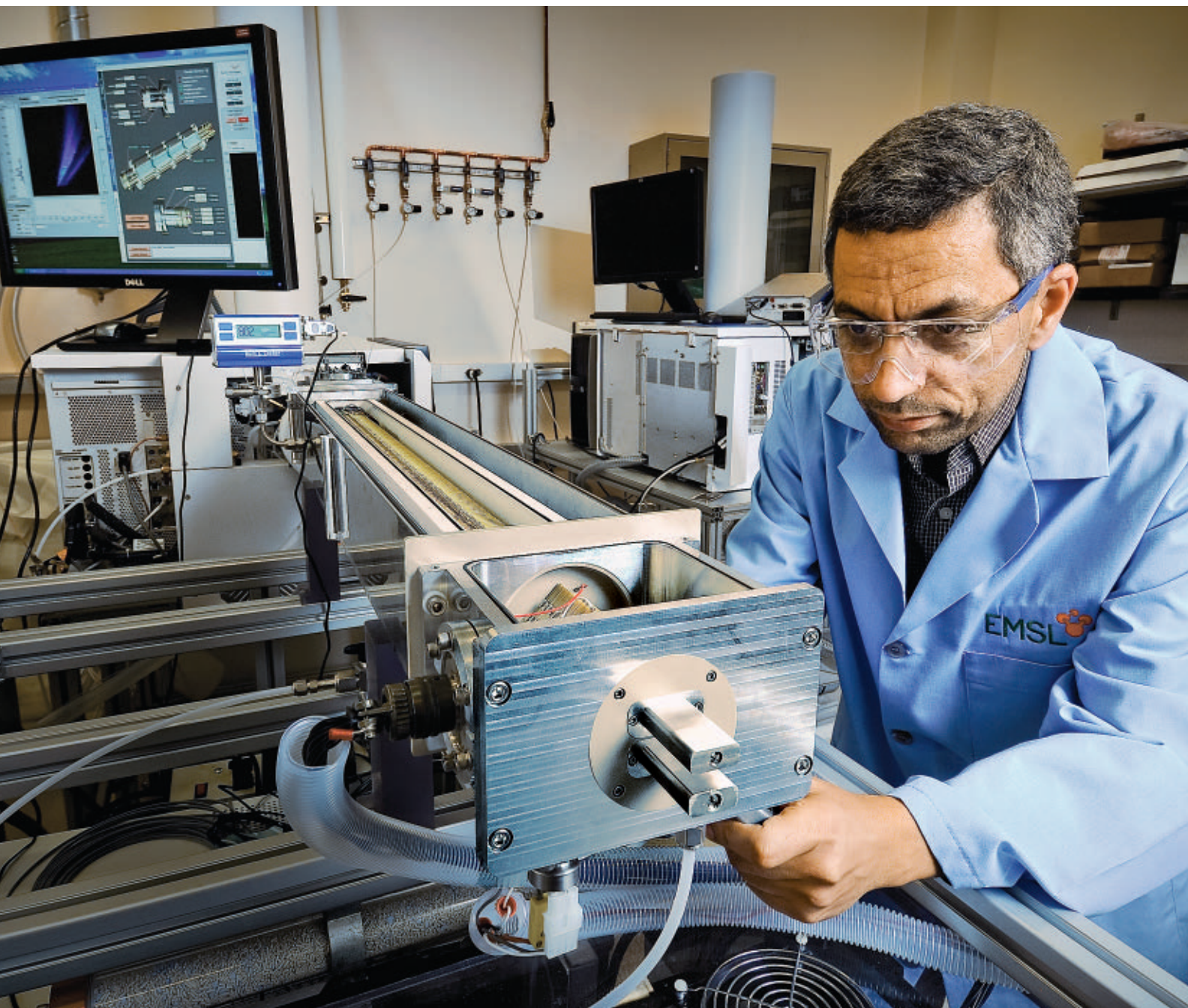
JUNE 21, 2010

C&EN

CHEMICAL & ENGINEERING NEWS

DRUG SAFETY
Recall triggers push for new legislation **P.22**

PREVENTING CANCER
The hunt for natural agents is still on **P.28**



MASS SPECTROMETRY

New options for high resolution **P.10**

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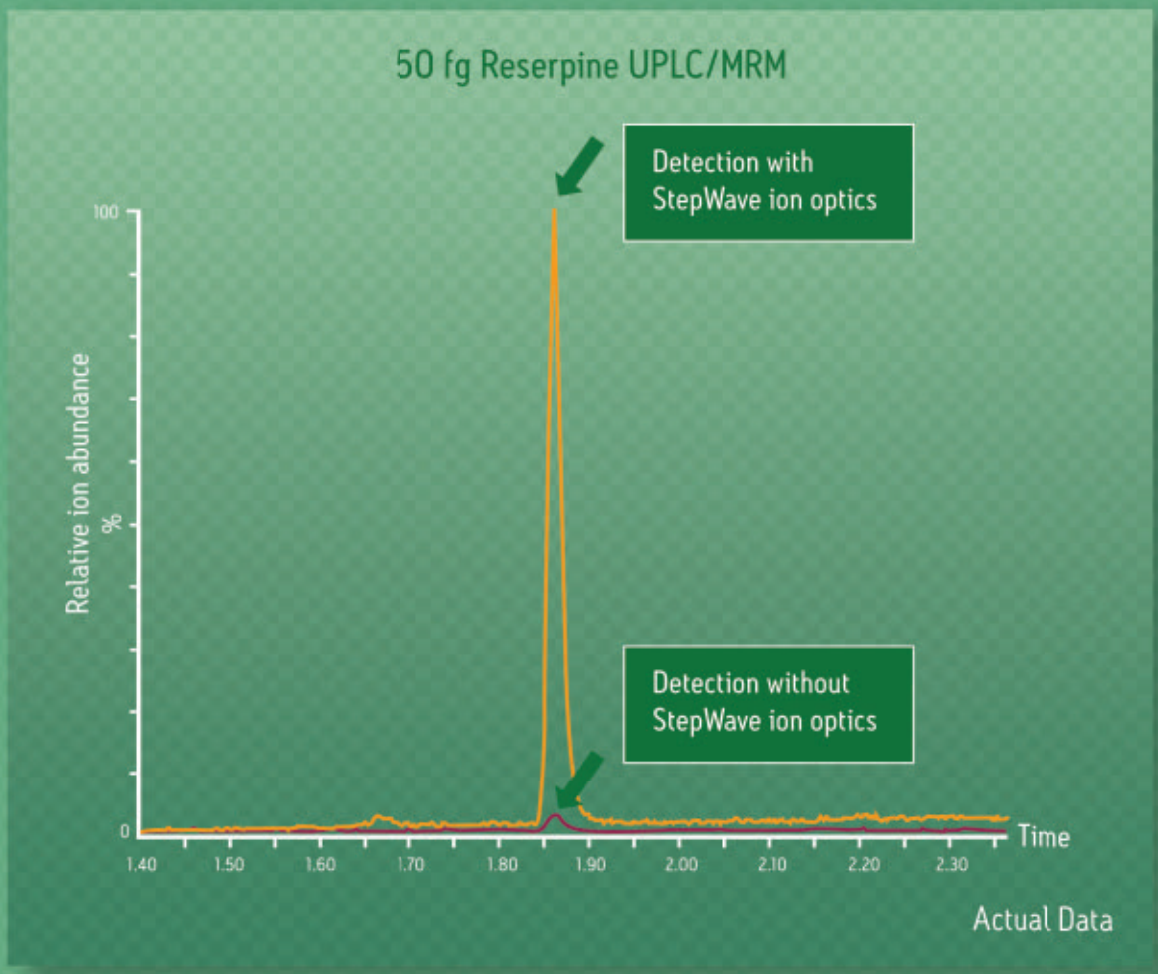

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JUNE 21, 2010

C&EN

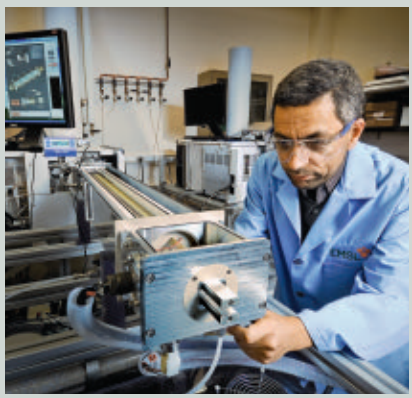
CHEMICAL & ENGINEERING NEWS

Serving the chemical, life sciences, and laboratory worlds

COVER STORY

HIGH-RES MASS SPEC

Instruments with increased resolving power and accuracy give users more choices than ever before. PAGE 10



QUOTE OF THE WEEK

"We have to make sure that what we have invested in ourselves pays off."

GILLES A. COTTIER, PRESIDENT, SAFC

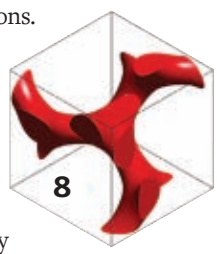
PAGE 19

NEWS OF THE WEEK

BUSINESS

GOVERNMENT & POLICY

SCIENCE & TECHNOLOGY



EDUCATION

THE DEPARTMENTS

COVER: *Yehia Ibrahim is part of a team that is coupling ion mobility with time-of-flight mass spectrometry for high-resolution proteomics measurements at Pacific Northwest National Laboratory's Environmental Molecular Sciences Laboratory. Scott Butner/PNNL*

& THIS WEEK ONLINE

WWW.CEN-ONLINE.ORG

BOSTON NATIONAL MEETING

Look for the Preliminary Program of the 240th ACS national meeting in the June 28 issue and find information online now at www.acs.org/boston2010.

PLUS: A collection of safety letters submitted by readers is available at www.cen-online.org/safety.

YOU'VE SOURCED A GREAT NEW SUPPLIER IN CHINA:

BUT WHO'S THEIR SHIPPER?

WHEN CAN THEY COLLECT? HOW MUCH?

HOW FAST? WHO'LL TRACK IT?

WHAT ABOUT DUTIES AND TAXES?

HOW MANY INVOICES?

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MERITS OF UNDERGRADUATE RESEARCH

ONE BENEFIT of teaching in a relatively small two-year college is the opportunity to seek out and challenge willing students to undertake undergraduate research (we call it independent study). Even with meager funds, and a bit of ingenuity, a teacher can come up with a project to engage a student willing to do a little extra. These small projects often pay off in a publication or at least an extra "bonus" on a transcript for transfer to a four-year college, or to a job. Two examples follow:

■ In one fascinating project, two students examined the effects of glucosamine and chondroitin on cartilage. (The cartilage was obtained, without cost, from a local grocery store). One student went on to study chemical engineering and the second went to pharmacy school.

■ In a second example, two students examined the UV-Vis spectra of Oriental teas: black tea, green tea, oolong tea, and white tea. These student researchers went on to study medicine.

Not only were such projects stimulating for students, they were also stimulating to their mentor. In education, we bemoan the lack of interest in science, mathematics, and engineering. Perhaps the way to stimulate students to consider science careers is to introduce short, easy-to-carry-out projects at the undergraduate level.

Jane Slezak
Johnstown, N.Y.

REVISITING NUCLEAR POWER

WARREN REYNOLDS' negative assessment of the status of nuclear power is badly out-of-date (C&EN, May 3, page 4). Sweden and Germany have indefinitely postponed (though not officially canceled) their scheduled phaseout of nuclear power. Spain has set no timetable for a phaseout. The Italian government has reversed its no-nuclear policy of 23 years and is in active discussions with French nuclear construction companies. The United Arab Emirates has contracted with the South Koreans for four new plants, and the Netherlands, Slovenia, and Vietnam are officially considering nuclear power construction. Finland is considering additional nuclear plants, despite the difficulties with the one presently under construction.

Meanwhile long-term construction programs are continuing in Russia, South Korea, Japan, China, and India, with several reactors completed each year. Argentina, France, Pakistan, Romania, and Taiwan each have one or two plants under active construction.

Construction costs have risen dramatically for all types of projects in recent years, which particularly affects nuclear and wind energy. Cost estimates in 2008 for new nuclear plants constructed in the U.S. were around $6 billion to $9 billion for a 1,000-MW Westinghouse AP1000 plant.

John E. Tanner Jr.
Idaho Falls, Idaho

NOT SO CURIOUS FLOW CHEMISTRY

"FIRMS ADVANCE Flow Chemistry" by Michael McCoy was quite interesting, but I was surprised to learn that continuous-flow chemistry is only now "growing beyond a laboratory curiosity" (C&EN, May 24, page 10).

On the basis of my limited exposure to bulk chemical manufacturing some 50 years ago, I assumed flow chemistry was widely used today in the high-volume chemical manufacturing business. In 1959, I began my career as an analytical chemist for Ultra Chemical Co., a small specialty chemical manufacturer in Paterson, N.J., and a subsidiary of Witco Chemical Co. One of the company's major products was sodium dodecylbenzene sulfonate, a major ingredient of the laundry detergents used in the 1960s. This material was routinely made in a 20,000-gal vessel by reacting dodecylbenzene with concentrated sulfuric acid. The resulting dodecylbenzene sulfonic acid was then neutralized with sodium hydroxide solution to form a viscous, opaque liquid termed "paste," which was then pumped to a spray tower to create the flakes or powder for packaging.

To increase productivity, the company's chemical engineers designed and built a pilot plant in 1961 to manufacture the material in a continuous-flow process. In that process, the reactants were separately pumped into a long stainless steel tube where the reaction took place. At the point along the tube where the sulfonation was complete, sodium hydroxide

solution was introduced and the resulting "paste" pumped up to the spray tower.

I analyzed samples of the reaction mixture at various points in the flow process so chemical engineers could make adjustments to reactant flow rate and temperature to optimize yield and throughput. The pilot plant was quite successful, and I believe this process was put into full production shortly thereafter. I left the company in 1962 for graduate school and spent the balance of my career in research and development. However, since that continuous-flow process went so smoothly all those years ago, I assumed the technique had spread throughout the industry for other bulk chemical production.

Joseph A. Castellano
San Jose, Calif.

WHAT'S IN A NAME?

I CONGRATULATE Carmen Drahl on her article on named chemical reactions, and especially for choosing a dramatic case: the Mizoroki-Heck reaction (C&EN, May 17, page 31). Both inventors had a cruel personal bend in their respective careers despite glamorous success and acclamation from the chemical community.

Tsutomu Mizoroki succumbed to pancreatic cancer only nine years after his breakthrough discovery of the palladium-catalyzed reaction. Richard F. Heck, despite an excellent publication record in ACS journals, lost funding, doesn't have a single entry in PubMed, and is relegated to the eternal waiting list for the Nobel Prize. I fully agree with Victor A. Snieckus that Heck's nomination for the Nobel Prize is overdue, also in remembrance of Mizoroki.

Raffaello Masciadri
Münchenstein, Switzerland

THE ARTICLE about named chemical reactions brought to mind my experience with a named reaction. More than 60 years ago, while trying to radiocarbon-label steroids, I chanced upon a previously unknown reaction. Hoping to retrieve a minuscule amount of product, I tried a method of direct introduction of radiocarbon into the steroid ring system.

Instead, the reaction went by an unusual intermediate directly into the steroid ring in almost quantitative yield and at the highest specific activity then possible. When I submitted this surprising finding in 1949 as a Comunication to the *Journal of the American Chemical Society*, it was turned down. I was asked to resubmit it as a Note.

That Note, which lay on the desk of the journal editor at Harvard, caught R. B. Woodward's eye and immediately I was called and asked for all the details. This reaction enabled him to introduce the last carbon into his steroid nucleus and go on to complete the total synthesis of cortisone. He gave me ample credit in his keynote talk and paper for my help. This reaction also made it possible for biochemists to establish cholesterol as the precursor of the steroid hormones in the body and to identify the intermediate steps in the biosynthesis of these hormones. Steroids labeled with C-14 by this method have found good use in biological science.

Perhaps because I was a lone organic chemist in a medical school, the only time I was asked to present my work to any department or established scientific group was at the International Congress of Organic Chemists in Zurich in 1955. I gave the opening paper attended by a front row of European Nobel Laureates. Also, although several footnotes mentioned the "Fujimoto reaction" in journals, it was probably not until a 1969 review article titled "The Fujimoto-Belleau Reaction" by J. Weil-Raynal was published in the journal *Synthesis* that this name appeared. This also recognized that Belleau had independently arrived at this reaction with a different compound and that his finding was published after my Note. As has been mentioned in your article, how a named reaction is received probably depends on science and politics.

George I. Fujimoto
San Diego

I ENJOYED the article on name reactions. I've admired these reactions ever since I ran my first Diels-Alder reaction in sophomore organic lab 50 years ago. I followed that up with dozens more both in undergraduate research (University of Minnesota, 1960–62, with W. E. Noland) and in grad school (Princeton, 1962–67, with E. C. Taylor). I guess this is my favorite reaction of all time along with other "no-mechanism" cyclization reactions. The latter would include the "ene" reaction (aka the Alder Ene reaction by J. J. Li).

I usually managed to get by on library copies of the name reactions books, but I did buy my own copy of Helmut Krauch and Werner Kunz's "Organic Name Reactions" in grad school, which I still have. More recently I managed to review Li's "Name Reactions," 3rd edition.

My first love in chemistry was organic synthesis, but my second was always chemical information. Prompted by a series of information-conscious mentors, I always eagerly did my own library/information research, even during my first two post-Princeton jobs when searching services were available. When those two jobs in pesticide synthesis dried up, I was offered a position as a technical information specialist at Amoco Corp. I've been a chemical info specialist ever since, even in (alleged) retirement.

My primary resource was *Chemical Abstracts*, and I helped grow the online chemical information industry from a user standpoint. This second and lasting chemistry love is probably why I've always been so fascinated with the likes of name reactions. Good to see someone else still is also.

Robert E. Buntrock
Orono, Maine

QUERY FOR READERS

C&EN is researching a story about the challenges and rewards of returning to the workforce after taking off an extended period of time to care for family members, including children or parents. If you have recently made this kind of move, C&EN would like to hear about your experiences. Please contact Susan Ainsworth at s_ainsworth@acs.org as soon as possible.

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C&EN
news of the week

JUNE 21, 2010 EDITED BY WILLIAM G. SCHULZ & ALICIA J. CHAMBERS

ZEWAIL WINS 2011 PRIESTLEY MEDAL

AWARDS: Nobel Laureate honored for development of ultrafast probe methods in chemistry and biology

AHMED H. ZEWAIL, the Linus Pauling Professor of Chemistry and Professor of Physics at California Institute of Technology and the 1999 Chemistry Nobel Laureate, has been selected to receive the 2011 Priestley Medal by the American Chemical Society Board of Directors at its June meeting. Zewail will be honored with ACS's most prestigious award in recognition of "his development of revolutionary methods for the study of ultrafast processes in chemistry, biology, and materials science."

Zewail's pioneering work in femtochemistry—the study of chemical processes on the femtosecond (10^{-15} second) timescale—established methodology for following the intricacies of chemical transformations as reactants evolve into products by way of fleeting reaction intermediates. His laser-driven "pump-probe" techniques, which were demonstrated initially on gas-phase reactions, captured "snapshots" of intermediates that existed for barely more than the femtosecond period of a molecular vibration.

The Zewail group's success in tracking gas-phase reactions with unprecedented time resolution motivated researchers worldwide to develop clever ways to apply pump-probe methodology to numerous chemical systems. The success also drove Zewail and his students to develop new types of ultrafast probe methods based on electron diffraction, crystallography, and microscopy (C&EN, Dec. 24, 2007, page 36).

Armed with this new generation of powerful tools, the Caltech team has captured spectra and close-up images and videos of crystal and surface phase transitions, hydration phenomena in biological macromolecules, and structural dynamics of bilayer membranes. And recently Zewail's group demonstrated a novel microscopy method for imaging protein vesicles and whole unstained cells with high contrast and nanometer resolution on the femtosecond timescale (*Proc. Natl. Acad. Sci. USA* **2010,** *107,* 9933).

"This work is changing not only what we know, but also how we think about the interplay of structure, dynamics, and function in molecular systems," says David A. Tirrell, a Caltech professor of chemistry and chemical engineering. Tirrell adds that the advances made by Zewail's group "are yielding qualitatively new insights into the atomic and molecular origins of complex chemical, physical, and biological behavior."

Rice University chemistry professor James L. Kinsey concurs. He notes that Zewail's discoveries are "opening up the new field of physical biology"—a discipline in which biologically important processes can be studied as never before at full atomic resolution on timescales ranging from femtoseconds to hours.

DOUGLAS A. LOCKHARD PHOTOGRAPHY

Even as Zewail's passionate commitment to fundamental science continues, in his words, to leave him awake at night thinking of ways to improve experiments, the Caltech scientist serves as a dedicated spokesman stressing the importance of science education. As a member of the President's Council of Advisors on Science & Technology and an enthusiastic science ambassador, Zewail travels widely, lecturing on what he describes as "the beauty and critical role of science in our lives."

