding and ulcers.—SE



Aspirin

DIAZOALKANE EXPANDS FLUORINE FOCUS ON ETHYL GROUPS

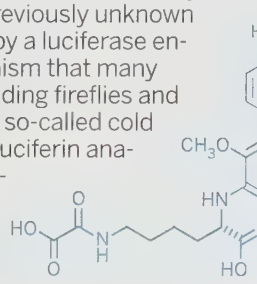
Developing new methods for introducing fluorine into complex organic molecules has been all the rage during the past few years. Researchers preparing drug candidates and crop protection chemicals typically seek to add a single fluorine atom or trifluoromethyl group and now have myriad ways to do so. But methods for adding longer, more lipophilic perfluoroalkyl groups such as pentafluoroethyl, $-C_2F_5$, to complex molecules are relatively scarce. The approaches tend to be direct additions of perfluoroalkyl groups using organometallic transfer reagents and don't use perfluoroalkyl-containing building blocks. Pavel K. Mykhailiuk of Enamine, a global supplier of research chemicals based in Kiev, Ukraine, has now developed a new building block for introducing C_2F_5 into organic molecules (*Chem. Eur. J.* 2014, DOI: 10.1002/chem.201304840). Mykhailiuk safely generates the fluorinated diazoalkane, $C_2F_5CH{=}N_2$, in situ from $C_2F_5CH_2NH_2{\bullet}HCl$ and $NaNO_2$. He demonstrated the utility of the reagent by using it in [3 + 2] cycloadditions with alkenes to prepare perfluoroethylated pyrazolines (one example shown) with better than 95% conversion rates. Mykhailiuk believes the diazofluoroalkane will also be as useful as other diazoalkanes for cyclopropanations, carbene insertions, and alkyne cycloadditions.—SR



Ph = phenyl | Diazofluoroalkane | Pyrazoline

EARTHWORM'S GLOW UNEARTHED

In the forest soils of Siberia, there is a tiny worm that will emit blue light if given a little tickle. The critter, known scientifically as *Fridericia heliota,* gets its glow via the oxidation of a previously unknown luciferin compound facilitated by a luciferase enzyme. This is the same mechanism that many bioluminescent creatures, including fireflies and certain jellyfish, use to produce so-called cold light. To date, only a handful of luciferin analogs have been chemically characterized. Researchers led by Ilia V. Yampolsky of the Russian Academy of Sciences' Institute of Bioorganic Chemistry wanted to know precisely which chemical made *F. heliota* glow. The team collected approximately 60,000 of the little worms, each of which is only about 15 mm long, and then extracted their bioluminescent components (*Angew. Chem. Int. Ed.* 2014, DOI: 10.1002/anie.201400529). The researchers were able to isolate only 0.005 mg of the color-giving chemical from which they could do limited NMR and mass spectral analyses. Using these studies, they narrowed down the structural possibilities to four isomeric peptides and then synthesized them. One of the synthesized compounds (shown) turned out to be a match with the natural Siberian worm luciferin and produced light when mixed with crude *Fridericia* luciferase.—BH



This Siberian earthworm glows blue when mechanically stimulated, thanks to its unique luciferin.

ANGEW. CHEM. INT. ED.

SOLID CONTRAST AGENT ENABLES LONG-TERM MRI

An injectable contrast agent for magnetic resonance imaging that coalesces into a solid now enables long-term monitoring of oxygen levels in tissues without the need for an invasive procedure, which is required to implant standard oxygen electrodes or a solid MRI contrast agent (*Proc. Natl. Acad. Sci. USA* 2014, DOI: 10.1073/pnas.1400015111). The new material maintains the concentration of the contrast agent in the tissue of interest for extended periods of time, permitting repeated quantitative measurements. Michael J. Cima and coworkers at Massachusetts Institute of Technology make the sensors from a saline suspension of oxygen-responsive dodecamethylpentasiloxane embedded in a support matrix of polydimethylsiloxane (PDMS). In rats, the injected PDMS particles coalesced into a solid sensor "depot" in muscle tissue, and there were no signs of an adverse tissue reaction. By using the right combination of MRI pulse sequences, the signal from PDMS is eliminated and the oxygen-responsive signal is preserved. The researchers used the sensors to measure partial pressure of oxy-

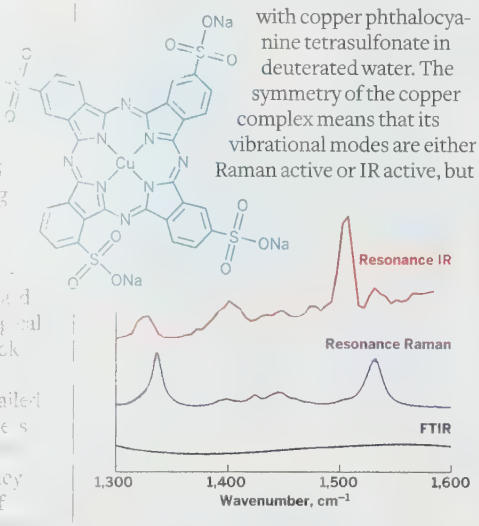
gen in the tissue of the rats as they l... gas streams containing different am... of oxygen or as they experienced res... blood flow to a limb. The sensors re... l functional for at least a month afte... i tion. By using different contrast ag... nts and support materials, the same strateg... would be used to make sensors opt...ized ... er analytes, the researchers su...gest.–

SQUEEZING MO... OF CORN LEFTOVE...

There's a lot more to corn th... s used as a sweetener and to ma...e eth... A characterization study o... products of corn processing, a con...ed liquid known as defatted corn sy...up (DCS), suggests that it has bee... overlooked as a potential valuable source of biobased chemicals (*ACS Sustainable Chem. Eng.* 2014, DOI: 10.1021/sc400508p). When corn is milled and processed, a major part of the starting material is drawn off to ferment into ethanol. Most of the leftover solids, called dried distillers grains, are repu... posed as animal feed. David R. Shonnard and coworkers at Michigan Technolo...gical University decided to take a closer look at DCS, which is often added to the dr... distillers grains, by carrying out a detailed compositional analysis. The researche... s found that the waste liquid is rich in f... carbohydrates, protein, and more. They then calculated the potential yields of various chemicals that could be m... fermentation processes using the r...oughly 700,000 metric tons of the materia... duced annually in the U.S. Although DCS doesn't appear useful for making fue...ls, it could be used to meet current U.S. demand for succinic acid (about 25,000 metric tons) or global demand for histidine (360 metric tons). Biobased chemical manufacturer Working Bugs, which was involved in the study, is considering options for capitalizing on the findings.—SR

INFRARED SPECTROSCOPY GETS A RESONANCE RAMAN ANALOG

In resonance Raman spectroscopy, matching the excitation frequency to an absorption frequency in the sample boosts the resulting Raman signal. But not all molecular vibrational modes are Raman active, and there has been no infrared version of resonance Raman. John C. Wright and coworkers at the University of Wisconsin, Madison, now report that a spectroscopic technique called triply resonant sum frequency (TRSF) spectroscopy provides that missing IR analog (*J. Phys. Chem. A* 2014, DOI: 10.1021/jp5018554). In TRSF spectroscopy, excitation pulses from three lasers interact with sample molecules to generate signals involving two vibrational states and an electronic state. When the laser pulses are in resonance with those coupled vibrational and electronic states, the signal from IR-active vibrational modes is enhanced. Wright and coworkers demonstrated the method with copper phthalocyanine tetrasulfonate in deuterated water. The symmetry of the copper complex means that its vibrational modes are either Raman active or IR active, but not both. The researchers observed features in the resonance IR spectrum that were not observable in either the FTIR spectrum or the resonance Raman spectrum, making the technique potentially useful for studying biomolecules such as hemes, as well as synthetic transition-metal complexes.—CHA



This region of the resonance IR spectrum of a copper complex (shown) differs from both the resonance Raman and the FTIR spectra.

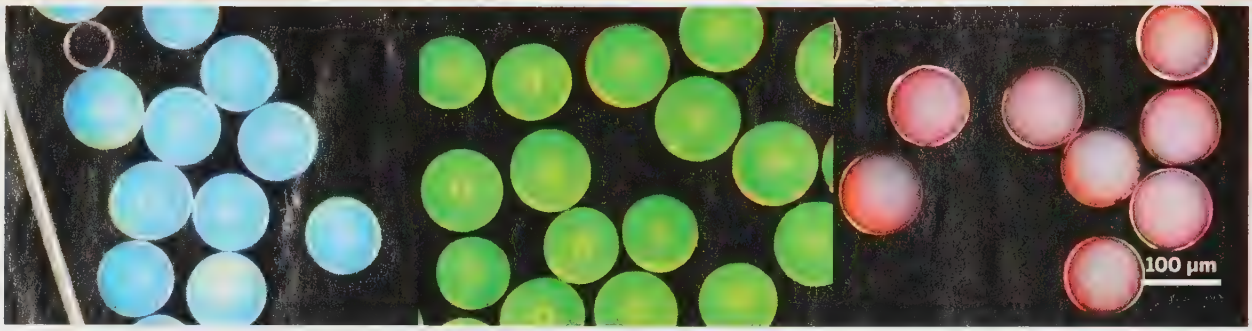
J. PHYS. CHEM. A

NEW ORGANIC DESIGNS FOR FERROELECTRICS

Using a newly developed computational technique to predict structural and electronic properties of as-yet-unsynthesized materials, chemists have designed a group of ferroelectric organic crystals that promise to outperform current state-of-the-art materials (*J. Am. Chem. Soc.* 2014, DOI: 10.1021/ja5017393). Ferroelectric materials have a knack for flipping electrical polarization when triggered by an electric field. That property makes them useful in random access memory devices, capacitors, and transistors. Common ferroelectrics such as barium titanate are inorganic. Because the range of applications could be broadened by lighter, more flexible, and less expensive materials, scientists have been searching for organic versions. Motivated by a 2012 study reporting success in synthesizing ferroelectrics based on tetrathiafulvalene (TTF), an electron donor, and pyromellitic diimide (PMDI), an electron acceptor, Shuang Chen and Xiao Cheng Zeng of the University of Nebraska, Lincoln, computationally screened tens of thousands of crystal structures based on TTF and PMDI motifs. The search turned up three highly stable compounds with predicted polarization values up to twice as large as today's top performers.—MJ

ZIPPING UP WOUNDS WITH NANOPARTICLES

Aqueous solutions of nanoparticles could one day replace sutures for healing cuts in skin and for certain surgical procedures, such as liver surgery, where stitches can be traumatic to soft tissues. Using aqueous solutions of silica or iron oxide nanoparticles, researchers in France led by Didier Letourneur of INSERM Paris and Ludwik Leibler of CNRS-ESPCI ParisTech found they were able to control bleeding and heal deep wounds in the skin and livers of rats (*Angew. Chem. Int. Ed.* 2014, DOI: 10.1002/anie.201401043). The wound closure occurs through a process known as nanobridging, wherein the nanoparticles adsorb to the tissue and biomacromolecules attach to the nanoparticles, ensuring that the wound surfaces adhere to one another. In addition to wound healing, the researchers used the nanoparticle solutions to fix medical devices and tissue-engineering constructs to organs, such as a rat's beating heart. They note that for skin and liver treatment, the procedure is fairly simple: Just dab the solution on the wound, push the wound edges into contact, and watch the wound seal in a matter of minutes. "Translation to clinical practice will require careful safety and toxicity investigations," the team notes.—BH



DYE-FREE COLOR Microcapsules with blue, green, and red structural color are prepared from core-shell nanoparticles with different shell thicknesses. These could be used to create a full-color display that doesn't need to be backlit.