The ACS Board also voted to award Michael E. Strem, president of high purity chemicals maker Strem Chemicals, the 2011 Charles Lathrop Parsons Award, and Zaida Morales-Martinez, emeritus professor of chemistry at Florida International University, the Award for Volunteer Service to ACS.

The Parson Award recognizes Strem for his contributions to the future of the chemical enterprise through innovative international programs for young chemists. It also acknowledges Strem's groundbreaking initiatives in forging new collaborations between business and education.

Strem is a cofounder of the Newburyport Education Foundation, set up in 1990 to foster collaboration between businesses in Newburyport, Mass., and local schools. Strem also helped create a U.S./German graduate student exchange program over the past decade through a joint effort of the German Chemical Society and the Northeastern Section of ACS.

Morales-Martinez has been a key figure in advancing diversity issues in ACS. She was instrumental in the establishment of the society's Committee on Minority Affairs in 1993 and has been an enthusiastic supporter of Project SEED and the ACS Scholars Program.—MITCH JACOBY AND MARC REISCH

"Even after all these years, the most rewarding thing for me is to see the sparkle in the eyes of all these young people learning about basic science. It still gets me very excited."
—AHMED ZEWAIL

CRITICAL PATH INSTITUTE

Woosley

DRUGMAKERS SHARE DATA

COLLABORATION: A collection of Alzheimer's disease trial results could speed drug development

SEEKING TO ACCELERATE the search for Alzheimer's disease cures, big pharma firms are drawing back the curtain on years' worth of patient data from clinical trials. The Coalition Against Major Diseases, a consortium that links drug companies, research foundations, patient-advocacy groups, and advisers from U.S. and European regulatory agencies, has established a publicly available database with information on more than 4,000 Alzheimer's disease patients from 11 clinical trials.

Companies contributing data include AstraZeneca, Abbott Laboratories, Johnson & Johnson, GlaxoSmithKline, Novartis, Pfizer, and Sanofi-Aventis. They are expected to eventually add data about patients with other brain diseases such as Huntington's and Parkinson's.

"Scientists from around the world will be able to analyze this new combined data from pharmaceutical companies, add their own data, and consequently better understand the course of these diseases," says Raymond Woosley, CEO of Critical Path Institute, a nonprofit funded by FDA that will manage the database.

The drug companies also have agreed to apply a common data standard for Alzheimer's disease when filing for drug approvals. The hope is that sharing data will improve clinical trial design and speed the identification of biomarkers of neurological diseases, helping to ensure that treatments are truly effective.

The participants' ultimate goal is to be able to identify people susceptible to neurological diseases before their symptoms emerge. After several failures of clinical trials involving patients with full-blown Alzheimer's, some neurologists have concluded that treatment can be effective only if started before the disease has advanced significantly.

The database is the latest in a string of collaborative efforts by pharmaceutical firms hoping to accelerate drug development. The scope and goals of the pacts vary. For example, Abbott, J&J, Eli Lilly & Co., Merck & Co., Novartis, and Pfizer are partners in Enlight Biosciences, a collaboration devoted to pulling transformative ideas out of academia.

Merck and AstraZeneca are conducting a trial to test a combination of two cancer drugs, AstraZeneca's AZD6244 and Merck's MK2206, that have yet to be approved. Recently, Lilly, Merck, and Pfizer said they would fund the Asian Cancer Research Group, a public pharmacogenomic database intended to speed development of treatments for cancer.—LISA JARVIS

ANTIBODIES AID NERVE REPAIR

NEUROSCIENCE: Lack of antibodies inhibits clearance of damaged tissue

STANFORD U.

Barres reports that myelin-targeting antibodies clear the way for repair of injured nerves.

ANTIBODIES ARE crucial for successful regeneration after nerve damage, reports a team led by Stanford University School of Medicine neurobiologist Ben A. Barres (*Proc. Natl. Acad. Sci. USA*, DOI: 10.1073/pnas.1001948107).

The finding may explain why nerve damage in the central nervous system (CNS), which lacks antibodies, isn't naturally repaired. By contrast, circulating antibodies can gain access to and help repair damage in the peripheral nervous system (PNS), which consists of nerve tissue outside the brain and spinal cord.

When the researchers began their study, they knew that myelin, a fatty insulator that coats the axon of nerve cells, is cleared rapidly from damaged nerves in the PNS but not the CNS. They also knew "the blood-nervous system barrier rapidly breaks down after PNS but not CNS injury," Barres says, enabling serum proteins to enter the degenerating nerve.

When the researchers assessed mutant mice that did not make antibodies, they found PNS myelin clearance was dramatically delayed. "In addition, the regenerative nerves grew back significantly slower," Barres says. "These findings show that degenerating myelin is strongly inhibitory to regenerating axons." Injecting the mice with an antimyelin antibody restored rapid myelin clearance.

"This is really important, elegant work," comments Zhigang He, a Harvard Medical School neurologist who studies nervous tissue regeneration. "Everybody's trying to understand what accounts for the difference between the capacities for repair in the peripheral versus the central nervous system. Now we have a possible mechanism, so we can start to think about some kind of strategy to speed up myelin clearance in the brain."

The results "imply that antibodies that target degenerating CNS myelin may be able to help clear degenerating CNS myelin, which otherwise will remain in the CNS forever, where it will continue to inhibit axon regeneration," Barres says.

Antibodies could be delivered to the CNS by injecting them into the cerebrospinal fluid, Barres says. "Alternatively, new ways are being developed to modify the antibody so that it can sneak into the brain across the blood-brain barrier," he adds, though "that has not been successfully done yet." Such methods could conceivably be used to treat conditions including stroke and spinal-cord trauma.—SOPHIE ROVNER

FIBER BUNDLES LINE UP

MATERIALS SCIENCE: Gel-like 'noodle' material could act as cell scaffolds

SCIENTISTS AT Northwestern University have discovered a mechanism for forming peptide-based liquid crystals that can be drawn by hand into long, highly aligned, gel-like nanofiber bundles with the shapes of noodles (*Nat. Mater.*, DOI: 10.1038/nmat2778). These soft and pliable materials could be useful as scaffolds for growth of cells in biomedical applications.

To make the new material, team leader Samuel I. Stupp and coworkers start with amphiphilic small molecules consisting of peptides with long alkyl chains. When heated in solution, these molecules organize themselves into two-dimensional plaques. As the solution cools, those plaques break into bundles of highly aligned nanofibers. These, in turn, form a liquid crystal that, when drawn through a salt solution, forms long noodlelike "monodomain" gels in which all the bundles are aligned in a single direction.

The drawing process occurs at "an extremely small shear rate that can be delivered by human hands," Stupp explains, whereas in a comparable process—electrospinning of polymers—strong mechanical and electrical forces are required to create oriented fibers.

The gel structures are robust enough to stand up to mechanical manipulations without breaking. For example, Stupp and coworkers showed they could make knots and spirals with them.

And the process is gentle enough that biological cells can be incorporated before forming the gel and drawing it into strings. "Normally, if you put cells in the liquids that people align by electrospinning, the mechanical and electrical forces can kill the cells," Stupp says.

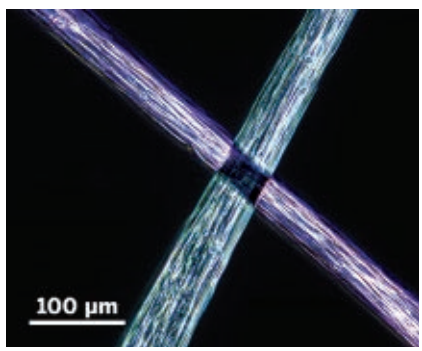
Only certain peptides attached to alkyl tails can form these monodomain gels, Stupp says. The peptide sequence must promote the formation of β-sheets, a type of protein secondary structure. In addition, the sequence must include charged amino acids to make it soluble in water.

Stupp and his coworkers hope to use the materials as scaffolds in biomedical repair applications for tissues such as nerves, blood vessels, and spinal cord. Stupp is particularly excited about the prospect of introducing the liquid directly into tissue. "The natural salts in tissue would cause the monodomain gel to form in place," he says.

Liquid crystals like those in the new material, have been difficult to orient over large areas, says Douglas L. Gin, a materials chemist at the University of Colorado, Boulder. Calling the work groundbreaking, Gin says that Stupp's success in a biomedical application "gives hope to researchers in the field that it should be possible to do so for other types of liquid-crystal materials for other applications."—CELIA ARNAUD

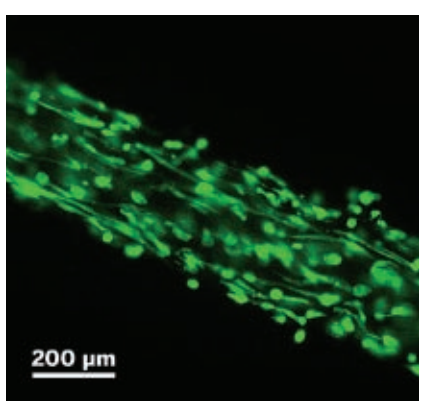
CROSSHAIRS

The extinction of light at the intersection of two crossed fibers viewed between cross-polarized filters demonstrates the fibers' uniform alignment.



LINING UP

Fluorescently labeled cells align themselves along the nanofiber string.



NAT. MATER. (BOTH)

ENVIRONMENT Obama continues push for energy, climate-change legislation

Speaking from the White House Oval Office last week, President Barack Obama once again pressed Congress for energy legislation as part of his program to control the damage from the BP spill in the Gulf of Mexico and to lower the risk and environmental threat of future oil-drilling accidents.

After outlining his Administration's "battle plan" to contain and clean up the spill, the President noted a "larger lesson" from the disaster—the high risk of drilling "a mile beneath the surface of the ocean" in a search for harder to find oil reserves. Saying the nation has known for decades that "the days of cheap and easily accessible oil were numbered," Obama urged Congress to act now on legislation to cut U.S. dependence on fossil fuels.

Obama said he endorsed legislation similar to the House-passed carbon dioxide cap-and-trade bill, but he said he would be "happy to look at other ideas and approaches from either party—as long as they seriously tackle our addiction to fossil fuels."

Republicans quickly responded with Senate Republican Leader Mitch McConnell (Ky.) accusing Obama of pressing for a "new national energy tax" to achieve the "ideological goal of passing global-warming legislation" while in the midst of the "worst environmental catastrophe in American history."

Only a few days earlier, a congressional fight over energy erupted on the Senate floor when Senate Republicans fell short in their attempt to pass a resolution by Sen. Lisa Murkowski (R-Alaska) blocking EPA from using regulations to cut greenhouse gas emissions.—JEFF JOHNSON

CONGRESS BLASTS OIL INDUSTRY

BP SPILL: Industry chiefs defend practices, while noting response plans' shortcomings

XINHUA/NEWSCOM

Top executives from five major oil companies testified before Congress last week.

IN PACKED HEARINGS last week before angry members of Congress, the heads of BP, ExxonMobil, Chevron, ConocoPhillips, and Shell Oil defended their industry in light of the April 20 BP oil rig explosion in the Gulf of Mexico, which has led to the worst environmental disaster in U.S. history.

Adding fuel to the hearings, a team of government and independent scientists last week revised estimates of the spill's size, raising the daily leak to up to 2.5 million gal, far higher than previous figures.

Triggering several of the hearings was a House of Representatives Energy & Commerce Committee investigation that found BP was far over budget and behind schedule as it neared completion of the well. Consequently, the report says, risky decisions were made over the objections of some BP personnel and contractors and in violation of industry guidelines in an attempt to speed completion of a difficult, "nightmare" well—in the words of one BP engineer.

Specifically, the report cited shortcomings in the well design and in preparations for the final cementing of the borehole to close the well, as well as several errors in construction, installation, and testing of the well casing.

BP found little support for its practices when quizzed by Congress members. Indeed, even the other oil executives took issue with BP's drilling practices for this well. "We would have drilled a different well," noted Rex W. Tillerson, ExxonMobil's CEO.

Energy & Commerce Committee members also challenged the value of oil industry response plans prepared by individual companies should an accident or spill occur. Committee Chairman Henry A. Waxman (D-Calif.) called them "cookie-cutter paper plans" and noted they were 90% identical. Several plans discussed how to protect walrus, a species not found in the Gulf, and the plans listed contact information for an oil-drilling expert who had died four years before the plans were written.

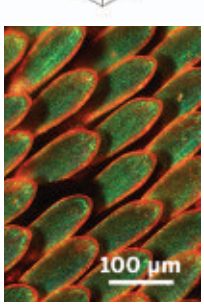
The oil executives acknowledged the response plans are inadequate. Tillerson called the mention of walrus an "embarrassment."

But Tillerson noted that when oil rig blowouts occur, "there will be impacts, and we never represented anything different than that."

"The emphasis has always been on preventing these things from occurring, because when they happen we are not well equipped to handle them," Tillerson said. "That is the fact of the enormity of dealing with them."—JEFF JOHNSON

THE BUTTERFLY EFFECT

NANOSCIENCE: Gyroid nanostructures give butterflies their glimmer



PROC. NATL. ACAD. SCI. USA

A nanoscale gyroid network (unit cell shown in red) of air and chitin gives these butterfly wing scales their vivid coloring.

A NEW EXAMINATION of butterflies' brightly colored wing scales has the photonics community all aflutter. For the first time, researchers have used small-angle X-ray scattering (SAXS) on single butterfly scales to characterize the three-dimensional photonic nanostructures that make butterfly wings so luminous (*Proc. Natl. Acad. Sci. USA*, DOI: 10.1073/pnas.0909616107).

Yale University's Richard O. Prum and coworkers looked at five different species from two butterfly families and found that the wing scales' nanostructure is a single network of gyroid photonic crystals made of air and chitin—the same stuff that makes up the exoskeletons of crustaceans and other insects.

Other scientists had previously predicted that the scales have a gyroid structure, but they studied the scales with transmission electron microscopy, which tends to shrink samples, altering their nanostructures. Prum's team turned to SAXS, a technique that's only recently been used to study natural photonics materials.

"To resolve structures this large," Prum says of the butterfly wing scales, "you need to look at scattered waves that are at very small angles to, and therefore very close to, the incident beam. Until recently, this capability was not available," he explains.

Prum's team also postulates a mechanism for gyroid formation based on the self-organizing physical dynamics of biological lipid-bilayer membranes. By mimicking the process, it might be possible to engineer superior photonic crystals, they say.

"Once again, advancements in nanocharacterization technologies have brought exciting new knowledge of materials on the nanoscale," comments Radislav A. Potyrailo, a principal scientist with GE Global Research, in Niskayuna, N.Y., who has studied the photonic properties of butterfly wings. "One of the significant aspects of this work is that it provides new insights on the formation of these photonic structures in nature. This new knowledge promises to propel the technologies focused on nanofabrication of 3-D nanostructures."—BETHANY HALFORD

TROJAN HORSE FOR B-CELL LYMPHOMA

SUGAR CHEMISTRY: Chemical synthesis yields agents that target cancer cells

BY USING CHEMICAL synthesis to add sugars to the surface of Trojan horse-like liposomes with a payload of anticancer agent, researchers have killed human B-cell lymphoma cells in blood and in live mice. This type of approach could lead to new therapeutics for B-cell lymphomas and other conditions.

B-cell lymphomas, cancers of immune-system B cells, are currently treated with doxorubicin and other chemotherapy agents or with monoclonal antibodies such as rituximab. These treatments have some moderate to severe side effects, and many patients still die from these cancers each year, so scientists continue to seek new medications.

Now, chemical glycobiologist James C. Paulson of Scripps Research Institute and coworkers have come up with a novel way to attack B-cell lymphomas (*Blood* **2010,** *115,* 4778). They synthesized a sialic acid-based glycan that serves as a ligand for CD22, a receptor found on the surface of B cells. They pinned a lipid tail onto the glycan via a polyethylene glycol linker. When they added the conjugate to liposomes, the glycans arrayed on the liposome surface. They then loaded the liposome cavity with the anticancer agent doxorubicin.

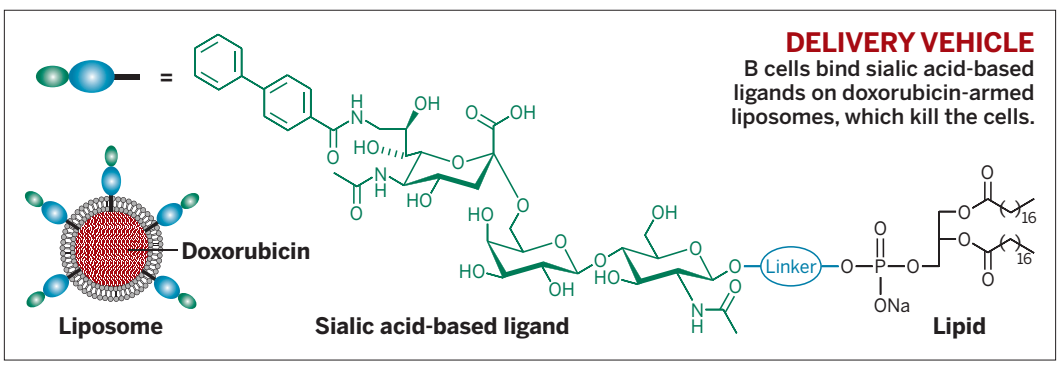
The glycan-studded liposomes act like Trojan horses when they encounter B cells. The B cells' CD22 receptors recognize and bind multivalently to the glycans, and the B cells then absorb the liposomes by endocytosis. Once inside the B cells, the liposomes deliver their doxorubicin cargo, killing the cells.

When the researchers administered a high dose of the liposomes to mice with human lymphoma, five of eight cancerous mice survived, whereas all of the mice in a control group died. Afterward, no tumor cells could be detected in the bone marrow of any of the treated mice. The treatment also destroyed B cells in blood samples from human patients with three types of B-cell lymphoma.

"This is a great example of how chemical synthesis can allow you to achieve a level of specificity that wouldn't be accessible with natural glycans," comments Laura L. Kiessling of the University of Wisconsin, Madison, a specialist in protein-glycan interactions.

The approach currently kills CD22-bearing macrophages as well as B cells, so Paulson and coworkers hope to refine it to further improve its selectivity. "But that doesn't detract from their having demonstrated that this kind of strategy can work," Kiessling says.

"We are very interested in moving this technology forward to see if it would be applicable to treatment of humans and to investigate other applications for this kind of targeting," Paulson says.—STU BORMAN



INTELLECTUAL PROPERTY Ohio appeals court rules against ACS in Leadscope case

The American Chemical Society has lost round two of its intellectual property dispute with Leadscope Inc., a Columbus, Ohio-based chemical informatics company. An Ohio appeals court, in a strongly worded decision released on June 15, upheld all counts against ACS that were determined by a jury in a 2008 lower court ruling (*C&EN Online* Latest News, March 28, 2008).

The appeals court decision could deal ACS a severe financial blow. The society may now have to pay Leadscope and three of its employees some $40 million in compensatory and punitive damages as well as attorney fees and court costs.

"ACS has not yet had an opportunity to carefully assess the details of the decision of the Court of Appeals," the society said in a statement. "Once it has done so, ACS will determine whether it is appropriate for ACS to seek further review of this matter by the Ohio Supreme Court."

The legal battle stretches back to 2002, when ACS brought suit against Leadscope and three former ACS employees who founded the company: Paul E. Blower Jr., Wayne P. Johnson, and Glenn J. Myatt. All three had worked in ACS's Chemical Abstracts Service division.

In the original suit, ACS alleged that the defendants improperly used ACS's intellectual property to develop, patent, and market Leadscope software products. The Leadscope defendants filed a counterclaim against ACS, charging defamation, tortious interference with business relations, unfair competition, and deceptive trade practices. The lower court found in favor of Leadscope on all but the last of the counterclaims.—WILLIAM SCHULZ

VERTICAL PATH Time-of-flight mass spectrometers, such as the one shown here, can now achieve high levels of resolving power.

AGILENT TECHNOLOGIES

HIGH-RES MASS SPEC

Mass spectrometry users have more **CHOICES FOR HIGH RESOLVING POWER,** from conventional ion cyclotron resonance to newer time of flight

CELIA HENRY ARNAUD, C&EN WASHINGTON

WHEN IT COMES TO high-resolution mass spectrometry, Fourier transform ion cyclotron resonance used to be the only game in town. FTICR MS still has the highest resolving power of all MS techniques, but improvements in other mass analyzers have made them suitable for some applications that previously required the big guns of FTICR.

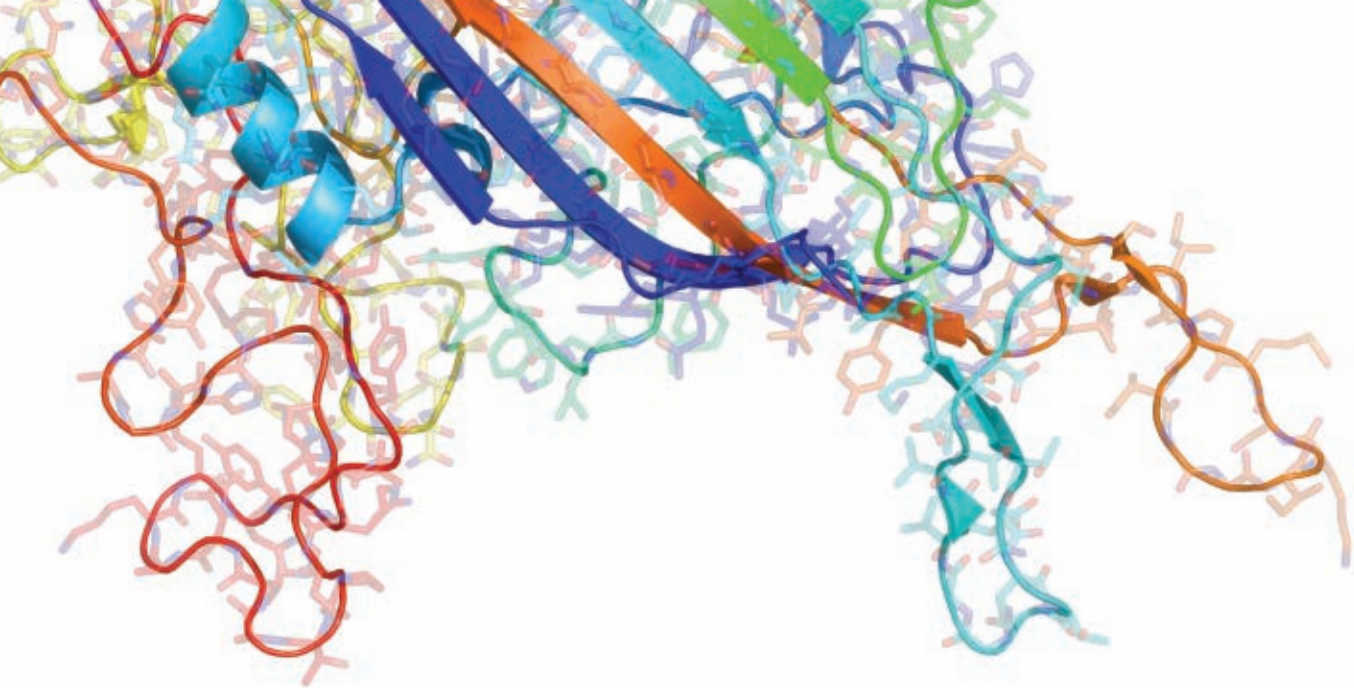
High resolution is particularly important as a means to obtain high mass accuracy and exact—as opposed to nominal—mass measurements. Resolution becomes especially important when overlapping sample components compromise the accuracy of mass measurements. "You need enough resolution to separate mixture components to enable getting high mass accuracy," says Richard D. Smith of Pacific Northwest National Laboratory (PNNL).

This idea of needing "enough" resolution means that improvements in mass analyzers that have traditionally not been considered high resolution are giving users more ways to obtain high-resolution, accurate mass measurements. Perhaps just as important, these newer instruments allow researchers to perform qualitative identification and quantitative analysis on the same instrument. These advances are making high-resolution MS attractive and accessible to more users than before.

In addition to FTICR, researchers can now also choose between mass analyzers such as Thermo Fisher Scientific's Orbitrap and time-of-flight (TOF) systems from several manufacturers. Picking the right mass analyzer for the job depends on what trade-offs are acceptable between resolving power and scan speed.

High resolution and the accompanying improved mass accuracy facilitate the analysis of complex mixtures in applications such as proteomics, metabolite identification, and petroleum research. In proteomics, the better mass accuracy made possible by high resolution allows researchers to be more confident about their protein identifications. In small-molecule applications, better resolution and improved mass accuracy can peg an identification to a single empirical formula instead of a range of possible formulas.

Resolution (Δm) is the mass difference needed to distinguish two peaks. As resolution improves, more components can be separated. However, when comparing the performance of different mass analyzers, people are more likely to talk in terms of resolving power, which is defined as $m/\Delta m$,



unprecedented

Only Orbitrap technology gives you the full complement of capabilities to solve real-world biological challenges in proteomics, metabolomics, drug metabolism, environmental/food residue analysis and clinical research applications. Nobody else can deliver the high resolution, superior dynamic range, unprecedented mass accuracy and unsurpassed sensitivity you need. Simultaneously. Thermo Scientific mass spectrometers. No trade-offs. No compromises.

mass accuracy

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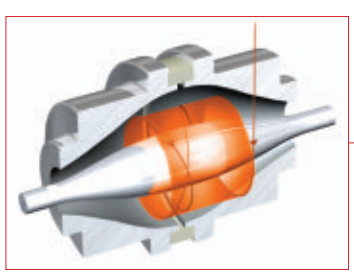

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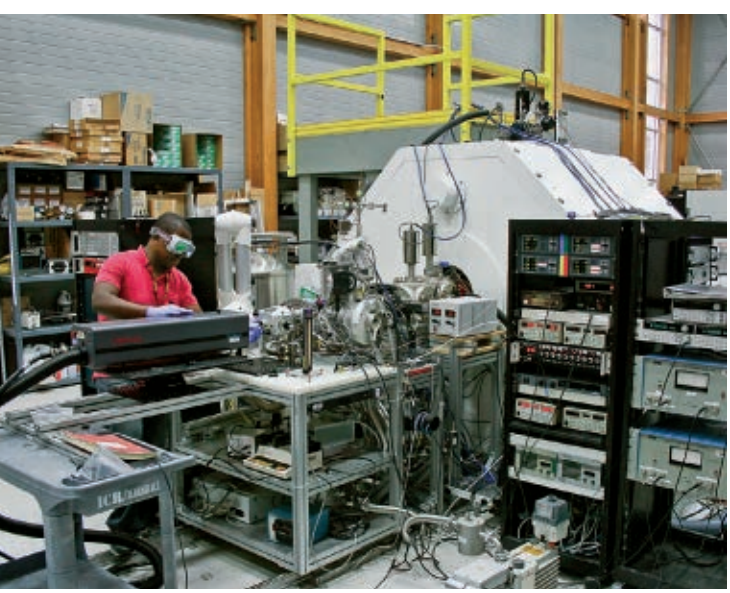
where m is the mass of an ion and Δm is the resolution. Both resolution and resolving power change as a function of the mass-to-charge ratio, and the extent of the change depends on the mass analyzer. Among mass analyzers now considered to have high resolution, resolving power ranges from tens of thousands for TOF to millions for FTICR.

RESOLVING POWER is especially important when dealing with unknowns, says Alan G. Marshall, a chemistry professor at Florida State University and director of the ion cyclotron resonance (ICR) program at the National High Magnetic Field Laboratory. "You only know there's more than one peak if you have enough resolution to tell them apart," he says. For simplicity, most discussions of resolving power focus on distinguishing two peaks of equal height. If the peaks are not of equal height, then more resolving power is necessary, Marshall says.



BIG GUNS FTICR mass spectrometers, such as this 9.4-tesla instrument at the National High Magnetic Field Laboratory, have the highest resolving power of any current mass analyzer.

COURTESY OF ALAN MARSHALL

Depending on the strength of the magnetic field used, FTICR, which uses superconducting magnets, can achieve resolving power of more than 1 million. But such levels can often be overkill. Thermo Fisher Scientific's Orbitrap, another type of Fourier transform mass analyzer, can achieve resolving power of 100,000, and TOF mass analyzers from a number of vendors can attain resolving powers of 40,000-plus. This lower—but still considered high—resolving power is sufficient for many applications.

TOF works by accelerating ions to the same kinetic energy and then measuring the time they take to travel through a defined path length. From this information, the mass of each ion can be calculated.

The two FT techniques differ in how they achieve their resolving power. ICR measures the motion of ions rotating around a magnetic field, whereas the Orbitrap measures the oscillation of ions back and forth within an electrostatic field. In both cases, the frequency of motion depends on the mass and charge of the ion and the strength of the magnetic or electrostatic field. A Fourier transform is a mathematical operation used to convert those frequencies to a mass spectrum.

FTICR instruments rely on big magnets to obtain high resolution. The magnetic field strengths of commercial systems start at 7 tesla and currently reach as high as 18 tesla. Bruker, with its solariX line of instruments, is the main FTICR vendor. Thermo Fisher Scientific also sells some FTICR instruments, but the company steers most users to the Orbitrap family of mass spectrometers, which tend to be less expensive because they don't use large superconducting magnets. Varian also sold FTICR spectrometers, but Agilent Technologies, which closed its acquisition of Varian late last month, has not yet decided the fate of the product line, according to Gustavo Salem, vice president and general manager of Agilent's Biological Systems Division.

The availability of less expensive high-resolution instruments such as the Orbitrap XL and TOF spectrometers has reduced the demand for FTICR, which was already a niche market. "A lot of people who were on the lower fringes of the FTICR market went to the Orbitrap," says Darwin Asa, marketing manager at Bruker Daltonics. "That's skewed our FTICR business more to the higher end." Bruker offers 7- or 9-tesla magnets in its low-end FTICRs and 12-, 15-, or 18-tesla magnets in its high-end instruments, Asa says.

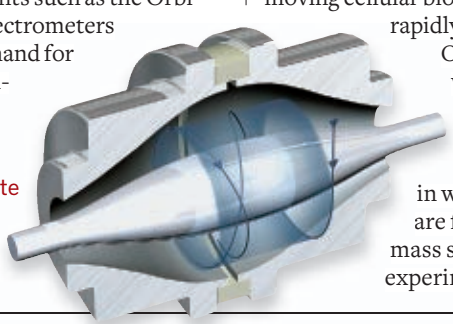
Despite the narrowing market for FTICR, Bruker continues to improve its systems. At the American Society for Mass Spectrometry meeting, which was held late last month in Salt Lake City, Bruker announced the addition of a MALDI ionization source to its solariX FTICR system. The matrix-assisted laser desorption/ionization source is aimed at imaging small molecules in tissue, particularly for pharmaceutical applications. "It's the only system that can give you small-molecule imaging at therapeutic doses," Asa says.

A drawback of both FT techniques—ICR and Orbitrap—is that high resolving power comes at the expense of scan speed. For example, the Orbitrap achieves a resolving power of 100,000 at one scan per second. Such scan speeds can't keep up with the increasingly narrow peaks generated by today's fast separations techniques. Doubling the scan speed to two scans per second cuts the resolving power in half.

FOR MANY USERS, as long as the resolution is above a certain threshold, the scan speed takes priority. Doubling or tripling the scan speed while maintaining current resolving power would be more beneficial to users than would an equivalent improvement in resolving power, says Ian D. Jardine, vice president of global R&D at Thermo Fisher Scientific.

The Orbitrap is making its mark in biological applications, Jardine says. He used to focus presentations on the Orbitrap technology itself, but he now emphasizes the research employing the Orbitrap that is published in journals such as *Science*, *Nature*, and *Cell*. "Mass spectrometry is moving cellular biology forward incredibly rapidly," Jardine says.

One application in which high resolution is particularly beneficial is "top down" proteomics, in which intact proteins are fragmented in the mass spectrometer. For such experiments, "you want high



CIRCLING In the Orbitrap, ions oscillate through the electric field around an electrode in the center.

THERMO FISHER SCIENTIFIC

"Mass spectrometry is moving cellular biology forward incredibly rapidly."

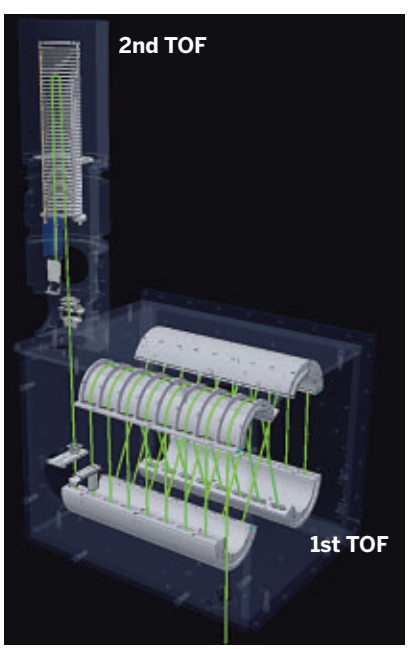
resolution, if you can get it," says Neil L. Kelleher of Northwestern University. "If you want the maximal level of information, 50,000 resolving power is just barely enough to resolve isotopes at 50 kilodaltons," he says. He uses the term "precision proteomics" to describe proteomics experiments with high levels of resolving power and mass accuracy that provide "hyperconfident" identifications.

For top-down proteomics, Kelleher currently uses high-resolution tandem MS systems, with ICR or ion traps for the first stage and either ICR or Orbitrap to record fragment ion spectra. But for top-down proteomics to catch on more broadly, it will have to be possible to carry it out in a "plug and play" manner on less expensive systems, he says. Kelleher says he would like to try to use cheaper "benchtop" Orbitrap systems to simplify and lower the cost of top-down proteomics experiments.

Kelleher also advocates precision proteomics for "bottom up" proteomics, a more common type of experiment in which proteins have been digested first. Given the relatively small masses of peptides produced by protein digestion, high precision can be achieved with less resolving power than is required for top-down proteomics. "For bottom-up, 100,000 is overkill," he says. With 50,000 resolving power, users can confidently identify unmodified peptides, he says.

John R. Yates III, who studies proteomics at Scripps Research Institute in La Jolla, Calif., finds that the accuracy of peptide identification in bottom-up proteomics is not dramatically improved by obtaining high-resolution data. The mass assignments do become more accurate with higher resolution, but "there's probably a limit to how much mass accuracy is usable," he says. Yates and coworkers run their proteomics experiments on an Orbitrap backed off to 60,000 resolving power. If that were insufficient for his analyses, "we would probably bite the bullet and scan slower," he says.

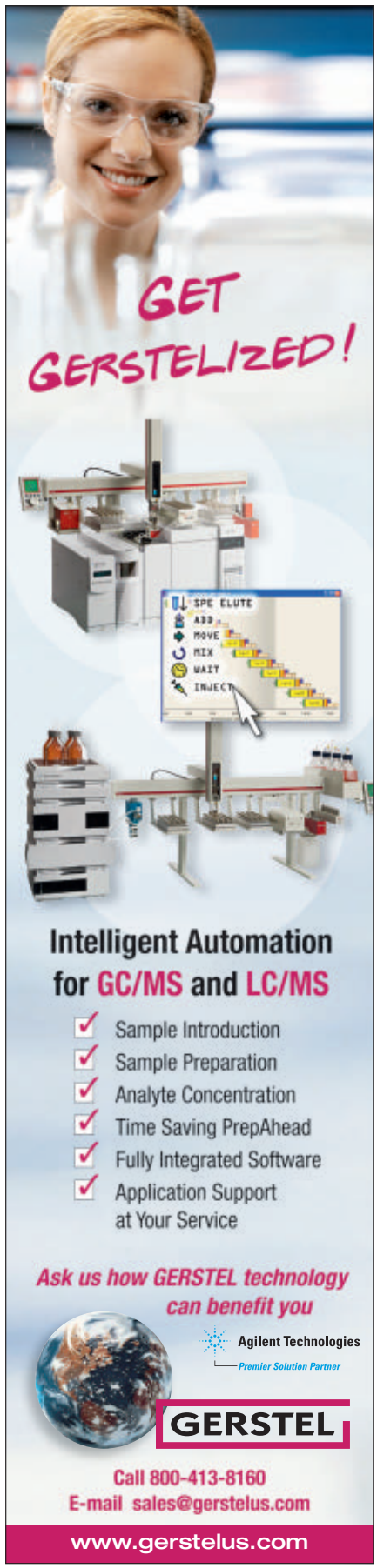
EVEN LONGTIME FTICR users are shifting to other high-resolution mass analyzers for some applications. In fact, Florida State's Marshall—perhaps the most vocal advocate for FTICR—has found applications for which he needed to use other techniques. For example, when he needed to analyze singly charged ions with a mass-to-charge ratio too high for FTICR, Marshall turned to TOF, which is faster, more sensitive, and has a wider mass range than either of the FT methods, he acknowledges.



JEOL

COMPACT PACKAGE A staggered figure-eight design gives the SpiralTOF a long flight path in a small space. The figure-eight analyzer (1st TOF) can be used alone or in combination with a linear TOF unit (2nd TOF).

Smith, another longtime FTICR user, has recently been relying increasingly on TOF. His lab has been pairing it with fast multiplexed ion-mobility separations, a combination he sees becoming his mass analyzer of choice for most applications. As his research has shifted more toward biological questions, he has realized that he doesn't always need the highest mass-resolving power. For bottom-up proteomics analysis of peptides with chromatographic and ion-mobility separations in front of the mass spectrometer, "the number of cases where you'd have mixtures of peptides that you can't resolve with 50,000 resolving power is extremely small," Smith says. Although his lab still uses FTICR for some experi-



ments, he expects the new high-resolution platforms to become dominant for broad applications.

The real advantage of TOF relative to the FT methods is speed, especially with the rise of fast chromatographic techniques. "People don't buy mass spectrometers and just inject samples," says Lester Taylor, LC/MS platforms and programs manager at Agilent. "They put something in front of it." Fast chromatography requires that the mass spectrometer scan quickly to collect enough points to define each chromatographic peak. "I've been in situations where you have to relax the chromatography constraints to make your peak wide enough to sample sufficiently" by MS, Taylor says.

A major application area for high-resolution TOF MS is metabolite identification. "A lot of drug metabolism people are heavily committed to UHPLC," Asa says, referring to ultra-high-pressure liquid chromatography. The speed of TOF lets researchers get high throughput from their UHPLC systems, and the resolution and mass accuracy enable them to confidently identify unknown metabolites.

IN RECENT YEARS, mass spec vendors have greatly improved the resolution of TOF mass analyzers. Bruker's maXis achieves a resolving power of 50,000, and instruments from AB Sciex, Waters, and Agilent achieve values of more than 40,000. JEOL's new SpiralTOF, which has an unusual ion trajectory, obtains 60,000 resolving power. In each case, the level of resolving power has been reached by a combination of system geometry and electronics.

"There's no one magic modification that makes it happen," Asa says. "It has a lot to do with focusing the ions, cooling the ions, and making sure that we're not losing the signal, resolution, and accuracy as those ions are going through the system and making it to the detector."

Vendors have also focused on developing instruments that can allow users to perform high-resolution qualitative identification and sensitive quantification on the same instrument. "Until now, customers have done their high-resolution, accurate-mass work on one dedicated platform and then moved to a triple-quadrupole platform for quantitation," says Dominic Gostick, director of biomarker MS, pharmaceutical, and proteomics businesses at AB Sciex.

At the American Society for Mass Spectrometry meeting, AB Sciex launched its new TripleTOF 5600, which achieves more than 40,000 resolving power across the mass range without loss of sensitivity or scan speed, the company says. "Our customers told us they needed 30,000 resolving power for most of their applications," Gostick says. "We wanted to develop an instrument that maintained high resolution and mass accuracy while delivering the speed—up to 100 scans per second—and sensitivity of a high-performance triple quad for robust quantitative analysis," he says.

Waters' entry into the quantitative, high-resolution TOF market, the Synapt G2, was introduced last year. The high resolution—routinely accessible at UHPLC-compatible speeds—is achieved by a combination of flight-tube geometry and detector electronics, according to Ronan O'Malley, group manager for TOF product management at Waters.

But the Synapt adds another type of resolution with the inclusion of an ion-mobility cell, in which ions can be separated on the basis of size and shape, as well as mass-to-charge ratio. "The second-generation Synapt's detector electronics provide enhanced dynamic range and allow for exact mass measurement of components separated by the high-resolution ion-mobility cell, enabling quantitative analysis of previously unresolvable isobaric species," O'Malley says. Isobaric species are chemically distinct entities that have the same nominal mass.

Another important factor for resolution and sensitivity is the capability to shepherd ions produced by an ionization source so they reach the mass analyzer and detector. For example, Agilent uses ion-beam compression technology in its 6540 and 6538 Q-TOF systems. The technology shapes the ion beam, "making sure that it's spatially compact and energetically homogeneous, so you haven't got an energy spread and spatial spread that degrade resolution," Taylor says.

JEOL's new SpiralTOF, which has a staggered figure-eight design, takes a new multipass approach to TOF. A danger with multipass systems, in which ions retrace the same path multiple times, is that the heavy ions can eventually catch up with the light ions and become indistinguishable. With the SpiralTOF, each trip around the figure eight is slightly offset, so the ions don't catch up with each other, says Robert B. Cody, product manager at JEOL. "That gives us a 17-meter flight path in a 1.3-meter package," he says.