COLLOIDS YIELD FULL COLOR PALETTE

Core-shell nanoparticles within microcapsules create novel pigments that get their color from a **PHYSICAL PHENOMENON**

BETHANY HALFORD, C&EN BOSTON

VINOTHAN N. MANOHARAN holds up a small vial of liquid. It looks something like milk—white and opaque and otherwise unremarkable. But the particles that make up this suspension could one day be used to create paints and inks that won't fade or full-color displays that don't need to be backlit. The key, says Manoharan, a professor in Harvard University's physics department and School of Engineering & Applied Sciences, is using some clever chemistry to bring about a physical phenomenon known as structural color.

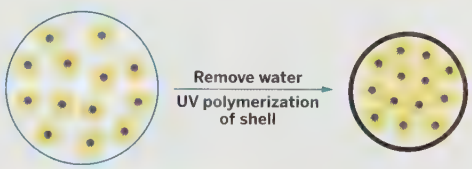
Much of what we see gets its color from colored molecules. There are, for example, aniline dyes, such as mauve, and metal compounds, such as cobalt blue, that give color to objects. There's a relationship between these molecules' electronic structures and how they absorb and reemit certain wavelengths of light.

Structural color has nothing to do with a molecule's electrons. Instead, structural color arises on the supramolecular level when a material's nanostructures selectively reflect certain wavelengths of light while letting all other wavelengths pass through.

"With structural colors you can make different colors from exactly the same material," explains Sofia Magkiriadou, a graduate student in Manoharan's lab. Because structural colors aren't based on molecules, which can react and change color, they tend to be more resistant to fading and bleaching.

During Magkiriadou's first week working with Manoharan, he asked her to take the white liquid and remove water from the colloidal suspension. When she did, the material turned blue, a result of the colloidal particles packing together in such a way that they reflected wavelengths of blue light.

This came as no surprise to Manoharan. Other researchers had made so-called photonic pigments, or pigments based on structural color, by making arrays of nanoparticles. Ordered nanoparticle arrays give rise to iridescent pigments, which physicists describe as anisotropic. Disordered arrays, physicists had recently learned, would also produce colored pigments. But these have a matte appearance, which physicists describe as isotropic. For paint or display applications, it's the matte appearance that everyone is after.



ALL TOGETHER NOW When the Manoharan lab removes water from microcapsules filled with core-shell nanoparticles, the microcapsule shrinks, bringing the particles close together. The average distance between the particles gives rise to a certain color, so it's possible to change the microcapsules' colors depending on how much water is removed. Ultraviolet polymerization of the microcapsule shell locks the color in.

Manoharan was pleased to see that the colloids Magkiriadou had dehydrated took on a blue matte appearance. But other researchers had already made isotropic blue and green photonic pigments. Manoharan and his students had bigger plans: They were hoping to use the same colloids to make a rainbow of pigments through structural color—a feat no one had accomplished yet.

TO UNDERSTAND the Manoharan lab's system, one must envision spheres within spheres within spheres. The smallest, innermost spheres are polystyrene nanoparticles. These make up the core of the core-shell nanoparticle colloids, and they are what physically scatter the light in Manoharan's photonic pigments.

The polystyrene nanoparticles are surrounded by a shell of poly(*N*-isopropylacrylamide-*co*-acrylic acid) or poly(NiPAm-AAc). This shell is transparent, so light can pass through it. It is also soft and can squish as the core-shell particles pack together. Modifying the distance between the polystyrene cores, by varying the shell thickness, makes them reflect different wavelengths of light, thereby producing different colors.

Jin-Gyu Park, a postdoc in the Manoharan lab, and Shin-Hyun Kim, currently a professor at Korea Advanced Institute of Science & Technology, came up with a way to use microfluidics to encapsulate an aqueous suspension of the core-shell nanoparticles within an ultraviolet-curable monomer, ethoxylated trimethylolpropane triacrylate. "That monomer shell is permeable to water, so you can shrink it down, and

…were inspired by bluebirds. Those … structural color to get that blue."

as you shrink it down you compress the particles," Manoharan explains. "As you suck more water out, you actually change the distance between the particles. So you can tune in color that way." The … is to polymerize the monomer … capsule, nanoparticles, and …

Using this system, Manoharan's team was able to produce structural … the full visible spectrum (*Angew. Chem. Int. Ed.* 2014, DOI: 10.1002/anie.…). That's impressive, says Eric … physicist at Yale who studies … color and soft materials. "In … we tried to make deep greens … structural color it just didn't work," says. "The Manoharan lab has … ferent architecture and designed … thesized new colloidal materials … ou to make red. I think that's potentially going to be very exciting."

Getting the red photonic pigment was probably the biggest hurdle, Manoharan says. "These things were inspired by bluebirds. Those birds use structural color to get that blue," he says. Red birds, however, don't use structural color. Instead they get their hue from colored molecules in their feathers. It occurred to Manoharan and his team that because nature doesn't make isotropic red with structural color it simply might not be possible for them to do it.

But this work, Manoharan says, shows that it is possible to make isotropic structural color in red, albeit a red that the researchers would like to look more saturated.

If you can make red, green, and blue, you can make all the colors you need for a color display that doesn't need to be backlit and therefore has a longer battery life. That's just one of the applications Manoharan has in mind for these photonic pigments. He says they could also be used in fade-resistant paints and inks, although he's quick to add they haven't yet shown that the pigments can go for years without losing their color.

"What we have now is a proof of concept," Manoharan says. "There's still some work that needs to be done before we can put these into applications." ■

COLOR THEORY

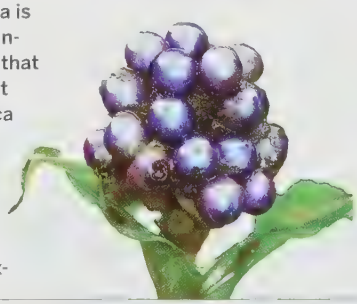
Structural Co…

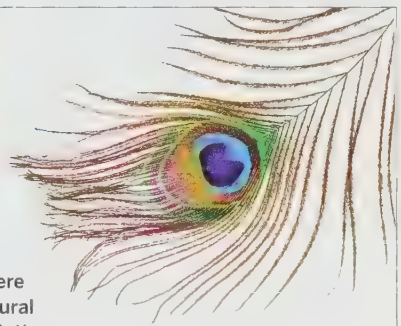
Bluebirds, butterflies, and berries of *Pollia condensata* all get their vivid blue hues from a phenomenon known as structural color. Structural color comes about on a supramolecular level when a mate…

…rial's nanostructures scatter light in such a way that certain wavelengths get reflected and amplified through constructive interference. This is different from dyes, which achieve color from their molecules' electrons. In fact, the …ecule… …in st… …y col… …bjects are usually colorless. Grind up these materials and that nanostructure is lost along with the color.

…opal is a classic example of an object …chieves …kable …s via …tural …fer- … Opals … silica …eres, about …) nm in diameter, …t are arranged in a highly …lered fashion. The silica is inherently colorless, but interference from the light that scatters through different parts of that ordered silica structure gives rise to an opal's color.

Physicists describe opals, peacock feathers, *Morpho* butterflies, and even compact discs as examples of anisotropic structural color. That is, their color changes with viewing angle. There is also isotropic structural color, in which the color doesn't change with viewing angle. The blue feathers of the eastern bluebird, for example, get their vivid hue from isotropic structural color. Isotropic structural color also arises from nanoscale structures, but they must be disordered to keep the color independent of the viewing angle.





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Objects with structural color tend to resist fading. A couple of years ago, researchers at England's Royal Botanic Gardens discovered that the blue color of *P. condensata* fruit comes from the nanostructure of its cellulose fibers, accounting for the fact that the fruit is as bright today as the day it was picked 40 years ago. This suggests that man-made structural color could also be fade-resistant, making such materials attractive for paint and ink applications.

C&EN WEBINARS

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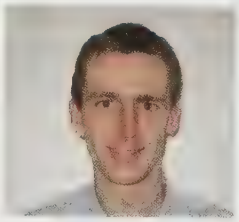
Trace Elemental Analysis of Waste Associated with Power Generation

MAY 15, 2014 8:00 a.m. PDT / 11:00 a.m. EDT / 15:00 GMT

SPEAKER



Matthew Cassap,
AA & ICP-OES Product Manager
Thermo Fisher Scientific

MODERATOR

Jyllian Kemsley, Ph.D.,
Senior Editor
C&EN

OVERVIEW

The analysis and handling of waste products associated with traditional forms of power generation is of critical importance. In this webinar, we will present simplified methods for trace elemental analysis of waste materials related to power generation using ICP-OES (Inductively Coupled Plasma-Optical Emission Spectroscopy). The primary focus will be on the analysis of wastes related to traditional power generation methods such as coal-fired power stations, where elemental analysis of both the coal and fly ash is required. We will also discuss the effluents connected with these power generation methods. Attendees will learn how to gain maximum performance from the latest ICP-OES instrumentation to enable their organizations to adhere to stringent environmental regulations.