EFFORTS ARE ALSO under way to push the resolving power of TOF beyond its current limits. Virgin Instruments, based in Sudbury, Mass., is developing an instrument with 200,000 resolving power, says Marvin L. Vestal, chief executive officer. The instrument is about 20 feet high and gets a two-story installation, with the ion source on the first floor, the ion mirror on the second floor, and a hole in the floor between. "Our major limitation is the mechanical vibration of the second floor," Vestal says. "If you walked across the room, you could see it on the mass spectrometer." Such unforeseen complications have kept them from hitting the predicted 200,000 resolving power, Vestal says.

One reason for constructing such an instrument is "just to establish that we know what all the limitations really are," Vestal says. Over the past several years, he has developed a detailed theory of what is feasible with current TOF technology. He finds that resolving power should increase in direct proportion to the flight path. "If a 20-foot tube gives us 200,000 resolving

MULTIPLE CHOICE

Mass spectrometry users have several options for mass analyzers with high resolving power

	MECHANISM USED TO SEPARATE IONS	RESOLVING POWER
Ion cyclotron resonance	Frequency of ion motion in magnetic field	>1,000,000
Orbitrap	Frequency of ion motion in electrostatic field	~100,000
Time of flight	Length of time for ions of defined kinetic energy to travel through defined flight path	Up to 40,000–60,000

"There's probably a limit to how much mass accuracy is usable."

power, then a 100-foot one should give us a million," he says. Vestal doesn't know whether Virgin will ever actually build such an instrument—even the more modest 20-foot one—commercially.

Even as TOFs continue to improve, there will always be a place for instruments with the highest levels of resolving power. Thus, advances continue in FTICR as well.

For example, the National High Magnetic Field Laboratory and the Environmental Molecular Sciences Laboratory at PNNL are collaborating on the development of new 21-tesla FTICR mass spectrometers. Projects and funding exist at both laboratories, and exploratory discussions are ongoing with potential magnet manufacturers. Such magnets would require two to three years to build, given the long lead times required for obtaining the necessary specialized superconducting wire materials.

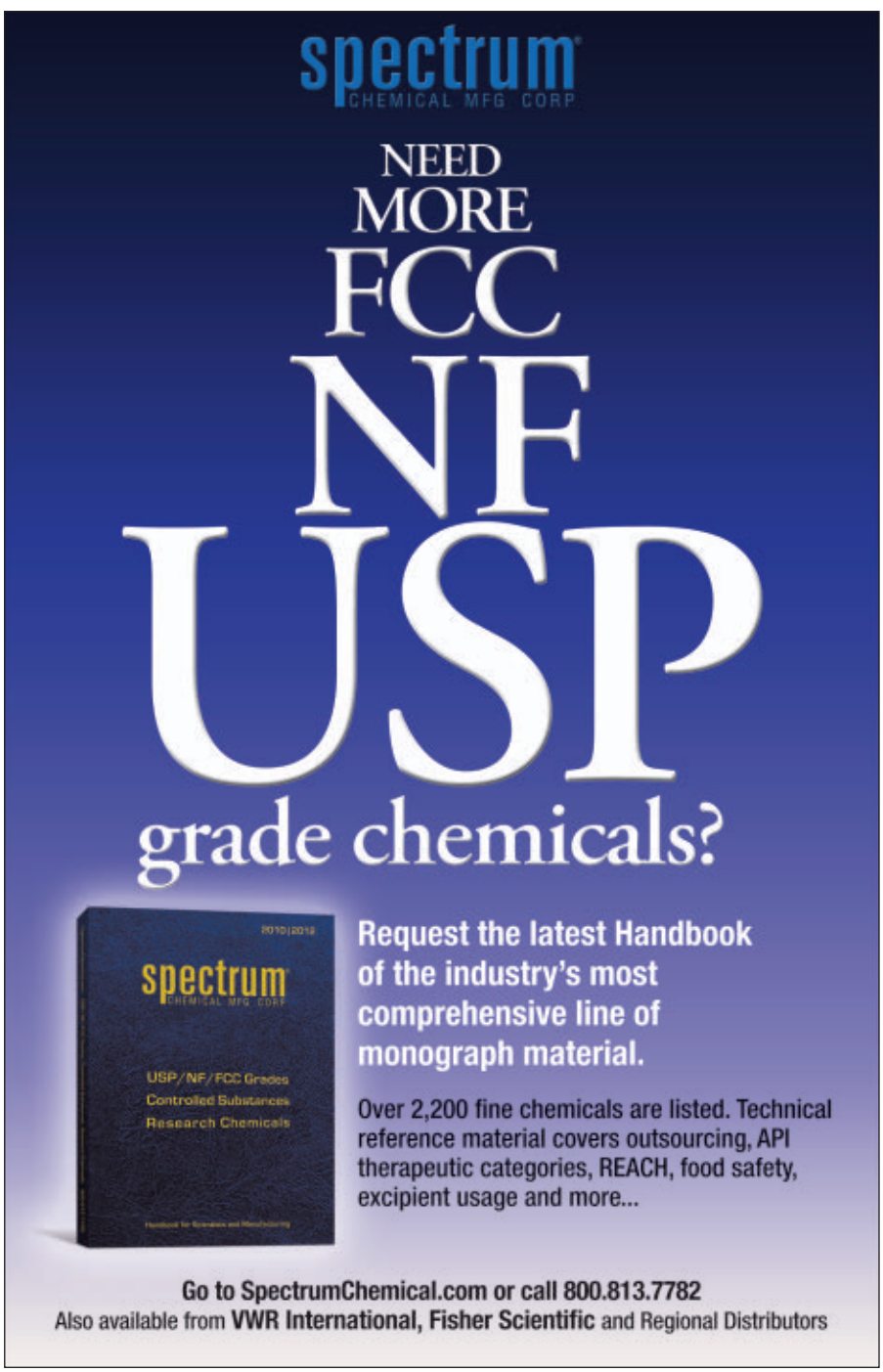
THIS TYPE OF INSTRUMENT is "not going to be common," Smith says. There's going to be only a couple of them in the U.S., he adds. "I don't think it will ever be broadly marketed and used." Instead, he says, the appropriate place for such instruments is a national laboratory, where users can bring samples when they need extreme resolving power, or in places where a critical mass of applications can justify the cost.

Smith already knows how he hopes to use the instrument in proteomics studies. "The very-high-end platforms will be used for initial identification, particularly in top-down proteomics applications," he says. "Once we've identified the parent protein, we don't need to dissociate it and identify it every time we make a measurement. We can establish what we call an accurate mass and time tag, and then use that information with an ion-mobility TOF platform to make routine, high-throughput measurements. With the information provided by the high-end FTICR, we can then do this much faster, with greater sensitivity, and on a much less expensive platform."

The main focus for the new instrument at the National High Magnetic Field Laboratory will be identification of protein modifications by top-down proteomics. "You never can figure out what's there unless you look at the whole protein to start with and then chop it up," Marshall says. "The difficulty is that proteins are big, and it's hard to do that." The average mass of a human protein is about 50 kilodaltons, Marshall notes. With current instruments, Marshall can capture only about half of the proteome in a single spectrum. "At 21 tesla, we should be able to get most of the rest of the way," he says.

Marshall also plans to apply the instrument to questions in petroleum research. His team can identify the components of petroleum up to about 800 or 900 Da, but the spectrum actually extends out to about 1,300 or 1,400 Da. Again, for this application, he expects the 21-tesla instrument to enable him to resolve all of the components.

The current crop of instruments gives users a variety of options for high-resolution MS. What is certain is that in the future mass spec will offer scientists even more choices. ■



RHODIA TO BUY CHINESE SURFACTANTS FIRM

Rhodia has agreed to acquire Feixiang Chemicals, a Chinese maker of fatty amines and surfactants, in a deal valued at $489 million. With headquarters in Zhangjiagang, near Shanghai, Feixiang has annual sales of about $250 million and has been growing at 20% per year. Rhodia says Feixiang's amines capability will reinforce its position in surfactants for home, agrochemical, and industrial markets. Rhodia's last sizable acquisition was McIntyre Group, a Chicago-area specialty surfactants maker, in 2009. After the Feixiang acquisition, CEO Jean-Pierre Clamadieu says, Rhodia will generate around one-third of its sales in Asia.—MM

HUNTSMAN ADDS TO RACING-CAR APPEAL

A racing car that finished first among gasoline-powered vehicles at the 24-hour Le Mans endurance race earlier this month included rearview-mirror housings that incorporate Huntsman Advanced Materials' encapsulants and adhesives. On Oreca 01, the mirror housings sport flexible organic light-emitting diodes that are encapsulated in a newly developed Huntsman ultraviolet light-curable polymer. The firm's Araldite epoxy adhesive is also used to affix the polyester-backed OLEDs to the carbon/epoxy contoured housings.—MSR

ORECA

A Huntsman encapsulant protects OLEDs on Oreca 01 from oxygen and moisture degradation.

INVISTA SUING BUTANEDIOL COMPETITOR

Invista has filed a lawsuit against Houston-based technology provider Frontech for allegedly stealing its process to make butanediol. The suit, filed in U.S. District Court in Houston, says Frontech and its president, Ming D. Wan, copied Invista's hydrogenation process design "right down to the millimeter" and used those trade secrets to secure two licenses with Chinese companies and to bid for three additional licenses. Invista has asked the court for injunctions and an award equal to three times Frontech's profits from licenses based on Invista technology.—MSR

ALBANY MOLECULAR ACQUIRES HYALURON

In a move to add finished-dosage manufacturing to its active pharmaceutical ingredient (API) services, Albany Molecular Research Inc. has acquired Hyaluron, a contract manufacturer of sterile syringe and vial fillings, for approximately $27 million. AMRI says the acquisition will allow it to offer a comprehensive manufacturing process for sterile injectable drugs, including the development and manufacture of the API, formulation, and the production of the finished-drug product. "We believe that the unique capabilities of both organizations will quickly assimilate into a larger, fully integrated [current Good Manufacturing Practice] manufacturing provider," says Thomas E. D'Ambra, CEO of AMRI, pointing to efficiencies and cost benefits of eliminating a technology transfer step between separate API and formulation contractors. Consultant James Bruno, president of Chemical & Pharmaceutical Solutions, says moving into finished-dose formulation is becoming an attractive option in API contract work as firms try to compete for fewer opportunities. "For a company like Albany Molecular, I think it's a natural fit," he says, noting that AMRI specializes in oncology drugs, which are often injectable, and already does some small-scale solid-dose formulation work. Filled-syringe formulation will also differentiate AMRI from other contract firms moving into formulation services, according to Bruno. "It's an attempt to stay at the high end as opposed to basic tablets and capsules," he says.—RM

SASOL BUILDING COCATALYST PLANT

Sasol is constructing a plant to make purified triethylaluminum at its facility in Brunsbüttel, Germany, and is entering the merchant market for the chemical, which is used as a cocatalyst in polyolefin production. Sasol uses triethylaluminum as a precursor for detergent alcohols. The company says it is the largest producer of triethylaluminum, with production for captive use at its detergent alcohols plants in Brunsbüttel and Lake Charles, La. The new unit will have a capacity of 6,000 metric tons per year and will be completed in 2012.—AHT

INEOS BIO WINS GRANT FOR U.K. ETHANOL PLANT

Ineos Bio, the biofuel division of Ineos, has been offered a $10.8 million grant from two U.K. government-sponsored clean fuel development agencies. One North East and the Department for Energy & Climate Change will fund the construction of a waste-to-ethanol plant in the Tees Valley, in northern England. The facility, planned for completion in 2012, will be able to convert more than 100,000 tons of biodegradable household and commercial waste per year into 24,000 tons of ethanol and 3 MW of electricity. Ineos will derive the fuel from fermentation by anaerobic bacteria and the power from cogeneration.—MV

NOVOZYMES AND LIGNOL DEVELOPING BIOFUEL

Danish enzyme maker Novozymes has signed a research and development agreement with Canadian cellulosic ethanol firm Lignol to make ethanol from wood chips and forestry residues. The companies say their goal is to reduce production costs to $2.00 per gal. Lignol's technology focuses on pretreatment of woody

biomass, and Novozymes makes enzymes to convert cellulosic sugars into ethanol. The firms plan to optimize their processes at Lignol's pilot plant in Burnaby, British Columbia.—MV

ABBOTT LICENSES NEUROCRINE DRUG

Abbott Laboratories will pay $75 million up front for access to Neurocrine Biosciences' elagolix, which has completed Phase II trials to treat endometriosis. The San Diego-based biotechnology company could get up to $500 million more if elagolix hits certain clinical and commercial milestones. Elagolix blocks gonadotropin-releasing hormone (GnRH) receptors in the pituitary gland, lowering the levels of sex hormones in circulation. The drug candidate differs from currently marketed drugs, which are peptides that act as GnRH agonists, in that it only partially suppresses estrogen and thus prevents the bone loss associated with other drugs.—LJ

GSK HAS ACQUIRED LABORATORIOS PHOENIX

To extend its reach into Latin America, GlaxoSmithKline has bought the 70-year-old Argentine pharmaceutical firm Laboratorios Phoenix for about $253 million in cash. Argentina ranks eighth among emerging markets for pharmaceuticals, with annual sales of $3 billion, and it has the third-highest annual growth rate at 22%, according to market research firm IMS Health. Existing GSK operations in Argentina had sales of about $148 million in 2009, and Laboratorios Phoenix reported sales of just over $100 million. Together they will rank third in Argentina, GSK says. The acquisition gives GSK a portfolio of generic drugs and a manufacturing facility near Buenos Aires.—AMT

PFIZER UNVEILS RARE-DISEASES UNIT

Taking a page from GlaxoSmithKline's playbook, Pfizer has created a research unit devoted to finding new medicines to treat rare diseases. A rare or "orphan" disease is defined as one that impacts fewer than 200,000 patients. More than 6,000 diseases are classified as orphan diseases, but less than 10% have dedicated treatments, Pfizer says. GSK established its unit focused on rare diseases in February. The moves come as pharma firms scour the landscape for untapped commercial opportunities.—LJ

CORRUPTION PROBED AT CHINA'S FDA

A senior official at China's State Food & Drug Administration has been suspended from his duties for suspected corruption. China's state media reported that Zhang Jingli, one of the agency's four deputy commissioners, is under investigation for "disciplinary violations," a phrase that usually means accepting bribes. Several senior SFDA officials have been involved in corruption cases in recent years. In 2007, Zheng Xiaoyu, the director of the agency, was executed for approving unsafe drugs in exchange for kickbacks (C&EN, July 16, 2007, page 9). In April of this year, state media reported that five drug safety officials, mostly responsible for vaccines, had been arrested for taking bribes.—JFT

BASF ESTABLISHES FOOD LAB IN NEW YORK

BASF has added a nutritional ingredients laboratory at its technical center in Tarrytown, N.Y. The company says the new facility will support application development for vitamins and colorants in vitamin-enhanced waters, carbonated soft drinks, nutritional bars, baked goods, and other products. The 160,000-sq-ft technical center in Tarrytown came with BASF's purchase of Ciba last year.—AHT


BASF

BASF will test food ingredients in its new lab.

BUSINESS ROUNDUP

DOW CHEMICAL has won a $61.7 million patent suit against Nova Chemicals in a federal court in Delaware. In the suit, originally filed in 2005, Dow alleged that Nova was infringing on patents for polyethylene blends for film and other products.

FMC has acquired the fluthiacet-methyl businesses of the Tokyo-based firms Kumiai Chemical and Ihara Chemical. FMC distributes fluthiacet-methyl, which is used to control glyphosate-resistant broadleaf weeds, in the U.S.

INTERNATIONAL Specialty Products has formed a sunscreen manufacturing alliance with India-based Vivimed Labs. Beginning on Oct. 1, Vivimed will produce a range of ultraviolet light absorbers that ISP will supply to makers of sun-protection sprays and lotions.

OCI plans to invest about $180 million to expand capacity for polysilicon by 5,000 metric tons per year at its plant in Gunsan, South Korea. The expansion is expected to be completed next year. OCI will then have 32,000 metric tons of polysilicon capacity.

DSM has agreed to pay $25 million to settle a civil price-fixing suit brought by customers that purchased ethylene propylene diene rubber between 1997 and 2001. A federal judge in the U.S. District Court for Connecticut must approve the class-action settlement before it becomes effective.

ENAVAIL plans to construct a facility in Abilene, Texas, that will provide commercial-scale particle engineering technology to the pharmaceutical industry. To open later this year in the Abilene Life Sciences Accelerator, the 1,800-sq-ft operation will enhance drug candidates that have poor water solubility.

MP BIOMEDICALS has agreed to acquire the protein biologics manufacturer ICPbio International. MP, a Santa Ana, Calif.-based provider of life sciences, fine chemicals, and diagnostic products, says ICPbio's New Zealand facility uses chromatographic extraction to produce high-purity serum protein materials such as thrombin and transferrin.

DSM will manufacture an antibiotic at its Capua, Italy, microbial fermentation facility for the U.K. biotech firm Novacta Biosystems. The antibiotic, a naturally derived compound known as a lantibiotic, will be used in trials as treatment for hospital-acquired *Clostridium difficile* infections.

A HEIGHTENED AGENDA

With regulatory threats growing, the AMERICAN CHEMISTRY COUNCIL steps up advocacy

MICHAEL MCCOY, C&EN NORTHEAST NEWS BUREAU

TO HEAR IT from executives attending the American Chemistry Council's annual meeting, it's both the best of times and the worst of times for the association and the industry it represents. Chemical companies are recovering from the recession nicely, and ACC is doing great, but many in the industry feel besieged on the legislative and regulatory fronts.

"In all of my 34 years in this industry, I've never seen a more challenging time," J. Brian Ferguson, chairman of Eastman Chemical and head of ACC's executive committee, told attendees at the event, which was held earlier this month at the Broadmoor Hotel in Colorado Springs, Colo.

Ferguson described an erosion of public faith in institutions ranging from banks and large corporations to government and labor unions. The BP oil spill in the Gulf of Mexico has only accelerated this public discontent. "All of our institutions face a crisis of trust," he said, "and as we all know, the chemical industry and our products remain at the front—or very near the front—of that line."

Zealous regulators and legislators are adding to the chemical industry's woes. At a briefing for reporters, Ferguson said he and his colleagues feel "under siege" from the Obama Administration's agenda.

"We face a barrage of legislative and regulatory initiatives that we feel will damage the industry," Ferguson said. "We anticipated that this would be the most aggressive policy environment many of us have faced in our entire careers, and that has been borne out."

As ACC sees it, the challenging initiatives include a draconian modernization of the Toxic Substances Control Act (TSCA), implementation of chemical safety legislation mandating that dangerous manufacturing processes be replaced with safer ones, and Environmental Protection Agency regulation of greenhouse gas emissions. Meanwhile, the drumbeat of bad publicity on bisphenol A, phthalates, and plastic bags is accompanied by the possibility of state-level product bans.

ACC's response to threats against chemicals that it believes are safe and effective has been to ratchet up its product advocacy efforts and to mobilize politically in congressional districts to an unprecedented degree. Overall, the association says it is devoting 58% of its resources to this kind of advocacy, up from only 28% just two years ago.

Lisa B. Harrison, ACC's vice president of communications, explained that the district-level effort is largely the brainchild of Calvin M. Dooley, ACC's president and chief executive officer, who was a Democratic member of the House of Representatives from 1991 to 2005. "Cal knows from his days as a congressman that what he reads in the local paper is more important than what he reads in the *Washington Post*," she said.

Harrison recently reorganized ACC's communications department so that it can better support what she calls "in-district advocacy." Also supporting such advocacy, she said, is the association's new drive for small-company members, because legislators are highly attuned to the voices of small businesses in their districts.

A third initiative is ACC's political mobilization department, which was formed about six months ago and now has four staffers. At the press briefing, Dooley said the new department is targeting districts led by legislators who are not necessarily industry backers but who are open to talking with ACC.

For example, the department recently facilitated a meeting in the Georgia district of Rep. John Barrow (D) that was attended by executives from a local ACC member company. The topic discussed, Dooley said, was the pain firms would feel if TSCA reform draft legislation now in the House Energy & Commerce Committee gets enacted into law.

Barrow, who is on the committee, is a member of the Blue Dog Coalition, a group of fiscally conservative Democrats. "We anticipate that the Republicans will align with us, and we need eight Democrats," Dooley said. "We have defined the universe of Democrats who we think are potential supporters of our priorities."

ACC'S FOCUS ON district-level initiatives is at the expense of broader public-outreach efforts. A year ago, the association wound down its $20 million-per-year national advertising program, conducted under the "essential$_2$" banner. In its place ACC started a more modest Web-oriented outreach campaign orchestrated by Racepoint Group, a public relations agency. But even that has been shut down, Harrison said. Instead, ACC will launch short-term outreach efforts as issues crop up in important states and districts.