KEY LEARNING OBJECTIVES:

- Sample preparation methods for solid waste from power generation
- Optimization of methods using advanced software
- Streamlining of sample analysis using advanced instrument hardware

WHO SHOULD ATTEND:

- Lab managers & technicians
- Environmental monitoring and in-house industrial labs
- Labs operating under EPA methods 200.7 and 6010C

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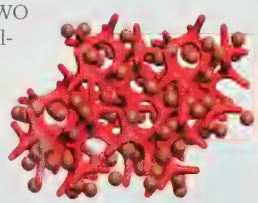
patentpicks

A look at recent patenting activity in electrode materials for **LITHIUM-ION BATTERIES,** brought to you by C&EN and CAS

In 1991, Sony rolled out the first commercial rechargeable lithium-ion battery. Soon after, patenting activity for Li-ion battery technology exploded. In such batteries, a conductive electrolyte shuttles Li^+ between the positive electrode (cathode) and negative electrode (anode) during charging and discharging. Small, lightweight Li-ion batteries are now found in many small portable electronics. But there's still room for improvement: Li-ion batteries do not charge as fast as other battery technologies. They also have limited power densities. Much of the current patenting in this area revolves around the development of more efficient electrodes, according to a recent analysis by the American Chemical Society's Chemical Abstracts Service. Here we highlight a few of the many strategies battery scientists are pursuing.

NANOTUBES GIVE ELECTRODES A BOOST

With Li-ion batteries, increasing the interfacial surface area between cathodes and anodes typically boosts power density and charging rate. A 2012 patent application outlines another strategy: dope the electrodes with carbon nanotubes (WO 2012159111). Ahmed Busnaina and colleagues at Northeastern University describe electrodes built on a carbon nanotube scaffold coated with a layer of a nanoparticulate electrochemically active substance. Thanks to the electrodes' alternating layers of carbon nanotubes and nanoparticles, Li-ion batteries built from them have a power density 100 to 10,000 times as great as that of conventional Li-ion batteries, the researchers claim. Even with these improvements in charge density, there is no sacrifice in charging and discharging rates. Instead, the researchers claim charging rate improvements of up to 100 times that of conventional electrodes.



Polyaniline network (red) features embedded Si nanoparticles (brown) coated with the conductive polymer.

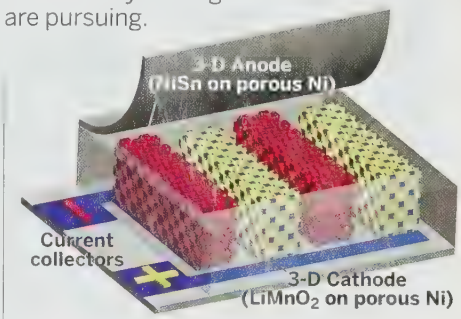
NAT. COMMUN. 2013, DOI: 10.1038/NCOMMS2941

SILICON SURPASSES CARBON

Graphite is the most common anode material used in Li-ion batteries. But its energy density is limited, making silicon—with a charge storage capacity more than 10 times that of carbon—an appealing alternative. Si-based anodes, however, have their own problems. When Li-ion batteries incorporating such anodes are charged and discharged, silicon particles embedded in the anodes expand and crack, destroying vital electrical connections. Researchers at Stanford University and Nanjing University, in China, hope to rectify this shortcoming. In a 2014 patent application, Stanford's Zhenan Bao and Yi Cui and their colleagues offer up a novel polymerization strategy as a solution (WO 2014026112). Si-based anodes are normally made by fashioning a matrix of silicon and carbon particles and then wrapping it in a polymeric material. Instead, the team seeded silicon nanoparticles into a conducting polymer hydrogel as it was forming. The result is a highly interconnected 3-D polyaniline network featuring embedded silicon nanoparticles coated in the polymer. Li-ion batteries that incorporate anodes made of this Si-based material boast a high storage capacity through 5,000 cycles of charging and discharging, the researchers report.

3-D IS BETTER THAN 2-D

Imagine computer chips containing tiny, embedded batteries. Miniature Li-ion battery designs under development at the University of Illinois, Urbana-Champaign, could one day make that possible. A 2013 patent application from Paul V. Braun, William P. King, and James H. Pikul describes a method for fabricating microscale batteries with porous three-dimensional electrodes (WO 2013019489). Compared with standard electrodes, porous 3-D electrodes have a far larger surface area. This makes room for more chemical reactions to take place, expediting the free flow of electrons and lithium ions, boosting both discharge and recharge rates. Taking inspiration from a fast-charging cathode developed by Braun, the researchers built a matching anode and then designed a way to integrate the two components to create a microscale battery. Even when the cathode and anode use entirely different chemistries—say porous nickel coated with $LiMnO_2$ or a NiSn alloy—the researchers managed to fabricate the microscale electrodes in close proximity on a single substrate. Not only do the tiny batteries pack in more power than competing technologies, but they also can be recharged 1,000 times as fast. They could potentially power personal electronics as well as miniaturized medical implants and distributed sensor networks, the researchers suggest.



Microscale Li-ion batteries are assembled from porous 3-D electrodes.

ADAPTED FROM NAT. COMMUN. 2013, DOI: 10.1038/NCOMMS2747

Patent Picks is a collaborative effort by C&EN and CAS. This feature reports on trends CAS scientists observe from patents in CAS databases. Patents now generate more than 70% of the new substances appearing in the literature.

CELEBRATION Former WRRC directors (from left) James Seiber, Antoinette Betschart, and Arthur Morgan and current director Zhang attended the landmark designation ceremony for flavor chemistry.

USDA LAB NAMED LANDMARK

ACS honors Western Regional Research Center again, this time for contributions to FLAVOR CHEMISTRY

ELIZABETH K. WILSON, C&EN WEST COAST NEWS BUREAU

DURING WORLD WAR II, food scientists at the Western Regional Research Center (WRRC) in Albany, Calif., were busy developing freezing and dehydrating methods for preserving foods. Ultimately, the need to preserve not only the food but also the flavor became a paramount goal.

Thanks to more than 60 years of research on flavor, we now know which compounds make an orange taste like an orange or rice taste like rice. We understand how they can be affected by processing and storage.

Much of this flavor knowledge comes from research performed at WRRC, which is run by the Department of Agriculture's Agricultural Research Service.

And so during a ceremony on Aug. 29, 2013, at WRRC, the American Chemical Society designated the facility a National Historic Chemical Landmark for its pioneering research in the chemistry of flavor.

This is the second time WRRC has been designated an ACS chemical landmark: In 2002, the facility was honored for its research advances in frozen-food technology (C&EN, Jan. 13, 2003, page 43).

As the only facility to receive two such awards, "this is a unique testament to WRRC's outstanding research," 2013 ACS President Marinda Li Wu said at last year's ceremony.

The flavor compound research has made it possible for frozen strawberries to taste fresh, for jelly beans to mimic flavors of a wide variety of foods, and for scientists to understand components of aroma and taste and learn how compounds react to preservation, Wu said. "Their work enables the widespread availability of high-quality, safe, and flavorful foods."

At the ceremony, Wu presented Howard Q. Zhang, WRRC director, with a plaque commemorating the designation. "We're extremely honored to be receiving such an award," Zhang said. "I think it shows the significance of the work that has been done here in the past and that we continue to build on."

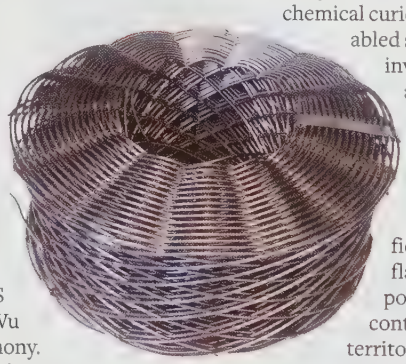
The strawberry was the focus of WRRC's first flavor project. In the late 1940s, flavor chemist Keene P. Dimick began devising analytical techniques to distill the flavor of strawberries into a concentrated oil. In 1953, Dimick built one of the earliest gas chromatographs, allowing researchers to separate flavor compounds. By 1956, Dimick's team had solved the mystery of strawberry flavor: The key compound is 4-hydroxy-2,5-dimethyl-3(2H)-furanone.

IN THE 1960S, WRRC was one of several facilities that pioneered the coupling of gas chromatography with mass spectrometry. With the analytical power of GC/MS, researchers moved on to identifying the main source of myriad other flavors: oranges (α- and β-sinensal), bell peppers (2-isobutyl-3-methoxypyrazine), rice (2-acetyl-1-pyrroline), and more.

Not only did this knowledge satisfy chemical curiosity, but it also enabled scientists to begin investigating topics such as odor thresholds and flavor potency and their importance in processing foods.

Today, flavor chemists have identified more than 7,000 flavor and aroma compounds, and WRRC continues to explore new territory, said Tara McHugh, research leader of WRRC's Food Processing Research Unit.

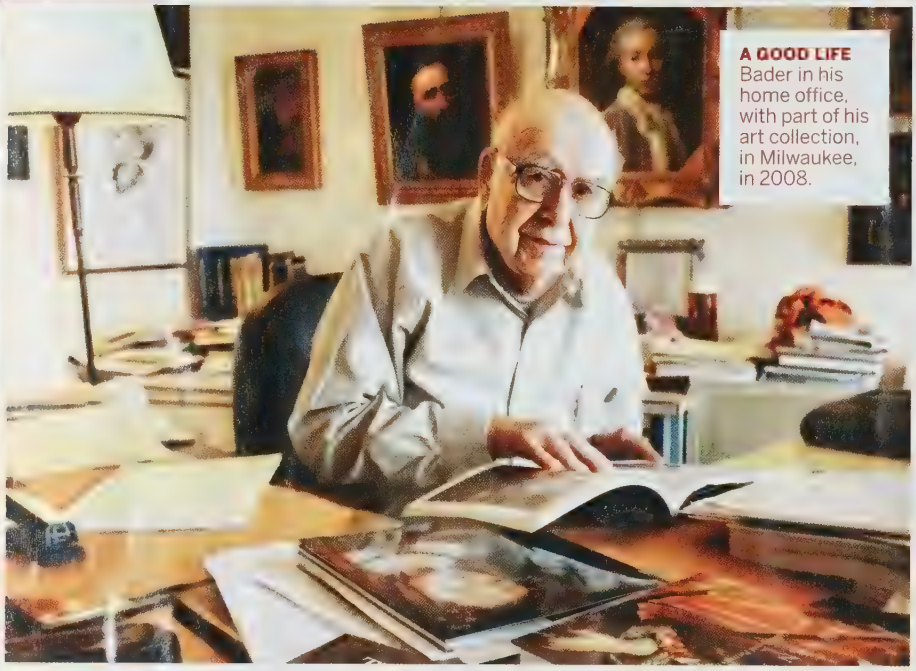
In a statement, she added, "Processed foods are an important part of the nation's food supply, and the technology developed [at WRRC] will continue to help us ensure that the supply is safe, marketable, and of high quality and that the food tastes good to even the most discriminating palates." ■



FLAVOR FINDER An early gas chromatograph coil developed at WRRC helped chemists separate flavor compounds.

ELIZABETH WILSON/C&EN

The flavor compound research has made it possible for frozen strawberries to taste fresh.



A GOOD LIFE Bader in his home office, with part of his art collection, in Milwaukee, in 2008.

DAVID BADER PHOTOGRAPHY

"Eighty years ago, when Alfred and I were in the same class in Vienna, I would never have imagined that he would become one of the great polymaths: scientist, yet religious; spectacular entrepreneur as well as even more spectacular philanthropist; sophisticated art dealer as well as major collector: all these boats sailing on a sea of chemistry!"

—CARL DJERASSI, EMERITUS PROFESSOR OF CHEMISTRY, STANFORD UNIVERSITY

CELEBRATING ALFRED BADER AT 90

C&EN lauds the **MYRIAD CONTRIBUTIONS** of the chemist, art collector, and philanthropist

LINDA WANG, C&EN WASHINGTON

ALFRED BADER MAY BE BEST KNOWN for cofounding Aldrich Chemical Co. (now part of Sigma-Aldrich) in 1951, and for being a preeminent art collector, but it's his enormous body of charitable work that may be his greatest legacy.

With his wife, Isabel, Bader has given millions of dollars to causes he's passionate about, including the American Chemical Society's Project SEED program, which provides scholarships to economically disadvantaged high school students to conduct hands-on research. In addition, since 1986, the Baders have supported an ACS national award, the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry.

In celebration of Bader's 90th birthday this month, C&EN reflects on the contributions of this multifaceted chemist, businessman, art collector, and champion for chemistry education. ■

CHEMICAL HERITAGE FOUNDATION

***The Aldrich Handbook,* which lists research chemicals for sale, is recognizable by the beautiful artwork on its covers. The 1967-68 edition of the catalog was the first to feature a painting from Bader's art collection: "The Quill Cutter" by Paulus de Lesire.**

"No one on this planet has done more to further chemists' capabilities and all chemical industries' ability to grow."

—K. BARRY SHARPLESS, W. M. KECK PROFESSOR OF CHEMISTRY, SCRIPPS RESEARCH INSTITUTE, CALIFORNIA

"Alfred Bader's name is synonymous with helping chemists to make molecules; furthermore, his support through awards, fellowships, and scholarships is unwavering. But more than that, Alfred, with Isabel at his side, has touched all whom he has met with enthusiasm about their work and a zest for life."

—VICTOR SNIECKUS, BADER CHAIR EMERITUS IN ORGANIC CHEMISTRY, QUEEN'S UNIVERSITY, ONTARIO

"Please bother us."

THIS STATEMENT BY ALFRED BADER BECAME ASSOCIATED WITH ALDRICH CHEMICAL CO., WHICH TOOK PRIDE IN TALKING WITH ITS CUSTOMERS.

"The Bader Scholarship was instrumental in allowing me to put more emphasis on my classes instead of thinking of the financial burden I might be to my parents. Thank you, Mr. and Mrs. Bader, for investing in my education."

—ANITA HURTADO, FORMER BADER SCHOLAR, NOW ASSOCIATE DIRECTOR IN THE SUPPLY-CHAIN ORGANIZATION AT MERCK & CO

JOHN STALEY PHOTOGRAPHY

Alfred and Isabel (center) are surrounded by former Bader Scholars during a reunion reception at the spring 2005 ACS national meeting in San Diego.

"Alfred and Isabel Bader's generosity has manifested itself at ACS in countless ways—and there are countless successful chemists who owe their careers to the investments that these two astonishing philanthropists made in Project SEED and the Bader Scholarships."

—MADELEINE JACOBS, ACS EXECUTIVE DIRECTOR AND CEO

JOHN STALEY PHOTOGRAPHY

Alfred with Isabel (left) and ACS Executive Director and CEO Madeleine Jacobs during the Bader Scholars reunion reception at the spring 2005 ACS national meeting in San Diego.

$1.7 million

The amount Alfred and Isabel have donated to ACS since 1986, with $1.3 million going toward the Alfred & Isabel Bader Scholars under the Project SEED program. Roughly 20 students each year receive one of these $5,000 scholarships.

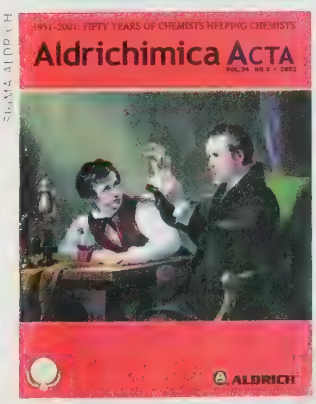
385

Number of Alfred & Isabel Bader Scholars to date.

68,000

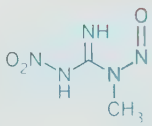
Approximate number of research chemicals in the Aldrich Handbook today.

SIGMA-ALDRICH



In addition to the Aldrich Handbook, Bader also started the journal Aldrichimica Acta, *which focuses on organic chemistry research.*

ALDRICH CHEMICAL CO.'S FIRST CHEMICAL:



N-Methyl-*N*′-nitro-*N*-nitrosoguanidine, which was used in the preparation of diazomethane. MNNG was marketed through the company's first catalog, in 1951, a one-page document that grew to become the Aldrich Handbook. Sigma-Aldrich no longer sells MNNG, a potent mutagen and carcinogen.

"It would seem unlikely that any person could be a renowned authority on paintings and fine artworks, synthetic chemistry, science history, and running a major science-based corporation. But I can say, 'Yes, it's possible,' and that person is Alfred Bader."

—ELIAS J. COREY, EMERITUS PROFESSOR OF CHEMISTRY, HARVARD UNIVERSITY

& MORE ONLINE Watch chemists share fond, and sometimes funny, recollections of the Aldrich Handbook, http://cenm.ag/bader.

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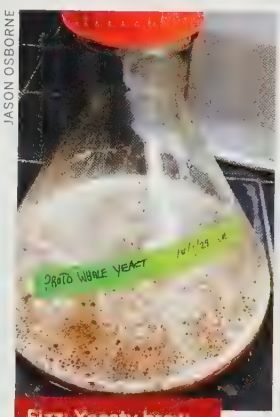
FOSSIL-INFUSED BEER, 75 MILLION-YEAR-OLD TURTLE BONES

If you're an aficionado of **CRAFT BEERS** made from ancient relics, then you will be happy to know that Lost Rhino Brewing in Ashburn, Va., is cooking up 650 gal of beer made with yeast teased from a 35 million-year-old whale fossil. It should be on tap at the end of May.

To be known as Bone Dusters Paleo Ale, the thirst-quenching mind-bender is the brainchild of two scientists: Jason Osborne and Jasper Akerboom. Osborne, a mechanical engineer at the Janelia Farm Research Campus of Howard Hughes Medical Institute, was looking for a way to get people to talk about science while throwing back a cold one. As an amateur paleontologist and cofounder of the fossil-hunting group Paleo Quest, he hit on the idea of trying to recruit some yeast residing on fossils to make the beer.

For that task he enlisted Akerboom, a microbiologist at Janelia Farm, who has a passion for home-brewed beer made with the wild yeast he collects. Akerboom swabbed Paleo Quest's collection in search of yeast with just the right stuff for making a good brew. He found it hanging on to a protocetid whale fossil: a yeast variant he has named *Saccharomyces cerevisiae* var. *protocetus* after the whale.

& VIDEO ONLINE



JASON OSBORNE

Fizz: Yeasty brew from a whale fossil.

Oddly, Osborne and Akerboom already have some competition from a brewer who claims to have captured 45 million-year-old yeasts from the gut of an amber-enrobed bee. In 2008, medical mycologist and Fossil Fuels Brewing Co. co-owner Raul J. Cano launched a line of beer from his Manteca, Calif., brewery using the antediluvian organisms. Osborne questions the likelihood of reviving 45 million-year-old yeast, but he says it sounds "pretty damn cool."

Still, such a yeasty froth of beer-brewing possibilities makes for a heady mix. In September, Akerboom plans to go full-time at Lost Rhino and hopes one day to have his own business: JasperYeast.

Analytical chemist Gregory Harpel doesn't have a bone to pick with anyone, and he wasn't having a cold one when he found a **TURTLE BONE** fossil that was missing for nearly 200 years. Like Osborne, he is also an amateur paleontologist.

Looking for fossilized shark teeth along a creek in Monmouth County, N.J., Harpel says he saw an odd protuberance in the grass. He thought it looked like a rock at first, but he went to examine at it anyway. "It wasn't a 'Lord of the Rings' moment," he says, referring to the ring-finding scene in the blockbuster fantasy movies based on the works of author J. R. R. Tolkien. "But it had the characteristics of a bone."

ACADEMY OF NATURAL SCIENCES/DREXEL U

Reunited: Bone fragments found almost 200 years apart are a match.

So he took the bone to the New Jersey State Museum. There, David Parris, the museum's curator of natural history, joked that it must be the other half of a limb now at the Academy of Natural Sciences at Drexel University in Philadelphia. First described in 1849 by naturalist Louis Agassiz, the limb at the academy was the only known specimen of a giant sea turtle, *Atlantochelys mortoni*. As it turns out, Parris was right. The two halves were a match.

The discovery gives scientists more information about *A. mortoni* than they had before. With the complete limb, they figure the animal, which roamed Earth 75 million years ago, was 10 feet from tip to tail, making it one of the largest sea turtles ever known.

Harpel donated the bone to the New Jersey museum. "I didn't want it sitting in my sock drawer," he says.

MARC REISCH *wrote this week's column. Please send comments and suggestions to newscripts@acs.org.*

Project SEED offers a bright high school student from an economically disadvantaged family the rare opportunity to engage in college-level research under the supervision of a volunteer scientist mentor. When you donate to Project SEED, you give 100% to a student stipend. Without your help, a student who could have had this life changing experience will not. Provide a pivotal scientific opportunity for an eager young mind.

Special Thanks to the Baders

On behalf of Project SEED students and mentors, we extend our deepest gratitude to Alfred and Isabel Bader for their long-time and dedicated support of summer research stipends and college scholarships.