MICHAEL MCCOY/C&EN

FACING CHALLENGES Harrison (from left), Dooley, and Ferguson address reporters at the recent ACC annual meeting.

The challenges facing the industry might be many, but the association contends that it has the financial and membership strength to confront them. At the press briefing, Dooley noted that ACC has signed up 13 new members over the past year, many of them the smaller companies it is pursuing. Retention of existing members—now about 145—is high, he added.

Over the past two years, the association has cut dues by almost 28% and reduced its own expenditures by 20%, Dooley said. At the same time, its reserves have risen from $9 million in 2008 to $34 million today. "I don't think ACC has ever been in stronger financial shape," he said, "and I don't think ACC has ever had stronger support from its members." ■

SAFC

READY FOR FIVE MORE

Sigma-Aldrich's **FINE CHEMICALS BUSINESS** sets its sights on the next five years of operation

JUST OVER five years ago, research chemicals provider Sigma-Aldrich launched a fine chemicals business under the SAFC brand. Through a series of business and technology acquisitions, coupled with steady internal investment, the business tripled in size and today has about $600 million in annual sales. From its start as a custom manufacturer of pharmaceutical chemicals, SAFC has also become a major supplier of cell-culture products for biomanufacturing and advanced materials for electronics.

"We are a 'fine molecules' supplier, meaning that we are in both small and large molecules, and not only in chemistry but biology, materials science, and analytical chemistry, as well," SAFC President Gilles A. Cottier explained at a recent briefing for reporters. SAFC's goal is to help customers make products by providing science-based tools and high-tech manufacturing. As the business strategizes for its next five years, this goal "translates into what we are and what we want to be," he added.

SAFC's desire for differentiated technical capabilities is apparent in its approach to synthesizing highly potent active pharmaceutical ingredients (APIs). These operations originated in the 2004 acquisition of Tetrionics, a small firm with annual sales of about $15 million. Tetrionics' chemistry was developed at the University of Wisconsin, Madison, and used to make paricalcitol, a vitamin D analog that is the API in Abbott Laboratories' parathyroid drug Zemplar.

By January 2005, SAFC had broken ground on its first expansion, spending $12 million to double capacity of highly potent compounds in the former Tetrionics plant at the University Research Park, in Madison. Within two years, it added pilot-plant and kilogram-scale lab capacity at the facility and added suites in St. Louis for conjugating potent compounds to antibodies.

All told, SAFC has invested more than $75 million in the high-potency area. Included in the total is $29 million to expand fermentation-derived potent API capacity in Israel, which is due to come onstream in the third quarter. And in April, SAFC opened a $30 million, 51,000-sq-ft highly potent API facility near Madison, in Verona, Wis.

SAFC still makes the vitamin D analog and 15 other commercial products at its Madison site. The expectation is that large-scale projects will soon populate the Verona facility, which was designed to support customers' needs for drugs that are on the market or in Phase III clinical trials. In two large-scale suites, reactors can accommodate batches in volumes of up to 4,000 L.

Roughly one-third of SAFC's API business is related to high-potency manufacturing, said David Feldker, vice president of SAFC Pharma, who maintains that the capacity buildup, although rapid, wasn't rash. "We have to be very judicious of what we are building and when, and that is mostly driven by customer timing on demand," he said. The market for highly potent compounds should continue to experience double-digit growth, according to SAFC.

STRONG MARKET SAFC has expanded its facilities for synthesizing highly potent drug compounds.

Indeed, double-digit growth in many target markets meant that SAFC had no reason to alter its strategy, despite the economic downturn, Cottier told C&EN. This strategy included the Verona and Israel expansions and a $12 million investment in viral manufacturing in Carlsbad, Calif., that added commercial-scale capability to make biologics, vaccines, and gene therapy products.

THAT ISN'T TO SAY the company didn't feel an impact from the recession. "Like every company, we took a look at our cost structure and discretionary spending and may have accelerated some decisions, but these were not cost-containment exercises only," he said. For example, SAFC consolidated production of dry-powder media in Lenexa, Kan., but it is spending more than $6 million to expand the site into a "center of excellence." SAFC recently announced it will expand production of reagents for liquid cell culture in St. Louis and Scotland.

Cottier pointed out that the fine chemicals industry underestimated the negative impact of some market trends, such as the decline in generalized outsourcing and the extent of the economic downturn. He believes that geographic, technological, and customer diversification helped SAFC continue to grow in 2009. "If you only bring pots and kettles, or undifferentiated capacity, and try to compete only on price, you are not going to succeed in this market," he said.

In a June 5 report, analysts at the investment advisory firm Standard & Poor's said they expect 8% organic growth for the SAFC business in 2010. Factors at play include a relatively stable life sciences market and improving demand trends from customers.

Looking ahead, Cottier said SAFC won't seek to play in every segment of the $60 billion-per-year fine chemicals market. Instead, he anticipates expanding in faster growing applications and geographic regions. Despite its past history, "we are not going to be on an acquisition spree, although we will look at opportunities as they come along," he said. "We have to make sure that what we have invested in ourselves pays off."—ANN THAYER

SEEDING A PROVINCE

GOVERNMENT OF QUEBEC partners with venture capital firm on a seed fund to spur biotech innovation

IT'S ROUGH OUT THERE for the budding biotech entrepreneur. These days, finding cash to pull a project out of an academic lab or to conduct tests that prove an idea's merit can be nearly impossible. For venture capitalists, the value generated from a start-up business is low, and the risk is often too high.

Officials from Quebec are trying to shake up the funding model in hopes of spurring innovation—and job creation—in the Canadian province. The government has handed over a pot of money to GeneChem, a Montreal-based venture capital firm run by scientists, to find and fund the best and brightest minds in the region.

For years, Quebec has been one of the top 10 biotech hubs in North America, but the province's government recently noticed a decrease in the number of start-up firms emerging from the region. And the environment for new companies seems only to be getting worse. The economic crisis created a capital crunch throughout the biotech industry in which early-stage funding has become particularly hard to come by.

"To the extent that there's capital available, in most venture capital firms a lot of that money is going to later stage companies," says G. Steven Burrill, chief executive officer of the investment firm Burrill & Co. The gap in funding for entrepreneurs who want to do the first few experiments to validate an idea "is probably greater than it's ever been," he adds.

Last fall, recognizing the economic and industry forces that entrepreneurs were up against, Quebec's government unveiled a biopharmaceuticals strategy designed to help new and existing companies adapt.

As part of a package that includes the usual R&D tax credits and calls for collaboration, the government created a $40 million biotech seed fund to be run by a private venture capital group. That group would also raise its own cash contribution. The fund would provide small amounts of money to Quebec-based start-ups culled from local universities and research institutes, with the goal of reviving innovation in the region. In October, the government asked interested venture capitalists to compete for the right to run the fund.

GeneChem came up with the winning proposal, a fund called AmorChem, after analyzing its own funding activities since its 1997 launch. The results surprised the financiers: Although most of the $300 million they invested over the years had gone to U.S. companies, when they gave out seed funding to start-ups, about half of it went to Canadian firms. Furthermore, local firms receiving funds had been the best performers.

GENECHEM

Holzbaur

Drilling down into those local investments, GeneChem assembled a list of "lessons learned" to apply to the government fund. The firm found that it had the most success when it was one of only a couple of investors in a start-up and when the investment was small. When a company is launched with a small amount of cash, a healthy return on the investment is more easily achieved, and the pool of potential future investors is larger. The venture capital firm also learned that there isn't much to be gained financially from conducting a Phase I trial for most therapeutic indications. Better to sell a molecule and let someone else do the toxicity screening.

However, the most important lesson, says Inès Holzbaur, a GeneChem vice president and one of several Ph.D. chemists on staff, is that the bigger the infrastructure, the harder it is to pull the plug on a project that isn't yielding results.

The gap in funding for entrepreneurs is "probably greater than it's ever been."

Those lessons informed GeneChem's strategy for AmorChem. The seed fund will be open for 10 years, although GeneChem hopes to make most of the 40 investments it has planned within the first five years. Each recipient will get an initial injection of no more than $500,000. Leftover cash from failed projects will be funneled to other companies in the fund's portfolio. The maximum investment per project will be $3 million, and the therapeutic concept must be validated within 18 to 24 months.

TO LOWER COSTS and avoid duplicating infrastructure, GeneChem plans to establish a small medicinal chemistry company to screen compounds for its start-up firms. "Drug targets are abundant at universities, but chemistry screening is not," Holzbaur says. Hiring a dozen chemists to make analogs doesn't make sense for a start-up, yet drug development chemistry needs to be tightly controlled, she adds. The GeneChem-run chemistry company will address those needs.

Once a molecule or technology has been validated, AmorChem expects to either license it or bundle it with other projects into companies with more robust financing. "We believe the licensing will really drive our returns," Holzbaur says.

Licensing promising projects might seem antithetical to the goal of reinvigorating Montreal's biotech cluster, but Holzbaur sees an upside for the region. "In order to have a biotech hub, you need to have success stories—like a company raising $50 million or being sold," she acknowledges. "But you also need people who are in the game a short time, make some money, and catch the bug and want to do it again."

Holzbaur has seen GeneChem's previous seed investment funds spread the entrepreneurial fever. This time she believes the process will lead not only to wealth creation in Quebec but also to a community of new, prosperous biotech firms.

GeneChem hopes to raise its contribution for AmorChem by the beginning of the fourth quarter. Once the fund is launched, the next step will be to scour the labs of local universities for winning ideas.—LISA JARVIS

WYOMING REQUIRES CHEMICAL DISCLOSURE

Wyoming has become the first state in the nation to require the energy industry to disclose which chemicals are used in hydraulic fracturing, a controversial drilling technique used to release hydrocarbons locked deep underground in shale rock formations. The process involves blasting chemically treated water and sand into a wellbore at high pressure to stimulate natural gas production. Industry maintains that the practice is safe, but environmental activists have raised concerns that it could contaminate drinking-water supplies. "People should be able to find out what chemicals they may have come in contact with, and emergency room doctors need this information in order to treat their patients and protect their staff," says Dan Heilig, staff attorney with Western Resource Advocates, a conservation group. New reporting rules require state regulators to keep information about the chemical mixtures confidential if a company can prove it is proprietary. In March, EPA launched a two-year research effort to examine the impacts of hydraulic fracturing on water quality and public health. And Democrats in Congress have proposed legislation (H.R. 2766, S. 1215) that would use the federal Safe Drinking Water Act to require companies to disclose the chemicals they use.—GH

SENATE VOTES TO LIMIT FORMALDEHYDE

The Senate approved legislation last week amending the Toxic Substances Control Act to establish emission limits for formaldehyde in composite wood products. The new health-based standards would apply to domestic products and foreign imports. A similar measure is pending in the House of Representatives. "High levels of formaldehyde are a health threat," Sen. Amy Klobuchar (D-Minn.), a bill cosponsor, said in a statement on June 14. "This bill will establish national standards that, when fully phased-in, will be the strongest in the world." Under the legislation, by Jan. 1, 2013, plywood and other new composite wood products sold in the U.S. would have to meet a formaldehyde emission standard of about 0.09 ppm. The wood products industry has adopted voluntary standards to limit formaldehyde emissions, but domestic products face competition from cheaper imported wood products, primarily from China, that may contain high concentrations of the chemical. "These standards will protect public health and ensure an even playing field between domestic wood products and foreign imports," Klobuchar said.—GH

Formaldehyde fumes in trailers used for emergency housing sparked congressional interest in cutting emissions.

FEMA

EPA DELAYS RISK STUDIES

EPA has put four of its ongoing human health risk assessments on hold because they rely heavily on tests conducted by the Ramazzini Institute, an animal testing laboratory in Italy that evaluates cancer-related effects of chemicals. The quality of data from the Ramazzini Institute was brought into question by the National Toxicology Program in a recent report that found major differences in opinion between NTP scientists and the Italian lab regarding an animal study on methanol. The four chemicals affected by the delay include methanol, methyl *tert*-butyl ether, ethyl *tert*-butyl ether, and acrylonitrile. EPA is currently determining whether to revise those four risk assessments or take action to verify the data used in the assessments. The agency is also investigating how best to ensure the integrity of completed risk assessments on vinyl chloride and 1,1-dichloroethylene, both of which relied on Ramazzini data. The Methanol Institute, an industry group, has long been pressuring EPA to review Ramazzini's methods.—BEE

INDUSTRY GETS FUNDS FOR CARBON CAPTURE

The Department of Energy announced it would provide $612 million—to be matched by $368 million in private funding—for three projects to capture and sequester CO_2 from industrial sources of greenhouse gases. The projects are large-scale, DOE notes, and are expected to be on-line by 2012 to 2014. Funded projects include a new methanol plant in Lake Charles, La., run by Leucadia Energy, which will capture 4.5 million tons of CO_2 per year. Air Products & Chemicals' Port Arthur, Texas, plant will capture 1 million tons of CO_2 annually from existing steam-methane reformers. The CO_2 from both of these projects will be piped through a Denbury Resources interstate pipeline; used for enhanced oil recovery at the Hastings West oil field, in Texas; and then sequestered underground. The third project will capture 1 million tons per year of CO_2 from the Archer Daniels Midland ethanol plant in Decatur, Ill., and sequester it in a deep saline reservoir near the plant. All government funding came through the American Recovery & Reinvestment Act of 2009.—JJ

FIGHTING DRUG RESISTANCE

Drug-resistant diseases are on the rise globally, and action is needed now to ensure that lifesaving drugs continue to work, a report by the Center for Global Development (CGD) concludes. To combat the problem, the report recommends that the World Health Organization take the lead and establish a network of laboratories dedicated to tracking the emergence and spread of drug-resistant microorganisms. The report also calls on pharmaceutical companies to provide a secure supply chain and ensure that high-quality medicines reach patients, particularly those in developing countries where counterfeit and substandard drugs are prevalent. Worldwide drug safety laws and enforcement of those laws should also be strengthened. Lastly, the report calls for research-funding agencies to create a Web-based network for researchers to share data that can accelerate the discovery of new drugs and diagnostics. "We know what actions are needed to fix the problem," Nancy Birdsall, president of CGD, said in a statement. "We just lack the incentives, institutions, and global leadership to get on with it."—BEE

DRUG SAFETY REFORM

Recall of **CHILDREN'S MEDICINE** prompts lawmakers to consider new authorities, resources for FDA

BRITT E. ERICKSON, C&EN WASHINGTON

WHEN MCNEIL Consumer Healthcare, a subsidiary of Johnson & Johnson, recalled more than 40 types of widely used children's medicine on April 30, confidence in the safety of the U.S. drug supply took a nose dive. American consumers and members of Congress, already wary of the quality of imported medicine, began questioning whether drugs manufactured in the U.S. are any better than those made overseas.

As J&J tries to rebuild its tarnished reputation and fix McNeil's quality control problems, lawmakers in the House of Representatives are examining what went wrong and what can be done to prevent such problems in the future. At a hearing on May 27, members of the House Committee on Oversight & Government Reform questioned executives from J&J and the Food & Drug Administration, the federal agency responsible for ensuring the safety and effectiveness of drugs.

Committee Chairman Edolphus Towns (D-N.Y.) stressed the need to know the health risks associated with the recall, whether the problems were an isolated incident or are widespread at McNeil, and whether FDA has sufficient resources and authorities to carry out its core mission of ensuring drug safety.

The recall, which included about 136 million bottles of liquid pediatric Tylenol, Motrin, Zyrtec, and Benadryl products, was conducted because of quality, purity, and potency problems, Towns noted. Some medicine was found to contain foreign particles, and some batches were found to have too much active ingredient.

"Almost every household in this country has these children's products in their medicine cabinets," Towns emphasized. "And everyone has the same questions: Are these products safe? And what are we doing to ensure safety in the future?"

Officials from both FDA and J&J testified that there is no evidence of serious adverse health effects related to the use of the recalled medicine. However, Joshua M. Sharfstein, principal deputy commissioner of FDA, told lawmakers that FDA's investigation of the health risks is still ongoing.

"Our experts believe the risk for any child in the U.S. was remote," he noted. "So far, FDA has no cases with evidence that a product quality issue contributed to a significant adverse health outcome."

Similarly, Colleen A. Goggins, worldwide chairman of J&J's Consumer Group, emphasized that "the recall was not undertaken on the basis of adverse medical events." Echoing Sharfstein's comment, she said that "the health risks to consumers from the recalled products were remote."

Nonetheless, "the quality and process issues that we found at McNeil, those which led to the recall and others, are unacceptable," Goggins acknowledged. She apologized "to the mothers, fathers, and caregivers for the concern and inconvenience caused by the recall."

RECALLED
The largest recall of children's medicine in U.S. history has Congress taking a closer look at drug safety.

SHUTTERSTOCK

This is not the first time McNeil has issued a recall because of quality problems, Sharfstein testified. "Over the last several years, FDA has had growing concerns about the quality of the company's manufacturing process," he said. "These concerns have led to a number of unsatisfactory inspections and consumer recalls."

FOR EXAMPLE, in spring 2009, FDA found that McNeil failed to meet its own quality standard when it used cellulose from a master lot that tested positive for the gram-negative bacterium *Burkholderia cepacia*, Sharfstein noted. Although the partial lot used in manufacturing did not test positive and no final products tested positive for the bacteria, the company violated FDA's current Good Manufacturing Practices (cGMP). As a result, McNeil recalled nearly 8 million bottles of children's medicine in August 2009.

And last fall, FDA became aware of consumer complaints that products from McNeil's Las Piedras, P.R., facility had a musty odor, Sharfstein said. "McNeil had

SUSAN MORRISSEY/C&EN

not fully investigated these reports for about a year and did not notify FDA despite the requirement that such reports be referred to the agency within three days," he pointed out.

The odor was eventually attributed to 2,4,6-tribromoanisole (TBA), a breakdown product of the fungicide 2,4,6-tribromophenol, which was used on wood pallets that stored empty medicine bottles. Risks from exposure to TBA include the potential for temporary gastrointestinal problems, but the small amounts transferred to the drugs did not pose a serious risk to health, Sharfstein testified. Nonetheless, McNeil conducted a series of recalls because of the contamination.

Another incident, which involved a dissolution problem with Motrin tablets, was particularly troubling to lawmakers. According to FDA documents, McNeil identified the problem in November 2008 and sent out contractors to perform "statistical sampling" of retailers to determine whether to initiate a recall. When FDA learned that McNeil had hired contractors to buy back the inferior drugs from retailers rather than recall them, the agency confronted the company. In July 2009, McNeil initiated a recall.

This pattern of noncompliance with FDA's cGMP convinced the agency to step up the frequency of inspections at McNeil's facilities, Sharfstein noted. And it is because of those inspections that McNeil's Fort Washington, Pa., facility—the one responsible for the latest recall of children's medicine—is currently shut down, he said. FDA is working with the company to ensure that it implements a corrective action plan that includes "significant enhancements to its quality system, organizational changes, and senior management oversight," he added.

FDA has also referred the case to its criminal unit, which will decide whether the company faces criminal liability charges for not complying with cGMP.

"This is a story of an agency that identified a problem, confronted a company, and eventually forced major changes to protect the public," Sharfstein noted. "A vigilant FDA is essential for drug safety in the U.S."

BUT WHEN ASKED whether FDA needs additional resources or authorities to ensure the safety of drugs, Sharfstein told lawmakers that the agency does need more authorities to do its job. He pointed to food safety legislation (H.R. 2749 and S. 510) working its way through Congress, which would give FDA the authority to require quality systems and preventive controls, to recall unsafe products, to access company records, and to impose civil penalties (C&EN, May 24, page 29). Those provisions, however, would only apply to food. "We don't have those authorities for drugs," he noted, adding that they would greatly enhance FDA's ability to ensure the safety of drugs.

FDA

Sharfstein

Chairman Towns pledged to introduce legislation that would give FDA the ability to order a recall of unsafe drugs. Currently, the agency relies on companies to voluntarily initiate recalls. If a company refuses, FDA must resort to court-ordered seizures, injunctions, and criminal prosecution, all of which are time-consuming. With respect to the latest McNeil recall, if the company had not cooperated with FDA, the products would still be on store shelves today, Sharfstein noted.

FDA and consumer groups are pushing for such legislation. In a June 1 letter to Towns, William Vaughan, health policy analyst with the nonprofit Consumers Union, recommended mandatory recall authority as well as more resources for FDA. "Consumers Union believes that the FDA needs more resources to ensure a more adequate level of inspections, especially internationally," he wrote.

Darrell E. Issa (R-Calif.), the ranking Republican on the committee, offered to work with Towns to give FDA additional authorities, including mandatory recall authority for drugs. "I am deeply concerned that the J&J recall is just the tip of the iceberg," Issa said, questioning whether FDA has the ability to ensure the safety of imported medicine.

"The safety of imports is extremely important to us," Sharfstein stressed. "There are certain things that we need to do better, including holding each person in the supply chain accountable."