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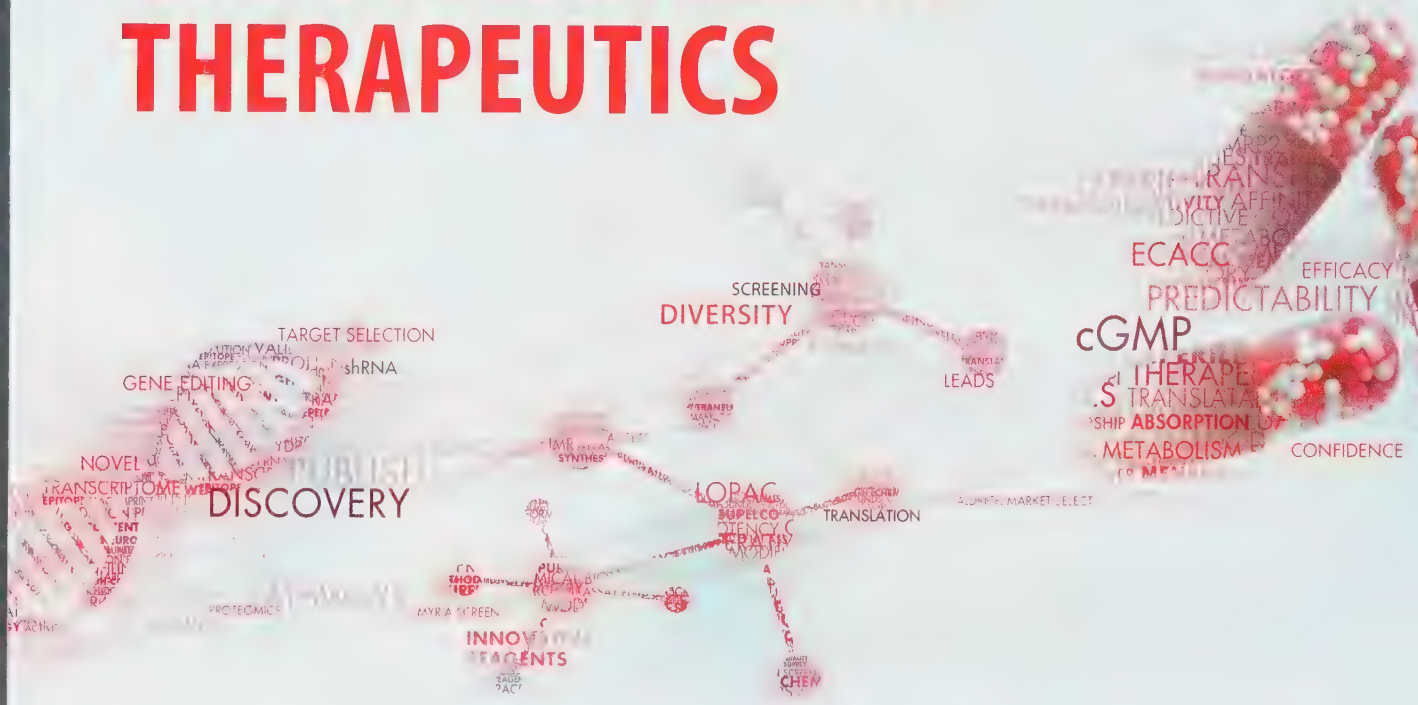

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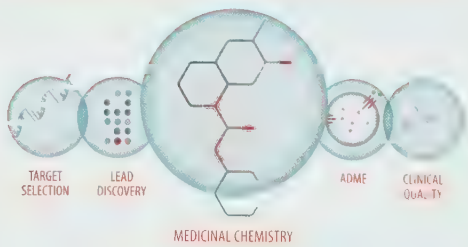

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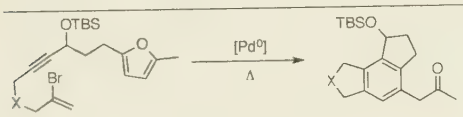
A new approach to the synthesis of highly substituted aromatic rings: the palladium mediated cascade approach.

Philip J. Parsons*, James A. Pryke, Alex C. Padgham, Clive S. Penkett, Matthew Renshaw and Steven Baker

Department of Chemistry, Imperial College of Science and Technology, London SW7 2AZ.

Supporting Information Placeholder

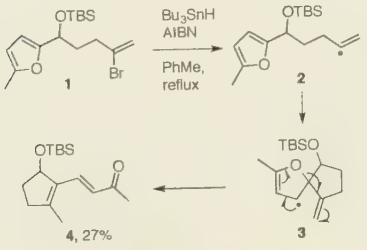
Dedicated to Dr.Alfred Bader on the occasion of his 90th Birthday



ABSTRACT: Pentasubstituted aromatic rings to serve as templates for drug design can be conveniently prepared by a palladium mediated cascade reaction. Treatment of a range of substituted forms bearing an alkenyl bromide linked to an alkyne tether were found to undergo palladium mediated cascade cyclisation reactions to form highly substituted benzene rings.

The discovery of cascade reactions has played an important role in shaping modern organic synthesis;[1] this technique has highlighted the concept of "atom economy"[2] and has made available routes to highly complex structures that have hitherto been more difficult to access. Numerous schemes have been devised to carry out cascade sequences, including radical,[3] thermal,[4] photochemical[5] and metal catalysed[6] reactions, as well as the more recent use of organocatalysis.[7] We have previously reported that carbon centred radicals can add in an intramolecular fashion to furans.[8,9,10] These investigations showed that substituted cyclopentenes can be formed following a cascade sequence which involved dearomatisation of the furan unit (Scheme 1).

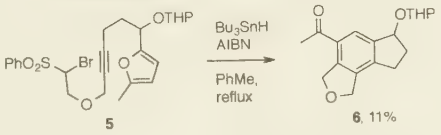
Scheme 1. Strategy for the synthesis of cyclopentadienes



Intramolecular addition of the alkenyl radical (2) to the furan resulted in the isolation of (4) which was formed by fragmentation of the spirocyclic intermediate (3). Pattenden et al. subsequently used this finding in an approach to fused tetracyclic ring systems.[11]

We further discovered that the sulfone (5) undergoes a radical mediated cyclisation to afford the pentasubstituted aromatic ring, albeit in very low yield (Scheme 2).[12]

Scheme 2. A radical cascade for the synthesis of polysubstituted benzenes



In view of the limited success of the radical mediated cascade, we elected to study the corresponding palladium catalysed reactions. Other groups had successfully used palladium salts in cascade reactions,[13] and we reported the use of palladium to form highly substituted aromatic rings and polycycles (Figure 1).[14]

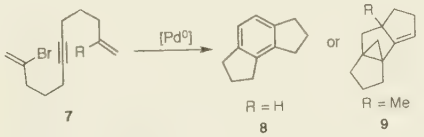


Figure 1. Palladium mediated polycyclic compound synthesis.

On the basis of these findings, we elected to evaluate the palladium assisted cascade cyclisation of substituted furans (Figure 2).

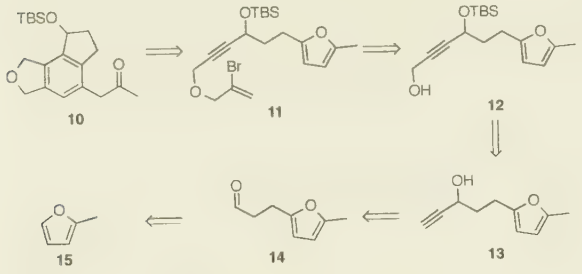
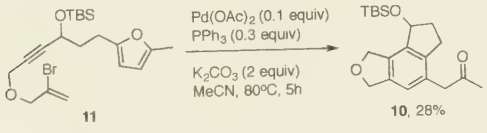


Figure 2. Retrosynthetic analysis for the construction of a pentasubstituted benzene.

Gold (III) mediated addition of methylfuran (15) to acrolein,[15] gave the aldehyde (14) (70%) which was converted into the alkyne (13) (69%). Conversion of the alcohol (13) into its TBS ester (73%) followed by base mediated addition of formaldehyde gave the alkynol (12) (69%). Treatment with sodium hydride in the presence of 2,3-dibromopropene gave the ether (11) (64%). With the desired cyclisation precursor (11) in hand, we investigated the palladium mediated cyclisation. We found, to our delight, that the desired cyclisation had taken place (Scheme 3).

Scheme 3. The palladium mediated cascade



Analysis of the reaction mixture by thin layer chromatography showed two major products, but on continued heating under reflux one product diminished and the ketone (10) was isolated in 28% yield. Further investigation of this interesting reaction suggested that the reaction proceeded through the cyclopentadiene (16) to furnish the ketone (10).

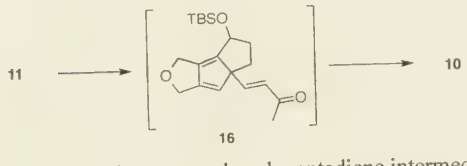
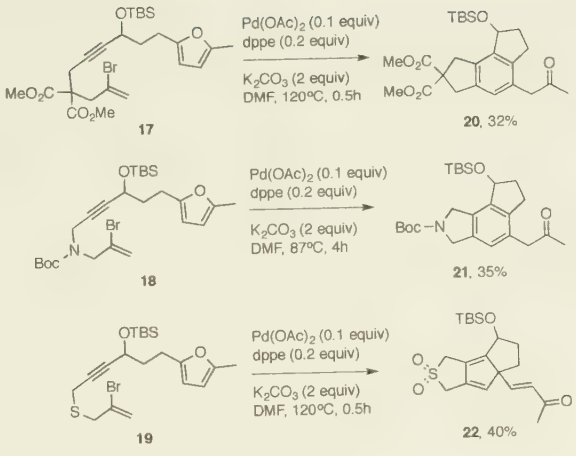


Figure 3. The proposed cyclopentadiene intermediate

Similar observations were made with the carbon (17) nitrogen (18) and sulfur (19) analogues (Scheme 4).

Scheme 4. Other examples of palladium mediated cascade reactions



The palladium mediated cyclisation of sulfide (19) was of particular interest; the cyclopentadiene (22) was the sole product. Oxidation of the sulfide had occurred during the cyclisation and further ring expansion was prevented due to increased ring strain induced by the presence of the sulfone moiety. The mechanism of the palladium mediated cyclisation is suggested in Figure 4.

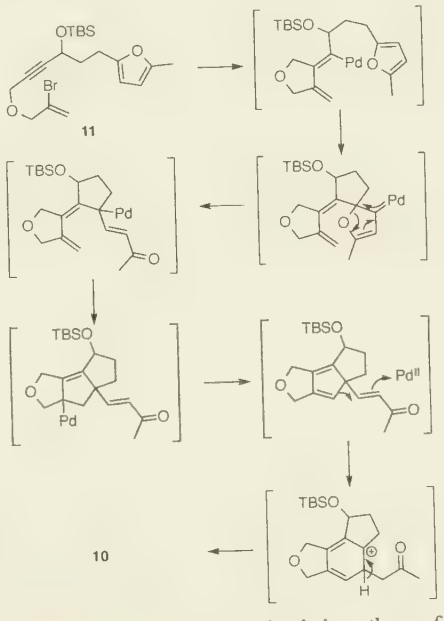


Figure 4. A proposed mechanistic pathway for the formation of substituted benzene rings.