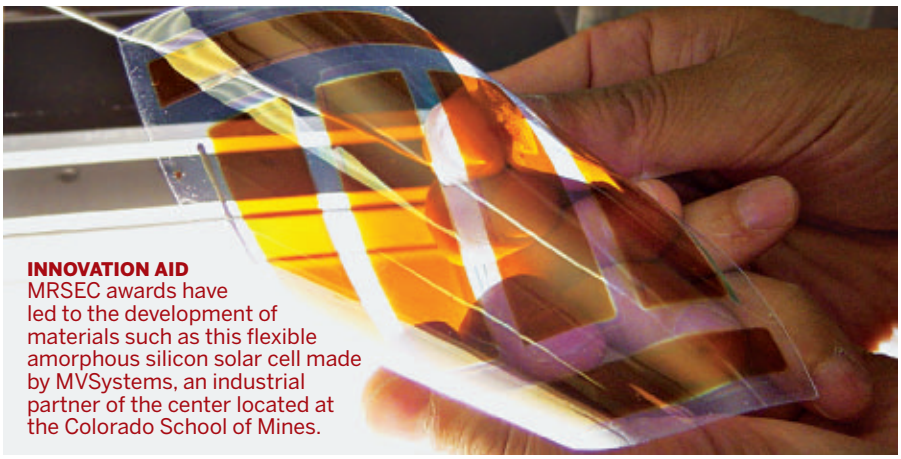
Sharfstein made similar comments at a March hearing on drug safety held by the House Energy & Commerce Committee's Subcommittee on Health. "Globalization has created new risks and challenges for the safety of the drug supply," he said. "Up to 40% of the drugs we take are imported, and up to 80% of the active pharmaceutical ingredients in the drugs we use are from foreign sources."

In addition, "the supply chain from raw material to consumer has become more and more complex, involving a web of repackagers and redistributors in a variety of locations," Sharfstein told lawmakers. "This makes oversight significantly more difficult and leaves weaknesses through which counterfeit, adulterated, and misbranded products might infiltrate the legitimate supply chain."

Also at the March hearing, John D. Dingell (D-Mich.), chairman emeritus of the Energy & Commerce Committee, was confident that Congress will pass drug safety legislation this year. "The safety of imported pharmaceuticals and supplies as well as the raw materials from which these are made is a matter of safety and great concern that must be addressed in this Congress," Dingell emphasized. "Last year, the House unanimously passed the bipartisan bill with regard to our food safety supply. I believe that we can and should and will pass similar legislation" for drugs this year. ■

"This is a story of an agency that identified a problem, confronted a company, and eventually forced major changes to protect the public."

MVSYSTEMS



INNOVATION AID MRSEC awards have led to the development of materials such as this flexible amorphous silicon solar cell made by MVSystems, an industrial partner of the center located at the Colorado School of Mines.

RESTRUCTURING NSF'S MATERIALS CENTERS

Division of Materials Research revamps centers program to EXTEND PARTICIPATION

RESEARCHERS ARE increasingly looking to tackle large-scale problems that require many players to solve. To better aid this pursuit, the National Science Foundation's Division of Materials Research is restructuring its Materials Research Science & Engineering Centers (MRSEC) program, which currently involves 27 centers and 807 faculty participants.

The revised program—Materials Research Centers & Teams—includes a new component, Materials Interdisciplinary Research Teams (MIRT), with a funding mechanism that is intended to be less onerous for participants by having fewer requirements than MRSEC. The names of the centers are also changing and will now be called the Centers of Excellence for Materials Research & Innovation (CEMRI).

"The goal of and motivation behind this restructuring is to broaden participation in this program," says Zakya H. Kafafi, director of NSF's Division of Materials Research. "We wanted to open up this competition to people and institutions who have never competed before."

The two options, CEMRI and MIRT, are intended to better meet the demands of the materials research and education community, and they come in response to a 2007 National Research Council report on MRSEC. Specifically, Kafafi tells C&EN, the report recommended the addition of a mechanism to support a single interdisciplinary team as well as a cluster of teams, which constitutes a center.

The division requested an overall budget for the two pieces of the program of about $36 million for fiscal 2011. Of that, $20 million to $24 million will go to fund an expected eight to 10 CEMRI awards, and $10 million to $12 million will go to support an estimated eight to 12 MIRT awards. CEMRI awards will be given for a six-year period, whereas MIRT grants will be awarded for an initial three-year stint.

Under the CEMRI part of the program, the division is looking to fund interdisciplinary materials research that addresses fundamental problems in science and engineering and requires a campus-based center. To be eligible, centers must include at least two, but no more than five, interdisciplinary research groups, which don't have to be located on the same university campus.

CEMRI grantees are expected to integrate education with research and develop appropriate outreach activities. They are also expected to include the development of experimental and computational facilities that support the long-term health of the U.S.'s materials research infrastructure.

But CEMRI applicants will have a new requirement to meet. Proposals will now have to include international collaborations—something that was optional for MRSEC. These types of working arrangements are "becoming very important as science is increasingly global," Kafafi explains.

THE NEW MIRT part of the program will also have a research and education emphasis but will have fewer requirements. For instance, MIRT grantees must involve at least five faculty-level participants, but they do not need to have a formal international collaboration. And MIRT grantees will not need to develop research and computational infrastructure, although they are tasked with operation and maintenance of such equipment. The goal is to open the program to smaller groups of researchers, many of which eventually become part of a larger center, Kafafi notes.

In addition to increasing participation from researchers and institutions that haven't previously competed in this type of mechanism, the restructured program also aims to increase participation by underrepresented groups.

"A goal is to broaden participation by including underrepresented majorities—namely women—and underrepresented minorities and people with disabilities," Kafafi says. To do this, she points out, proposals will need to include a strategic plan for increasing diversity at all levels, complete with metrics to measure progress over the award period.

JAMES MARSHALL/NRL

Kafafi

Preliminary proposals for both awards are being accepted by the division until Sept. 1 for CEMRI and Sept. 3 for MIRT. After peer review, a subset of applicants will be invited to submit full proposals. Final award announcements are expected next summer.

"I would like to invite the scientific community to cross new boundaries, interact with members of new and different disciplines, and connect globally via a cyberinfrastructure to address many of the 21st-century challenges and solve fundamental scientific problems," Kafafi says. "These centers will have overarching goals to achieve and will educate the materials researchers of the future in working in new interdisciplinary and emerging areas of science."—SUSAN MORRISSEY

CLIMATE CHANGING

UN talks begin **REBUILDING PROCESS** to craft an emissions treaty following Copenhagen letdown

INTERNATIONAL TALKS on climate change earlier this month attempted to re-establish political momentum for a legally binding treaty on greenhouse gas emissions. The original treaty was derailed at last year's United Nations summit in Copenhagen.

Negotiators got down to two weeks of business in Bonn, Germany, that concluded on June 11. These negotiations followed a minor three-day round of discussions in April that marked the official start of the 2010 climate talks. At the end of the June meeting, discussion leaders presented a draft treaty document to serve as the starting point for more talks that are scheduled for later this year. That draft suggests industrialized countries should aim to reduce their greenhouse gas emissions by 25 to 40% by 2020 but does not specify a base year.

The draft will undergo further refinement before the next round of talks in August. Jonathan Pershing, U.S. deputy special envoy for climate change, says the Obama Administration will insist that the new negotiating text build on the Copenhagen Accord, a nonbinding political agreement that emerged at last December's climate summit in Copenhagen.

That meeting was expected to produce a legally binding treaty that would control emissions of greenhouse gases and provide financing to help developing countries adapt to climate change and install cleaner energy technologies. However, the UN-sponsored discussions stalled over the course of the two-week meeting.

Closed-door talks at the meeting among a group of world leaders convened by President Barack Obama produced the Copenhagen Accord. It calls on countries to set their own goals for controlling domestic greenhouse gas emissions. Industrialized countries also pledged to supply $30 billion per year between 2010 and 2012 to help developing nations (C&EN, Jan. 4, page 8).

The major question for this year's climate negotiations is whether countries still intend to craft a new, legally binding international treaty on climate change, says Yvo de Boer, the UN's top climate-change official. A legally binding agreement "creates accountability" that less formal pacts lack, he explains.

In addition, de Boer says, "one of the main priorities for this year is to rebuild trust, to rebuild confidence in that negotiating process." Copenhagen "was a pretty horrible conference and did a lot of damage to the atmosphere of the negotiating process," he adds.

A key part of that rebuilding will be for industrialized countries to begin supplying the money they pledged under the Copenhagen Accord, de Boer says.

A related issue that negotiators are struggling with is how to get the money to developing countries. Saleemul Huq, a senior fellow at the London-based International Institute for Environment & Development, says that the developing world favors channeling the money through the UN bureaucracy that administers the 1992 global climate-change treaty. But donors from industrialized countries would rather funnel it through the World Bank or through their own development assistance programs, Huq says.

CLIMATE NEGOTIATIONS will resume in Bonn in August, with another round of discussions scheduled for October. Negotiators are preparing for a major climate conference in Cancún, Mexico, from Nov. 29 to Dec. 10. However, climate-talk observers say that they expect no new legally binding treaty before a 2011 climate conference that will take place in South Africa.

The recently ended Bonn meeting marked the last climate negotiation session that de Boer will oversee. Effective July 1, he will become global adviser on climate and sustainability for financial and accounting firm KPMG and will work in academia. Costa Rican diplomat Christiana Figueres has been tapped to replace him.—CHERYL HOGUE

DATING PHARAOHS

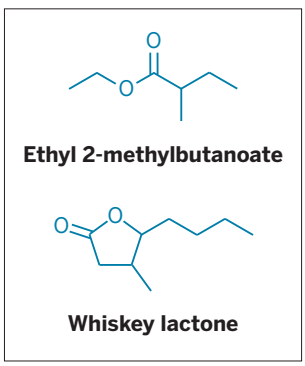
University of Oxford researchers have come up with the most comprehensive chronology thus far of Egypt's dynasty of pharaohs by radiocarbon-dating some 211 artifacts (*Science* **2010,** *328,* 1554). Until now, when Egyptologists have talked about when different pharaohs reigned, the dates they discussed were primarily determined using historical documents. The results of the project, led by Christopher Bronk Ramsey, director of a radiocarbon-dating facility at Oxford's Research Laboratory for Archaeology & the History of Art, correlate well with historically derived dates—with a few exceptions. For example, new radiocarbon dating puts the start of the New Kingdom—ancient Egypt's golden age—between 1570 and 1544 B.C., several decades earlier than historical estimates. The revised chronology will also enable experts to compare and contrast the timing of important events in other ancient societies such as those in Mesopotamia, Sudan, and Central Asia. Ramsey's team sampled baskets, plant-based textiles, seeds, and other plant remains from museum collections around the world that were clearly associated with the reign of a particular pharaoh and used statistical methods and calibrated samples to ensure that the dating was accurate.—SE

EZRA MARCUS

Ancient documents such as this papyrus from El-Lahun, Egypt, were radiocarbon-dated as part of the pharaoh chronology project.

MÉLANGE OF VOLATILES DISTINGUISH BRANDIES

Researchers in France trying to tease out the chemical "je ne sais quoi" that distinguishes apple, grape, and plum brandies are reporting that the secret is the relative concentrations of the fruit-based volatile compounds (*J. Agric. Food Chem.,* DOI: 10.1021/jf9045667). A team led by Jérôme Ledauphin of the University of Caen used mass spectrometry to compare the volatiles in Calvados (apple), Mirabelle (plum), Cognac (grape), and Armagnac (grape) brandies. Many of the more than 200 compounds they detected were found in all the fruit brandies. But each type of beverage has its own relative concentrations of these compounds that set it apart. For example, higher concentrations of methyl branched esters such as ethyl 2-methylbutanoate are measured in apple-based Calvados. In plum-based Mirabelle, higher concentrations of aldehydes such as hexanal, heptanal, and nonanal distinguish the brandy and give it what expert tasters call "vegetal and green aromatic notes," Ledauphin explains. The zest of grape-based brandies comes from so-called whiskey lactones, which give rise to coconut-like odors. Next up in the French group's research is to figure out when in the fermentation process the distinguishing aromas and tastes develop.—SE



MOLECULAR MACHINES SPOTTED ON THE MOVE

The molecular machines synthesized by Northwestern University's J. Fraser Stoddart and coworkers have long held promise as switches in molecular electronics and other nanoscale devices. But the researchers have only been able to infer the movements of these tiny devices from spectroscopic data—until now. Teaming up with UCLA's Paul S. Weiss and coworkers, Stoddart's group is reporting the first direct observation of the movement of a molecular machine using scanning tunneling microscopy (*ACS Nano,* DOI: 10.1021/nn100545r). The machine is a bistable rotaxane—a ring wrapped around a dumbbell-shaped structure tethered to a gold surface. Depending on the rotaxane's redox state, the cationic ring moves from a tetrathiafulvalene moiety at one end of the dumbbell to a 1,5-dioxynaphthalene unit at the opposite end. The researchers found that both the conformation of the dumbbell and interactions with the gold surface and with neighboring molecules influence the motion within these interlocked molecules. "To realize the full potential of these functional molecules at the nanoscale, it is imperative to understand their operation at the single-molecule level under environments relevant to actual device operation," the researchers note.—BH

MODIFIED GOLD PARTICLES SERVE AS CHIRAL ADSORBENTS

Gold nanoparticles decorated with chiral molecules can serve as enantioselective separation media for other types of chiral molecules, according to researchers at Carnegie Mellon University (*J. Am. Chem. Soc.,* DOI: 10.1021/ja908219h). In addition to demonstrating the potential for use in chiral separations, the study may lead to advances in enantiospecific catalysis and sensing applications. Nisha Shukla, Melissa A. Bartel, and Andrew J. Gellman treated suspensions of gold nanoparticles with D-cysteine, L-cysteine, and the racemic mixture. The team then exposed the coated nanoparticles to propylene oxide. Next, they conducted a series of control experiments in which they measured the optical rotation of bare nanoparticles (which are not chiral), cysteine-modified particles, and coated nanoparticles that had been exposed to enantiomerically

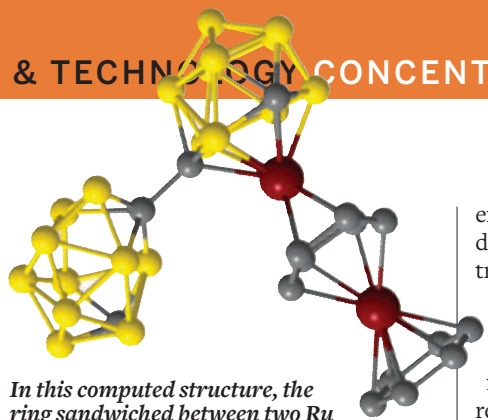
pure propylene oxide. They observed that L-cysteine-modified gold particles selectively adsorb (*R*)-propylene oxide and that the D-enantiomer selectively adsorbs (*S*)-propylene oxide. Exposing a racemic mixture of propylene oxide to one type of modified gold particle results in an enantiomerically enriched solution, they say.—MJ

THE MOON IS 'WETTER' THAN FIRST BELIEVED

Geologists studying moon rocks have found evidence that water once existed on the lunar surface at levels 100 times greater than previously thought (*Proc. Natl. Acad. Sci. USA*, DOI: 10.1073/pnas.1006677107). Using secondary ion mass spectrometry, Francis M. McCubbin and coworkers at Carnegie Institution for Science, in Washington, D.C., looked for hydroxyl groups in the mineral apatite from lunar samples collected during Apollo missions in the 1970s. The team extrapolated its findings to estimate the water content for the region of the moon from which the samples were collected at 64 ppb to 5 ppm. Previous estimates were less than 1 ppb. "The presence of hydroxyl in apatite from a number of different types of lunar rocks indicates that water may be ubiquitous within the lunar interior," McCubbin and coworkers note in the paper. The researchers ruled out contamination of samples after they had been collected, observing that hydroxyl groups would have a tough time binding to and penetrating the moon rocks' surface. The Carnegie Institution study complements the work of Alberto E. Saal of Brown University, who published a paper two years ago in *Nature* that first countered conventional wisdom that the moon was dry as a bone (C&EN, July 14, 2008, page 34). Saal's work examined glass beads from one type of lunar volcanic rock.—DP

CAGEY ARENE CLEAVAGE

A carbon-boron cage compound has been discovered doing some challenging chemistry at room temperature—breaking the carbon-carbon bond of an aromatic ring. If a catalytic version of this chemistry could be developed, it might be useful for removing impurities in crude petroleum, the reaction's discoverers say (*Angew. Chem. Int. Ed.*, DOI: 10.1002/anie.201001555). Chemists have previously cleaved a C–C bond on an aromatic heterocycle at elevated temperatures (C&EN, Feb. 1, page 10). For Stuart A. Macgregor and Alan J. Welch of Scotland's Heriot-Watt University, their room-temperature arene bond-breaking came unexpectedly. With a ruthenium *p*-cymene species, their team was trying to add a ruthenium vertex to each of the cages on a bis-carborane. But instead, one cage incorporated two ruthenium *p*-cymene fragments, and an aromatic C–C bond on one *p*-cymene was cleaved. Density functional theory calculations carried out by the team suggest that this happened because the *p*-cymene becomes sandwiched between two ruthenium atoms atop one carborane cage. The other carborane reduces the arene, disrupting its aromaticity and triggering bond-breaking. Adaptations of this chemistry to other arenes are in progress, Welch says.—CD



In this computed structure, the ring sandwiched between two Ru atoms (red) has been reduced; one of its C–C bonds will later be cleaved. (C is gray and B is yellow.)

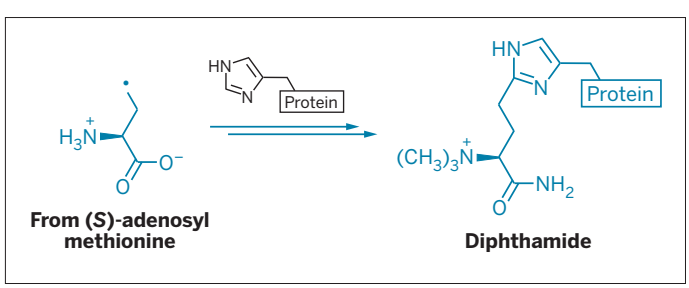
ALAN WELCH

NANOWIRES NOW DELIVER

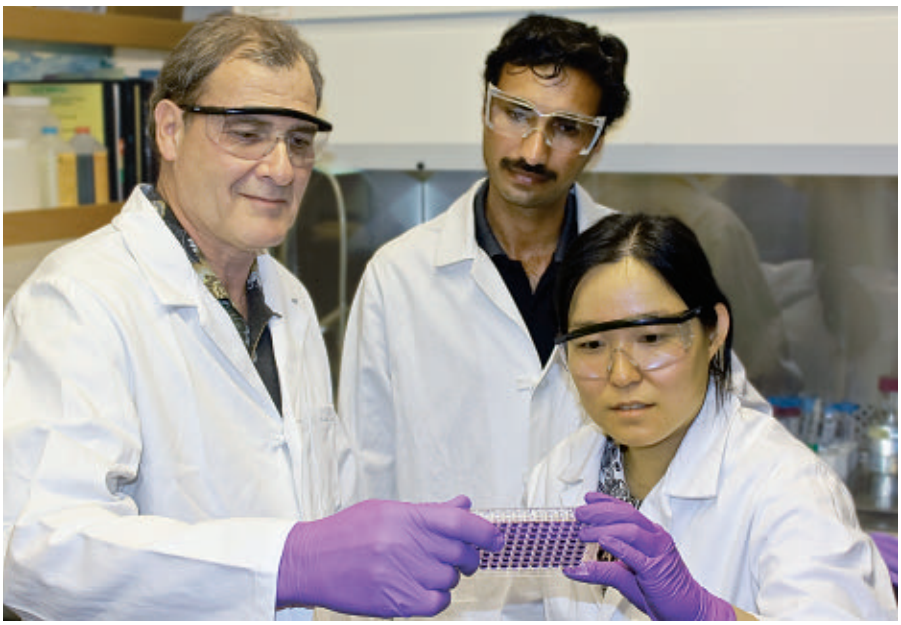
Researchers can now precisely manipulate nanowires to deliver molecules to individual cells and even to specific regions within cells (*Nat. Nanotechnol.*, DOI: 10.1038/nnano.2010.104). Andre Levchenko, Chia-Ling Chien, and coworkers at Johns Hopkins University showed that they can control the trajectory of cytokine-loaded gold nanowires with a combination of alternating and constant electric fields. The alternating fields regulate the nanowire orientation, whereas the constant fields dictate the direction of motion. Using this method, the researchers manipulated nanowires to deliver tumor necrosis factor-α (TNFα), a biological molecule involved in cell signaling, to targeted cells. They monitored the effects of TNFα delivery by imaging the distribution of nuclear factor-κB (NF-κB), a transcription factor released in response to TNFα. In cell culture, NF-κB was activated only in cells that were in direct contact with the nanowires. The researchers also found that they could increase the cellular response by delivering multiple nanowires to a single cell. The team expects that other biologically active compounds can be delivered in the same way and that the method will be useful for a variety of biological applications.—CHA

RADICAL START FOR IRON-SULFUR ENZYME

A modified amino acid that is the target of diphtheria toxin is assembled through some unusual enzyme reactivity, a multi-institution team has found (*Nature* **2010,** *465*, 891). Researchers have known for decades about the molecular target, called diphthamide. But its biosynthesis had remained unclear. Steven E. Ealick, Jack Freed, and Hening Lin of Cornell University in collaboration with Carsten Krebs of Pennsylvania State University and coworkers have revealed the structure and chemistry of a novel iron-sulfur enzyme that they say catalyzes the first step of diphthamide biosynthesis in a microorganism. Diphthamide, which is found on a protein factor used during translation, is a histidine residue modified with help from the cofactor (*S*)-adenosyl methionine (SAM). The team's work suggests the new enzyme's 4Fe-4S cluster transfers an electron to SAM to generate a 3-amino-3-carboxypropyl radical intermediate, which goes toward making diphthamide. Similar iron-sulfur enzymes all generate a 5′-deoxyadenosyl radical from SAM instead, so the new enzyme represents "a remarkable adaptation of hallmark reactivity," Krebs says. Eventually, the team hopes to understand how many different enzymes generate different reactive species from SAM.—CD



MAGGIE MORRIS



NATURAL EXPLORERS Pezzuto (from left) examines assays with visiting scientist Ihsan-ul-Haq and postdoc Eun Jung (Amy) Park.

CANCER PREVENTION, NATURALLY

The **DIFFICULT SEARCH** for cancer-preventing natural products takes several paths

CARMEN DRAHL, C&EN WASHINGTON

CANCER IS A major killer, with each type of cancer a different beast, and molecules from nature have become some of medicine's most powerful cancer treatments. But rather than fighting cancer that's already raging, many scientists are seeking ways to prevent or delay it.

Cancer prevention has seen a few molecular success stories so far, although none of the compounds has come straight from nature. For example, the synthetic drugs finasteride and dutasteride, which treat enlargement of the prostate gland, have proven effective at deterring prostate cancer. Both the osteoporosis drug raloxifene and the breast cancer treatment tamoxifen, also synthetic agents, have cut the breast cancer rate in half among women at high risk. Nevertheless, some research groups believe natural products might prove to be a fruitful source of future preventive drugs for cancer.

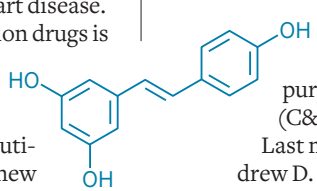
By and large, chemoprevention has lagged behind preventive-drug development in other areas, such as heart disease. The pipeline of cancer prevention drugs is woefully thin, especially when compared with the pipeline of experimental drugs for treating cancer, and most pharmaceutical companies aren't pursuing new chemopreventive agents.

John M. Pezzuto of the University of Hawaii, Hilo, is among those trying to fill the cancer prevention pipeline with Mother Nature's help. "When we got into this field, there were programs in natural products focused on chemotherapy but almost nothing focused on chemoprevention," he says.

Most existing cancer prevention agents didn't come from a ground-up discovery and medicinal chemistry effort, Pezzuto says. Instead, they were developed from drugs that were already on the market for other uses, sometimes stemming from epidemiological observations about a cancer prevention trend. For instance, aspirin, which has proven efficacious at preventing colon cancer in several randomized clinical trials, was first recognized for its ability to relieve pain and prevent heart attacks and strokes. If useful cancer prevention agents have been developed by such indirect routes, still more new agents might come from a dedicated discovery platform, Pezzuto contends.

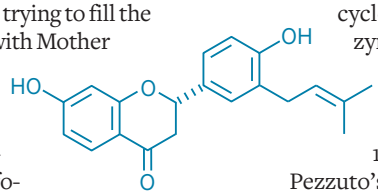
FOR NEARLY 20 YEARS, Pezzuto has led a multi-institution team dedicated to finding natural-product agents and new molecular targets for cancer prevention. The team, which is funded by the National Cancer Institute (NCI), combines experts in natural-product isolation, organic synthesis, structural biology, mass spectrometry, and animal testing.

The program has evolved over the years. The group's discovery efforts began with terrestrial plants. That approach uncovered several molecules with promising cancer prevention activity, most notably resveratrol, the red-wine compound made by a range of plants that has been the subject of controversy because of its purported antiaging properties (C&EN, Dec. 14, 2009, page 36).



Resveratrol

Last month, team member Andrew D. Mesecar of the University of Illinois, Chicago, solved the structure of resveratrol bound to cyclooxygenase-1, an enzyme thought to mediate resveratrol's chemopreventive activity (*Biochem. J.*, DOI: 10.1042/BJ20091857).



Abyssinone II

Pezzuto's team was the first to show that resveratrol might have cancer prevention activity (*Science* **1997,** *275,* 218), and today, the agent has reached clinical trials for this purpose.

Another agent the team is working with, abyssinone II, is from a plant used in

As preventive agents, "natural products haven't been as successful as one might like, but that doesn't mean the next one won't be."

traditional Chinese medicine. It has been selected for further studies under NCI's Rapid Access to Preventive Intervention Development (RAPID) program, which assists academic investigators with preclinical and early clinical drug development. Team member Mark Cushman of Purdue University has been preparing abyssinone derivatives for additional testing.

Pezzuto's team is now starting to look beyond plants. Relatively little is known about the potential of compounds from deep-ocean microbes, Pezzuto says. So, in collaboration with William Fenical of Scripps Institution of Oceanography, who is a pioneer in this area, the team has started exploring these microbes as a source of natural-product agents for cancer prevention.

At Ohio State University, Gary D. Stoner is studying the cancer prevention potential of natural products in foods. He bases his work on the concept that although the amount of a natural product in a specific food is small, a complex mixture of foods might provide a favorable chemopreventive effect. "We've worked mainly with berries, a little bit with beets," Stoner says.

His current focus is on a freeze-dried and powdered black raspberry mixture his team has developed that blocks formation of esophageal and colon cancers in rats. Preliminary studies of the powder on human volunteers with premalignant lesions in their mouths indicate that the berry powder is safe to consume. More studies are needed to show that it truly slows or halts the onset of cancer. To that end, Stoner's team has received funding from NCI to conduct a randomized, placebo-controlled clinical trial on the berry powder, which the researchers hope to begin soon. "The food-based approach to cancer prevention has been hurt" by companies that have made health claims for foods "on the basis of very little research," Stoner says.

FARTHER EAST, at Dartmouth College, in Hanover, N.H., Michael B. Sporn has been researching chemopreventive agents for decades. In fact, he coined the term "chemoprevention" in the 1970s. Like Pezzuto, Sporn believes in the potential utility of isolated natural products in cancer prevention. To Sporn, natural products are less of a solution themselves and more of an inspiration for analogs. "Finasteride and dutasteride are not natural products," he points out. "They are testosterone analogs."

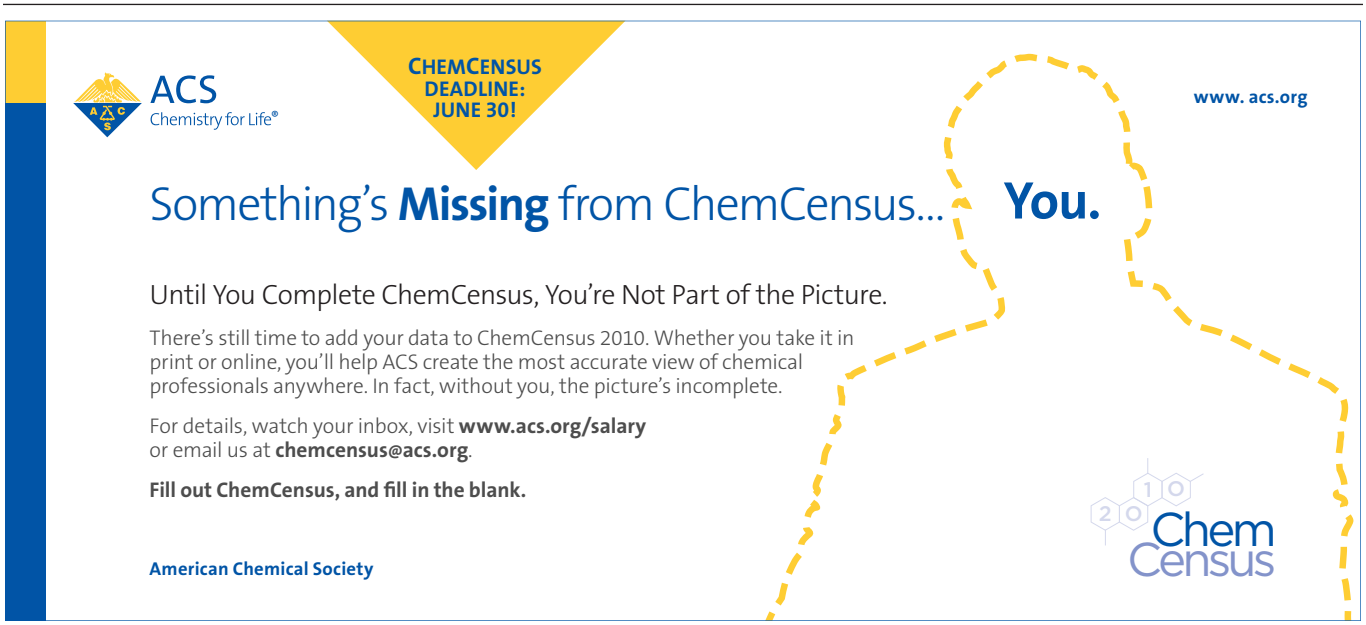
Sporn's own research has largely focused on making chemical improvements to retinoids and related molecules that have potential as cancer prevention agents. "Many natural-product scaffolds give us important clues about what might be useful," he says, and organic chemists can make such molecules into much better chemoprevention agents.

No matter how good a molecule might look in early studies, it's still tough for an experimental chemoprevention therapy to make it through the drug approval process, especially when compared with a drug already on the market for something else. Any agent for preventing cancer is going to be given primarily to healthy patients, says Barnett S. Kramer, associate director for disease prevention at the National Institutes of Health. "When you're dealing with healthy people, there's a very high bar to clear," he says. "It's good to have a sense of what the potential harms will be going into a study. If you have information from previous trials, then it's very helpful background."

In that sense, it helps that repurposed drugs such as aspirin had already been studied extensively in other contexts. "It is difficult to make a healthy person better off than they already are," Kramer says. Studies of new entities need to be undertaken with the appropriate amount of caution, he adds.

Large-scale cancer prevention studies of the natural products beta-carotene and vitamin E have been disappointing because neither turned out to be an effective cancer prevention agent, Kramer notes. But that doesn't mean prevention researchers should give up on studying molecules from nature, he says. As preventive agents, "natural products haven't been as successful as one might like, but that doesn't mean the next one won't be," he says. "We have to judge them on a case-by-case basis."

Natural products are a good idea for chemoprevention, Sporn says. He and others believe it's only a matter of time before that potential becomes reality. ■



HUMAN GENOME SEQUENCE MILESTONE

Health care improvements come into focus as human sequence marks its 10TH YEAR

STU BORMAN, C&EN WASHINGTON

HAPPY BIRTHDAY to the human genome sequence, or at least human knowledge of it. This week marks the 10th anniversary of the completion of the draft human genome sequence by the international Human Genome Project (HGP) and the private company Celera Genomics.

That artificial finishing point, announced on June 26, 2000, at the White House, has turned out to be a commencement. Since then, advances in collecting, organizing, and interpreting genetic data and dramatic reductions in the cost of gene sequencing have made it possible for genomics to have a growing influence on human health care.

It's been said that a truly transformational technology will always have its immediate consequences overestimated and its long-term consequences underestimated, noted National Institutes of Health Director Francis S. Collins at a recent meeting. "I think that's turning out to be true for what we are learning from the human genome. This science is driving a lot of the excitement right now in biomedical research, and that's likely to continue for some time," he said.

Collins, who led the U.S. component of HGP as director of the National Human Genome Research Institute (NHGRI) from 1993 to 2008, spoke at "The Human Genome: A Decade of Discovery, Creating a Healthy Future," an anniversary symposium held in Washington, D.C., on June 7.

The cost of genome sequencing has plummeted so much over the past decade that companies are now marketing sequence data on disease risks directly to consumers. Collins recently tested this out by submitting his own DNA (under an assumed name) to three genotyping companies.

"All three of these companies seemed to have highly accurate lab methods in terms of their sequence data," he said. "All three agreed that I had an increased risk of diabetes, maybe something like 50% higher than the average person. That was actually a bit of an eye-opener and caused me to change my health behaviors a bit. But they were all over the place in terms of other predictions, like prostate cancer, where one said [my risk] was lower than average, one said I was average, and the other said I was above average.

"That's obviously unsettling if these are in fact recommendations that people are going to pay attention to," Collins said. "There will be no doubt rather intense discussion over the course of the coming months over the degree to which this kind of direct-to-consumer marketing needs more oversight."

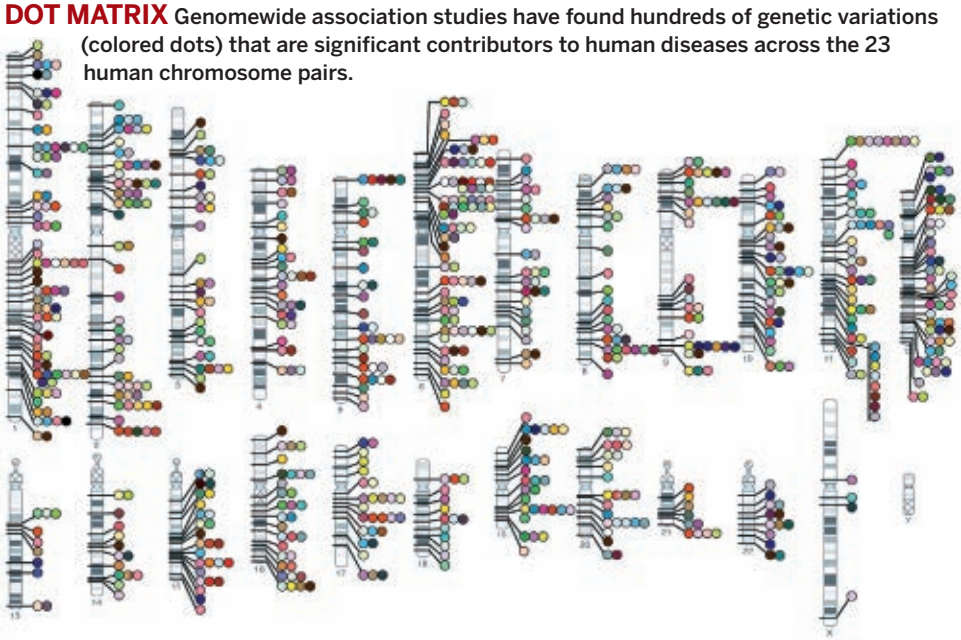
IN ADDITION TO the 10th anniversary of the draft sequence, it's close to the 20th anniversary of HGP, which was launched in October 1990. There was no sequencing of the human genome in a serious way for about the first six years of the project. Pilot projects for human genome sequencing began in 1996, and 20 centers in six countries then worked together to generate the June 2000 draft sequence. Over the next three years, scientists continued to work on the draft sequence to improve its completeness and enhance its accuracy, and in April 2003, the high-quality reference human genome sequence was declared complete.

Improvements in sequencing technology eased the way to those sequences and are now beginning to affect human health care in ways "we could hardly have imagined 10 years ago," Collins said. He noted that the cost of sequencing 1 million base pairs, which was about $20,000 in 1999, is now 20 cents and continues to drop. "There is no end in sight," Collins said. "No laws of physics have to be violated for this to continue, and it's continuing in a dramatic way."

HGP's human genome sequence cost about $400 million. But Illumina Inc. announced earlier this month that it is now charging $9,500 to sequence the genome of an individual with a serious medical condition. "The expectation is that we will reach the $1,000 genome, certainly in the next four to five years," Collins said.

As genome sequencing has gotten cheaper, a variety of projects have been established to find out

DOT MATRIX Genomewide association studies have found hundreds of genetic variations (colored dots) that are significant contributors to human diseases across the 23 human chromosome pairs.



NHGRI

more about the genome and expand medical applications of genomics. For example, the Cancer Genome Atlas is currently being assembled "to understand at the most detailed molecular level for the 20 most common cancers what is driving them" and how that information can be used diagnostically and therapeutically, Collins said.

Encode, the Encyclopedia of DNA Elements, is collecting information on how proteins tell genes whether they should be on or off, on epigenetic (nonsequence) effects on gene function, and on how genetic variations contribute to disease.

The International Knockout Mouse Consortium is developing in stem cells a knockout of every single mouse protein-coding gene and then making those stem cells available for research. The aim is to improve the ability to determine the function of different working genes.

Researchers studying particular genes often want to obtain actual copies of those genes (called cDNAs), but it can take months of work to obtain each one. So the Mammalian Gene Collection is assembling and making available a complete set of cDNAs for both the human and the mouse.

THE 1000 Genomes Project plans to sequence the genomes of at least 1,000 participants from different ethnic groups. It's an international effort to establish a detailed catalog of human genetic variation to support future biomedical studies.

The Human Microbiome Project is creating a catalog of all the microorganisms living in and on our bodies to better understand how those microbes contribute to human health and disease.

And the International HapMap Project is identifying the contributions of sequence variations to human disease. It focuses on the roughly 0.4% of the genome that differs among individuals—99.6% of different people's gene sequences being identical—and on mapping these sequence variations to specific locations on chromosomes. HapMap data facilitate genome-wide association studies, in which hundreds of genome-sequence associations with common diseases have now been validated. Many of these associations are weak or partial, but they nevertheless serve as pointers to potential drug targets.

Genomic data are also beginning to be used for personalized medicine—not only to provide the kind of data Collins obtained on his personal DNA but also to identify individualized responses to drugs. For example, in March, the Food & Drug Administration added a black-box warning to the anticlotting medication Plavix (clopidogrel) to warn patients and health care professionals that the drug is less effective in individuals with a variant gene for a liver enzyme that catalyzes formation of the drug's active form.

Genomics will continue to get "closer and closer to patients" and will increasingly influence the way medicine is practiced, said the current NHGRI director, Eric D. Green, at the anniversary symposium. "You can just start to imagine all the projects that will spin out as you begin to sequence not dozens of human genome sequences, but hundreds, thousands, tens of thousands—because the technology is absolutely driving this." ■

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BETTER ROUTE TO HARD-TO-GET ISOMERS

PEPTIDIC CATALYST yields access to chiral biaryl compounds

A NEW SYNTHETIC path to atropisomers—a class of chiral compounds that includes drugs, natural products, and ligands for asymmetric catalysis—could open the door to creating a wider range of such compounds, which until now have been difficult to synthesize.

Atropisomers are stereoisomers that can be enantiomeric, owing to a steric barrier to rotation about a single bond. Examples include biaryl compounds with bulky substituents, natural products such as the antibiotic vancomycin, and BINAP, a ligand widely used as a catalyst in asymmetric synthesis.

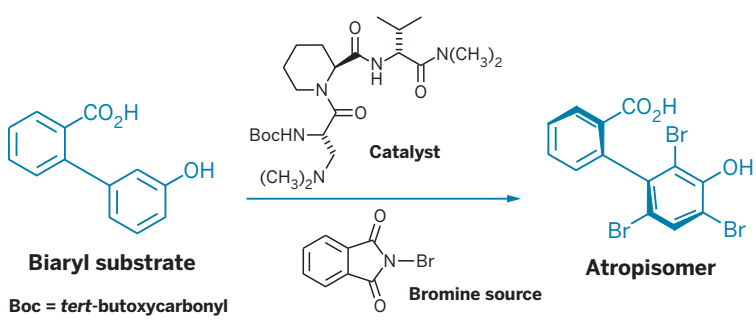
Previous techniques for creating atropisomers relied on capturing them with selective reactions of rapidly equilibrating compounds or forging new bonds between biaryl fragments. But catalytic reactions that can produce specific atropisomeric enantiomers from equilibrating racemic mixtures have not been extensively developed.

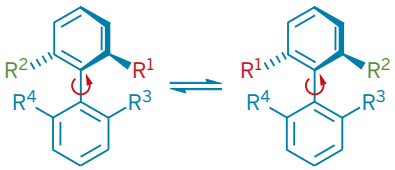
Now, synthetic chemist Scott J. Miller and coworkers Jeffrey L. Gustafson and Daniel Lim of Yale University have crafted what could prove to be a more general approach (*Science* **2010,** *328,* 1251). They designed and optimized a small-molecule tripeptide-based catalyst that trihalogenates enantiomeric but rapidly interconverting biaryl compounds stereoselectively, forming stable atropisomeric products.