Further investigations into the construction of highly substituted aromatic compounds are the subject of ongoing research.

ASSOCIATED CONTENT

Supporting Information

Experimental procedures and compound characterization data. This material is available free of charge via the Internet at http://pubs.acs.org.

AUTHOR INFORMATION

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ACKNOWLEDGMENT

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DOWNLOADING DISTANCE ED IN INDIA

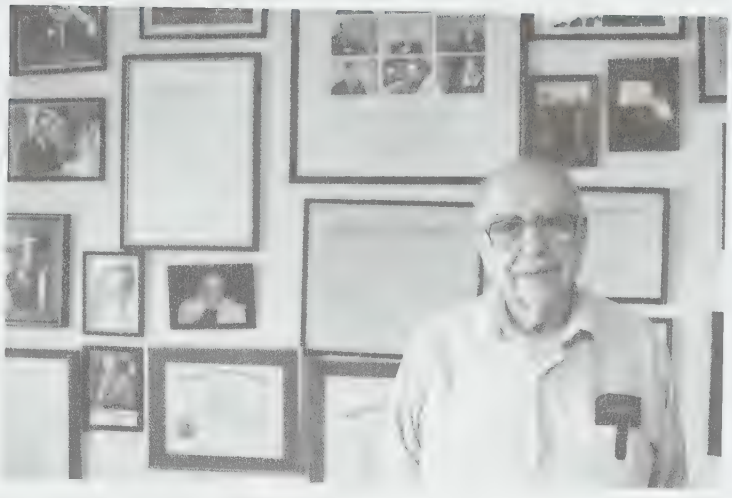
Wisconsin Distinguished Professor Pradeep Rohatgi visited India in March to expand collaborative agreements between UWM and Indian institutions. An agreement with R.V. College of Engineering in Bangalore was signed, providing engineering students the opportunity to study in Bangalore for three years and come to UWM for their final year.

Rohatgi brought back a draft agreement from the Council of Scientific and Industrial Research (CSIR), which runs a chain of 40 laboratories throughout India. Rohatgi had served as a founder-director of two of these laboratories, in Trivandrum and Bhopal.

Rohatgi visited the Central Scientific Instruments Organization (CSIO), one of the CSIR laboratories, in Chandigarh, Punjab. CSIO has offered its training center to start UWM educational activities in Chandigarh. CSIO has the capacity to download Internet courses relayed from UWM and provide adjunct instructors for UWM courses in Chandigarh.

R. K. Bajpai, director of CSIO and an internationally known researcher in advanced materials, will visit UWM to negotiate final agreements.

Also during his visit, Rohatgi did joint research and gave a seminar on recent advances in cast metal matrix composites at the Indian Institute of Technology in Kanpur. He established links to deliver UW System courses in Kanpur. Finally, he visited IIT Delhi. UWM signed a collaborative agreement with IIT Kanpur and IIT Delhi last year.



Joseph Neumann

Alfred Bader will teach a class on the Rembrandt Research Project in September.

I spy a Rembrandt! BADER PUTS PAINTINGS TO THE TEST

by Cathy Prescher

Alfred Bader's marriage of complementary professional pursuits has given him a unique set of skills to trace the authenticity of fine works of art.

As the founder of Aldrich Chemical Company in Milwaukee, which later became the Sigma-Aldrich Corporation, Bader traveled worldwide in his quest to add rare research chemicals to his catalog. Intertwined with his ventures were visits to antique stores, art galleries, and auction houses.

Bader, who is known throughout the world as a chemist-writer-lecturer, also is a respected art collector and dealer. He is exceptionally qualified to unravel the complexities of art world mysteries. After leaving Sigma-Aldrich eight years ago, he opened Alfred Bader Fine Arts in Milwaukee. While his gallery is known for its moderately priced selections representing several eras and styles, its specialty is Dutch masters.

University Outreach is pleased that Bader has agreed to contribute his time to teach "The Rembrandt Research Project and the Collector" for the Arts & Liberal Studies Program, 7 to 8:30 p.m. on Monday, Sept. 18, at the Grand Avenue.

Bader will discuss how the Rembrandt Research Project, led by eminent Rembrandt scholars, has examined almost all of the works attributed to the painter.

The project has published three volumes, grading the paintings "A" for accepted, "B" for in doubt, and "C" for not by Rembrandt. Their ratings have impacted the paintings' values.

During his talk, illustrated with slides, Bader also will discuss some of the decisions made by the scholars and their impact on the collector.

Registration for the program is $10. To register, call 227-3200 or 800/222-3623. For more information, call 227-3320.

Pradeep Rohatgi (left) and R. K Bajpai, director of India's Central Scientific Instruments Organization (CSIO), in the CSIO's Advanced Materials Laboratory at Chandigarh, Punjab. CSIO is interested in providing UWM courses at its training center over the Internet

UWM NEWS ON FILE

Recent clippings that relate to UWM, along with press releases generated by News Services and Publications, are available in the Golda Meir Library in a binder titled "UWM News" at the two-hour reserve desk (first floor, east wing).

RENEWED INTEREST IN NORSE CULTURE – NATIONWIDE AND AT UWM

were interacting with other cultures, perhaps as mercenaries," says Davis. "It points to a metropolitan situation."

The standard theory is that runes were derived from the Romans' Latin alphabet. But the papers presented at GLAC6 cast doubt on that and place the use of runes before Latin.

■ Based on the inscriptions on two bronze helmets discovered in the early 19th century in Slovenia, Tom Marky of Arizona State University believes that runes can be traced to language and symbols borrowed from the Etruscans (an ancient culture centered in northern Italy that predated the Roman civilization). His research suggests that runes also may have been influenced by Celtic writing and had their origins in an urban melting pot where several cultures would have mingled over long periods. Because of their mobility, ancient Germanic peoples who were the ancestors of the Vikings most likely shared company with Celts and Etruscans beginning about 200 A.D.

■ Seiichi Suzuki of Kansai Gaiai University in Japan presented his belief that the earliest written use of one runic symbol found on a bracteate in Suffolk, England, in 1981 can be traced to a cultural identity symbol of Lower Saxony. Suzuki, one of the conference keynote speakers, determined that the symbol was created to represent an evolved sound in the language and believes it was actually made far south of where it was found.

The research is important because it helps identify where Norse people traveled and what routes they took to return home: Their everyday accoutrements, emblazoned with writing, were left along the way.

In her summer course, "Vikings and Violence," Watson-Madler and her students are studying culture, history, and legends of the Viking age. "Ultimately," she says, "the course is meant to give a more honest picture of the Vikings than just the violence."

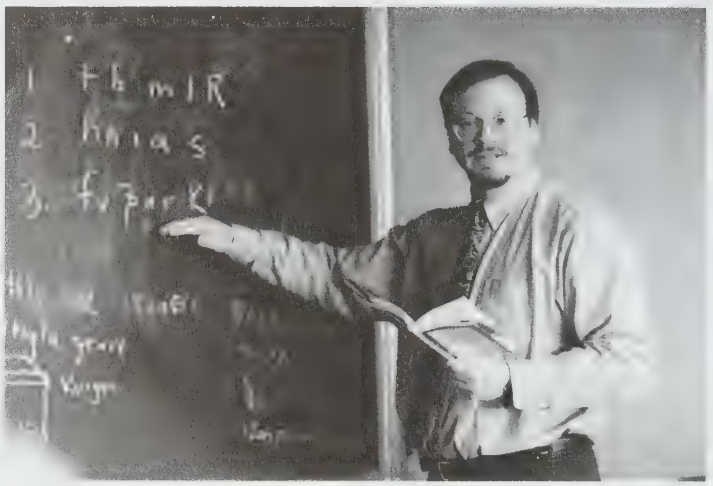
Vikings are often stereotyped, says Davis, since the term "Viking" derives from the Norse term for "raider." The Vikings were a segment of a much larger population, the Norse people, most of whom were traders, explorers, and farmers. The Norse constitute the descendants of the northern branch of the Germanic peoples, and are related to the Anglo-Saxons and Germans.

True, Vikings did attack foreign outposts and monasteries. It was considered a great honor to go abroad and an even greater honor to die in battle.

Not all sailed for the thrill or piracy of it. Many traveled simply to trade. They traded with the East and met other traders from as far away as Arabia.

Iron was the source of their strength because it allowed them to forge tools and weaponry, but they also liked to adorn themselves with jewelry, belts, and other personal items.

By the year 800 the people had become geographically separated. Gradually, their use of runes gave way to the Latin alphabet as more and more were converted to Christianity. Ironically, what we know of the Vikings was recorded beginning in the 14th century by writers who were using the Latin alphabet to translate the Norse language.



Photography by Alan Magayne-Roshak

Garry Davis, coordinator of the German program, discusses the new scholarship on runes, ancient Germanic writing, with a summer class.

WHAT'S HAPPENING?

Up-to-date information on campus and community events can be found on the Web at **www.uwm.edu/events** or by clicking on the UWM calendar link on the "News and Events" page.

WHAT'S THE CONNECTION?

UWM's Urban Connection Web site focuses on the university's urban partnerships and community work. The site can be accessed through the "Welcome" button on the UWM homepage, or directly at **www.uwm.edu/UrbanCon/collab.html/**.

The site includes a roster of some 200 community collaborations representing every school and college on campus. Entries can be sorted by topic, contact person, title, or school/college.

MOVIES UNDER THE STARS

FIFTH ANNUAL MILWAUKEE OUTDOOR EXPERIMENTAL FILM FESTIVAL

Milwaukee's Fifth Annual Outdoor Experimental Film Festival will be held Saturday, July 15, in Pere Marquette Park, corner of Old World Third and State Streets. The two-hour festival begins at sundown (approximately 9:30 p.m.) and is free and open to the public. UWM's Film Department is among the festival sponsors.

The program features short experimental films rarely seen outside museums and universities. The artists represented include the renowned and the yet to be discovered.

Among the works to be presented are "The Life of a Yeti" by the California painter Megan Whitmarsh; New York filmmaker Julie Murray's "Domain," and filmmaker and curator Brian Frye's "The Anatomy of Melancholy." Also on the bill are works by Matt McCormick, Naomi Uman, Mark Street, and others.

People are encouraged to come early with picnic baskets, lawn chairs, and blankets. For more information, phone Stephanie Barber, 374-4135; Carl Bogner, 229-4758; or the UWM Film Department, 229-6015.