The approach—which has high enantioselectivities (enantiomeric ratios of about 95:5) and high yields (in most cases 65 to 87%)—could make a wider range of potentially useful enantiomeric compounds more accessible synthetically. Miller and coworkers also propose a possible mechanism for the reaction, enabling them to rationalize its stereochemical outcome.

BROMINATION

Catalytic reaction adds bromines, yielding atropisomeric product.





ATROPISOMERISM

Biaryl atropisomers like these two can be isolated if there is a high barrier to rotation around the central bond (curvy arrows), such as when the R-group substituents are very bulky.

The technique could lead to "selective reactions of other interconverting, axially chiral compounds, promoted by simple peptide-based catalysts," the researchers write.

"I was mesmerized by the paper," says T. Ross Kelly of Boston College, who has worked with atropisomers. "I never would have predicted that this would have worked"—that a small peptide-based compound would catalyze atropisomer resolution—"and I never would have tried it. The wonderful thing about basic research is sometimes you hit amazing pay dirt, and I think this is one of those cases. The technique should have lots of utility," he says.

Jonathan Clayden of the University of Manchester, in England, who developed an earlier atropisomer synthesis method, says: "The Miller paper's key breakthrough is conceptually simple—it uses a peptide to capture one conformation of a molecule, which is then trapped by having its rotational freedom clamped down. It's a proof of concept which, because the catalysts are peptides, will be readily extendable to a range of substrates, I'm sure. I think this is the key advantage—potential flexibility."

"The results are exciting and important because they provide a new way to control a very subtle form of isomerism in organic molecules," says Samuel H. Gellman, a specialist in designed peptides at the University of Wisconsin, Madison. "Although the creation of isomerically pure biaryl compounds is very important," until now scientists have found it extremely difficult to form one or the other enantiomer predominantly, he continues. Many scientists will be drawn to these results, Gellman says.—STU BORMAN

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ASSESSING SAFETY

Survey characterizes the safety culture in ACADEMIC LABORATORIES

JYLLIAN KEMSLEY, C&EN WEST COAST NEWS BUREAU

THE AMERICAN Chemical Society Division of Chemical Health & Safety (CHAS) has released the results of an April survey aimed at evaluating the laboratory safety culture within hundreds of academic chemistry departments. Intended to establish a baseline of knowledge about laboratory safety programs, the survey asked departments about administrative issues such as access to chemical hygiene plans and emergency equipment, as well as training and work practices of faculty, staff, and students.

Certain aspects of the survey make it difficult to obtain a clear picture of academic safety culture. For example, some questions refer only to "students" without specifying undergraduate or graduate, and answers to other questions about chemical hygiene plans may be influenced by differing state requirements.

Nevertheless, responses to some questions paint a relatively positive picture. The survey showed, for instance, that most faculty, staff, and students receive some form of safety training. Also, 75.9% of respondents answered "agree" or "strongly agree" when asked whether their institution's administration supports the development and enforcement of safety rules for laboratories.

Yet 8.9% of survey respondents answered "disagree" or "strongly disagree" to that question. And the survey indicated that 70.5% of faculty, 59.2% of professional staff, 52.1% of graduate students, and 20.1% of undergraduates work alone in laboratories "often" or "occasionally," a practice that health and safety professionals generally consider unsafe.

The survey also showed that safety considerations aren't usually included in the evaluation of faculty, staff, and students. "I think that's a bit problematic in terms of the school helping to instill a culture of safety," says Edward Miller, chair of the chemistry department at the State University of New York, Plattsburgh, and one of the survey developers. "There's an old adage that if no one's measuring it then it isn't important," he adds, acknowledging that his own performance assessments have never included safety.

The survey effort started at the August 2009 ACS national meeting in Washington, D.C. Miller attended the CHAS executive committee meeting there and asked if the division would consider looking into the state of safety in academic departments. "I had been thinking about all the things we've been struggling with over the years in my own department" in terms of fostering a safety-conscious environment, Miller says. "I was wondering how other departments were faring."

With the blessing of CHAS, Miller teamed up with Ralph Stuart, secretary of CHAS and the University of Vermont's environmental safety manager, to develop the survey. They were starting from scratch, Stuart notes, since, as far as anyone could tell, no survey of academic laboratory safety culture had ever been done before. Miller and Stuart wrote an initial set of questions, which were then reviewed by the CHAS executive committee as well as the ACS Committee on Chemical Safety.

Miller and Stuart contacted 922 chemistry department chairs for the survey and heard back from 45.4% of the schools. Of the respondents, 81.4% were department chairs as opposed to safety committee members or chemical hygiene officers.

ALTHOUGH THE ANSWERS to the survey may look promising, the devil may be in the details. The survey responses indicate that the vast majority of students receive safety training, for instance. "It's clear that training is being delivered," Stuart says. "Now we need to think about how to collect information from the people receiving the training" to evaluate whether the training is effective.

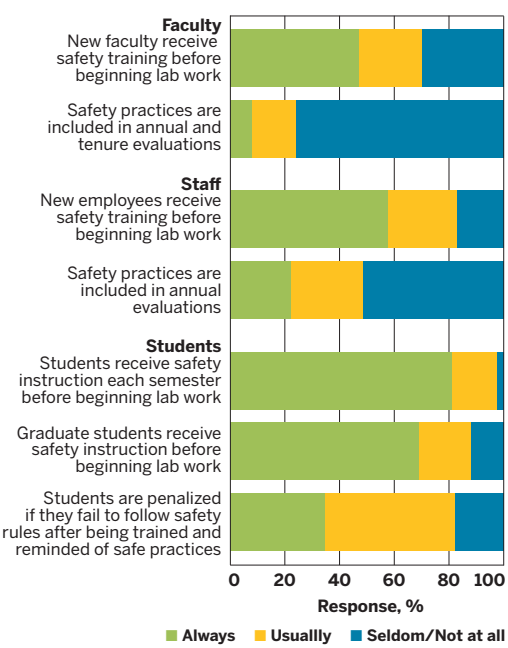
In addition to collecting answers to set questions, the survey allowed respondents to comment on various questions or aspects of the survey. The submitted comments were mixed. Regarding institutional policies, a respondent at one school noted that "the university-level safety office provides little guidance and oversight," while another described a program involving surprise lab inspections. Regarding student safety, comments varied from "students are poorly supervised" to "students are kicked out" for not following safety rules.

The survey results are available on the CHAS website (dchas.org, click on "Culture Survey"). The division is also soliciting comments on the results. That information will help determine the next steps. Focus groups are under consideration, as well as additional surveys to target and compare the responses of students and health and safety professionals. "The more feedback we get the better and more useful we can make it for people," Miller says.

"I'm pretty excited that the conversation is going on," he adds. "Safety is a tough subject sometimes to get people to focus on." ■

SAFETY CULTURE METRICS

Safety training and evaluation are uneven across academic populations



SOURCE: ACS Division of Chemical Health & Safety survey, April 2010

CHEMIST SUES COLLEGE

ZAFRA LERMAN says she was fired from Columbia College Chicago because of her religion and gender

A $20 MILLION discrimination and breach of contract suit was filed against Columbia College Chicago and four of its administrators in early April by one of its longtime tenured professors, Zafra Lerman. A noted science educator, human rights activist, and familiar face in various American Chemical Society governance positions over the years, Lerman was fired by the college in October 2009 after it accused her of misappropriating grant funds.

At the college, Lerman, a professor of science and public policy, was founder and head of the Institute for Science Education & Science Communication (ISESC). She says she brought innovative science teaching methods to educators in Chicago public schools and also to people on the margins of society, such as prisoners and homeless children. A Columbia College performance evaluation for Lerman dated April 2009 and included as an exhibit in her lawsuit is filled with high praise for her programs and accomplishments and indicates that she "exceeds expectations."

In the suit, Lerman charges that she was discriminated against because she is Jewish and female. Moreover, as a tenured professor, she claims that she was denied due process in fighting her dismissal. She says she was never given a written reason for her dismissal, as is required by Columbia College's own guidelines on terminating employment of tenured professors.

A faculty committee that reviewed the college's decision, Lerman adds, was denied access to key documents and administrators in its investigation of her appeal. The committee agreed that she was not given an appropriate written reason for her termination in accord with the college's guidelines. The American Association of University Professors has also appealed Lerman's termination and warned Columbia College that it has violated the terms of her tenure.

Officials at Columbia College have declined to comment on the case. However, the college has responded to her suit with its own detailed court filings. In those documents, the college denies that Lerman was discriminated against because of her religion or gender, that she was denied due process, or that the terms of her tenure were violated. The filing claims that she was given a written reason for her termination.

The response by Columbia College further states that Lerman has misrepresented the findings of the faculty committee that reviewed her termination and that the performance evaluation Lerman cites was a draft. The college also says that at the time of her termination, Lerman was given a choice to resign or be fired.

RUDY BAUM/C&EN

Lerman

But Lerman is adamant in her charges against Columbia College. "Nobody at Columbia College was ever treated like I was treated," she says. On the day of her dismissal, she adds, she was locked out of her office and told not to return to campus. Her pay and benefits were immediately suspended. To this day, she says, she has not been allowed to retrieve even personal belongings.

OTHER COLUMBIA COLLEGE tenured professors accused of wrongdoing—especially male and non-Jewish faculty members—have not been treated in such a harsh manner, says Lerman's attorney, Laurel Bellows of Bellows & Bellows, in Chicago. It is unprecedented, Bellows adds, that a tenured professor at the college would have pay and benefits terminated before a full appeals process had been completed. For example, she claims that pay and benefits for a certain Columbia College professor accused of possessing child pornography on a work computer were continued while his case was under appeal.

Former ACS president E. Ann Nalley says that Columbia College, after firing Lerman, wrongfully held on to funds raised by Lerman for the conference series "Frontiers of Chemical Sciences: Research and Education in the Middle East—A Bridge to Peace," also called the Malta Conference. Lerman is a leading proponent and organizer of the conference, and Nalley is deputy chair of the organizing committee.

Nalley had to negotiate transfer of the funds from Columbia College to the International Union of Pure & Applied Chemistry, which now operates the conference, she says. Because of the college's delays, "we almost had to cancel the Malta Conference" in 2009, Nalley adds. The college denies that it wrongfully retained the funds.

Columbia College "violated every principle of tenure we see in higher education," says Nalley, a chemistry professor at Cameron University, in Lawton, Okla. "I can't imagine any situation that wouldn't at least allow a person to get their things out of their office."

ISESC brought in millions of dollars in grants for Columbia College, Nalley says. "It's unbelievable what Zafra accomplished. It will never be duplicated—it was unique, especially for chemistry," she says. "I can't imagine what the people at Columbia College were thinking."

"A lot of the older people have been fired, especially some of the bigger names like Zafra," Jeffrey Wade, a former assistant to Lerman, says of recent personnel moves at Columbia College. Wade's position was terminated on May 28. He had been with the college for 30 years. He says ISESC has been restructured and downgraded to a project within the science and math department. Under Lerman's leadership, the institute had been an entity unto itself at the college.

"Zafra was not the kind of person they wanted around," says a longtime faculty member about the Columbia College administration. This source, who has requested anonymity for fear of retaliation, says he knew that the faculty who reviewed her dismissal found it unwarranted and that their findings would be disregarded by administrators.

Columbia College "used to be a school with a heart," the faculty member says. "Now it's become a more corporate kind of" environment. He specifically blames Columbia College President Warrick L. Carter and Board Chairman Allen M. Turner.

If Turner "gets away with what he did to Zafra," the faculty member says, "many more will follow."—WILLIAM SCHULZ

Building A Diverse Profession And Inclusive Community

THOMAS H. LANE, 2009 ACS PRESIDENT, AND JOSEPH S. FRANCISCO, 2010 ACS PRESIDENT

AS ACS CORE VALUES, diversity and inclusion are the foundation of the society's strategic plan. These values indicate that as an organization, we are passionate about building a diverse and inclusive community of highly skilled chemistry professionals.

Is our commitment to these values transparent to our membership and the chemistry community? What must ACS do to take a greater leadership role in developing a community of chemistry professionals that reflects the diversity of the U.S.?

These are important questions that have been asked for many years within the society, and they have an even greater urgency today. Both research and business benefit from diverse perspectives within the technical workforce because many of the toughest problems are solved best by teams of individuals with diverse scientific and cultural backgrounds. The landscape of chemistry employment is changing rapidly, and we have an obligation to prepare our members to be successful in this ever-evolving marketplace.

Promoting the development of a diverse and inclusive workforce that reflects the demographics of the nation will ensure that ACS remains vibrant and relevant, serving the chemical enterprise and promoting innovations and advances in the chemical sciences. Over the past two decades, ACS has led efforts both to increase the participation of minorities and women and to enhance their stature within the society and the profession.

& MORE ONLINE

In 2009, we appointed the Task Force on Implementing the ACS Diversity Reports. The reports, from a series of three workshops focused on increasing participation of African American, Hispanic, and Native American undergraduate students in chemistry, included a total of 86 recommendations for units across ACS.

The task force began its work by articulating a vision of what a society like ACS should be, by preparing an inventory of existing activities focused on underrepresented racial and ethnic groups, and by determining which workshop recommendations would have the highest potential impact. Task force recommendations—for enhancing the impact of ACS activities on diversity and inclusion and for strengthening ACS's position as a national leader in diversity in science, technology, engineering, and mathematics (STEM) education—fell into four categories:

PETER CUTTS PHOTOGRAPHY (BOTH)

■ **Developing & Sustaining a Long-Term Vision & Coordinating New & Existing Activities.** Ensuring that the chemistry profession remains vibrant and relevant requires purposeful, committed, and coordinated efforts by ACS, the primary steward of the profession. To achieve the goal of a diverse, representative, and highly qualified workforce in chemistry, ACS must enhance the impact and visibility, both internally and externally, of its diversity and inclusion efforts. This effort requires the development of a shared vision and strategic leadership at all levels of the organization. Activities must be prioritized and aligned to maximize the potential of the human and capital resources invested in them.

■ **Developing & Maintaining Relationships & Partnerships.** No organization, including ACS, has the resources or the connections to develop a diverse workforce alone. All parts of the chemistry enterprise have to be involved. Underrepresented communities must be engaged. In addition to partnering with minority advocacy organizations, ACS should strengthen its relations with academic institutions, including but not limited to minority-serving institutions. Industry, which has realized the benefits of and developed strategies for building a diverse workforce, must be part of the equation.

■ **Engaging Communities.** Every facet of ACS must be positioned to take maximum advantage of the full talent pool in chemistry. By sharing strategies, ACS divisions, local sections, and committees can leverage the successful programs and activities already in place. Strategies for becoming more inclusive will increase the impact of volunteer contributions and foster greater involvement. As core values, diversity and inclusion should be reflected across the society.

■ **Measuring Progress & Celebrating Success.** Building a diverse community requires sustained efforts. The extensive inventory of activities prepared by the task force indicates that significant progress has been made since 1991, when then-ACS president S. Allen Heininger appointed the Task Force on Minority Affairs. By updating the inventory and collecting more data, the impact of future activities can be demonstrated.

AT THE 2010 ACS spring national meeting, the task force shared its report with the ACS Board of Directors. In response, the Committee on Professional & Member Relations' Subcommittee on Professional Advancement, chaired by ACS President-Elect Nancy B. Jackson, was charged with prioritizing the task force's recommendations and assigning accountability and developing timelines to implement them. Immediate strategic action will position ACS to align the demographics of the chemistry enterprise with those of the nation's citizens and to assume a national leadership role in broadening participation in the STEM disciplines.

Your insights are needed. Please visit www.acs.org and click on the "Diversity" link, where you can read the workshop reports, review the inventory, and send your suggestions to the Professional & Member Relations Committee at p&mr@acs.org. ■

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Three Faculty Positions in Photovoltaics

One Endowed Chair and two Junior Positions

The Department of Physics & Astronomy at the University of Toledo (UT) invites applications for three faculty positions to begin August 2010.

One position, the **Ohio Research Scholar Endowed Chair in Photovoltaics (PV),** may be connected to one or both of the Junior Positions if appropriate, though this is not required. The successful applicants are expected to participate in a broad statewide initiative in PV as members of the **Wright Center for Photovoltaics Innovation & Commercialization (www.pvic.org).** Joint appointments in other departments/colleges and in UT's School of Solar & Advanced Renewal Energy are likely and some teaching at the undergraduate and graduate level will be expected as well. Candidates are sought with exceptional experience and qualifications in any area(s) of PV. Successful candidates will desire to collaborate broadly with university colleagues and industrial partners on PV science and technology and plan to establish world-class infrastructure and capabilities to fabricate and/or analyze PV materials, interfaces, and/or device structures. They will also be expected to involve graduate and undergraduate students in their research program.

The Ohio Research Scholar Endowed Chair and the Junior positions will be supported by significant start-up packages with funds from the Ohio Department of Development and UT. These positions are part of an ongoing effort by the State of Ohio and UT to maintain and grow PV excellence and leadership in Northwest Ohio.

A Ph.D. in Physics, Chemistry, Materials Science or a closely related field is required, as well as research experience beyond the Ph.D. A strong track record of external research support is required for the senior position, whereas candidates for the other two positions must demonstrate considerable potential for attracting external support (an existing track record is a plus). We encourage women and minority candidates to apply.

Requests for more information and application packages should be sent to:

pvic_hiring@utoledo.edu
or mail to:
Physics Search
Department of Physics & Astronomy
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Toledo, OH 43606-3390

The application package (one PDF document) should include a cover letter stating the position(s) of interest, a CV, a research plan (three pp max), a teaching statement (one pg max), and the names and contact information of at least three references who have been requested to submit letters on behalf of the applicant. Consideration of complete applications, including three reference letters, will begin on June 15, 2010, and continue until the positions are filled.

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newscripts

SUPERVEGGIES, TREADMILL MULTITASKING, LIFESAVING UNDIES

It's safe to say that most people have the desire to live a long, healthy life. Along those lines, Newscripts has come across some intriguing research and two newfangled contraptions designed to help people attain that goal.

An apple a day keeps the doctor away, but beets might keep chronic diseases at bay, according to new research by Rui Hai Liu and coworkers at Cornell University. The researchers measured the cellular **ANTIOXIDANT ACTIVITY** of 27 common vegetables—including such childhood favorites as brussels sprouts and green beans—to establish which of them had the most potential for health benefits.

"Increased fruit and vegetable consumption is an effective strategy to increase antioxidant intake and decrease oxidative stress and may lead to reduced risk of developing chronic diseases, such as cancer and cardiovascular disease," the researchers write.

Using a fluorescence-based cellular assay, the Cornell team found that beets, broccoli, and red peppers had the highest amount of cellular antioxidant activity, and veggies such as cucumbers, spinach, and lettuce ranked lowest. So if you want a leg up in the fight against diabetes, Alzheimer's disease, and cataracts, don't forget to eat your beets. The findings were published in the *Journal of Agricultural & Food Chemistry* (**2010,** *58,* 6621).

ISTOCK (ALL)

Superveggies: Beets, broccoli, and red peppers could stave off chronic diseases. Don't just sit there: Walking while working could help you live longer.

Now that Newscripts has passed along its best diet advice, let's tackle the other key component to living well: exercise. For working men and women, finding time during the day to get the recommended hour of exertion can be difficult, especially when you consider how long some people are trapped behind a desk.

Enter the **TREKDESK,** a computer table designed to fit over any basic treadmill that lets you walk while you tap away on your keyboard, check your e-mail, or surf the Internet.

"Chairs are the enemy," the TrekDesk website declares under a list of 52 supposed benefits of the product. The list promises perks that vary widely in grandeur, such as improvements in blood lipid profiles, decreases in the incidence of impotence, and reduction in the risk of colon cancer.

The walking-while-working concept sounds rather difficult to juggle, but if you'd like to try out this fitness miracle for yourself, you can find the TrekDesk online at Amazon.com.

The final item in our health roundup is a handy article of clothing out of the University of California, San Diego. Reuters is reporting that nanoengineering professor Joseph Wang and colleagues have developed and designed new **MEN'S BRIEFS** that are more than just an undergarment.

The waistband, which remains in constant contact with the skin, comes equipped with an electrochemical biosensor that is designed to measure blood pressure, heart rate, and other general vital signs. The sensor is an array of carbon electrodes screen-printed directly onto the fabric.

Wang's research is being sponsored by the U.S. military with the intention that the technology might one day be used on the battlefield to monitor soldiers' health and well-being. However, the technology's application extends well beyond the military, Wang tells Reuters. For example, the biosensor could be programmed to monitor various cardiac markers in the elderly, alerting the user to any potential for stroke.

TREKDESK

FAITH HAYDEN *wrote this week's column. Please send comments and suggestions to newscripts@acs.org.*

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