APRIL 28, 2014

C&EN

CHEMICAL & ENGINEERING NEWS

CAPTURING CO_2
Enhanced oil recovery may be coal's unlikely savior **P.23**

NEW HUES
Exploiting nanostructure to create novel pigments **P.28**

HAPPY BIRTHDAY, DR. BADER

For more than 60 years, Dr. Alfred Bader has made his mark on the world of chemistry. But the Aldrich Chemical Company founder and avid art collector's impact has been far broader than the world of science. That's why we're proud to wish him a very happy 90th birthday.

Alfred, which he prefers over his more formal title, has made immeasurable contributions to the worlds of chemistry, art and biblical history, which he has studied for most of his life. He believes in the difference one person can make, and has used his considerable success to support organizations that make an impact in their communities.

Happy Birthday, Dr. Bader. Or, shall we say, Alfred. On behalf of Sigma-Aldrich, thank you for all you've done to make a difference in the scientific community and beyond.

Photo courtesy of Alfred Bader

Dr. Bader, 2005

To wish Dr. Bader a Happy Birthday, sign our electronic guest book:
Aldrich.com/acta471-bader

Acquisitions alter size, not ranking **P.10**

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SIGMA-ALDRICH

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CAPTURING CO_2
Enhanced oil recovery may be coal's unlikely savior **P.23**

NEW HUES
Exploiting nanostructure to create novel pigments **P.28**

TOP INSTRUMENT COMPANIES

Acquisitions alter size, not ranking **P.10**

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C&EN

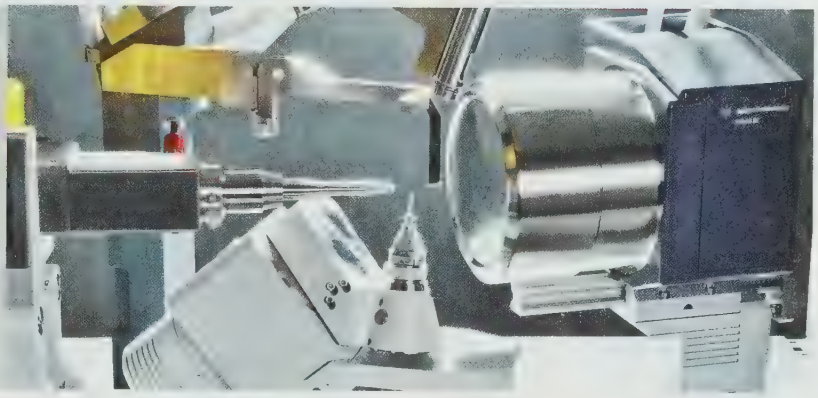
CHEMICAL & ENGINEERING NEWS

Serving the chemical, life sciences, and laboratory worlds

COVER STORY

TOP INSTRUMENT COMPANIES

The biggest firms in C&EN's annual ranking held on to top spots and grew organically and through acquisitions. PAGE 10



QUOTE OF THE WEEK

"It would seem unlikely that any person could be a renowned authority on paintings and fine artworks, synthetic chemistry, science history, and running a major science-based corporation. But I can say, 'Yes, it's possible,' and that person is Alfred Bader."

ELIAS J. COREY, EMERITUS PROFESSOR OF CHEMISTRY, HARVARD UNIVERSITY PAGE 34

NEWS OF THE WEEK

BUSINESS

GOVERNMENT & POLICY

SCIENCE & TECHNOLOGY

ACS NEWS

PEOPLE

THE DEPARTMENTS

COVER: *Close-up view of Agilent Technologies' GV1000 X-ray Diffractometer with the Atlas S2 CCD detector. Agilent*

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LETTERS

WHAT'S IN A NAME?

"OBSCURE CHEMICAL Taints Water Supply" features a timeline about MCHM (C&EN, Feb. 17, page 10). I remain mystified by the naming of the compound. The names of two separate compounds (4-methylcyclohexane and methanol) are simply joined together. Why isn't the name 4-methylcyclohexylmethanol a methanol derivative?
Charles Feldmann
Cincinnati

BREAKING GOOD, NOT BAD

ALTHOUGH the final episode of the Emmy Award-winning AMC television series "Breaking Bad" has aired, discussion of its influence on society continues. Questions range from "Will it increase interest in science generally among both U.S. students and the general public?" to "Will it encourage our younger generation to synthesize meth?"

Students sometimes can't distinguish between fact and fiction. Students see negative characteristics in Walter White, the fictional high school chemistry teacher portrayed on "Breaking Bad." Then they wonder if their own real-life high school teachers have similar characteristics. Students have reportedly asked high school teachers, "Do you make meth?"

Being confronted with such a negative parallel can be disappointing. But such a teachable moment can be transformed into an opportunity to demonstrate the good that chemists do.

One can point to personal experiences and those of other chemists in sometimes heroic efforts to improve human lives. The visibility and high-quality narrative of "Breaking Bad" could greatly impact the image of chemistry teachers.

Without commentary and interpretation, young people might infer that chemistry teachers spend their evenings cooking methamphetamine. What will be the perception of our students?

We can confront the issue head-on and inspire rather than apologize. We can point out the ways in which chemists and chemistry teachers have shaped our world, making our contemporary society possible. When students ask this type of question, we should be ready. We want to inspire them to reach positive goals by offering positive role models.

We hope high school chemistry teachers will respond to such questions with, "We inspire, we persuade, and we teach." Therefore, "we are proud to be chemistry teachers."
Donna J. Nelson
Norman, Okla.
Sally Mitchell
East Syracuse, N.Y.

Note: Donna Nelson, a professor of chemistry at the University of Oklahoma, Norman, served as a science adviser to the producers of "Breaking Bad." Sally Mitchell is a teacher at East Syracuse Minoa High School.

TRANSPARENCY IS A GOOD THING

REGARDING "For Transparency's Sake," I see H.R. 4012 as a good thing overall (C&EN, Feb. 24, page 28). Given events over the past several years, it has become increasingly clear that there are multiple standards for "transparency." The environment is an omnipotent yet fragile force that can affect the lives of everyone around the world. As such, we should not put our trust in black-box scientific results.

The article speaks of "patient privacy rules," but it is my understanding that, in order to have a patent, detailed disclosure is required so anyone can verify its claims. Software patents protect the methodology that the code uses to attain a result, and a copyright can protect the duplication of the code itself. With these protections in place, I see no problem with full disclosure.

It is surprising that Rep. Suzanne Bonamici (D-Ore.) proclaims that secret data or secret software is "valuable" and the "best available science to inform regulatory actions" when she and the rest of us do not and cannot know how the results are attained. I am equally surprised that the Environmental Protection Agency had been making policy since 1990 based on two key studies that weren't available for scrutiny. So on what basis do we make policy decisions? On the words of a few researchers?

How about we just accept the words of researchers from pharmaceutical companies instead of requiring proof of drug safety and efficacy before approval? The Food & Drug Administration requires complete information disclosure of all clinical subjects for drug approvals. EPA can require the same for the studies on which its policies are based. EPA can easily code subject

identity of any study for the purposes of public disclosure.

Whoever owns the modeling software leased (no doubt at a high price) to EPA should get a patent and a copyright and release the information required for public transparency. I want to know why I should trust their model, especially if it affects the environment. Frankly, I don't trust politicians or agencies that do not care to know the workings behind the science from which they make policy.

Pete Nirchio
Lebanon, N.J.

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RECONSIDERING ETHANOL

THE PATENT PICKS item "From Cellulosic Ethanol to Butanol" begins with the statement, "Blending ethanol into gasoline oxygenates the fuel, reduces pollution, and stretches petroleum supplies" (C&EN, Feb. 24, page 39). This statement is wrong on two counts.

First, ethanol-containing fuel may create less pollution per gallon of fuel burned, but because it requires more fuel to drive 1 mile, it actually calculates to create more pollution per mile driven.

Second, numerous studies show the total energy required to grow the corn, convert it to ethanol, transport it to the refiners, and blend it into the fuel is greater than the energy generated. So we actually end up having to import more petroleum when using ethanol in gasoline than when using straight gasoline.

Your statements are commonly made by the businesses that benefit from the ethanol and corn business, but I would hope a science magazine would get the science right.

David Berkebile
Landenberg, Pa.

A 'KNEADED' CONSIDERATION

AS INSIGHT into the desirability of using azodicarbonamide in bread making, consider how many of C&EN's readers would use this ingredient when making bread for themselves (C&EN, Feb. 17, page 9). Few would, I daresay. There are two reasons: First, it is unnecessary. Although it functions as a dough conditioner, azodicarbonamide's purpose is to decrease the cost of making large amounts of bread quickly. Second, with the notable exceptions of salt, water, and a few necessary minerals, many people, if not most, find the use of ingredients in their food that are not derived by simple processes from living things to be offensive.

The focus solely on the safety of ingredients is often used to frame the discussion of an issue so as to preclude consideration of this second point as a valid reason for opposition to their use. This is usually followed up by claims that the public is uneducated in such matters, implying that they are not fit to make decisions about what they eat.

David Lane
Davis, Calif.

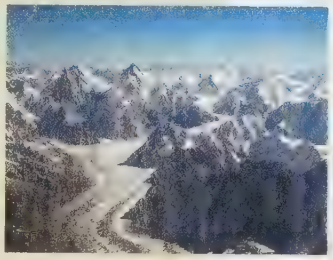
& THIS WEEK ONLINE

Speaking Of Chemistry

To showcase its most intriguing stories in minutes, C&EN has launched a Web-based program, Speaking of Chemistry. In the most recent podcast episode, C&EN Associate Editor Lauren Wolf and Senior Editor Carmen Drahl present highlights from stories on ways to make spider silk without spiders, the health risks of e-cigarettes, and milk proteins used as flame retardants.
http://cenm.ag/two43

Tracing The Loss Of Himalayan Glaciers

Scientists want to estimate how fast glaciers in the Himalayas are disappearing. But the task is difficult because of the region's treacherous terrain and high altitudes. Now, oceanographers report a new strategy that involves monitoring changes in the salinity and oxygen isotope composition of the Bay of Bengal, which receives most of the region's glacial meltwater.
http://cenm.ag/two44



GUILHEM VELLUT/ WIKIMEDIA COMMONS

Stories Of The Aldrich Handbook

When it's time to buy research chemicals, chemists usually reach for the Aldrich Handbook. But the catalog also has sentimental value for many chemists. This March, at the ACS national meeting in Dallas, C&EN Senior Editor Linda Wang asked chemists to share their favorite memories of using the ubiquitous catalog. Check out a video of their responses.
http://cenm.ag/bader

Antifungal Coating For Medical Devices

Fungal films coat surfaces around us, and a fog of microscopic spores permeates the air. For people with compromised immune systems, some opportunistic fungi species can start dangerous infections. To combat one hot spot for invading fungi, a team of researchers has developed a coating for the rubber surfaces of medical devices that releases antifungal drugs when fungi are present.
http://cenm.ag/two45

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OVERVIEW

Monitoring and maintaining water purity are important to the power and electronics industries. In the both of these industries, impurities must be minimized and monitored to prevent corrosion or scaling, and degradation in demineralization processes. Corrosion on a power plant scale can be catastrophic: broken pipes, leaks, contamination, costly unplanned maintenance, and power interruptions. In the electronics industries, the impurities can be just as catastrophic, causing contamination, production problems, and product failures.

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- Demonstrate Thermo Scientific IC innovations around simple analysis methods

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A GOOD LIFE Bader in his home office, with part of his art collection, in Milwaukee, in 2008.

DAVID BADER PHOTOGRAPHY

"Eighty years ago, when Alfred and I were in the same class in Vienna, I would never have imagined that he would become one of the great polymaths: scientist, yet religious; spectacular entrepreneur as well as even more spectacular philanthropist; sophisticated art dealer as well as major collector: all these boats sailing on a sea of chemistry!"

—CARL DJERASSI, EMERITUS PROFESSOR OF CHEMISTRY, STANFORD UNIVERSITY

CELEBRATING ALFRED BADER AT 90

C&EN lauds the **MYRIAD CONTRIBUTIONS** of the chemist, art collector, and philanthropist

LINDA WANG, C&EN WASHINGTON

ALFRED BADER MAY BE BEST KNOWN for cofounding Aldrich Chemical Co. (now part of Sigma-Aldrich) in 1951, and for being a preeminent art collector, but it's his enormous body of charitable work that may be his greatest legacy.

With his wife, Isabel, Bader has given millions of dollars to causes he's passionate about, including the American Chemical Society's Project SEED program, which provides scholarships to economically disadvantaged high school students to conduct hands-on research. In addition, since 1986, the Baders have supported an ACS national award, the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry.

In celebration of Bader's 90th birthday this month, C&EN reflects on the contributions of this multifaceted chemist, businessman, art collector, and champion for chemistry education. ■

CHEMICAL HERITAGE FOUNDATION

The Aldrich Handbook, which lists research chemicals for sale, is recognizable by the beautiful artwork on its covers. The 1967-68 edition of the catalog was the first to feature a painting from Bader's art collection: "The Quill Cutter" by Paulus de Lesire.

"No one on this planet has done more to further chemists' capabilities and all chemical industries' ability to grow."

—K. BARRY SHARPLESS, W. M. KECK PROFESSOR OF CHEMISTRY, SCRIPPS RESEARCH INSTITUTE CALIFORNIA

"Alfred Bader's name is synonymous with helping chemists to make molecules; furthermore, his support through awards, fellowships, and scholarships is unwavering. But more than that, Alfred, with Isabel at his side, has touched all whom he has met with enthusiasm about their work and a zest for life."

—VICTOR SNIECKUS, BADER CHAIR EMERITUS IN ORGANIC CHEMISTRY QUEEN'S UNIVERSITY, ONTARIO

"Please bother us."

THIS STATEMENT BY ALFRED BADER BECAME ASSOCIATED WITH ALDRICH CHEMICAL CO., WHICH TOOK PRIDE IN TALKING WITH ITS CUSTOMERS.

"The Bader Scholarship was instrumental in allowing me to put more emphasis on my classes instead of thinking of the financial burden I might be to my parents. Thank you, Mr. and Mrs. Bader, for investing in my education."

—ANITA HURTADO, FORMER BADER SCHOLAR, NOW ASSOCIATE DIRECTOR IN THE SUPPLY-CHAIN ORGANIZATION AT MERCK & CO.

JOHN STALEY PHOTOGRAPHY

Alfred and Isabel (center) are surrounded by former Bader Scholars during a reunion reception at the spring 2005 ACS national meeting in San Diego.

"Alfred and Isabel Bader's generosity has manifested itself at ACS in countless ways—and there are countless successful chemists who owe their careers to the investments that these two astonishing philanthropists made in Project SEED and the Bader Scholarships."

—MADELEINE JACOBS, ACS EXECUTIVE DIRECTOR AND CEO

JOHN STALEY PHOTOGRAPHY

Alfred with Isabel (left) and ACS Executive Director and CEO Madeleine Jacobs during the Bader Scholars reunion reception at the spring 2005 ACS national meeting in San Diego.

$1.7 million

The amount Alfred and Isabel have donated to ACS since 1986, with $1.3 million going toward the Alfred & Isabel Bader Scholars under the Project SEED program. Roughly 20 students each year receive one of these $5,000 scholarships.

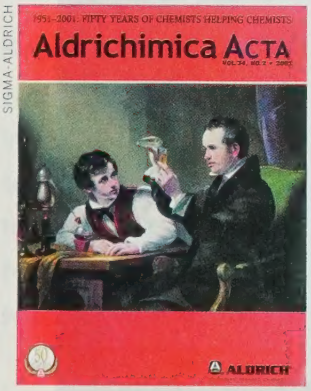
385

Number of Alfred & Isabel Bader Scholars to date.

68,000

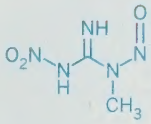
Approximate number of research chemicals in the Aldrich Handbook today.

SIGMA-ALDRICH



In addition to the Aldrich Handbook, Bader also started the journal Aldrichimica Acta, *which focuses on organic chemistry research.*

ALDRICH CHEMICAL CO.'S FIRST CHEMICAL:



N-Methyl-*N*′-nitro-*N*-nitrosoguanidine, which was used in the preparation of diazomethane. MNNG was marketed through the company's first catalog, in 1951, a one-page document that grew to become the Aldrich Handbook. Sigma-Aldrich no longer sells MNNG, a potent mutagen and carcinogen.

"It would seem unlikely that any person could be a renowned authority on paintings and fine artworks, synthetic chemistry, science history, and running a major science-based corporation. But I can say, 'Yes, it's possible,' and that person is Alfred Bader."

—ELIAS J. COREY, EMERITUS PROFESSOR OF CHEMISTRY, HARVARD UNIVERSITY

& MORE ONLINE Watch chemists share fond, and sometimes funny, recollections of the Aldrich Handbook, http://cenm.ag/bader.

Project SEED offers a bright high school student from an economically disadvantaged family the rare opportunity to engage in college-level research under the supervision of a volunteer scientist mentor. When you donate to Project SEED, you give 100% to a student stipend. Without your help, a student who could have had this life changing experience will not. Provide a pivotal scientific opportunity for an eager young mind.

Special Thanks to the Baders

On behalf of Project SEED students and mentors, we extend our deepest gratitude to Alfred and Isabel Bader for their long-time and dedicated support of summer research stipends and college scholarships.

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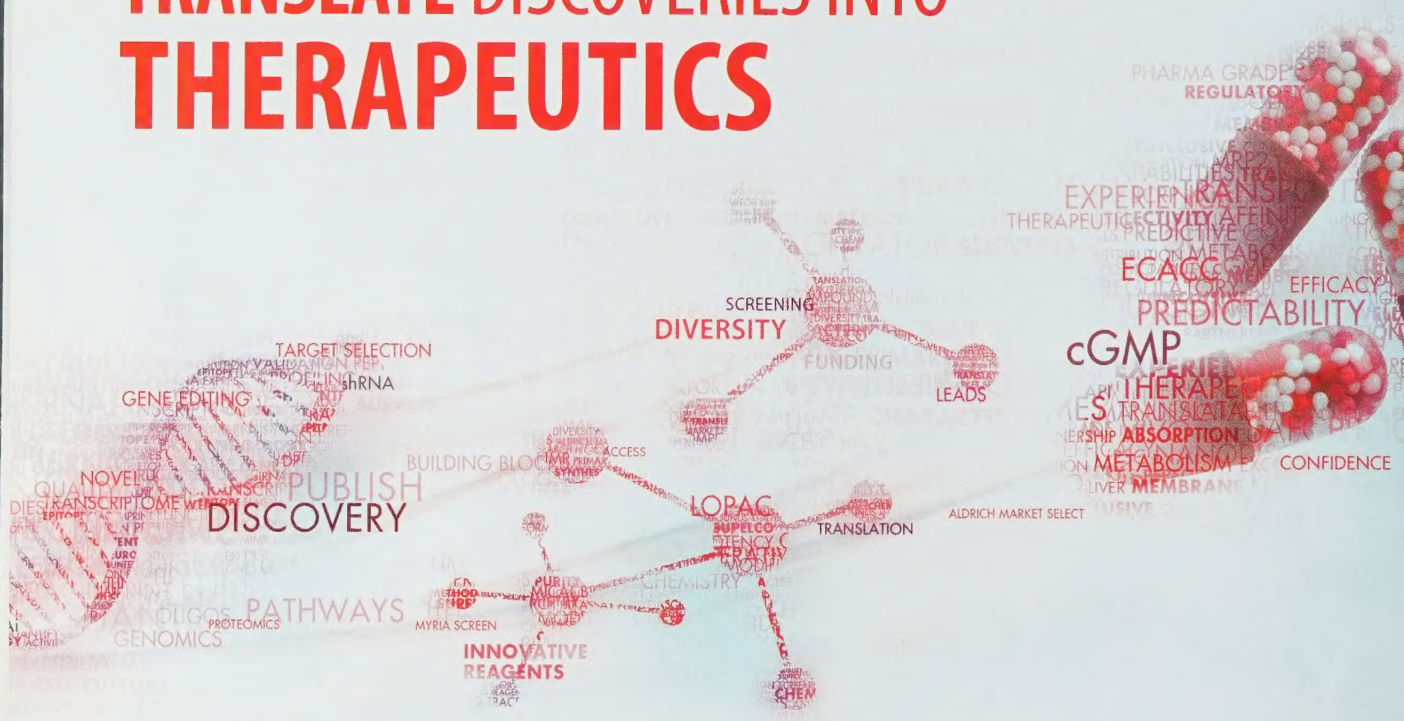

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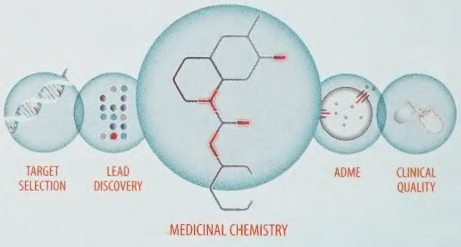

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